NAWI

National Alliance for Water Innovation

MASTER TECHNOLOGY ROADMAP

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CONTENTS

TABLE OF FIGURES

TABLE OF TABLES

1. INTRODUCTION

Clean water is critical to ensure good health, strong communities, vibrant ecosystems, and a functional economy for manufacturing, farming, tourism, recreation, energy production, and other sectors' needs.

Research to improve desalination technologies can make nontraditional sources of water (i.e., brackish water; seawater; produced and extracted water; and power sector, industrial, municipal, and agricultural wastewaters) a cost-effective alternative. These nontraditional sources can then be applied to a variety of beneficial end uses, such as drinking water, industrial process water, and irrigation, expanding the circular water economy by reusing water supplies and valorizing constituents we currently consider to be waste. As an added benefit, these water supplies could contain valuable constituents that could be reclaimed to further **a circular economy.**

1.1. Establishing an Energy-Water Desalination Hub

In 2019, the U.S. Department of Energy (DOE) established an Energy-Water Desalination Hub (part of a family of Energy Innovation Hubs to address water security issues in the United States. NAWI was funded to address this critical component of the DOE's broader Energy-Water Nexus portfolio to help address the nation's water security needs. NAWI's goal is to enable the manufacturing of energy-efficient desalination technologies in the United States at a lower cost with the same (or higher) quality and reduced environmental impact for 90 percent of nontraditional water sources within the next 10 years.

NAWI is led by Lawrence Berkeley National Laboratory in Berkeley, California and includes Oak Ridge National Laboratory, the National Renewable Energy Laboratory, the National Energy Technology Laboratory, 19 founding university partners, and 10 founding industry partners. This partnership is focused on conducting early-stage research (technology readiness levels [TRLs] 2–4) on desalination and associated water-treatment technologies to secure affordable and energy-efficient water supplies for the United States from nontraditional water sources. NAWI's five-year research program will consist of collaborative early-stage applied research projects involving DOE laboratories, universities, federal agencies, and industry partners. DOE is expected to support NAWI with $110 million in funding over five years, with an additional $34 million in cost-share contributions from public and private stakeholders.

As a part of the NAWI research program, this Master Roadmap was developed to identify research and development (R&D) opportunities that help address their particular challenges that the five water sectors (Power, Resource Extraction, Industry, Municipal, and Agriculture, or PRIMA) face in treating nontraditional water sources. Recognizing the important sector-specific variations in water availability and water technology needs, NAWI has also published five end-use water roadmaps with tailored R&D and modeling opportunities for each sector. These roadmaps have each been published as standalone documents that can inform future NAWI investments as well as provide insight into priorities for other research funding partners.

1.2. Pipe-Parity and Baseline Definitions

A core part of NAWI's vision of a circular water economy is reducing the cost of treating nontraditional source waters to the same range as the portfolio of accessing new traditional water sources, essentially achieving pipe-parity. The costs considered are not just economic but include consideration of energy consumption, system reliability, water recovery, and other qualitative factors that affect the selection of a new water source. To effectively assess R&D opportunities, pipe-parity metrics are utilized; they encompass a variety of information that is useful to decision makers regarding investments related to different source water types.

Pipe-parity is defined as technological and non-technological solutions and capabilities that make marginal water sources viable for end-use applications. Like the concept of grid parity (where an alternative energy source generates power at a levelized cost of electricity [LCOE] that is less than or equal to the price of power from the electricity grid), a nontraditional water source achieves pipe-parity when a decision maker chooses it as their best option for extending its water supply.

Specific pipe-parity metrics of relevance can include:

Cost

Cost metrics can include levelized costs of water treatment as well as individual cost components, such as capital or operational and maintenance (O&M) costs.

Energy Performance

Energy performance metrics can include the total energy requirements of the water treatment process, the type of energy required (e.g., thermal vs. electricity), embedded energy in chemicals and materials, and the degree to which alternative energy resources are utilized.

Water Treatment Performance

Water treatment performance metrics can include the percent removal of various constituents of concern and the percent recovery of water from the treatment train.

Human Health and Environment Externalities

Externality metrics can include air emissions, greenhouse gas emissions, waste streams, societal and health impacts, and land-use impacts.

Process Adaptability

Process adaptability metrics can include the ability to incorporate variable input water qualities, incorporate variable input water quantity flows, produce variable output water quality, and operate flexibly in response to variable energy inputs.

Reliability and Availability

System reliability and availability metrics can include factors related to the likelihood of a water treatment system not being able to treat water to a specified standard at a given moment, how quickly the system can restart operations after being shut down for a given reason, confidence in source water availability, the degree to which the process is vulnerable to supply chain disruptions, and the ability to withstand environmental, climate, or hydrological disruptions.

Compatibility

Compatibility metrics can include ease of operation and level of oversight needed, how well the technology integrates with existing infrastructure, how consistent the technology is with existing regulations and water rights regimes, and the level of social acceptance.

Sustainability

Sustainability metrics can include the degree to which freshwater inputs are required for industrial applications, the percentage of water utilized that is reused or recycled within a facility, and watershed-scale impacts.

To establish references on which pipe-parity metrics are most applicable in each sector, **baseline studies** for each of NAWI's eight nontraditional water sources have been conducted. These studies collect data about the use of each source water and evaluate several representative treatment trains for the targeted source water to better understand current technology selections and implementation methods. The baselines provide range estimates of the current state of water treatment pathways across pipe-parity metrics, which enable the calculation of potential ranges of improvement.

1.3. Nontraditional Waters and End-Use Sectors of Interest

NAWI has identified eight nontraditional water supplies of interest for further study:

Seawater and Ocean Water	Water from the ocean or from bodies strongly influenced by ocean water, including bays and estuaries, with a typical total dissolved solids (TDS) between 30,000 and 35,000 milligrams per liter (mg/L).
Brackish Groundwater	Water pumped from brackish aquifers, with particular focus on inland areas where brine disposal is limiting. Brackish water generally is defined as water with 1–10 grams per liter (g/L) of total dissolved solids (TDS).
Industrial Wastewater	Water from various industrial processes that can be treated for reused
Municipal Wastewater	Wastewater treated for reuse through municipal resource recovery treatment plants utilizing advanced treatment processes or decentralized treatment systems
Agricultural Wastewater	Wastewater from tile drainage, tailwater, and other water produced on irrigated croplands, as well as wastewater generated during livestock management, that can be treated for reuse or disposal
Mining Wastewater	Wastewater from mining operations that can be reused or prepared for disposal
Produced Water	Water used for or produced by oil and gas exploration activities (including fracking) that can be reused or prepared for disposal
Power and Cooling Wastewater	Water used for cooling or as a byproduct of treatment (e.g., flue gas desulfurization) that can be reused or prepared for disposal

These nontraditional water sources range widely in TDS (100 milligrams per liter [mg/L] – 800,000 mg/L total) as well as the type and concentrations of contaminants (e.g., nutrients, hydrocarbons, organic compounds, metals). **These different water supplies require varying degrees of treatment to reach reusable quality.**

When these nontraditional water supplies are treated with novel technologies created through the NAWI desalination hub, these remediated wastewaters could be repurposed back to one or more of the following five end-use sectors:

Power — Water used in the electricity sector, especially for thermoelectric cooling

Resource Extraction — Water used to extract resources, including mining and oil and gas exploration and production

Industrial — Water used in industrial and manufacturing activities not included elsewhere, including but not limited to petrochemical refining, food and beverage processing, metallurgy, and commercial and institutional building cooling

Municipal — Water used by public water systems (which include entities that are both publicly and privately owned) to supply customers in their service area

Agriculture — Water used in the agricultural sector, especially for irrigation and food production

NAWI identified these broad "PRIMA" sectors because they are major users of water with opportunities for reuse. Figure 1 expands on the industries included in NAWI's PRIMA broad end-use sectors. These areas are not meant to be exhaustive, as nearly all industries and sectors rely on water in one way or another.

END-USE SECTOR	INDUSTRIES INCLUDED
Power	Thermoelectric Renewable energy
Resource Extraction*	Upstream oil and gas Hydraulic fracturing operations Mining
Industrial†	Refineries Petrochemicals Primary metals Food and beverage Pulp and paper Data centers and large campuses
Municipal	Public supply for use by residential, commercial, industrial, institutional, public service, and some agricultural customers within the utility service area
Agriculture	Irrigation Livestock Upstream food processing

Figure 1. Industries covered in each PRIMA roadmap sector

* An important distinction for oil and gas and mining operations: upstream drilling operations fall under the Resource Extraction Sector and downstream refining operations fall under the Industrial Sector.

† This list of industries for the Industrial Sector is for baselining and initial roadmapping. This list will be reviewed in future roadmap iterations.

1.4. A-PRIME

Securing water supplies for multiple end-uses requires technology revolutions that will transition the United States from a linear to a circular water economy.

These desalination and reuse advances will be realized by developing a suite of Autonomous, Precise, Resilient, Intensified, Modular, and Electrified (A-PRIME) technologies that support distributed and centralized treatment at a cost comparable to other inland and industrial sources. Each aspect of this hypothesis has been vetted with water treatment professionals from each PRIMA industry sector as well as NAWI's Research Advisory Council (RAC) to ensure that it is a relevant means of advancing desalination and water treatment capabilities for nontraditional source waters. These areas may be modified as new priorities and opportunities are identified.

The NAWI A-PRIME hypothesis outlines the following six major challenge areas needing improvement for water treatment to reach pipe-parity for nontraditional waters.

A The **Autonomous** area entails developing robust sensor networks coupled with sophisticated analytics and secure controls systems.

P The **Precise** area focuses on a targeted treatment approach with precise removal or transformation of treatment-limiting constituents and trace contaminants.

R The **Resilient** area looks to enable adaptable treatment processes and strengthen water supply networks.

I The **Intensified** area focuses on innovative technologies and process intensification for brine concentration and crystallization and the management and valorization of residuals.

M The **Modular** area looks to improve materials and manufacturing processes and scalability to expand the range of cost-competitive treatment components and eliminate intensive pre/post-treatment.

E The **Electrified** area aims to replace chemically intensive processes with electrified processes that are more amenable to variable or fluctuating operating conditions.

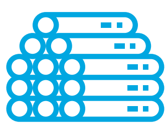
1.5. Desalination Hub Topic Areas

There are key technology areas of R&D, modeling, and analysis that cut across the water sources and sectors in the NAWI Hub.

They can be categorized under three interdependent topic areas, as summarized below:

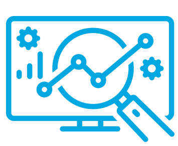
Process Innovation and Intensification R&D

Novel technology processes and system design concepts are needed to improve energy efficiency and lower costs for water treatment. New technologies related to water pre-treatment systems (e.g., upstream from the desalination unit operation) and other novel approaches can address associated challenges such as water reuse, water efficiency, and high-value co-products.



Materials and Manufacturing R&D

Materials R&D has the potential to improve energy efficiency and lower costs through improved materials used in specific components and in water treatment systems. Desalination and related water treatment technologies can benefit from materials improvements for a range of products (e.g., membranes, pipes, tanks, and pumps) that dramatically increase their performance, efficiency, longevity, durability, and corrosion resistance.



Data, Modeling, and Analysis

In order to consistently define, track, and achieve pipe-parity in the highest impact areas, strategic, non-biased, and integrated data and analysis is needed. This data, in addition to studies and analysis tools, is necessary to guide the Hub's strategic R&D portfolio. A centralized data system will also fill the void in industry for shared information and provide decision-making tools related to water treatment implementation. Multi-scale models and simulation tools can inform R&D via performance forecasting, design optimization, and operation of desalination technologies and related water-treatment systems, leading into improved energy efficiency and lowered costs.

2. MASTER ROADMAP OVERVIEW

Prior to developing a master roadmap, a team of researchers and water professionals engaged in a detailed process of evaluating water uses, state-of-the-art technologies, emerging technologies and existing uses of desalination and advanced water technologies within five major water user categories in the United States. The resulting Water User Sector Roadmaps were complemented by a Baseline Analysis of a suite of representative treatment systems conducted by NAWI researchers working in collaboration with the Hub's Industrial Partners. Over 400 experts and practitioners contributed to the NAWI roadmapping and baselining initiatives. This Master Roadmap, which synthesizes the findings from these different efforts as well as feedback from members of NAWI's RAC, serves as the basis for identifying NAWI's research Areas of Interest (AOIs).

During the roadmapping process, a total of 89 sector-specific AOIs were identified from which R&D have the potential to reduce the costs and energy intensity of desalination and fit-for-purpose water reuse and increase the availability and adoptability of nontraditional water sources. We prioritized these AOIs based on their impact across multiple water use sectors and their potential to expand the use of nontraditional waters. This evaluation involved quantitative analysis of current water reuse and desalination practices and a combination of quantitative and qualitative assessments of R&D priorities for enabling nontraditional water reuse. Underlying the decision-making process was a strategy of identifying a limited number of AOIs in which research conducted by NAWI could create synergies that combine to achieve the greatest progress in achieving pipe-parity in multiple areas. We also prioritized AOIs that leverage the unique data, analysis, modeling, simulation, characterization, manufacturing, optimization, and testing capabilities of DOE's National Laboratories.

The guiding principle behind NAWI is that research at TRLs ranging from 2 to 4 (i.e., concept identification through laboratory validation) can provide a basis for dramatic improvements in the performance of small-scale autonomous desalination and water treatment systems. Much of this research should also be applicable to existing, centralized desalination and advanced water treatment facilities, where they could combine to produce substantial reductions in capital costs, operating budgets, and energy consumption. Research at a very fundamental level (i.e., TRL 1; basic research) lies outside of NAWI's scope. In some cases, however, we identified basic research programs within DOE, the U.S. National Science Foundation, and other federal and state agencies' research portfolios that were well aligned with A-PRIME (e.g., in areas such as Intensified Brine Management and Precision Separation) and created links with them to assure that the knowledge that they were generating could be built upon in NAWI's research. Similarly, demonstration and optimization of system performance in pilot- and full-scale systems—an essential step to realizing NAWI's low-TRL research advances in operational systems—will require further R&D investment by federal, state, and industrial entities.

To assure that NAWI's research has the greatest possible impact, we prioritized research needs that were likely to have substantive pipe-parity impacts in several different water sectors. Research needs identified in the Water User Sector Roadmaps that were of primary relevance to only one or two sectors were given a lower priority in the master roadmapping process than those that were likely to affect multiple sectors. Similarly, research that offered incremental or moderate improvements over the state-of-the-art were lower priority than those offering the potential for paradigm-shifting approaches to water desalination challenges (Figure 2).

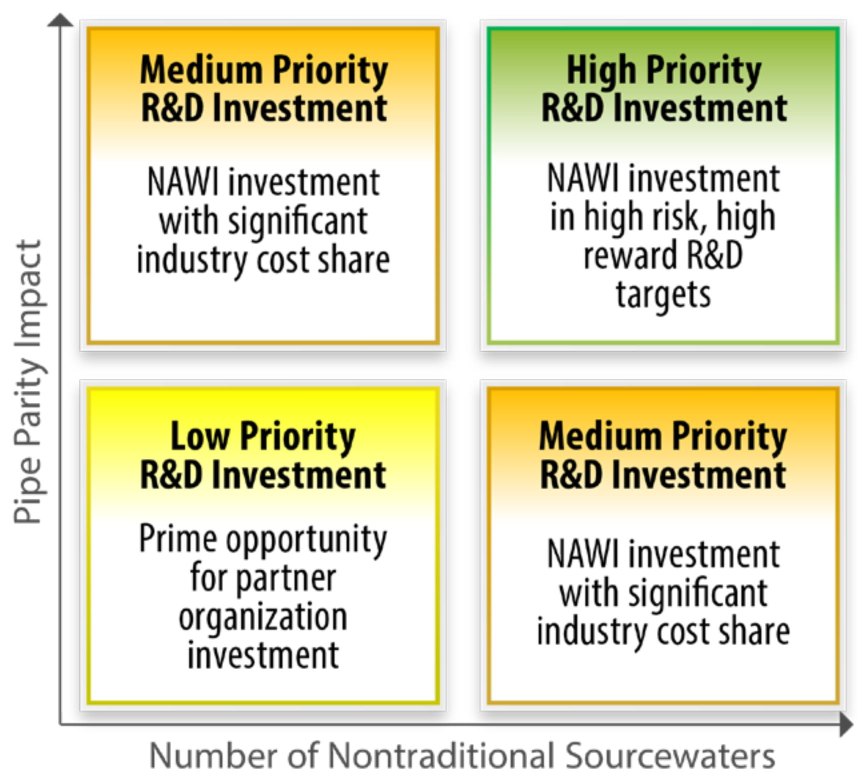


Figure 2. Overview of NAWI Master Roadmap investment priorities

2.1. Current Status of U.S. Water Users

2.1.1. Water User Sector Background

To gain insight into the Master Roadmap, it is helpful to consider current and future water recycling and desalination needs identified within the five water user sector roadmaps. The following section summarizes some of the key findings that informed development of the Master Roadmap. Readers who are interested in additional details should consult the relevant Water User Sector Roadmaps, available on NAWI's website (https://www.nawihub.org/roadmaps). This section provides a brief overview of water user sectors, their water withdrawals (Figure 3), the ways in which they use water, and other relevant information.

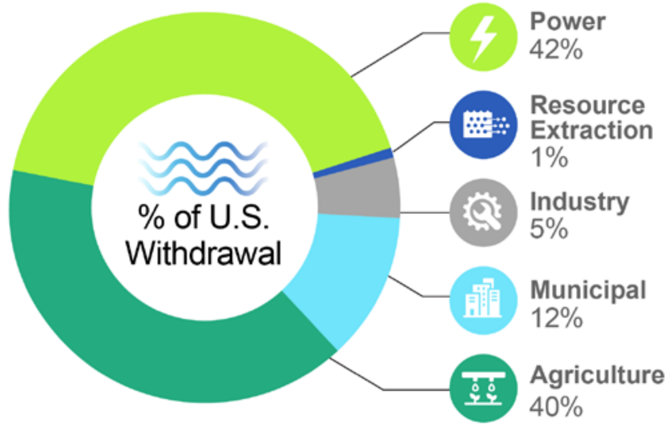


Figure 3. Overview of water withdrawals in the United States[1]

POWER

Thermoelectric power generation (e.g., natural gas, coal, petroleum, nuclear) in the United States accounts for 41 percent of the country's water withdrawals, or 500 million cubic meters (m^3) per day (130 billion gallons per day).[1] Most of these water withdrawals are associated with older, thermoelectric power plants that use once-through cooling—a process in which water passes through the main condensers in a single pass to remove waste heat. Evaporative cooling schemes, which account for less than seven percent of U.S. water withdrawals, consume almost all of the water withdrawn from the environment[2]. Due to regulations and the increasing popularity of renewable energy (e.g., wind, solar), many once-through cooling schemes are now being retired. The primary source of water for cooling thermoelectric power plants is fresh surface water. Seawater is employed for once-through cooling in many coastal areas, but its importance at the national scale is decreasing as California phases out its use.

AGRICULTURE

The Agriculture Sector is a significant water user in the United States; almost 280 million m^3 per day per day (75 billion gallons per day) of water are used to irrigate over 200,000 farms.[1] The demand for irrigation water in the United States is heterogeneous, varying with climate, time of year, crop type, and other factors. Western states, which typically have drier climates, accounted for 46 percent of the harvested cropland but used 84 percent of the irrigation water.

MUNICIPAL

Total water withdrawals for public supply, referred to as municipal water uses in our roadmap-ping process, accounted for about 148 million m^3 per day (39 billion gallons per day) in 2015. Municipal water systems delivered potable water to about 87 percent of the U. S. population.[1] The primary sources of water for municipal use are surface and groundwater supplies, with the majority of water drawn from fresh surface-water sources.

INDUSTRIAL

The Industrial Sector withdraws about 68.5 million m³ per day (18.1 billion gallons per day).[1] Because this sector is so heterogenous, NAWI focused on key industrial subsectors in our road-mapping process, including oil refineries, pulp and paper mills, primary metals factories, chemical manufacturing, and the food and beverage industries, as well as data centers and large campuses. These subsectors represent about 35 percent of the overall water withdrawals by industry. Most of the water for the Industrial Sector is self-supplied from surface and ground water. Municipal water is the first alternative source when self-supply of freshwater is impractical, because it is available in most industrial locations, is of consistent quality, and is relatively inexpensive.

RESOURCE EXTRACTION

The Resource Extraction Sector withdraws about 15.5 million m³ of water per day (4.1 billion gallons per day) for mining and extraction of petroleum products in the United States.[1] Resource extraction often employs proximal groundwater and surface water supplies. In particular, ample quantities of water are often obtained when mines are dewatered or when oil and gas are recovered from the subsurface. Internal reuse (i.e., recycled water) is also an important source of supply for resource extraction.

Considering water use from the perspective of the volume of water withdrawn provides insight into the relative demand of the different water user sectors. However, there are other helpful ways to conceptualize water use, especially when evaluating opportunities for impactful research on water recycling and desalination.

For example, the Power Sector, which withdraws the largest quantity of water in the United States, returns the majority of water that it uses to its original source through the discharge of once-through cooling systems. As a result of the low-intensity nature of this practice, there are not many opportunities for NAWI's research to affect these types of power plants. However, the gradual conversion of once-through cooling systems to recirculating cooling systems, which is driven by water scarcity and concerns about environmental impacts of thermal discharges, is accompanied by opportunities for application of desalination and advanced water treatment. For instance, the management of blowdown water (i.e., the waste from the recirculating cooling process) can be energy-intensive and may result in a brine that is challenging to manage. Therefore, R&D targeted at a small fraction of the water withdrawn by the Power Sector could enable more rapid reductions in the water withdrawals and ecological stress associated with once-through cooling by advancing pipe-parity for recirculating cooling.

In contrast to water use for thermoelectric power plants, the Municipal Sector, which currently withdraws only about a third as much water as the Power Sector, has numerous opportunities for advancing pipe-parity because a larger fraction of the water that it takes out of the environment is used in a consumptive manner (i.e., about half in arid regions where outdoor irrigation is common), and demand is stable or slowly growing in many water-stressed parts of the country. The Municipal Sector also includes users that are already paying some of the highest marginal costs for water world-wide due to their desire to avoid the economic damage associated with water scarcity. In other words, water-stressed cities are often the earliest adopters of desalination and advanced water treatment technologies because they need reliable, high-quality sources of water and are able to pay for it.

2.1.2. Water User Sector Regional Variations

Beyond the details of how a water user sector operates, it is also constructive to consider water use patterns on a regional basis, because water demand depends upon climate, population density, and locations of water consuming activities like irrigated agriculture and industry. As part of NAWI's roadmapping process, we considered regional variability in water use patterns and the likelihood that desalination and advanced water technologies would be employed in different water user sectors, as exemplified by the following brief summaries.

MUNICIPAL

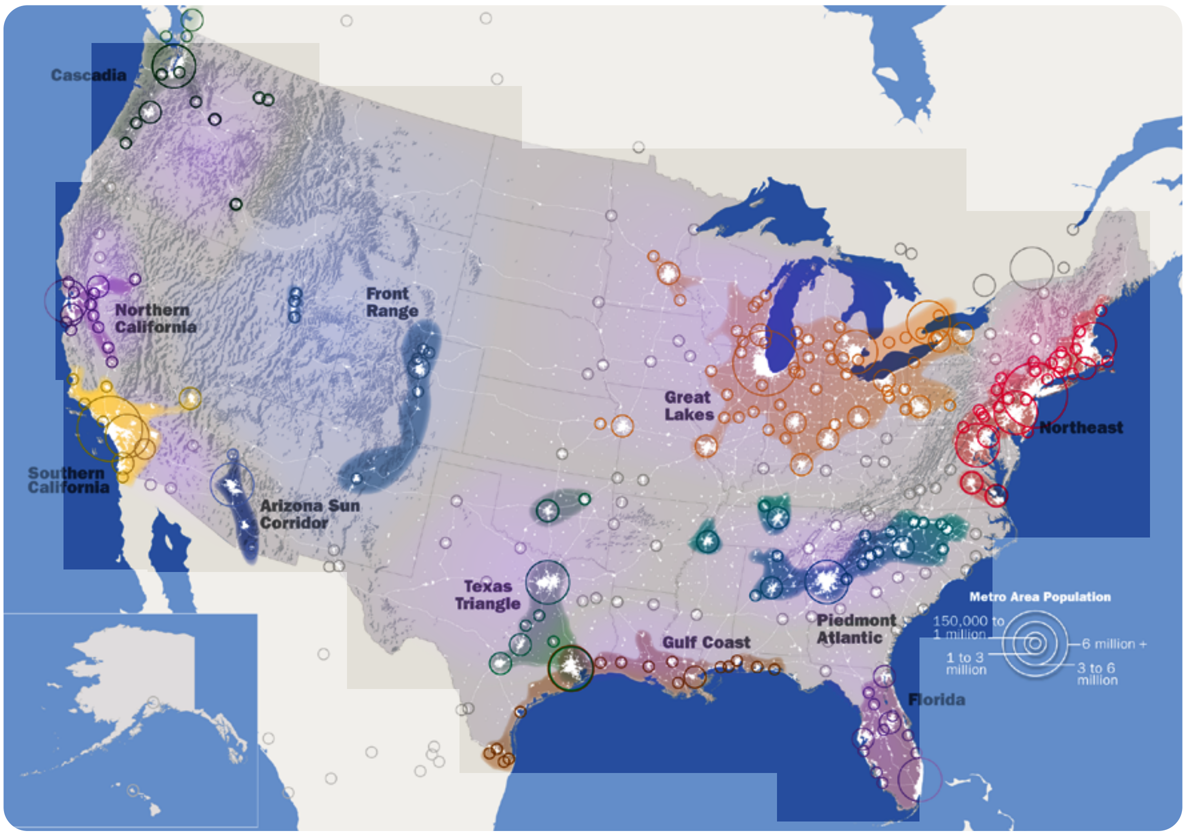


Figure 4. U.S. Megaregions[3]

In the Municipal Sector, water use is concentrated within major metropolitan areas (i.e., megaregions). The existing infrastructure, availability of local and imported water sources, and geography determine the types of water recycling and desalination technologies that are likely to be adopted and the timing with which investments are likely to be made.

For example, the Southern California Megaregion, encompassing the triangular area running from Santa Barbara in the north to San Diego in the south and east to Las Vegas, includes many of the country's early adopters of seawater desalination and potable water reuse. These municipal water sources have already achieved pipe-parity with traditional sources due to the high population density and the paucity of additional local or imported water. In particular, seawater desalination and potable water reuse are attractive in these regions because many users have access to deep ocean outfalls for disposal of brine.

The Arizona Sun Corridor, which includes Phoenix and Tucson, also faces considerable water stress, but it does not have access to the ocean for brine discharge. As a result, desalination of brackish groundwater has been hampered by limited options for brine management. Potable water reuse in the Arizona Sun Corridor tends to be limited to locations where reverse osmosis (RO) concentrate can be discharged to rivers that already have elevated salt concentrations. Cities in the Front Range and Piedmont Atlantic Megaregions also face water stress. However, the lack of suitable locations for brine discharge, coupled with relatively low salt levels in source waters, have incentivized potable water reuse projects that do not employ desalination. Potable water reuse projects in these megaregions tend to employ advanced water treatment technologies, like ozonation and activated carbon sorption, to eliminate the need for desalination and concentrate management.

AGRICULTURE

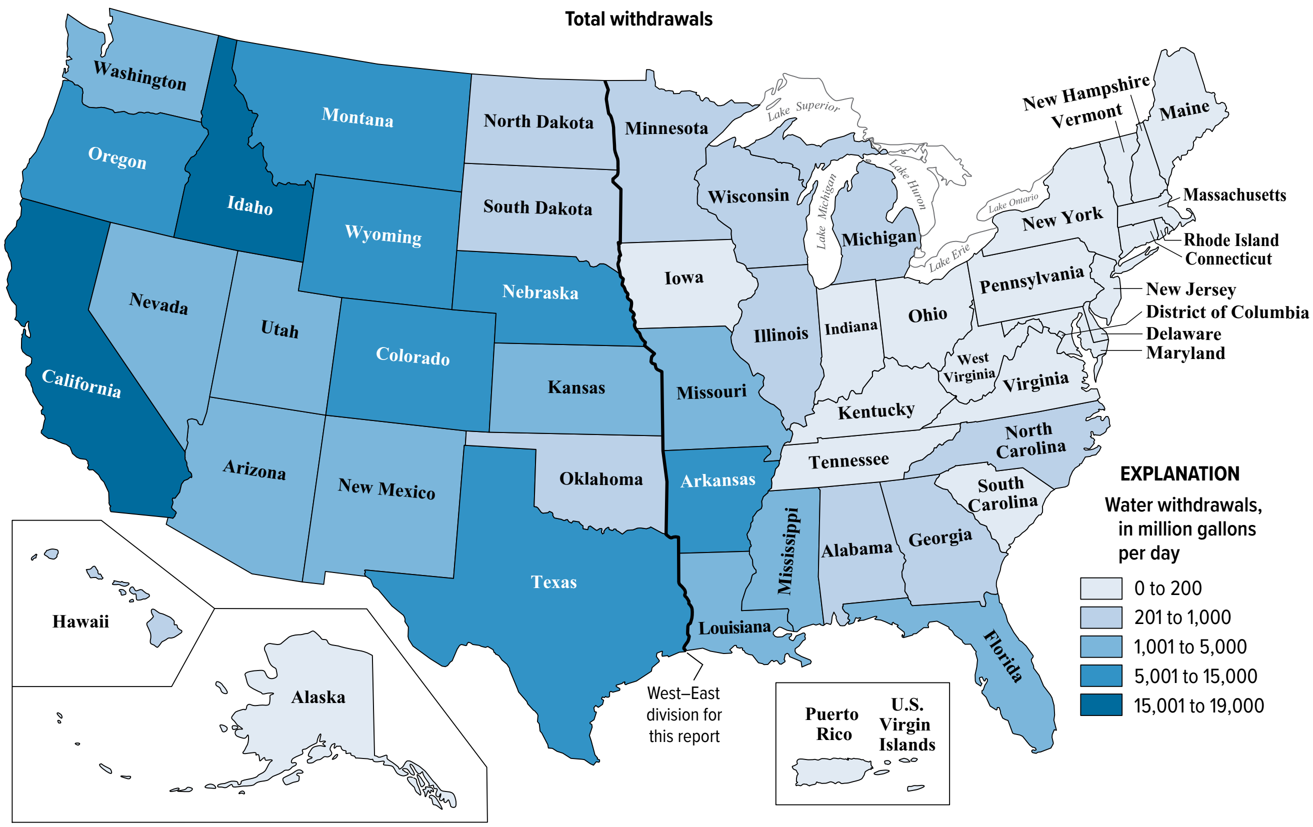


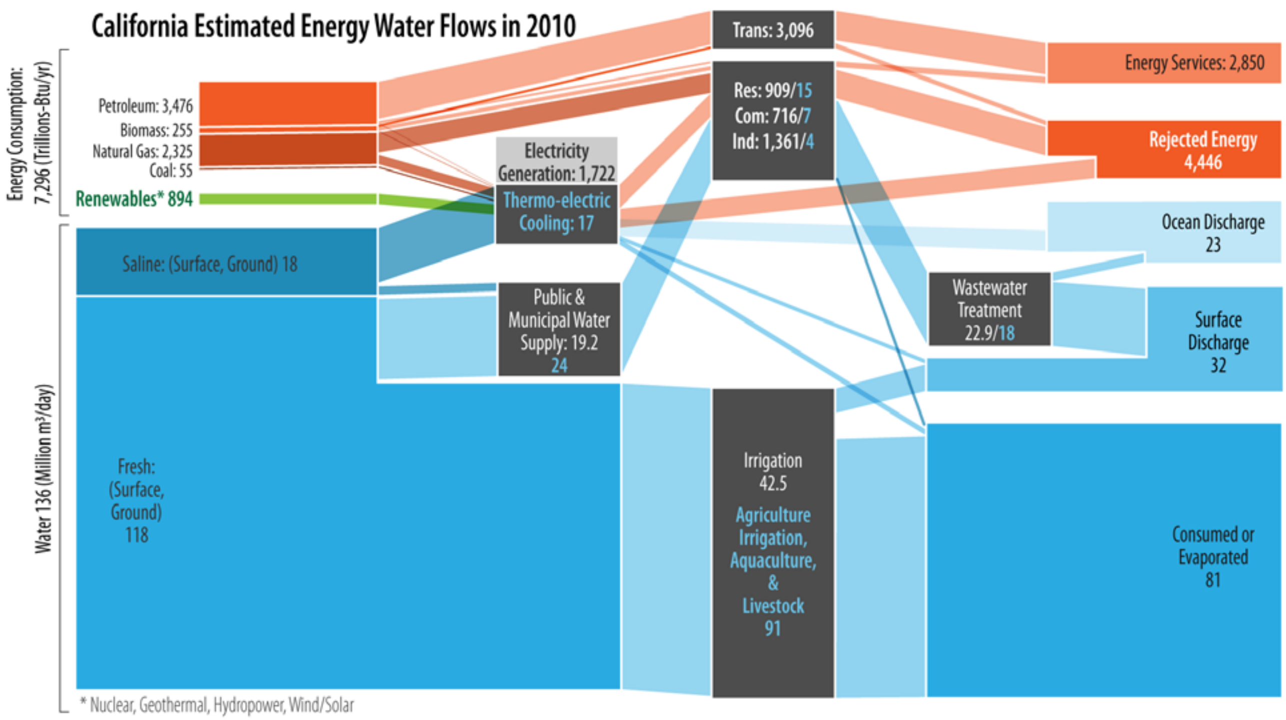
Figure 5. Irrigation water use by source and state, 2015[1]

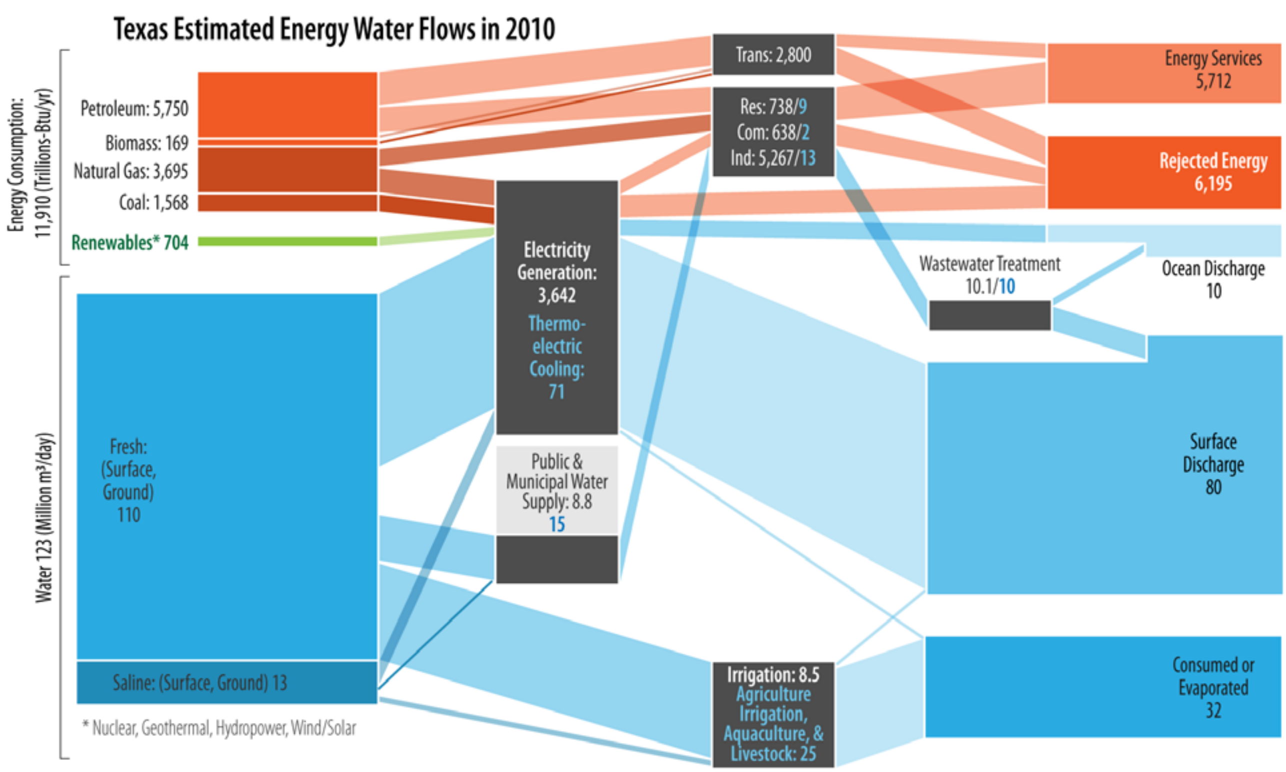
Similar regional differences are also evident in the Agriculture Sector, with irrigation practiced to a much greater degree in the western part of the country. Among the Western states, California struggles to control salinity and toxic geogenic species (e.g., selenium, boron, uranium) released when irrigation is used during the cultivation of high-value crops (e.g., fruits, nuts), while the states in the Great Plains tend to grow grain and forage (e.g., wheat, corn, alfalfa) under conditions in which salt management is less of a concern. As a result, there are more opportunities to apply desalination and water recycling technologies to treat drainage water from irrigated fields in California, where removal of salts and geogenic contaminants are critical to the long-term sustainability of high-value agriculture. Similar issues are of considerable interest to agriculture throughout much of the Southwest. Further east, where water resources are more plentiful, control of nutrients and pesticides in nonpoint source runoff originating in agricultural fields is a greater concern than salts and geogenic species.

From the standpoint of NAWI's research program, inexpensive treatment processes that are capable of removing nutrients and pesticides from tile drains or small streams would have considerable interest in this part of the country, even if those areas are not engaged in a substantial amount of irrigation.

POWER

Regional differences also affect water use patterns in the Power Sector. Among the three highest-populated states, considerable differences are evident in water sources and uses. California mainly relies on seawater for cooling its thermoelectric power plants; this has been decreasing in recent years as the state's electricity producers decarbonize, regulations on once-through cooling with seawater come into effect, and the state's nuclear power plants are decommissioned.





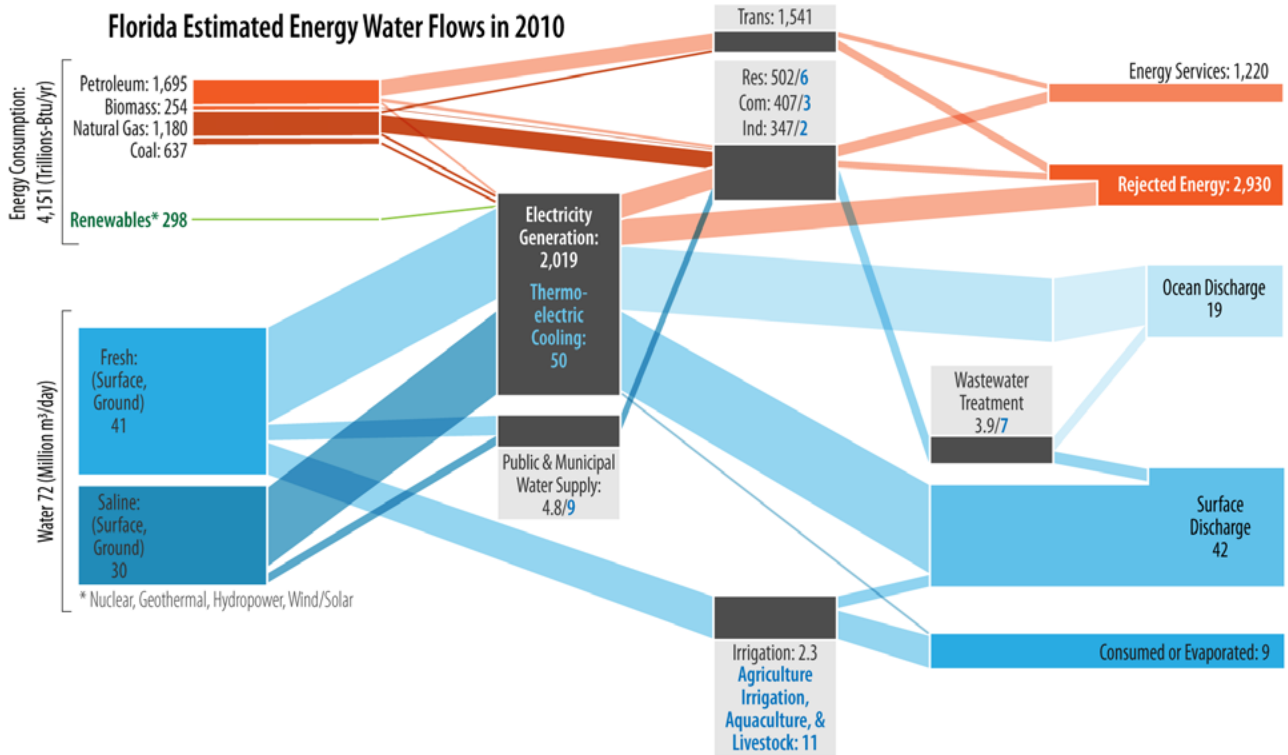


Figure 6. Annual state-level energy and water flows in 2010 for California, Texas, and Florida[4]
Adapted from Greenberg et al., 2017

In contrast, Florida uses a combination of surface water and seawater for once-through cooling of its thermoelectric facilities, and Texas, which lacks seawater access for many of its cities, relies almost entirely on freshwater for thermoelectric cooling. Although all three states face considerable water stress, their desalination and advanced water treatment needs are quite different. California is unlikely to increase its water use in the Power Sector, but it might have need for high-purity water if electrolysis for hydrogen production becomes popular, whereas Texas may convert some of its once-through power plants to recirculating cooling plans and Florida may increase its reliance on seawater cooling.

RESOURCE EXTRACTION

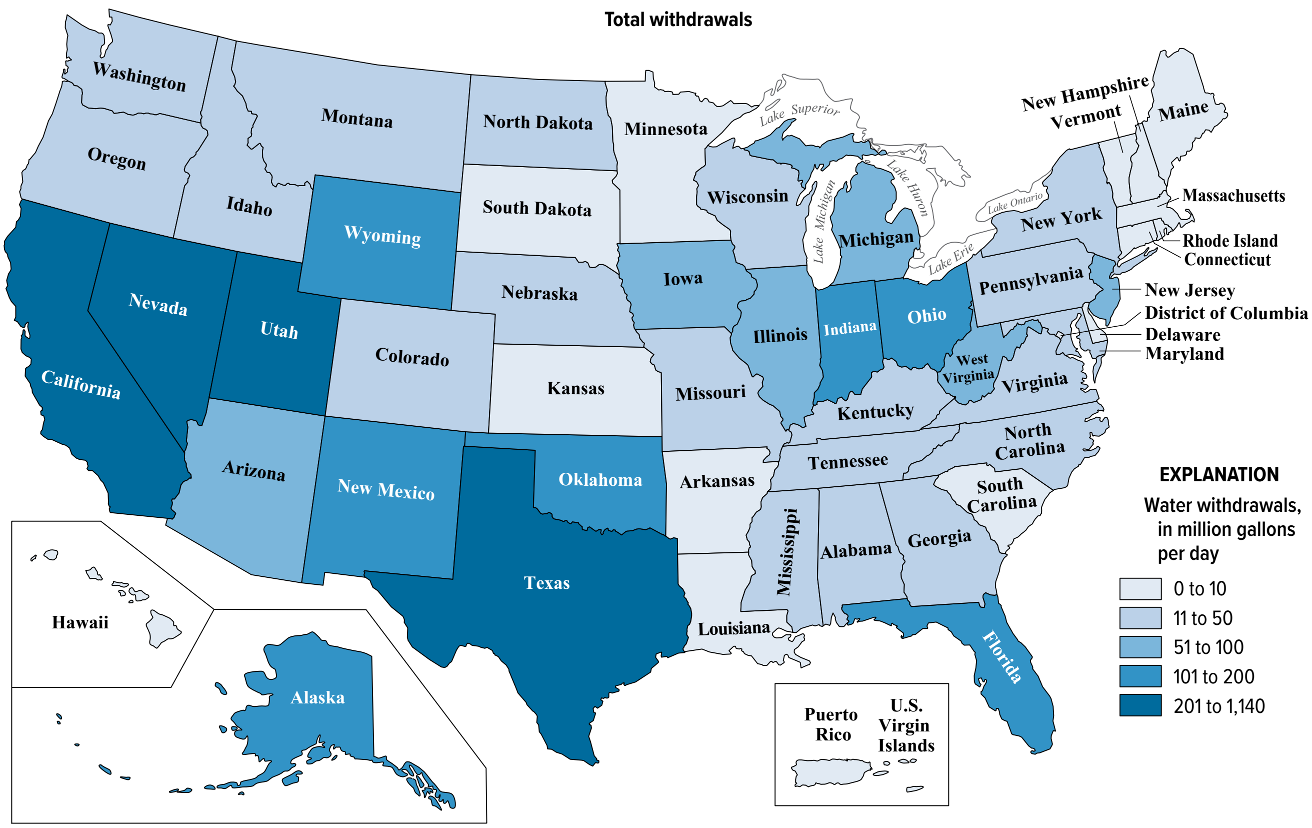


Figure 7. Resource extraction withdrawals by state in 2015[1]

Resource extraction also exhibits regional variation, with the greatest withdrawals for oil and gas and mining occurring in Texas, Oklahoma, and the Southwestern United States. An important feature of resource extraction is the fact that operations often take place in sparsely populated areas, far from existing infrastructure, for electricity, supplies and waste disposal. These characteristics increase interest within the industry in autonomous operations and treatment processes that do not require frequent supply of reagents. In addition, the Resource Extraction Sector must often source and treat its own water. In many cases, the activities involved in resource extraction itself make water available (e.g., large volumes of water are extracted from oil and gas wells and water is often generated when mine shafts are dewatered). This water often requires treatment prior to use and/or release to the environment. In some cases, the main concerns are associated with toxic constituents (e.g., metals, hydrocarbons) that are amenable to selective separation, whereas in other situations, the water contains high concentrations of ions and must be desalinated prior to use and/or disposal.

Given regional and temporal variations in water quality and water quantity, desalination of water from resource recovery operations will only be of interest in a limited number of locations, whereas selective removal of toxic ions or ions that cause scaling or clogging when discharged to the subsurface will be of broader interest.

INDUSTRIAL

	COOLING	BOILER	PROCESS	OTHER
Oil Refineries	55%	30%	10%	5%
Chemicals	60%	10%	25%	5%
Primary Metals	85%	2%	4%	9%
Food and Beverage	35%	5%	55%	5%
Pulp and Paper	5%	10%	80%	5%
Data Centers*	>95%	-	-	<5%

Figure 8. Fraction of water used within each industrial subsector for cooling water, boiler feedwater, process water uses, and other uses[5]

*Data Center onsite water use is primarily for cooling purposes, while Large Campus water use varies widely

Within the Industrial Sector, regional variation in water use patterns has some effect on water use and treatment technologies (e.g., industries that require large volumes of colling water, like primary metal manufacturers, tend to be located along rivers or lakes that provide an ample supply of freshwater). However, differences among industry types tend to play a larger role in water needs and the likelihood that a specific operation will adopt desalination or advanced water treatment.

The roadmapping effort indicated two main opportunities within the Industrial Sector: 1) technologies that enable or improve water use efficiency in boilers or cooling systems; and 2) approaches that lead to improved performance of treatment systems for process waters. With respect to the latter, research that supports process resilience or that employs sensors and actuators to reduce energy use and improve process performance would likely transfer among different industries. Within the topic of boilers and cooling systems, enabling autonomous operation, improving the removal of scale-forming ions, and managing residuals produced from recirculating cooling have great potential, especially if they can be implemented in small-scale, modular systems.

2.2. Approach to the Master Roadmap

The first step involved in identifying AOIs for the Master Roadmap was to screen the 89 AOIs in the Water User Sector Roadmaps to eliminate topics that pertained to only a single water sector. Although many of these topics are relevant to achieving our pipe-parity goals, they are more appropriately funded by industry groups (e.g., the Electric Power Research Institute [EPRI], Water Research Foundation [WRF]) and mission-driven government agencies (e.g., the U.S. Bureau of Reclamation [USBR], U.S. Department of Agriculture [USDA], Environmental Protection agency [EPA]), as noted in Figure 9.

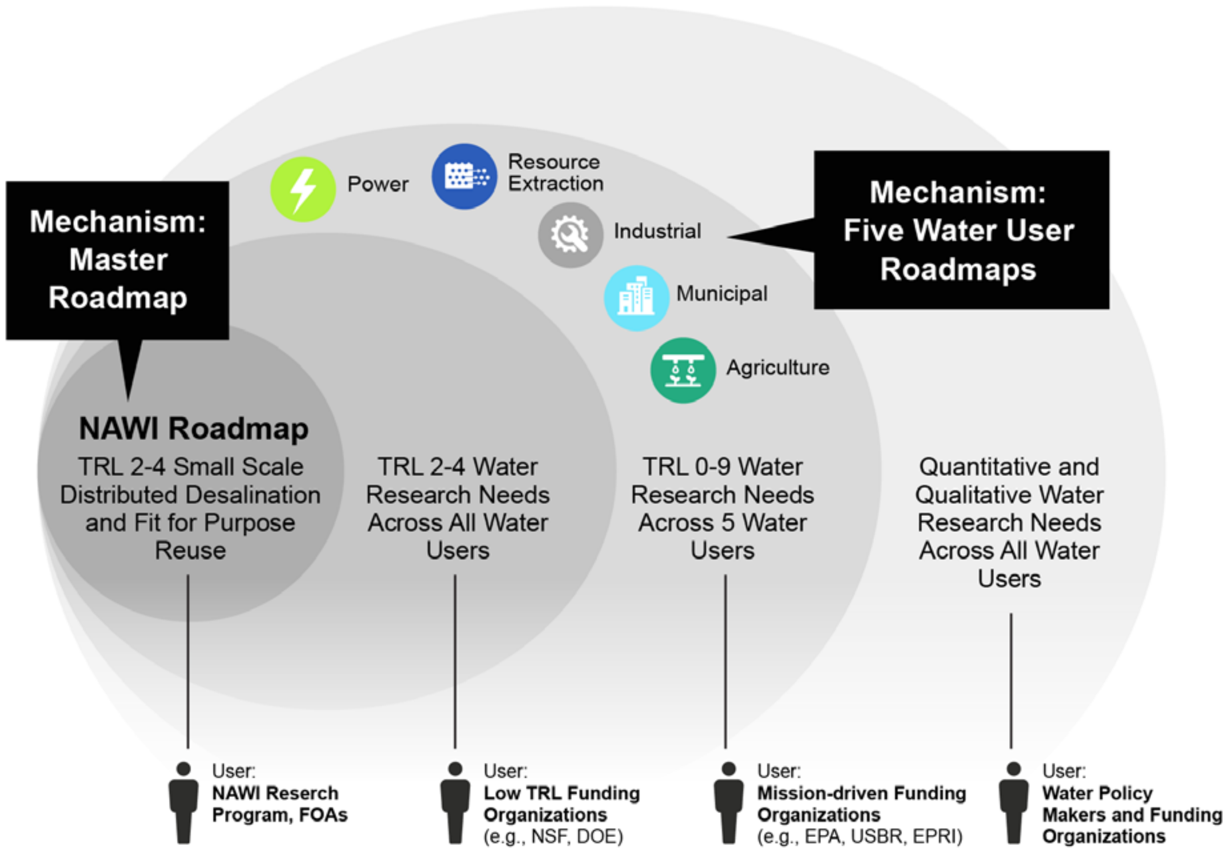


Figure 9. NAWI Master Roadmap in the context of other opportunities

Next, we screened to remove AOIs falling outside of NAWI's TRL 2–4 research mission. Finally, we consulted NAWI's RAC and Technical Team to identify cross-cutting AOIs omitted from the sector-specific roadmapping process. The final set of AOIs were then grouped according to themes within each of the A-PRIME Challenge Areas.

In the second screening step, we prioritized research that would benefit most from NAWI's research. AOIs where critical barriers to progress could be overcome by bringing established approaches into the water sector were of particular interest. AOIs that were well aligned with unique modeling, simulation, characterization, manufacturing, and testing capabilities of NAWI research consortium members were also prioritized. In contrast, AOIs that were unlikely to result in substantial advances within a five-year period (e.g., de novo development of water quality sensors) or exhibiting substantial overlap with research underway in support of other sectors (e.g., development of corrosion-resistant materials) were de-emphasized.

Finally, we analyzed the expected size of the opportunity and the potential for NAWI's research to make substantial contributions to pipe-parity. With respect to the size of the opportunity, we considered factors such as the volume of water that would likely be treated with the technology when it reaches maturity, the potential savings to users that could be realized by adoption of the technology, and the number of water user sectors that are struggling with the problem that would be addressed by the technology. Whenever possible, we attempted to use information from the Water User Sector Roadmaps, Baseline Analyses, or other well-respected sources to quantify these values. When this was not possible, we relied upon expert elicitation.

To analyze the opportunity for research to make substantial contributions to pipe-parity, we employed findings from the baseline analysis. The NAWI baseline case studies provided facility-level unit process details on cost and performance characteristics. NAWI evaluated 24 baseline case studies, addressing water issues across sectors and scales (Figure 10). In some cases, we employed scenario analyses to estimate the relative impact of research associated with some of the AOIs (e.g., how much would the levelized cost of water decrease if a new technology increased water recovery during desalination from 70 to 95 percent?). This approach was helpful in situations in which research had the potential to improve the performance of an existing unit process. For those topics in which research was more closely aligned with NAWI's mission of enabling small-scale, autonomous treatment systems, the analysis was focused on the potential for research to increase deployment of systems (i.e., we relied upon our previous analysis of the merits of distributed, autonomous systems described by Mauter and Fiske in their 2020 paper in "Energy & Environmental Science").[6]

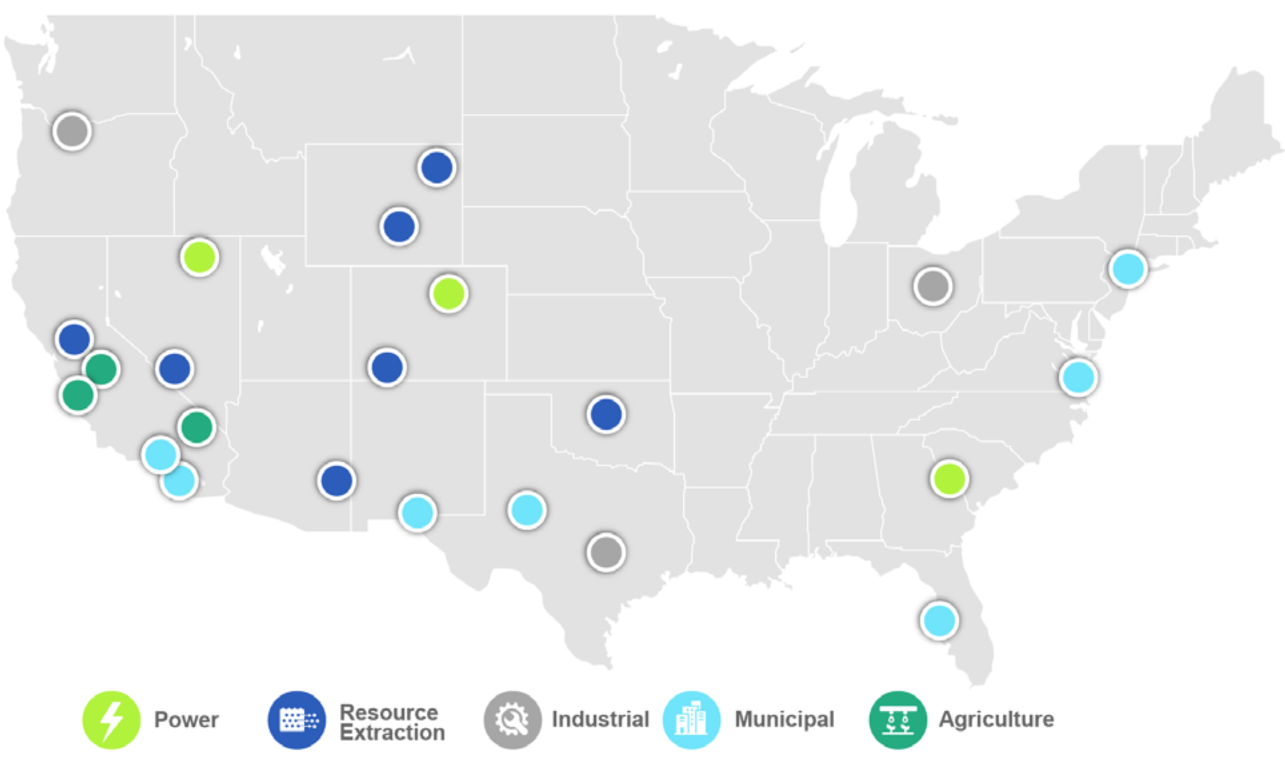


Figure 10. Map highlighting location and end-use type of NAWI baseline studies

A summary of NAWI's Priority R&D Investment priorities is depicted below (Figure 11). NAWI researchers assisted in quantifying and ranking the AOIs and the A-PRIME and Circular Water Economy Challenge Area priorities identified in the roadmapping effort. This analysis included estimates of the potential impact advancements on individual facilities combined with estimates of the extent to which issues and challenges are prevalent throughout end-use sectors. The potential for application for nontraditional water treatment was calculated by averaging the number of water-use sectors affected and the relative volume of nontraditional source waters affected if pipe-parity were to be achieved. The potential for pipe-parity improvement was based on quantitative analysis of NAWI baseline studies combined with experts' qualitative assessment of the ability for these technologies to improve pipe-parity across all metrics (e.g., lowering costs and energy use, increasing resilience and reliability). Assessment was informed by baseline analysis of existing system costs and energy performance as well as scenario analysis of future performance, whenever available. A mid-range ranking indicates NAWI research would have an estimated net improvement to pipe-parity metrics of about 25 percent for the targeted unit process and/or about 10 percent improvement to the overall system for a representative affected facility or facilities.

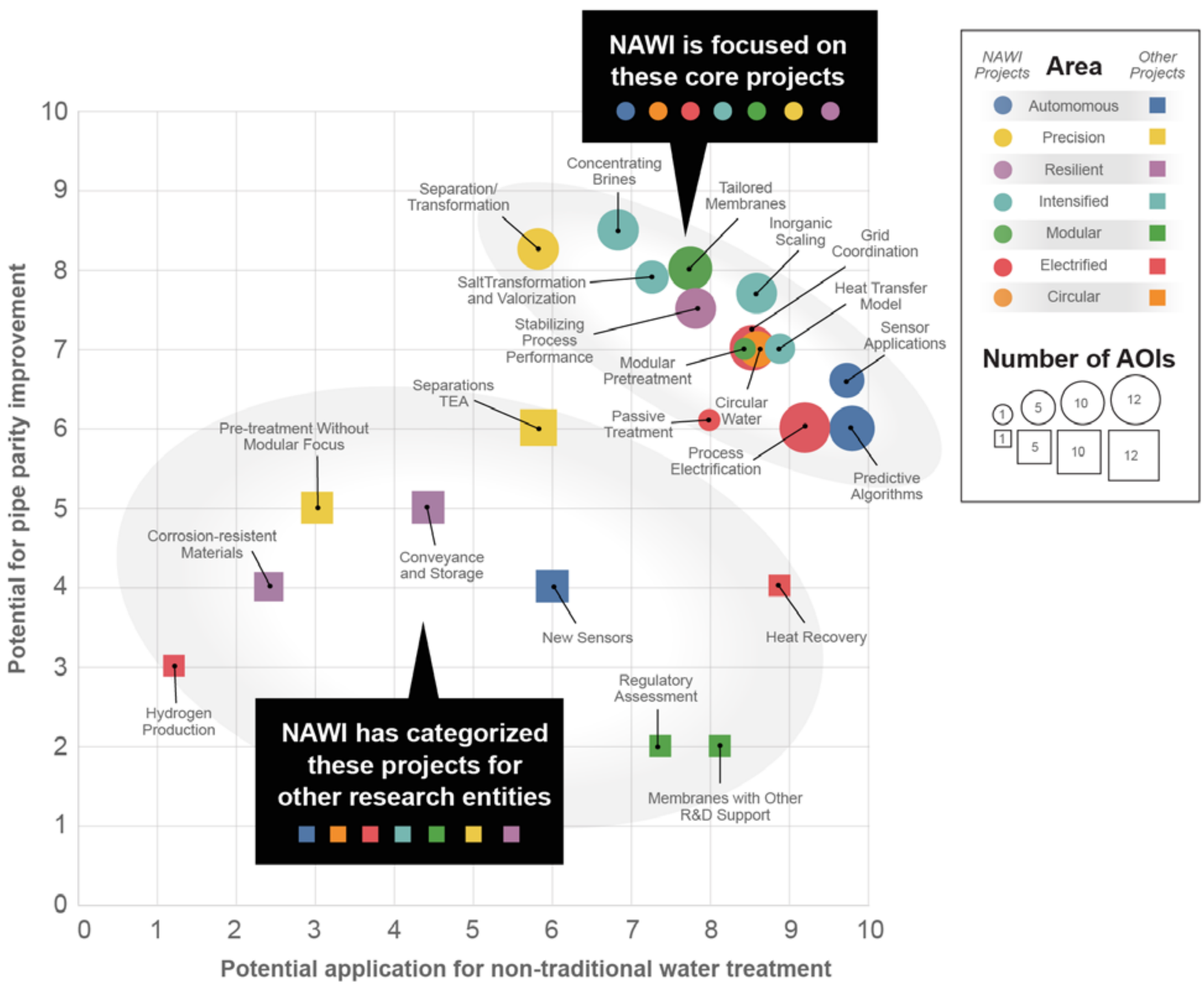


Figure 11. Prioritizing PRIMA roadmap AOIs for inclusion in Master Roadmap. PRIMA AOIs with similar scope are grouped for clarity. Marker color indicates the challenge area. Marker shape indicates whether it was determined to be in NAWI's scope. Marker size indicates the number of PRIMA AOIs that were relevant to this topic. Some PRIMA AOIs are included in multiple topics.

NAWI's Master Roadmap prioritization process produced 16 distinct AOIs that will guide NAWI's initial investments in high-priority research. Each Master Roadmap AOI draws from one or more Power[7], Resource Extraction[8], Industrial[9], Municipal[10], or Agriculture[11] roadmap AOI and can be mapped to an A-PRIME or Circular Water Economy Challenge Area (Figure 12). Each Master Roadmap AOI is described in detail in Section 4, and the NAWI PRIMA roadmaps are available on the NAWI website (https://www.nawihub.org/roadmaps).

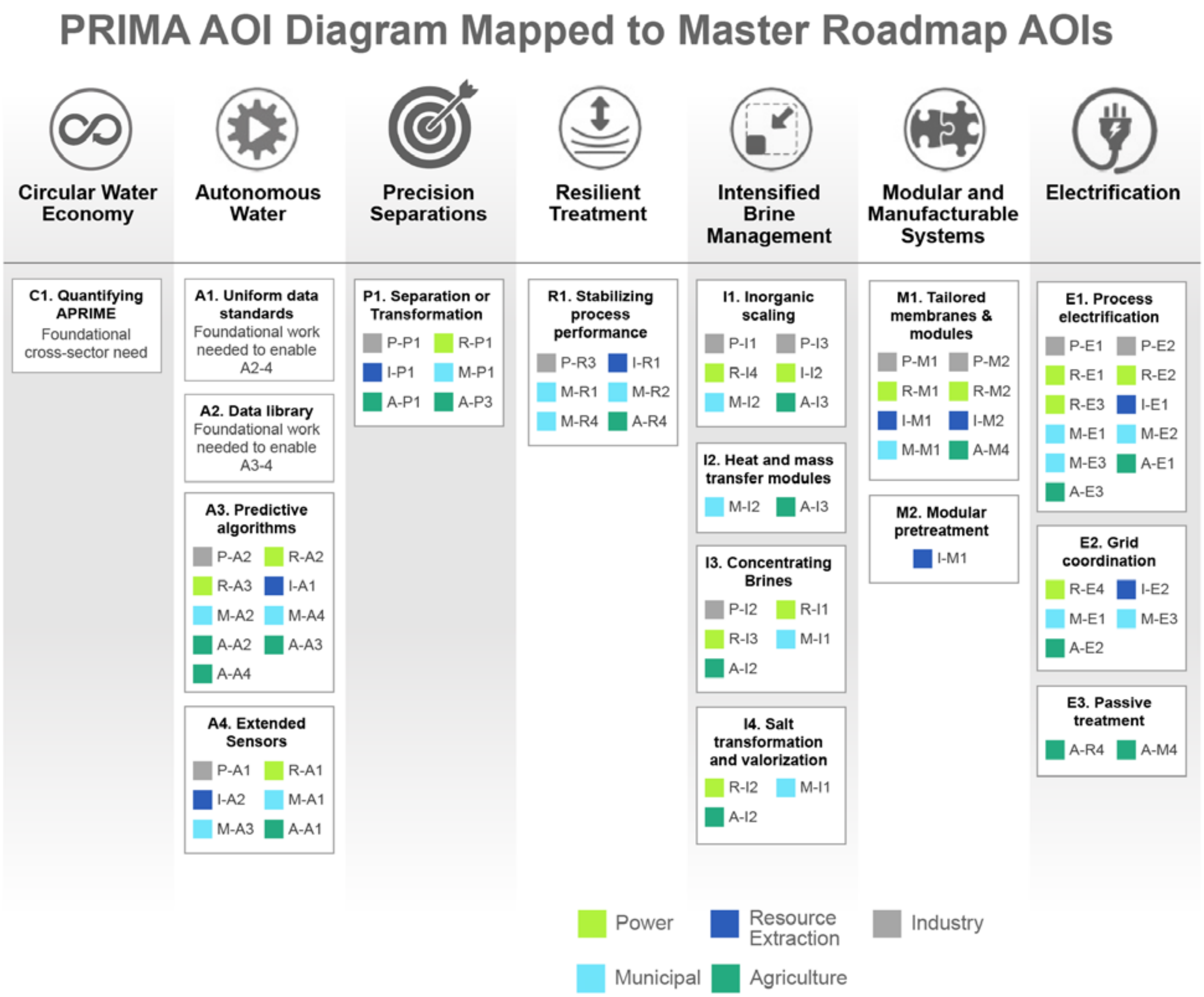
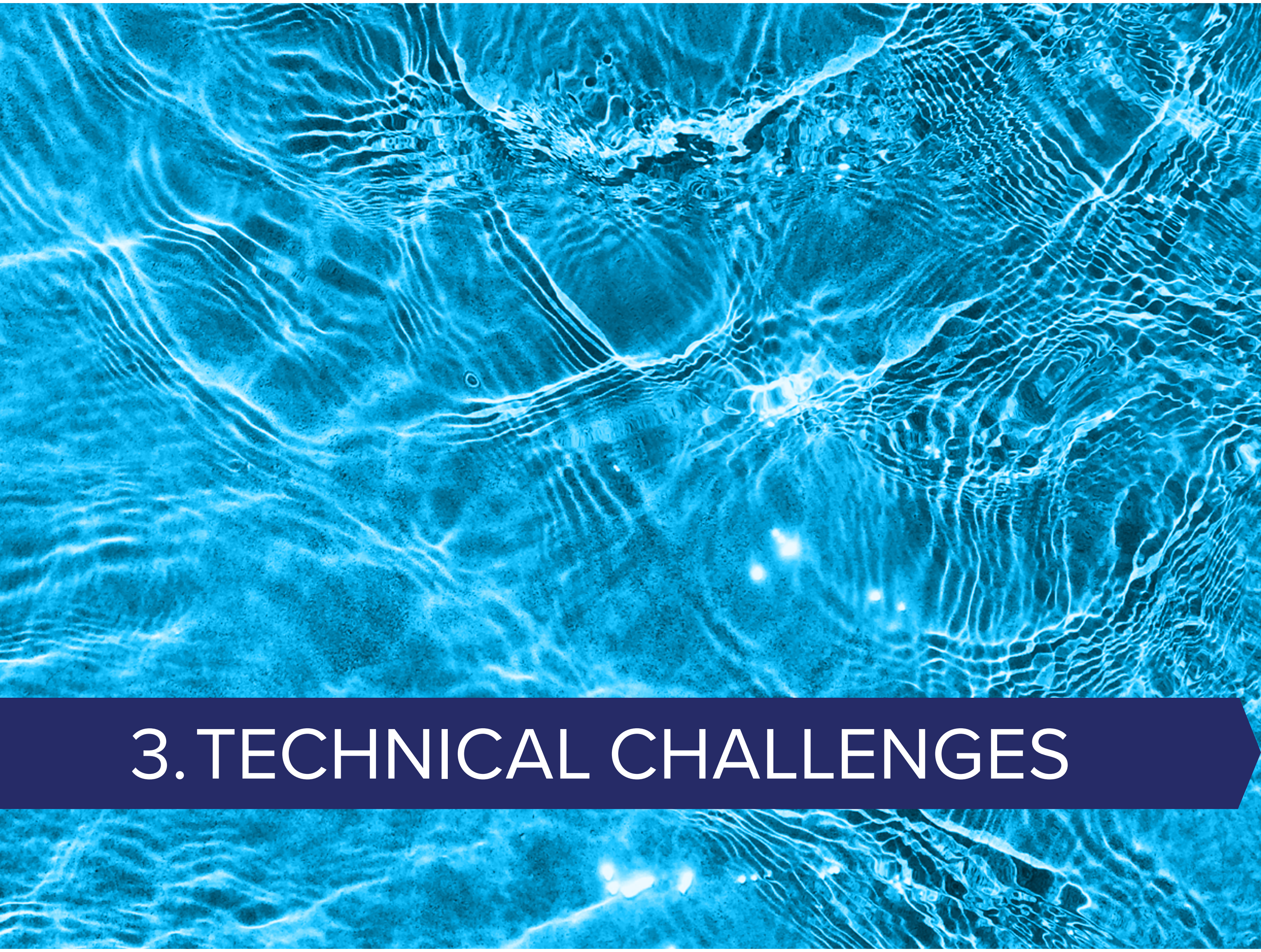
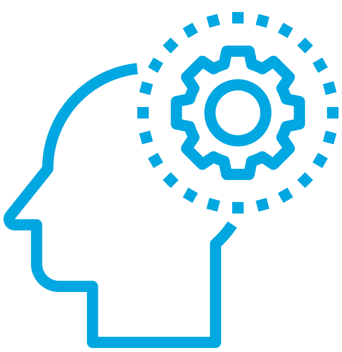


Figure 12. NAWI Master Roadmap AOIs mapped to PRIMA Roadmap AOIs



3. TECHNICAL CHALLENGES



Discussion of challenges and knowledge gaps associated with desalination and advanced water treatment can be divided into two categories: technical issues and non-technical issues. The technical issues are the focus of NAWI's research to promote the use of nontraditional water. Although they are not the primary focus of NAWI, non-technical issues are also important considerations in efforts to create desalination and water treatment technologies that are likely to be adopted. The individual roadmaps contain thorough discussion of these issues, which are summarized in the following section.

3.1. Technical Challenges

Infrastructure Integration

In some cases, an entity operating in a remote location may recycle water or install a desalination system that operates independently of existing infrastructure. More commonly, water recycling and use of nontraditional water sources are integrated into established water systems. As a result, their operation is enabled or constrained by the existing water system. In general, nontraditional water sources will be more easily and readily adopted if they are physically and technically compatible with existing plant and system designs, including piping, power supplies, and storage limitations.

Historically, water systems were often designed to capture economies of scale associated with treatment, water storage, and management. This resulted in conditions in which desalination and water recycling systems need to be compatible with centralized systems to ensure continued benefits from past investments and to integrate into existing management and regulatory institutions. This is particularly relevant in situations in which new water sources will be transported in existing water distribution systems. For example, the composition of drinking water produced by desalination must be adjusted (i.e., re-mineralized) in a manner that minimizes the leaching of lead and copper from distribution pipes and premise plumbing. To avoid added costs of replacing irrigation infrastructure, recycled water also needs to be treated to reduce the amount of labile organic carbon followed by addition of a disinfectant residual to minimize fouling of small-diameter pipes and irrigation nozzles.

The long service life of water treatment infrastructure magnifies the constraints that the need for integration puts on new technologies. New approaches face greater barriers to adoption if they disrupt the status quo and create stranded assets. This effect, often referred to as infrastructure lock-in, affects the timing, design, space constraints, water quality parameters, and other criteria for new water sources. Further, it can limit the timing for adoption of certain technologies. Water innovations that advance nontraditional water must consider both the effects of infrastructure lock-in that constrain their design and the ways in which these innovations exacerbate lock-in in the future.

In addition to these factors, water infrastructure in the United States has not been well maintained and needs significant investment, particularly in the municipal sector. As investments in infrastructure rehabilitation are made in the coming decades, an opportunity may arise to create hybrid municipal systems that allow distributed treatment systems to work in harmony with centralized systems. Such hybrid systems also may be adopted in the other water use sectors (e.g., industrial and agricultural water use).

For sectors located in remote areas (e.g., resource extraction, industry, water systems serving small clusters of homes), infrastructure to access, transport, and store water; dispose of waste; and provide related services (e.g., electric grid connection; internet) may not exist. It can be expensive to develop this support network, especially when it is needed to meet fluctuating water needs. Infrastructure is typically sized for peak water needs, which may only occur for periods of months to years in the Resource Extraction Sector or seasonally in the Agriculture Sector. These demands have limited flexibility, creating planning, storage, and/or treatment challenges that may be more significant for certain nontraditional waters. When distributed treatment technologies are adopted in any sector, their flexibility and modular nature may be an attraction: lowering costs, driving additional innovation, and promoting pipe-parity for desalination and advanced water treatment for nontraditional water sources.

System Variability

The diversity of water treatment requirements and site-specific differences among sectors increases the cost and complexity of treatment, especially of these is a lack of standardized technical solutions. This can be an impediment to technology adoption. The need for customization limits the potential for manufacturing efficiency for treatment technologies. Sectors with diverse water sources, treatment needs, technical and spatial constraints, and operating conditions have particular challenges, as there are limits on standardization that can occur within these sectors. This is particularly relevant in the Industrial Sector, where water uses vary considerably. It is also germane to the Power, Resource Extraction, and Agriculture Sectors.

Residual Management

In all sectors, management of brine produced during desalination and water reuse can be difficult and costly, especially in locations lacking convenient access to ocean outfalls or deep wells with conditions suitable for brine disposal. Storage, transport, and disposal of brines and other water treatment residuals (e.g., water treatment sludges) carry with them the risks of releases to the environment and associated impacts.

The degree of concern around residuals management varies geographically and by sector based on the composition and volume of the waste. Brine composition is affected by factors such as the local geologic conditions, nature of the activity (e.g., fossil fuel production often generates brines that are contaminated with hydrocarbons), and chemicals added to the water during industrial activities. The presence of toxic metals, organic chemicals, or other constituents (e.g., biocides, silica) can complicate treatment needs and the potential for valorization.

Concerns about residual management are relevant to pipe-parity in all five PRIMA roadmaps (Table 1). Existing brine management technologies are energy-intensive and often produce large masses of residuals, which are often contaminated with toxic substances. In many cases, experts indicated that this issue is the main factor slowing diffusion of desalination and fit-for-purpose water reuse.

ISSUE	POWER	RESOURCE EXTRACTION	INDUSTRIAL	MUNICIPAL	AGRICULTURE
Infrastructure Integration	4.1.3. 4.2.1. 4.2.2.		4.1.2.	4.1.1. 4.1.4.	4.1.4.
System Variability	4.1.1. 4.1.2.	4.1.1. 4.1.2. 4.1.3.	4.1.2. 4.1.4.		4.1.1.
Residuals Management	4.1.4.	4.1.4.	4.2.2. 4.2.4.	4.1.4.	4.1.4.

Table 1. Summary of References to Technical Challenges by PRIMA Roadmap Section Number

3.2. Non-Technical Challenges

3.2.1. Social Challenges

Economics

All five roadmaps described concerns about the low cost of water and its impacts on adoption of nontraditional sources. In most parts of the country, water is treated as an inexpensive and abundant commodity. As a result of past investments and water rights, many water users pay considerably less than what would be required to obtain additional water (i.e., the marginal costs of water). Across all water sectors, users expressed concern about their water costs increasing as they experience scarcity or adopt nontraditional water sources. As a result, nontraditional water sources must overcome the institutional inertia associated with continued access to low-cost water sources by users who have existing water resources.

Institutional conditions

Institutional fragmentation affects water users and often serves as an impediment to the adoption of new technologies or business models. For example, in the Municipal Sector, water utility managers often view distributed water treatment and fit-for-purpose reuse with suspicion because it falls outside of their purview. It also threatens their revenue streams. Water users in the Power Sector may find it challenging to partner with water and wastewater treatment utilities to manage their water treatment residuals, while industrial water users that could easily adopt new technologies may have little incentive to adopt recycling if they already have historic water rights that allow them to use large amounts of surface water. Policymakers have begun to advocate for a shift toward to a “One Water” approach, which encourages coordination between water users to facilitate additional reuse. However, this ideal will remain elusive as long as many different entities are responsible for different aspects of the water cycle.

Social acceptance

Even if advancements in water recycling and access to nontraditional water treatment succeed technically, a lack of public acceptance can preclude adoption. A lack of trust in authorities (i.e., industry, regulators, and utilities) can be regional, cultural, or societal. Historical controversies associated with water access and water quality have lowered trust in some sectors. These issues, whatever their source, can manifest as opposition to water supply projects or decreased value in products produced with the unfamiliar water sources. Gaining the public’s trust in the use of nontraditional water sources requires transparency, demonstrations of competence, and effective engagement with the full range of stakeholders to address pragmatic, moral, and cognitive concerns.

Workforce development

Adoption of nontraditional water sources also may require better education and training of the workforce. In the Municipal Sector, specific concerns were raised by stakeholders about the large portion of system operators that are nearing retirement. Increasing the complexity of water systems poses concerns in other sectors, because water is typically not the industry’s primary focus. If new water technologies require a substantial amount of new expertise among users, the high costs of workforce development may slow the rate of adoption and limit the functionality of systems. Alternatively, autonomous systems may reduce the need for additional training for operating complex water systems.

3.2.2 Regulatory Challenges

Public health

To protect public health, drinking water, water used for irrigation of crops, and water used for landscaping must comply with state and federal regulations. With respect to chemical contaminants, the presence of toxic metals (e.g., arsenic, uranium), organic compounds (e.g., 1,4-dioxane, NDMA, PFAS), and nitrate may necessitate additional treatment prior to water reuse or brine disposal. Pathogenic microbes also are a concern for public health (e.g., the use of recycled water or water from nontraditional sources could create inhalation risks with respect to Legionella in cooling towers and municipal water systems). Furthermore, worries that some yet-to-be-discovered contaminants that pose potential public health risks will occur in recycled water or water from a nontraditional source pose potential barriers to adoption of fit-for-purpose recycled water systems.

Environmental health

To protect aquatic organisms and wildlife, the potential for residuals produced by desalination and water recycling systems (e.g., RO brines) to pose ecological risks must be considered in the development of desalination and fit-for-purpose water recycling systems. For example, stringent discharge requirements for metals, nutrients and toxic trace organic contaminants may require frequent monitoring of discharges from water recycling facilities, power plants, and resource extraction operations. Furthermore, the discharge of brines can pose substantial risks for freshwater systems in which organisms are not adapted to high salt concentrations.

Water rights

Water rights dictate access to certain nontraditional water sources that could create challenges. Water rights are managed at the state level, with some states following riparian rights derived from common law, others (particularly in the water-scarce West) following appropriative rights and still others using a combination of the two. Surface and groundwater rights may be managed separately or in conjunction with each other as governed at a state level. The complexity of U.S. water rights also complicates plans for accessing nontraditional water sources. For example, in some Western states, downstream water rights and flow mandates may restrict the ability of an upstream user to recycle water that would otherwise be discharged to a river.

3.2.3 Environmental Challenges

Climate Change

Climate change is one of the biggest factors driving interest in water recycling and the exploitation of nontraditional water sources. Climate change impacts surface water supplies through more frequent droughts, increasing frequency of large storms (which may drive the operators of reservoirs to maintain lower water levels to avoid risks of dam failures), and warmer temperatures (which drive up water demand and reduce the amount of water-reaching reservoirs, rivers, or groundwater). Climate change also may complicate efforts to exploit nontraditional sources (e.g., through an increasing frequency of algal blooms near the intake of seawater desalination facilities or increasing salt levels in municipal wastewater and agricultural drainage water).

Concerns about climate change are also leading to greater scrutiny of direct and indirect greenhouse gas emissions associated with water-related operations. With respect to energy use, decarbonization of the energy sector will address many of the indirect emissions concerns, but the release of methane and nitrous oxide by advanced water treatment systems poses concerns even after fossil fuels are phased out. There are also opportunities for using desalination systems to support climate change mitigation (e.g., taking advantage of the capacity of certain brines to serve as sources of alkalinity and as carbon sinks and using them in carbon sequestration projects).

Sustainable Resource Use

Future water decisions may increasingly be constrained by expectations that resources will be used in a sustainable manner (i.e., ensuring future generations will continue to benefit from investments in water systems). This issue is particularly germane to the use of brackish groundwater in many locations. Because this "fossil groundwater" is not being recharged, these nontraditional resources will be fully depleted eventually, which might lower the attractiveness for exploiting this resource. Conversely, recovery of mineral resources like phosphorus and critical elements from desalination brines or industrial waste can contribute to sustainable resource use and might be valued by society when considering sustainability in the design of water systems.

Table 2. Summary of References to Non-Technical Challenges by PRIMA Roadmap Section Number

ISSUE	POWER	RESOURCE EXTRACTION	INDUSTRIAL	MUNICIPAL	AGRICULTURE
SOCIAL CHALLENGES					
Economic/Costs		4.2.1.	4.2.1.	4.2.1.	4.1.1.
Institutional Conditions					4.2.2.
Social Acceptance/ Equity	4.2.3.	4.2.6.		4.2.1 4.2.2.	4.2.1.
Workforce Training	4.2.4.	4.2.5.	4.2.5.	4.1.5.	
REGULATORY CHALLENGES					
Public Health		4.2.3.		4.1.5.	4.2.2.
Ecological Impacts	4.2.3. 4.2.5.	4.2.3.		4.1.5. 4.2.2.	4.2.3.
Water Rights	4.2.5.			4.3.	
ENVIRONMENTAL CHALLENGES					
Climate Change Adaptation	4.2.3.	4.2.3. 4.2.4.		4.4.	4.2.3.
Climate Change Mitigation					4.2.3.
Sustainable Resource Use				4.4.	

4. AREAS OF INTEREST

A-PRIME Enables Pipe-Parity

To overcome the challenges presented in Section 3, this roadmap identifies the following set of high-impact research priorities that NAWI will explore to expand the use of nontraditional source waters for the nation.

All the priorities are grouped under the A-PRIME categories: Autonomous, Precise, Resilient, Intensified, Modular, and Electrified. Advanced desalination and reuse will require a new generation of low-cost modular processes that are inexpensive to customize, manufacture, operate autonomously, and maintain. This shift to small, connected, “appliance-like” water treatment systems that are mass-manufactured cannot be achieved by simply scaling down existing treatment plant designs or introducing marginal improvements to current treatment processes. Instead, there is a need for a suite of next-generation desalination technologies that autonomously adapt to variable water chemistry, precisely and efficiently remove trace contaminants of concern, are robust to process upsets, desalinate water and concentrate brines in as few modular units as possible, are readily manufactured, and do not require a constant resupply of consumable chemical reagents. ***Investing R&D resources in the following priorities will lead to a revolution in desalination and treatment processes for the nation.*** Each identified AOI contains a short description, along with research targets and questions.

4.1. Autonomous Water

Sensors networks and adaptive process control for efficient, resilient, and secure water treatment systems.

In most situations, water treatment systems require human intervention (i.e., decisions made by operators) to adapt to variations in water quality, take into account the effects of component degradation, and correct operational failures. Coupling advanced sensing and control networks with models that account for interdependencies between unit processes will facilitate the deployment of a network of autonomous distributed water treatment systems. The innovations required to create such systems could also improve the performance of centralized treatment systems by enhancing process efficiency and reliability, while simultaneously reducing the number of trained personnel needed to maintain and operate treatment systems. Together, these innovations could significantly lower the cost of both centralized and distributed desalination systems.

Although considerable progress has already been made in the development of simple sensor and actuator systems for individual water treatment processes, numerous early-stage applied research challenges remain before integrated autonomous systems can reach their full potential. For example, existing Supervisory Control and Data Acquisition (SCADA) systems that control treatment systems are often unable to access data collected in pretreatment modules or data from grab samples collected by treatment plant operators. To realize the promise of the digital twin approach, a standardized and generalizable platform that can be used to manage data and assure that control systems are secure against manipulation by unauthorized users is needed.

This platform will enable researchers to access large amounts of data from operating water treatment trains in a manner that allows them to create robust process models capable of taking advantage of the power of information technology. By making large amounts of temporally resolved data from operating treatment plants available, researchers will be able to test new approaches for detecting process upsets and operating interdependent water treatment processes in a more efficient and robust manner. Finally, substantial improvements in addressing data sparsity or drift-through improvements in fault detection and self-calibration or improvements in sensor systems will further improve the performance and reduce the cost of autonomous water treatment systems. By taking advantage of the latest developments in sensor design and data processing and analysis, it will be possible to lower the cost of collecting data, which will provide a basis for continuously adjusting processes to make them more robust and cost-effective.

4.1.1 Summary Priority Areas of Interest.

1. Uniform metadata schemas for water treatment trains:

By adopting standardized metadata schemas, it will be possible to rapidly deploy advanced analytics and controls platforms that access all of the information being collected at water treatment facilities. Identification of such metadata will require the development of a data library and an informatics platform.

2. Water treatment data library:

The creation of an accessible data stream consisting of sensor and process operation data from approximately 20 full-scale treatment trains will provide a testing platform against which researchers can evaluate the potential for robust water treatment analytics to improve the overall efficacy of desalination processes.

3. Predictive algorithms for process control and fault detection:

With the assistance of the aforementioned data stream, researchers can generate and evaluate algorithms that optimize process control settings, prevent process upsets, optimize sensor placement, and predict process performance under a range of conditions.

4. Extended capabilities of deployable sensors:

Fundamental advances, including the development of more robust materials, lower-cost sensing platforms, and better communication capabilities, along with the development of sensors that do not come into contact with water, can reduce the costs of collecting data under the conditions encountered in water treatment systems.

4.1.2 Targets

1. **Develop a standardized metadata schema** that can be applied across diverse desalination facilities.
2. **Develop research infrastructure** in the form of high-temporal-resolution data streams from over 50 diverse facilities, enabling researchers and commercial entities to rapidly test alternative control schemas and assess their impact on pipe-parity metrics.
3. **Use autonomous detection** of critical water quality parameters to adapt process configuration and performance to reduce catastrophic failures and process upsets by 50 percent, reduce the frequency of routine maintenance, and lower the operational factor of safety by 50 percent.

4.1.3 Area of Interest Descriptions

AOI A-1: Uniform metadata schemas for rapid adoption of secure and functional digital infrastructure[1,2]

NAWI's vision for autonomous water treatment trains requires a robust, open-source, and secure infrastructure system that integrates hardware, software, communications, analysis, control, and operator oversight. Although SCADA systems and Programmable Logic Controllers (PLCs) currently support treatment plant operations, their current implementation is the result of piecemeal development over a period of decades. As a result, it is difficult to integrate the operation of treatment trains in a manner that allows plant operators to capture the process improvements that can be realized during autonomous operation. We seek a unified, open-source metadata schema (sometimes referred to as an Internet of Things [IoT] stack) that builds upon existing sensing and control platforms and promotes cross-sector collaboration to enable breakthroughs in performance for the entire water treatment train. Fundamental challenges associated with the development of an IoT stack for water include assuring that data remain safe, secure, and private; leveraging the tremendous quantity of data collected by sensors embedded in existing treatment trains; and enabling end users of varying technical abilities to manage, control, and program IoT-enabled treatment trains.

NAWI's research activities will focus on developing a uniform metadata schema that supports data integration from multiple sources (e.g., multiple SCADA systems, laboratory measurements, sensors, energy use data, weather predictions, distribution system monitoring). The developed metadata schema will support rapid deployment of advanced analytics and controls platforms at new and existing water treatment facilities. Our research in this area will also focus on translating and customizing IoT infrastructure developed for other applications (e.g., building controls) to water treatment systems, with emphasis on new end-user open-source tools that address the critical data management needs of water users.

AOI A-1.
RESEARCH QUESTIONS (RQS):

- What are the characteristic types, formats, and frequencies of data collection at desalination facilities?
- What consistent relational features exist across facilities?
- How will changing influent water conditions, degradation of component performance, or sensor quality issues such as drift, fouling, etc., be represented and documented in this schema?
- What types of data will utility operators need to improve real-time decision-making?
- What would a "standard of practice" applicable to municipal water data collection, storage, and dissemination include, and is there a need for one?

1. Ag.A3. Develop automated digital network (e.g., IoT, SCADA, digital twins, artificial intelligence) systems for integrated water quality data analysis, data-driven decision-making, process monitoring, and control for optimized water treatment.

2. Ind.A1. Automate decision-making and control of water treatment processes based on big data and using machine learning algorithms. Ind.A1.4 (seamless integration between data collection and process control devices and to ensure cyber security), Ind.A1.5 (Digital twin system of existing water treatment system for large data collection, parallel comparison, supervised learning of algorithms, and calibration of mechanistic models)

AOI A-2: Water treatment data library: A virtual testbed for evaluating process control applications

A comprehensive, high-temporal-resolution water treatment plant database has been a critical barrier to the development of autonomous process control applications (e.g., analytics, predictive control, fault detection) for water treatment plants. We seek a diverse and representative library of treatment plant data to rapidly accelerate R&D progress for desalination. Data should be described using the uniform metadata schema described in AOI A-1 and should fully represent a complete treatment train at appropriate temporal resolution for a minimum of one year of operation. We seek to build a library consisting of at least 20 water desalination and reuse treatment trains, based at 15 or more locations. The data should be stored in NAWI's Water Data Analysis and Management System (WaterDAMS), the secure, flexible, and adaptable data management system enabling both private and public dataset access. A minimum of 50 percent of the uploaded data should be available to the public.

AOI A-2.
RESEARCH QUESTIONS (RQS):

- What facility characteristics (e.g., treatment train unit processes, scale of facility, duration of data set) constitute a representative sample of plants for a NAWI data set?
- Given the reality of changing influent water conditions, degradation of component performance, or sensor quality issues such as drift, fouling, etc., at desalination plants what is the minimum duration of data that might constitute a complete data set?
- What degree of anonymity will be required for data-sharing consent?
- What fee-for-use or other structure might be adopted for the data set to sustain its long-term curation and maintenance?

AOI A-3: Predictive algorithms for process control and fault detection[3,4,5,6,7,8]

Autonomously managed water treatment systems are particularly well-suited for responding to variable water quality, especially during the period when treatment trains are first deployed or when source water quality fluctuates in an unanticipated manner. Although many water treatment systems are outfitted with arrays of sensors, presently the data are used mainly for detecting system failures. NAWI's research in this area is intended to shift the paradigm for data use in water treatment systems from preventative monitoring to adaptive control. Research shall focus on developing: 1) real-time, data-driven tools that optimize process control settings for improved treatment train performance (e.g., reducing the cost or energy needs of treatment processes by continuously adjusting settings) and adaptability to variable influent composition or required treated water quality; 2) methods for early detection, attribution, and correction of system faults (e.g., sensor drift; cyberattacks, upset recovery); and 3) methods to assess model predictive ability, robustness, interpretability, and interoperability across treatment trains to reduce the need for extended calibration and training periods. Researchers are expected to employ the NAWI data stream (i.e., AOI A-2) to develop and test algorithms for a variety of water treatment trains and operating modes (e.g., intermittent operation) of relevance to NAWI's vision of autonomous, distributed treatment systems.

The potential savings associated with predictive control are difficult to quantify without grounding in actual facilities. At one end of the spectrum is the prevention of plant shutdown by predictive control, which could have substantial benefits in many applications. At the other end is autonomous control, allowing operations to be optimized. This has the potential to decrease energy use and improve system performance, but the overall impact on operations and pipe-parity will depend upon current practices and efficiency gains that can be realized by automation.

3. Power.A2. Develop artificial intelligence and algorithms to integrate sensor data with dynamic system operation and control.

4. ReEx.A2. Develop automated data collection and processing programs and platforms to identify trends in process performance and anomalies; trends in feed, product, and brine chemistry; and early warning signals of changing influent water quality that allow adjustments to process performance.

5. ReEx.A3. Develop model-based control and data-driven models (digital twins) to enable optimization of process set-points and process dynamics, leading to energy reduction, fit-for-purpose quality, and optimal water productivity and recovery.

6. Ind.A1. Automated decision-making and control of water treatment processes based on big data and using machine learning algorithms.

7. Muni.A4. Develop digital twins of water treatment plant and artificial intelligence to drive the autonomous operation of the treatment plant.

8. Ag.A2. Apply machine learning models and algorithms to data from sensors and other sources to develop crop, process, and source water-specific agricultural water quality standards, and to minimize the costs of alternative source water treatment, storage, and delivery.

AOI A-3.

RESEARCH QUESTIONS (RQS):

- What controls and autonomous process optimization approaches are most reliable, effective, and facile to implement at representative desalination facilities?
- What are the most cost-effective strategies for mitigating the effects of sensor errors, drift, fouling, etc., on controls schema performance?
- Are preferred controls approaches a function of system size, installed treatment trains, operational mode (e.g., steady state; non-steady state), etc.?
- What are the optimal or improved sensing configurations for representative water treatment processes that enable controls approaches that optimize performance?
- Are there hardware shortcomings in water treatment systems or data availability limitations that prevent implementation of various control schema?
- What level of autonomy can be achieved at certain costs? Do cost and energy savings from sensing and controls schemas exceed these costs?
- How can control algorithms be implemented effectively enough to reduce operating expenses by more than 20 percent, energy use by 10 percent, time out of compliance by 90 percent, and downtime for maintenance by 10 percent over long durations and in several operational “challenge” conditions (e.g., changing influent water conditions, degradation of component performance, or sensor quality issues such as drift, fouling, etc.) at operational NAWI desalination testbeds?

AOI A-4: Extend capabilities of existing sensing platforms to support autonomous desalination[9,10,11,12,13,14]

Existing sensor platforms provide inadequate information for process control applications or are expensive and require considerable effort to maintain. To support autonomous desalination and water reuse systems, NAWI seeks innovative approaches for augmenting sensor capabilities by deploying new types of sensors or by using existing sensors in new ways. These include approaches for extending the lifespan or dramatically lowering the cost of sensor deployment and reducing the need for calibration (e.g., self-calibrating sensors) under conditions typical of water treatment systems (e.g., in the presence of salts, microbes, particles, or elevated temperatures). Low TRL research that supports autonomous operations through the deployment of new types of sensors, including non-intrusive load monitoring approaches, soft sensors, smart cloud enabled sensors, and sensors that do not come into contact with water (e.g., vibrational sensors, light sensors) are also topics of considerable interest.

AOI A-4.
RESEARCH QUESTIONS (RQS):

- Develop approaches for monitoring critical treatment train performance parameters (e.g., sensors external to the plant or those that do not come in contact with water), parameters that are not routinely monitored (e.g., Parallel Factor [PARAFAC] analysis of organic matter) or process performance (e.g., acoustic sensors that monitor equipment status) that have the potential to circumvent many of the limitations of existing real-time monitoring systems. We seek sensor innovations that demonstrably improve the balance of automation system costs relative to operational cost savings relative to the status quo.

9. Power.A1. Develop sensors and sensor groups for bulk assessments of diverse water quality parameters that can indicate organic, inorganic, biological fouling propensity, surface corrosion, and water quality violations.

10. ReEx.A1. Develop reliable, robust sensors suitable for the complex, harsh environments and varying water quality present in oil and gas and mining applications. Sensors should be developed to enable advanced autonomous control systems in distributed and often remote produced water and mining wastewater treatment plants and to reduce the cost and turnaround time of water analysis.

11. Ind.A2. Use advanced sensors to monitor water quality online.

12. Muni.A1. Develop inline or near real-time sensors for monitoring the removal of pathogens and contaminants of emerging concern (CEC) for municipal wastewater reuse.

13. Muni.A3. Create sensors or sensor groups that can report the propensity for fouling and inorganic scaling.

14. Ag.A1. Develop and use rapid, real-time, low-cost sensor groups and associated monitoring and control systems to detect target pollutants/constituents (e.g., pathogens, selenium, phosphorus, nitrogen), with a focus on elements with fluctuating concentrations.

4.2. Precise

Targeted removal of trace solutes for regulatory compliance, enhanced water recovery, and resource valorization.

Most water treatment systems rely on inefficient bulk separation processes (e.g., pressure-driven membranes) to remove solutes that occur at trace levels. Although they are effective, they create a waste management problem by also removing other solutes. A more targeted approach to trace contaminant removal can reduce the cost and energy intensity of treatment processes while simultaneously reducing system complexity and waste management costs. Precision separation also enhances the likelihood of profitable recovery and valorization of brines, thereby offsetting the overall costs of desalination systems.

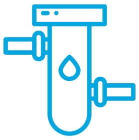
In recognition of the potential benefits of precision separation, considerable effort has been directed at contaminants that must be removed to enable specific water uses. For example, selenium—a contaminant that is often found in high concentration when water from locations with high levels of certain naturally occurring minerals evaporates—often undergoes biological treatment processes or treatment with anion exchange resins to remove it from agricultural drainage and mining wastes. However, the complexity of biological processes and the need to convert selenate to selenite prior to separation, as well as the high costs of sorbent materials, limits the application of such processes. For seawater desalination, the need to remove dissolved boron during RO often necessitates additional treatment steps that increase the cost, energy consumption, and size of treatment plants.

Over the past three decades, chemical oxidation (i.e., advanced oxidation processes) has emerged as a cost-competitive process for transforming or mineralizing contaminants that are not removed during desalination (e.g., 1,4-dioxane). However, the nonselective nature of the hydroxyl radical—the main oxidant employed in these processes—greatly reduces the efficiency of this approach when it is used to treat water that contains organic matter, bicarbonate, or other radical sinks. In contrast, reductive processes can exhibit much greater precision. For example, inexpensive scrap iron has been employed in permeable reactive barriers to dehalogenate solvents like trichloroethylene in contaminated groundwater. Likewise, solvated electrons produced from water radiolysis or by photolysis of precursors like sulfite can selectively reduce recalcitrant contaminants like per- and polyfluoroalkyl substances (PFAS) in the presence of other solutes, provided that dissolved oxygen is removed prior to treatment. Although they offer great potential, selective reduction of trace contaminants is not widely used in water treatment because it is energy-intensive and capital-intensive.

NAWI is interested in early-stage applied research to improve the selectivity of materials for precision separation and to enable the use of precision reactions to transform trace contaminants. We seek novel materials with high selectivity and affinity for target species, fast uptake kinetics, and efficient regeneration steps that are amenable to manufacturing at scale. We also seek new approaches for employing chemical reactions to transform trace contaminants in the presence of high concentrations of other solutes.

4.2.1 Summary Priority Areas of Interest

1. Trace contaminant separation or transformation:



By developing novel approachesfor the removal (and possible recovery) of metals, metalloids, nutrients, and trace organic contaminants, pipe-parity can be advanced by reducing the complexity of treatment trains and increasing the potential for valorization of wastes.

4.2.2 Targets

1. **Develop technological solutions to address contaminants** within at least one of four priority classes of contaminants: oxyanions, nutrients, metals, and organics. Priority classes of contaminants/end-use water sectors outside of this list will be considered if they present a sufficiently strong case for game-changing impact.
2. **Develop technological solutions that apply to contaminant problems** in at least one of five PRIMA water end-use sectors (Power, Resource Extraction, Industrial, Municipal, and Agricultural).
3. **Develop technological solutions that are adaptable** and are not one-off sorbents/solutes for a niche application.
4. **Develop technological solutions that demonstrate substantive improvements** over state-of-the-art approaches across multiple pipe-parity metrics relative to status quo technologies without seriously compromising other pipe-parity metrics.
5. **Encourage material development or process improvements** that advance a separations platform from TRL 2 (technology concept and/or application formulated) to TRL 4 (component and/or system validation in a laboratory environment).

4.2.3 Area of Interest Descriptions

AOI P-1: Trace contaminant separation or transformation[15,16,17,18,19,20,21,22,23,24,25]

Precision separation of trace constituents during water treatment may provide substantial cost and energy savings for desalination systems by avoiding energy-intensive bulk separations, reducing the size and complexity of the treatment train, reducing the cost of managing residual wastes, or valorizing recovered materials. NAWI seeks precision separations platforms applicable across a range of selective inorganic and recalcitrant organic constituents, including metals, metalloids, nutrients, and trace organic contaminants that hinder specific water reuse applications. Approaches that exhibit small footprints, fast kinetics, and process stability when encountering variable water quality are particularly attractive because they may be well-suited for distributed treatment trains.

As with other projects, the research must demonstrate substantive improvements over state-of-the-art approaches across multiple pipe-parity metrics. Supporting analysis for precision separations projects will aid in minimizing overall costs by considering the amount, type, and purity of feed, concentrate, and product streams. The approach should explicitly consider the transportation, treatment, concentration, use, and/or disposal of each constituent, as well as the impact of widespread adoption of valorization on the market for relevant products under conditions relevant to parts of the United States, where desalination is likely to become important. The analysis should also account for relevant factors such as geological conditions, regulations, and social acceptability of the environmental release of constituents in the waste materials. Where appropriate, the approach should employ or be capable of being integrated within existing NAWI efforts such as WaterTAP and ProteusLIB.

15. Power.P2. Create effective methods for purification and extraction of valuable compounds in power plant discharge water.
16. Power.Plus2. Identify market value of specific compounds with detailed techno-economic assessment.
17. ReEx.P2. Develop and expand selective separation technologies (e.g., membrane, sorption, ion exchange) for selective separation of metal ions and nutrients that inhibit downstream processes or selected end uses and to recover valuable minerals while treating complex produced waters, mining waters, and their concomitant brine streams.
18. Ind.P2. Investigate selective separation and recovery of metal ions and nutrients from waste and brine streams (porous materials and membranes with precise control of morphology, pore dimension, surface chemistry that enable selective transport or binding; selective catalytic and electrocatalytic materials and processes).
19. Ag.P2. Develop low-cost, selective separation for valorization of wastewater (e.g., meat processing water, tile drainage) by for instance extracting nutrients such as nitrogen, phosphorus, calcium, and protein.
20. Ag.P4. Explore selective removal of sodium and chlorine using electrochemical/electro-membrane processes to reduce the sodium absorption ratio (SAR) for irrigation or recover salt and add back to brining during meat processing.
21. Power.P1. Develop novel adsorbents and absorbents that integrate physiochemical and biological processes with regenerative capabilities for efficient and enhanced removal of contaminants.
22. ReEx.P1. Develop and expand selective separation (e.g., membrane, sorption, ion exchange) and destruction (e.g., catalytic, electrochemical, and advanced oxidation) technologies for the selective separation/destruction of recalcitrant, soluble organic pollutants.
23. Ind.P1. Develop selective separation and destruction of recalcitrant organic pollutants in industrial wastewater.
24. Muni.P1. Develop technology and engineered materials for selective adsorption, destruction, or removal of target constituents and in situ regeneration of selective adsorption sites on engineered material surfaces.
25. Ag.P1. Develop low-cost, selective separation of contaminants that can adversely affect agricultural production or meat and dairy processing, or negatively impact public health and/or agro-ecosystems (e.g., boron, selenium and other oxyanions, emulsified oil, naturally occurring radioactive materials [NORM] such as radium, biocides, surfactants, halogenated components, disinfection-by products, microbially resistant genes, and contaminants of emerging concern such as pharmaceuticals, personal care products, endocrine disrupting chemicals, and fluorinated organics).

AOI P-1.

RESEARCH QUESTIONS (RQS):

- Estimate the cost of target constituent removal technologies as a function of species concentration, removal efficacy, and cost for specific PRIMA water users.
- Which separations platforms are most adaptable to a range of either metal, metalloid, or organic constituents impeding water reuse? At what species concentrations? In the presence of which competing constituents?
- What strategies optimize the removal of contaminants of concerns without requiring extensive additional pretreatment (e.g., to avoid reactions with organic matter and other redox-active solutes)?

4.3. Resilient Treatment and Transport

Enhanced reliability and longevity of water treatment equipment and distribution systems through development of adaptable processes that are not adversely affected by feedwater variability and robust materials that are resistant to fouling and corrosion.

In most places, municipal water infrastructure relies upon centralized water treatment, storage, and distribution systems that are energy-intensive and costly to maintain. Water treatment in the Power, Resource Extraction, and Industrial Sectors often employs scaled-down versions of centralized systems or relies upon transport of water and wastes by truck. NAWI's vision of distributed water recycling and desalination systems have the potential to dramatically reduce costs and energy intensity in many settings if they can operate effectively over the range of conditions encountered in different applications. In particular, temporal fluctuations in influent water quality and demand for water pose challenges to small-scale treatment systems because transient conditions increase the likelihood of fouling, scaling, or process upsets. To ensure that distributed treatment systems and their associated distribution networks can operate effectively, adaptable treatment processes and robust materials are needed.

Much of the prior research on fouling, scaling, and process upsets has either focused on steady-state conditions or has been empirical in nature. To advance pipe-parity efforts, new tools, better predictive models, and approaches for assuring resilient operation under fluctuating inlet water composition are needed. NAWI's early-stage applied research in this area will span molecular- to systems-scale applications. Building upon developments in the autonomous water area, we will apply robust materials design and process-design principles to ensure compatibility of distributed water systems with a wide variety of conditions. We will test materials and process designs in laboratory systems and employ state-of-the-art in-operando characterization tools with materials that resist corrosion and fouling in distributed desalination systems. By developing a fundamental understanding of the factors that lead to fouling and scaling under non-steady-state conditions, it will be possible to achieve substantial improvements in treatment system resiliency. This new knowledge will inform the deployment and use of sensors and actuators and will support development of better antifouling materials and new operating modes. Taken together, research on resilient treatment and transport coupled with other NAWI research outputs will make it possible to deploy small-scale treatment systems that operate closer to their optimal levels over a wide range of feedwater conditions.

After water is desalinated, its composition is adjusted before it is distributed through the control of pH, addition of ions (e.g., calcium), and corrosion-control chemicals (e.g., orthophosphate). It also may be disinfected or treated to remove chemical contaminants. The approach for preparing water for distribution was adapted from practices that had been developed for systems for conveying treated surface or groundwater. As demand grows and prices drop, a larger fraction of desalinated water will not be blended with water from other sources prior to distribution. The challenges associated with widespread distribution of desalinated water will merit development of a better understanding of the factors affecting corrosion and fouling when desalinated water is distributed. **Identifying better approaches for storing, remineralizing, and removing chemical and biological contaminants will enhance resiliency, extend the lifetime of pipes, and protect public health.**

4.3.1 Summary Priority Areas of Interest

1. Stabilizing process performance to variable feedwaters:

Leveraging advanced understanding of fouling and scaling phenomena will stabilize process performance against variable water quality and flow rates.

4.3.2 Targets

1. **Decrease the frequency of cleaning needed** in distributed desalination systems by 50 percent.
2. **Decrease the frequency of component replacement** or system failure by 50 percent in water recycling or desalination systems subjected to fluctuating water quality.
3. **Expand the range of water qualities** that can be treated by a system by 50 percent.

4.3.3 Area of Interest Descriptions

AOI R-1: Stabilizing process performance to variable feedwaters[26,27,28,29,30,31]

Fouling and scaling are fundamental issues that have been studied for decades. Although sophisticated approaches for surface modification, interfacial texturing, and embedded antimicrobials have been studied as means of mitigating fouling and scaling on membranes and other surfaces, little progress has been made toward the development of durable solutions that can be applied across diverse feedwater qualities and module designs employed in distributed desalination systems. Indeed, manufacturers of desalination systems have found the greatest success in addressing these issues through pretreatment[32] targeted at removal of specific precursors and the use of dynamic operating modes that disrupt the development of biofilms and mineral scale.[33,34]

We seek research on fouling and scaling phenomena that extends beyond previous efforts, which were mainly targeted at steady-state operating conditions with water that did not fluctuate substantially in composition, by providing actionable insight into relationships between monitorable source water quality parameters, flow conditions, and the stability and propensity of surfaces for foulant and scalant growth. Projects may leverage and adapt state-of-the-art computational methods (e.g., coupled mass transport and reactivity models, microbial population dynamics models), sensing platforms (e.g., real-time operando surface characterization), and process control models to simulate and test alternative module flow patterns, inform next generation spacer designs, identify critical foulant and scaling precursors, and inform the operation of control systems used for autonomous desalination systems.

26. Power.R3. Design pretreatment and desalination processes that can tolerate water quality variability and provide reliable treatment.
27. Ind.R1. Enhance chemical and biological resiliency of materials and process components in water treatment.
28. Muni.R1. Improve and evaluate materials and surface capabilities for resisting fouling, scaling and corrosion. Materials can be developed that are more compatible with chemical cleaning that resolves fouling and scaling.
29. Muni.R2. Develop materials with longer lifetimes and that can be designed for easier reuse, remanufacture, or recycle.
30. Muni.R4. Advance understanding of fundamental mechanisms of fouling, scaling, and corrosion.
31. Ag.R4. Develop engineering and materials science approaches that address material/system stability, lifetime, and durability challenges based on mechanistic understanding of degradation/stability/durability.
32. Power.R3. Design pretreatment and desalination processes that can tolerate water quality variability and provide reliable treatment.
33. Power.R1. Design materials, processes, and treatment components that can maintain integrity throughout periods of operation in non-steady-state regimes.
34. ReEx.R1. Develop autonomous water treatment systems that can quickly respond to and recover from changes in water quality, environmental conditions, and flow rates

AOI R-1.

RESEARCH QUESTIONS (RQS):

- How flexible, resilient, electrified, autonomous, energy-intensive, and costly are different types of prototypical packaged systems for distributed water treatment? To what degree can innovation in pretreatment, process operation (e.g., non-steady state operation), or controls enhance the performance of these systems?
- What are the primary failure modes for unit processes subjected to variable water quality?
- Are sensing and automation techniques sufficient to adapt to fluctuating water quality, or are alternative process or treatment train designs required?
- What are the cost and energy implications of expanding pretreatment to address fluctuating water quality?

4.4. Intensified

Dramatic reductions in the cost and energy intensity of concentrate management by maximizing brine valorization, developing novel processes for brine concentration, and reducing the costs of small-scale brine management systems.

Current brine management technologies (e.g., thermal treatment, evaporation ponds) are energy-intensive and complex, occupy large areas, and are poorly suited for the modest flows of small-scale desalination systems. At the same time, the increasing popularity of brackish water desalination; unconventional oil and gas development; new regulatory requirements for effluent discharge at power generation, mining, and manufacturing facilities; and plans for carbon storage in saline reservoirs are creating new demands for more efficient brine and concentrate management. Innovative technologies for brine concentration and crystallization would dramatically reduce the costs and energy intensity of small-scale desalination facilities by eliminating the need for brine conveyance, lowering energy intensity, reducing dependence on finite injection well capacity, and enhancing water recovery from nontraditional sources.

NAWI's early-stage applied research on intensified brine management will focus on developing alternatives to thermally driven brine management technologies, materials innovations to improve the efficiency of existing processes, and approaches for valorizing residuals produced from desalination. To advance our pipe-parity efforts, we seek innovative brine management solutions for high-salinity streams, with particular focus on halving the treatment cost of saline brines (i.e., 75,000 and 250,000 ppm TDS). These solutions could involve system designs that couple brine treatment with resource recovery, chemical synthesis, and flexible operations for grid integration; modeling and simulation efforts to understand and overcome heat and mass transfer barriers to process and materials performance; process configurations that combine multiple driving forces to dramatically lower the cost of modular brine crystallization units and control inorganic scaling; and materials and manufacturing innovations that extend the pressure tolerance of spiral-wound RO membranes/modules, reduce the membrane structural parameter, reduce the synthesis and processing costs of ion exchange membranes, and enable prediction and operando characterization of chemical and material properties in brine concentration systems.

4.4.1 Summary Priority Areas of Interest

1. Novel processes and operational modes that leverage a fundamental understanding of the thermodynamics and kinetics of inorganic scaling processes in ultra-high salinity brines:

Enable more effective brine management by leveraging state-of-the-art models describing molecular-to-macroscopic properties of hypersaline solutions under conditions relevant to brine concentration to elucidate mechanisms and predict kinetics of homogeneous and heterogeneous nucleation and growth of crystalline (e.g., calcium, barium, and strontium sulfates) and amorphous (e.g., silica) scales.

2. Experimentally validated computational models for optimizing heat and mass transfer rates in hypersaline conditions and complex geometries:

Leverage an improved understanding of heat and mass transfer at high salinities to optimize component design (e.g., feed spacers, heat exchangers) and process operation (e.g., non-steady state operation) for reduced process cost and improved separation performance.

3. Process and material innovations enabling low-cost concentration of high-salinity waters:

Use advances in process engineering and materials science to enable brine concentration to 250 g/L TDS for direct input into a brine crystallizer.

4. Bulk constituent transformation or valorization:

Enhance the value of residuals produced by brine management processes.

4.4.2 Targets

1. **Develop predictive models** that employ state-of-the-art mechanistic understanding of the kinetics of nucleation and growth of crystalline and amorphous scales in brines enable the design of brine management systems that are at least 25 percent less costly than currently available systems.
2. **Develop component and process designs** that mitigate concentration and thermal polarization and reduce the cost of brine concentration systems by at least 25 percent.
3. **Develop brine valorization processes** that yield net revenues that are at least 25 percent higher than existing systems without substantially increasing system complexity.

4.4.3 Area of Interest Descriptions

AOI I-1: Novel processes and operational modes that leverage a fundamental understanding of the thermodynamics and kinetics of inorganic scaling processes in ultra-high salinity brines to improve system performance[35,36,37,38]

Brines typically contain high levels of sparingly soluble species (e.g., silica and divalent cations such as calcium, barium, and strontium).[39,40] Precipitation of these species during brine concentration can significantly hinder process efficiency. Current solution models exhibit limited accuracy in describing chemical speciation and precipitation kinetics of brines over wide concentration ranges, over a range of temperatures and pressures relevant to process conditions, or in the presence of other colloidal, organic, or biological species. Next-generation solution models must describe the molecular-to-macroscopic properties of hypersaline solutions under conditions relevant to brine concentration and elucidate mechanisms of homogeneous and heterogeneous nucleation and growth of crystalline (e.g., calcium, barium, and strontium sulfates) and amorphous (e.g., silica) scales. **NAWI seeks to leverage next-generation solution models to inform the design and operational modes of brine treatment process design and operation.**

AOI I-1.

RESEARCH QUESTIONS (RQS):

- What is the most computationally tractable way to represent validated solution property models for density, viscosity, solubility, osmotic pressure, precipitation kinetics, etc., in ProteusLib across the range of feedwater chemistries represented by baseline studies and recoveries up to zero-liquid discharge (ZLD)?

35. Power.I1. Understand reaction kinetics for complex solution chemistries, including nucleation and crystal growth at high salinity and/or temperatures and chemical models to predict precipitation of recoverable pure salts—exploiting gradients, freeze/thaw, nucleation, and solute activity in high-salinity waters.
36. Ind.I2. Optimize prediction and chemical modeling of concentrate waste and brine streams.
37. Muni.I2. Develop advanced geochemical modeling and operando monitoring tools to characterize, understand precipitation, nucleation, crystallization, solute activity, and heat transfer in high-salinity waters.
38. Ag.I3. Develop advanced modeling and operando monitoring tools to understand precipitation, nucleation, crystallization, solute activity, and heat transfer in high-salinity waters to control scaling and intensify process design for brine treatment.
39. Power.I 3. Integrate brine characterization with sensor/control systems and whole-plant operations.
40. ReEx.I4. Optimize the prediction and characterization of brine streams.

AOI I-2: Experimentally validated computational models for optimizing heat and mass transfer rates in hypersaline conditions and complex geometries[41]

Heat and mass transfer limitations hinder the efficiency of high-salinity brine concentration processes. Methods for computationally describing and experimentally validating heat and mass transfer coefficients in hypersaline environments and complex geometries relevant to brine concentrators or crystallizers may lead to novel process designs and operational modes. NAWI will leverage an improved understanding of heat and mass transfer at high salinities to optimize component design (e.g., feed spacers, heat exchangers) and process operation (e.g., non-steady-state operation) to reduce process cost and improve brine concentrator performance.

AOI I-2.

RESEARCH QUESTIONS (RQS):

- What spatial and temporal resolution is required for experimental measurement techniques to validate heat and mass transfer rates within +/- 10 percent?
- How representative are the heat and mass transfer rates measured in test cells to full scale modules?
- How do manufacturing constraints limit the deployment of optimized structures for heat and mass transfer?

41. Power. I2. Modify to existing processes to improve ZLD systems and development of integrated or hybrid processes to improve ZLD systems (i.e., modify thermal techniques using electrified approaches).

AOI I-3: Process and material innovations enabling low-cost concentration of high salinity waters[42,43,44,45,46,47]

One of the most capital- and energy-intensive parts of brine management involves concentrating brines produced during desalination, which typically contain from 10–70 g/L TDS up to hypersaline conditions (e.g., 250 g/L TDS) that are typically subject to further dewatering in a brine crystallizer. NAWI seeks innovations in the concentration of brines that offer substantial cost reduction over the best available process (e.g., mechanical vapor compression) in both small-scale and large-scale operations. Because of the inherently low energy efficiency of evaporative technologies, we are especially interested in processes that leverage hydraulic pressure, osmotic pressure, electric potential, or other driving forces that are well suited for modularization. Innovations suitable to this AOI may be a standalone single process or a hybrid treatment train that combines several processes operating with different driving forces in new ways that yield substantial improvements in process performance. We are also interested in materials innovations that substantially reduce the capital and operating costs of existing processes. **Proposed innovations may enhance the performance (e.g., thermal conductivity, permeability), durability, and cleanability of materials in contact with hypersaline brines and must have a viable pathway to scalable manufacturing.**

AOI I-3.
RESEARCH QUESTIONS (RQS):

- How can compaction and failure modes be characterized at the selective layer-support interface?
- What materials or manufacturing innovations will enable cost-effective polymer and composite membrane structures that resist compaction up to 200 bar, maintain seawater RO A and B parameters, and can be readily integrated into high-pressure modules with costs less than five times those of current RO modules?
- What advances in permeate spacer design and implementation can be used to mitigate/minimize embossing of membranes when operating at high pressure?
- What are current costs and performance attributes of best-available processes (e.g., mechanical vapor compression [MVC]) under conditions that are most relevant to ZLD applications? How do these compare with emerging technology performance?

42. Power.I2. Modify to existing processes to improve ZLD systems and development of integrated or hybrid processes to improve ZLD systems.

43. ReEx.I1. Develop hybrid treatment trains (across scales) to further enhance water recovery from brines from desalination processes, high salinity produced water, or mining wastewater.

44. ReEx.I3. Develop cost-effective methods for brine management and solidification.

45. Ind.I1. Cost-effective waste/brine management and solidification.

46. Muni.I1. Develop innovative technologies to reduce the volume of concentrate for disposal, achieve ZLD, and couple brine management with resource recovery (e.g., metals, energy, and other commercial products) and chemical synthesis (e.g., bleach, hydrogen peroxide, acids, and bases).

47. Ag.I1. Develop technologies for cost-effectively producing and managing low-volume, high-concentration brines, or high volumes of desalination waste, to avoid the use of dilution for their disposal.

AOI I-4: Bulk constituent transformation or valorization: Enhancing the value of residuals produced by brine management processes

We propose a novel schema for bulk constituent transformation or valorization of crystalline solids or brines over 250,000 ppm TDS that is economically viable for one or more of the PRIMA roadmap baseline sites and does not increase net carbon emissions by more than 10 percent. **Economical management of concentrated brines may be facilitated by identifying valuable uses or low-cost disposal options for each brine constituent.**

AOI I-4.
RESEARCH QUESTIONS (RQS):

- What bulk constituent disposal options are deployed today, and how will future policy or technological constraints limit these options in the future?
- How will fluctuating water quality, treatment train design, product purity, and market prices for commoditized goods influence the economic viability of transformation and valorization schema?
- How universal is the proposed valorization schema across PRIMA water users and geographic locations?

4.5. Modular

Materials and manufacturing innovations that substantially reduce the cost of small-scale desalination and fit-for-purpose reuse applications.

Most of the water treatment systems built during the 20th century were custom-built for the specific application for which they were intended. As a result, engineering design, permitting, pilot testing, and adjustment of design shortcomings slowed the deployment of treatment systems and ultimately increased costs. The commercialization of RO membranes represented more than just an advance in water desalination; it was one of the first examples of the way in which advances in manufacturing and modularization of unit processes could simplify water treatment processes and lower the cost of advanced water treatment. More recently, progress toward modularization has gained momentum as other aspects of water treatment (e.g., microfiltration, advanced oxidation processes) have been designed as standardized units. Coincident with the increasing popularity of modular treatment systems, manufacturing has undergone a shift that has been referred to as the fourth industrial revolution (i.e., Industry 4.0). By adopting sensors, artificial intelligence, and advances in manufacturing technology, it is becoming easier to create materials and parts that are tailored to specific needs. These advances will open up opportunities to manufacture water treatment modules that are better serve the specific needs of a user (e.g., by considering the composition of the water being treated and the uses of the treated water).

The production of more effective membrane materials and modules is an area in which advances in modular manufacturing can advance NAWI's pipe-parity goals. Innovations in manufacturing are necessary to enable the deployment of cost-competitive membranes that provide substantial advantages over the existing polymeric membranes that currently account for the vast majority of desalination systems. New membrane materials also may decrease the cost and complexity of functionalized membranes capable of selective sorption, degradation, or rejection of specific contaminants. In addition, new materials and manufacturing processes have the potential to reduce costs and extend the range of pressures at which desalination processes can be operated, thereby increasing water recovery and decreasing the volume of brine produced during membrane treatment.

Processes employed for pretreatment of water prior to desalination represent another important opportunity for modularization. Although some modular forms of pretreatment (e.g., microfiltration, ultrafiltration) recently have become more popular, less compact processes, such as sand filtration and chemical softening, are still very common in centralized desalination systems. In some circumstances, the preference for these processes is related to more than simply habit. For example, part of the choice of the designers of Israel's Ashkelon Seawater Desalination Plant (design capacity 330,000 m^3/day) to use mixed media filtration as a pre-treatment step instead of membrane filtration was related to the ability of microbes on the filters to remove assimilable organic carbon that contributes to biofouling of the RO membranes. Modularized pretreatment systems that can provide performance comparable to or better than existing processes used at centralized treatment plants are particularly important to small-scale, autonomous desalination systems because modular units tend to have smaller footprints, require fewer chemicals, cost less to maintain, and generate less waste.

4.5.1 Summary Priority Areas of Interest

1. Manufacturing platforms for tailored membranes and modules:

Leverage advances in manufacturing and prior research on membrane materials, fouling, and transport to enable the development of tailored membranes and module designs that can provide substantial advantages over existing membranes in the treatment of specific feedwaters and water treatment applications.

2. Enhancing pretreatment kinetics through modular design:

Develop and employ knowledge about factors affecting the efficacy of pretreatment processes to develop modular designs that prepare water for desalination while reducing the cost and shrinking the physical footprint of treatment systems.

4.5.2 Targets

1. **Develop a manufacturing platform** that dramatically increases the range of polymers and the tunability/control of membrane properties (e.g., permeance, selectivity, and organics rejection) in all dimensions.
2. **Tailor membranes for high recovery softening** via divalent selectivity for brackish water applications.
3. **Develop chlorine-tolerant, high boron-rejecting membranes** for seawater RO applications.
4. **Use membranes with selectivity** against trace concentrations of low MW, polar compounds for wastewater reuse applications.
5. **Hybridize and modularize pretreatment unit processes** for organics, oil and grease, and particulate removal to reduce weight, size/footprint, and complexity in one or more distributed, small-scale PRIMA treatment trains.

4.5.3 Area of Interest Descriptions

AOI M-1: Manufacturing platforms for tailored membranes and modules[48,49,50,51,52,53,54]

Economies of scale in manufacturing have led to low-cost modules for seawater desalination but have not produced membranes tailored to applications such as industrial water reuse or wastewater recycling. Although market diversification in membrane and module designs has increased recently and may continue to do so as the market expands, the design and deployment of low-cost, tailored membranes is progressing too slowly for NAWI's objectives of diverse distributed reuse. NAWI seeks to shift the paradigm in membrane and module design and manufacturing through the development of cost-effective membranes and modules that can be customized for specific feedwater and process applications.

Early-stage applied research is needed to advance the cost-effective manufacturability of customized membrane materials and modules.[55,56,57,58] These advances could include a better understanding of polymer chemistry that enables more precise control of membrane properties and manufacturing innovations (e.g., additive, roll-to-roll, spray coating), as well as scalable and cost-competitive deployment of novel membrane materials or spacers, in operando characterization techniques that inform the design of membranes and spacers suited for varying solute conditions, and computational fluid dynamics models that enable design of modules with module geometries and flow patterns that are less susceptible to fouling. In recognition of the fact that displacing incumbent membrane and module designs will require order-of-magnitude cost reductions that are only likely to be achievable through focused research on manufacturability, our investments in this AOI will be limited to the materials and applications with the greatest potential for substantial gains in manufacturability over the time scale of a decade.

48. Power.M1. Develop flexible and reliable water treatment systems built on modular components to address nonsteady-state operation, reliability, and reactor-in-series needs at power plants.

49. Power.M2. Advance dual-function membrane manufacturing approaches that enable their cost-effective production at scale.

50. ReEx.M1. Increase flexibility, scalability, and portability of modular treatment systems and characterize operating limitations to enable cost-effective solutions and increase industry adoption.

51. ReEx.M2. Innovate membrane module design for improved durability against various stress factors (e.g., chemical, temperature, pressure) and application in high-salinity, high-pressure, and high-flow waste streams.

52. Ind.M2. Improve membrane module design and fabrication techniques and enhance bench scale and industrial pilot testing programs to objectively verify performance. Also, increase flexibility and scalability to develop cost-effective modular treatment systems.

53. Muni.M1. Manufacturing innovations for on-demand production of treatment components.

54. Ag.M4. Develop manufacturing approaches to advance design aspects of modularity: collaborations to design correctly (modularity with natural systems).

55. Muni.M2. Advance technologies that can improve the performance of building-scale on-site water treatment and reuse systems.

56. Ag.M1. Develop high-rate and high-recovery desalination processes (e.g., over 98 percent) for agricultural applications, such as electrodialysis.

57. Ag.M2. Create a hybrid system combining water treatment with onsite production of fertilizers from municipal wastewater or centrate, agricultural, and food wastewater (e.g., osmotic membrane, electrochemical processes, ion exchange, pervaporation).

58. Ag.M3. Create a hybrid system combining water treatment with onsite production of fertilizers from municipal wastewater or centrate, agricultural, and food wastewater (e.g., osmotic membrane, electrochemical processes, ion exchange, pervaporation).

Advances are also needed in materials that will allow membrane modules to be operated at higher pressures. We anticipate that prior innovations made in other industries in materials including ceramic, polymeric, and carbonaceous materials will be critical to achieving this objective. For example, low-cost ceramic membranes could fundamentally change the economics of pre-treatment, enabling process intensification by eliminating several energy-intensive and large footprint treatment steps. Ceramics also offer an advantage over other materials because they can withstand exposure to chemicals (e.g., chlorine, concentrated acids) that would otherwise damage polymeric membranes. Similarly, advances in spray coating technologies and high-tensile-strength carbon fiber spinning could enable new types of desalination membranes that extend the pressure tolerance and water recovery of traditional RO membranes. Finally, adaptation of roll-to-roll processing techniques for ion exchange membrane materials has the potential to yield order-of-magnitude cost reductions and performance improvements in electrochemically driven separation processes advantageous in energy-efficient brackish water desalination.

AOI M-1.

RESEARCH QUESTIONS (RQS):

- What are the limitations that prevent the manufacturing of tailored desalination membranes for high recovery softening, high boron-rejection, high chlorine tolerance, or high trace organic rejection applications, and how can these limitations be addressed?
- What tunable parameters in the manufacturing process will confer control over desired membrane properties?
- How do we ensure quality control (at a molecular level) during manufacturing? Is there an economically viable role for online metrics, including assessing the presence of defects and consistency of thickness, crosslink density, surface charge, and chemical functionality?
- What are the costs and benefits associated with manufacturing membranes tailored to the specific needs of individual treatment systems (i.e., what is needed to create custom designed membranes)?
- How do we measure concentrations of inorganic and organic components in membrane materials (e.g., partition coefficients) under conditions relevant to treatment systems (i.e., in a hydrated state and under pressure)?
- What are the most promising approaches for reducing the costs and tailoring the performance of ceramic membranes?

AOI M-2: Enhancing pretreatment kinetics through modular design[59]

Conventional pretreatment processes account for about 25 percent of a seawater desalination plant capital and operational costs. Slow separation mechanisms (e.g., gravitational settling) provide energy efficient and cost-effective pretreatment in many situations, but these same attributes make them a poor fit for deployment in small-scale systems. Although membrane-based microfiltration and ultrafiltration processes have displaced some conventional pretreatment processes, others (e.g., dissolved air floatation, softening) are not readily replaced by modular membrane systems. We seek innovative approaches to pretreatment that employ new materials and processes, enabled by sensors and actuators, to create modular, resilient pretreatment systems capable of removing suspended particles, assimilable organic carbon and ions that contribute to membrane fouling. In particular, processes that can achieve the objectives of pretreatment without the need for frequent replenishment of chemical reagents or the generation of solid wastes are desirable.

AOI M-2.
RESEARCH QUESTIONS (RQS):

- What are current costs associated with pretreatment across geographies, source water, end users, and treatment train types, and what are appropriate targets for pretreatment cost reductions?
- Develop high-throughput, modular processes that hybridize two or more treatment steps and operate efficiently and reliably in high-salinity waters. Examples of possible pretreatment technologies include chemical addition, chemical mixing, settling, flotation, and filtration units.
- Eliminate or fully replace chemical dosing for RO treatment trains through substitution of unit processes or in-situ generation of reagents. For on-site chemical generation systems, assess methods of chemical purity control for on-site generation with varying source water quality and evaluate the potential and impact of byproduct formation.
- Develop high-recovery, throughput, and divalent selectivity softening and silica removal processes to reduce scale formation in high-recovery membrane desalination processes. Specific technical targets to be defined through analysis on baseline studies.
- Cost-effective, modular pretreatment technologies that reduce the concentration of small molecule organics that reach membranes.
- How can sensors and actuators be used in concert with modular pretreatment systems to rapidly respond to fluctuating conditions and minimize the risk process failures?

59. Ind.M1. Define the level of wastewater treatment necessary to protect downstream membrane processes and develop economically scalable, modular pre- and post-treatment processes with reduced weight and footprints that can be flexibly integrated with membrane processes.

4.6. Electrified

Electrifying water treatment processes and facilitating their integration with a clean energy grid.

Many existing water treatment trains employ relatively large volumes of chemicals (e.g., acid, caustic, coagulants, antiscalants, chemical disinfectants). **In addition to increasing the cost and complexity of water treatment, the act of supplying chemicals and managing the residuals that that they produce pose substantial challenges to distributed water treatment systems.** Treatment processes that rely upon chemicals also are difficult to adjust in response to fluctuations in water quality and flow rates. In many situations, the functions provided by chemicals can be replaced by processes that require only electricity. For example, acidic and basic solutions can be generated at anodes and cathodes, respectively, during water electrolysis. Similarly, water can be disinfected with ultraviolet light or with ozone or chlorine produced on-site using electricity. Replacing chemically intensive, steady-state treatment processes with electrified processes has the potential to advance pipe-parity in small-scale desalination systems by reducing operating costs and providing a means of more rapidly adjusting treatment processes to fluctuations in water quality or flow. For small-scale operations and in centralized systems, increasing reliance on electricity also provides opportunities to more efficiently exploit renewable energy and temporal variations in the cost of electricity.

To realize the electrification of water treatment, early-stage research is needed. In particular, NAWI is interested in new approaches to support the design of more efficient and reliable electrified treatment processes and treatment trains. In many cases, these advances will require the development of low-cost, robust electrodes that can overcome some of the problems such as mass transport limitations, scaling, and limited electrode longevity. To meet the challenge of operating under conditions of variable flow and water quality, electrified treatment trains will need to be designed in a manner in which non-steady-state operating conditions (e.g., diurnal fluctuations in flow exceeding 50 percent) do not damage components (e.g., through scaling) or compromise water quality. Variations in the cost of electricity or the availability of solar and wind power also yield opportunities to advance pipe-parity. Early-stage research is needed to assess the viability of different systems-level strategies for moving and treating water in a manner that maximizes economic benefits and utilization of renewable electricity sources.

In addition to electrifying energy-intensive chemical treatment processes and adapting water treatment and distribution to renewable energy sources, NAWI has an opportunity to advance pipe-parity goals by increasing the reliability and capabilities of low energy, nature-based treatment systems. Replacing part or all of energy-intensive treatment processes like dewatering of desalination brines with nature-based processes has the potential to significantly reduce energy use while simultaneously improving water quality, providing ecosystem services and other benefits that are valued by society.

4.6.1 Summary Priority Areas of Interest

1. Water process electrification:

Reduce carbon emissions and complications related to chemical management by employing electrified processes for contaminant removal or reagent (e.g., acid, base, disinfectant) production.

2. Water and electricity grid coordination:

Support load-following and demand-response services through innovative design of treatment trains, water distribution, and storage systems.

3. High throughput passive treatment systems:

Use low- or no-treatment solutions that rely primarily on water conveyance and natural processes in land abundant settings.

4.6.2 Targets

1. **Develop electrified unit processes** on small-scale water treatment trains that are cost-competitive with the existing chemically intensive treatment trains.
2. **Reduce the life cycle carbon intensity of water desalination** by 30 percent under projected carbon intensity of the 2050 U.S. electricity grid.
3. **Develop water treatment trains** capable of reducing electricity costs by 20 percent without diminished performance through load following or demand response market participation.
4. **Achieve a 50 percent reduction in the cost of treating constituents of concern** in applications that are not limited by land availability (e.g., agriculture, mining) through the use of nature-based treatment systems.

4.6.3 Area of Interest Descriptions

AOI E-1: Treatment process electrification[60,61,62,63,64,65,66,67,68]

Electrification of water treatment processes will be critical to achieving NAWI's goal of enabling autonomous, small-scale water treatment systems, as well as efforts to lower costs and make centralized water treatment processes more resilient and adaptive. Electrified treatment processes also have the potential to contribute to reduce greenhouse gas emissions and environmental and health impacts associated with the mining, use, and disposal of water treatment chemicals. NAWI seeks novel approaches for decreasing or eliminating the need for water treatment chemicals through the use of electrified treatment methods (e.g., electrochemical production of reagents, use of ultraviolet (UV) light or electric fields for water treatment needs currently met by chemical means). Within the area of specific unit processes, we are particularly interested in research that supports the development of processes leading to fully electrified desalination treatment trains. Research should focus on overcoming barriers to the uptake of electrified treatment processes, such as the need to develop low-cost, long-lasting electrodes, overcoming mass transport limitations and scaling at surfaces. In the evaluation of pipe-parity metrics, researchers should consider life-cycle costs of materials and water treatment chemicals as well as the ways in which electrified treatment processes can support the operation of small-scale water treatment systems.

60. Power.E1. Develop electrified processes and the scientific basis for these processes that can provide chemical-free removal of specific constituents.

61. Power.E2. Lower chemical intensity of water management at power plants through electrified approaches to disinfection and scale inhibition.

62. ReEx.E1. Develop and optimize electrified treatment processes (e.g., electromagnetic field, electrocoagulation) to reduce chemical use and associated transportation logistics/costs.

63. ReEx.E2. Develop and evaluate performance, limitations, and implementation of electrical desalination processes.

64. ReEx.E3. Evaluate the use of water electrolysis/bipolar electrodialysis for generation of chemicals onsite and in situ, including bleach, acids, and bases, at resource extraction facilities.

65. Ind.E1. Develop chemical-free electrocatalytic processes for pollutant destruction.

66. Muni.E1. Develop innovative technologies and materials to improve system efficiency and reduce the costs and energy demand of the electrified processes.

67. Ag.E1. Develop innovative materials for advanced electro-membranes, electro-catalytic, and bio-electrochemical systems that can be used for pretreatment (e.g., chemical free scaling and fouling control, pH adjustment), treatment (e.g., removal of contaminants), and posttreatment (e.g., UV-light-emitting diode [LED] advanced oxidation processes [AOPs]) to improve system performance and reduce costs.

68. Ag.E3. Develop technologies to concentrate contaminants for more efficient treatment (e.g., smaller volumes, higher removal rates) by electrochemical and electrocatalytic processes.

AOI E-1.

RESEARCH QUESTIONS (RQS):

- What are life cycle energy and cost implications of electrifying treatment processes in large scale and distributed desalination applications? Set upper bounds for electricity consumption/grid performance in break-even assessment with current chemically intensive unit processes in five PRIMA treatment trains.
- What are the potential water quality benefits and limitations of deploying electrochemical treatment processes across the range of common constituents in PRIMA feed waters (e.g., chloride, sulfate, organics) and the challenges with integration of electrochemical treatment processes systems into existing treatment trains deployed in the NAWI baseline studies? Work should specifically address challenges in dose control, applicable salinity range, in-situ coagulant generation, fluid dynamics and mass transfer, corrosion kinetics, passivation, sludge production, and their influence on pipe-parity metrics, including levelized cost of water, carbon intensity, and reliability.
- How can a fundamental understanding of the inherent limitations of existing electrochemical water treatment processes (e.g., surface and electrochemical phenomena of electrodes that lead to the performance deterioration, mass transport limitations, expensive materials) be leveraged to develop strategies to minimize these phenomena and address the high costs of electrochemical water treatment systems through one or more innovations in materials composition, material structure (e.g., thickness, pore size distribution), surface coatings, cell designs (e.g., flow hydraulics, spacers), or operational modes?

  This effort may be facilitated by developing strategies for fast screening of a wide range of materials and modular cell designs to promote electrically driven process development and transfer to industry. These strategies could be pursued through: (i) mechanistic understanding of material behavior, (ii) development of a library of new catalysts such as cost-effective single atom (alloy) catalysts that enable selective electrode reaction, (iii) novel accelerated cell life testing protocols, and (iv) robust computational descriptors of process performance.
- How can novel, modular chemical-free pretreatments (e.g., electromagnetic field, ultrasonic) be developed for removing hardness and other weakly charged ions (e.g., dissolved silica and boron) on membranes, heat exchanger surfaces, pipelines, and other water treatment devices through an improved understanding of the science, mechanisms, and factors affecting the efficiency of these technologies for PRIMA water qualities?
- How can innovative, modular approaches be developed for cost-effective, small-scale, on-site production of chemicals used in the water treatment process (e.g., hydrogen peroxide) without precursor supplies?

AOI E-2: Water and electricity grid coordination[69,70,71,72,73]

The ability of electrified water treatment systems to adjust their flows in response to changes in electricity costs or the availability of renewable electricity is a potential benefit of NAWI's vision of automation, resilience, and small-scale distributed desalination systems. Fluctuations in the rate at which water is treated as well as storage have the potential to compromise water quality and stress components of the treatment system. NAWI seeks early-stage research that will enable reliable performance of water desalination and recycling systems through innovations in materials, processes, treatment trains, and distribution networks. Materials and process projects should leverage an understanding of the behavior of unit processes and treatment systems under intermittent operating conditions over short and long-time durations and variable operation under partial capacity conditions. Treatment train and extended network models also are needed to identify the best ways for realizing objectives for realistic water flow volumes, water quality requirements, electricity prices, storage capacity, and demand response compensation schema over both short (i.e., measured in hours) and long (i.e., seasonal) time durations.

AOI E-2.
RESEARCH QUESTIONS (RQS):

- What are the attributes of existing and emerging treatment technologies that make them best suited for taking advantage of variable operating conditions?
- What are the pipe-parity implications of operating treatment systems under various levels of intermittent and flexible operating schedules?
- How do the size, storage capacity, and size of treatment and distribution networks affect the ability to take advantage of fluctuating prices or availability of renewable electricity?
- What is the best way to develop treatment train controls strategies for reducing the cost of electricity by shifting load to non-peak electricity pricing hours or integrating it with renewable energy sources?
- How can modular desalination treatment trains be developed that seamlessly ramp capacity up and down based on energy cost and/or availability of renewable energy? These modules will allow water treatment to be easily toggled on and off without long startup or shutdown sequences, operator oversight, performance inefficiencies, or environmental emissions.

69. ReEx.E4. Investigate usage of alternative and renewable energy sources in electrified water treatment.

70. Ind.E2. Develop robust electrocatalytic processes and electrified treatment systems that integrate system operation with the electrical grid, optimizing for use of renewable energy and timing usage during periods of low electrical demands.

71. Muni.E3. Incorporate variable renewable energy into water treatment systems and leverage clean energy to replace chemical-intensive systems with electricity-intensive systems.

72. Ag.E2. Integrate renewable/alternative energy with electrified desalination and related processes for remote/farm locations. Develop techno-economic models to quantify the synergies between these two systems as well as the benefits gained in stability, reliability, and flexibility derived from electrification.

73. Ag.E4. Improve energy efficiency by waste heat recovery and systems optimization of electrified driven process (e.g., recover heat from boiling water or engines used in meat processing).

AOI E-3: High-throughput passive treatment systems[78]

Passive treatment systems requiring low energy for operation (e.g., ponds, wetlands, aquifers) will continue to provide a low-cost means of treating and storing water in areas where land costs are low or where conditions favor subsurface water storage. By integrating active management (i.e., sensors, actuators, control of substrates or flow paths) into nature-based systems it may be possible to greatly enhance their ability to augment NAWI's small-scale treatment systems and advances being made at centralized facilities. We seek early-stage research that makes nature-based treatment processes more efficient, predictable, and reliable by active management and the development of new approaches for more efficiently achieving treatment objectives that are energy-intensive or otherwise difficult to achieve with existing technologies (e.g., removal of contaminants from agricultural drainage). **We also seek analyses that support decision-making about how best to integrate nature-based systems into treatment trains for pretreatment, desalination, and water storage as a means of taking advantage of low-cost treatment and storage afforded by these systems.**

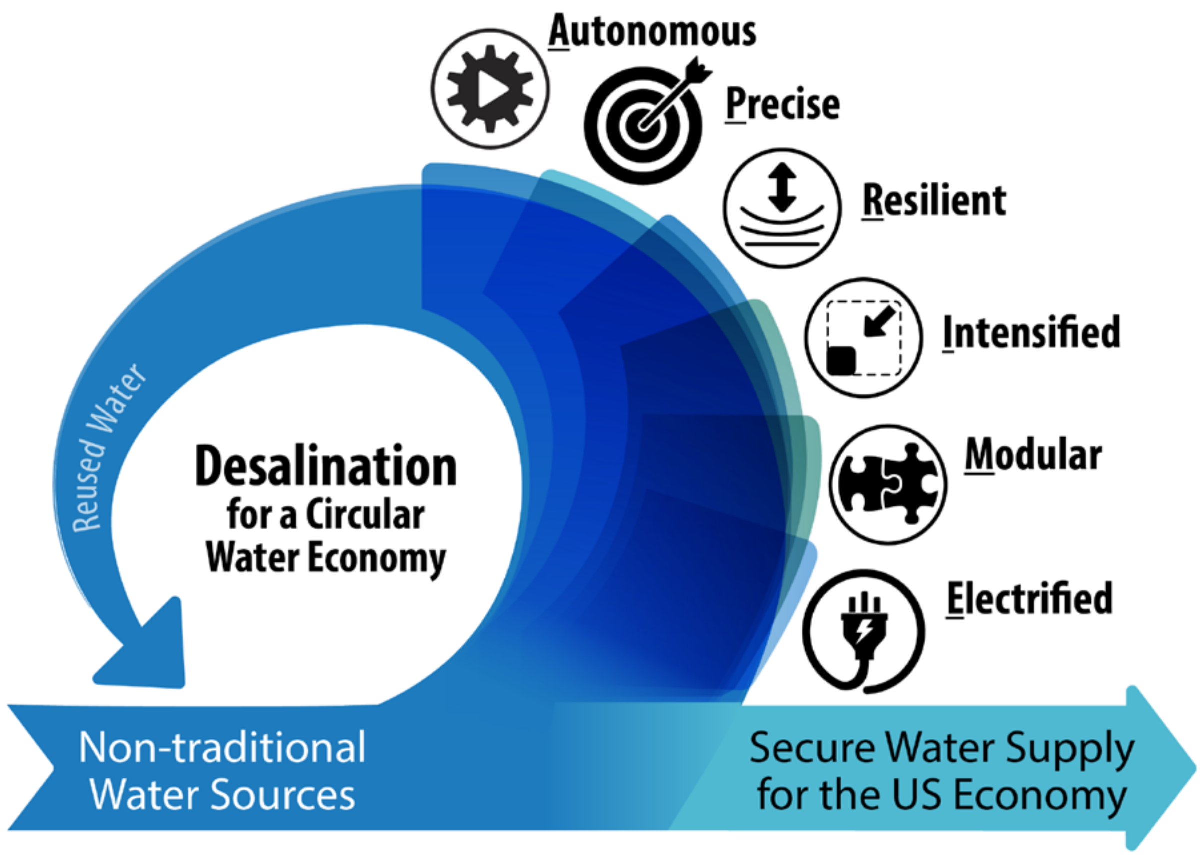
AOI E-3.
RESEARCH QUESTIONS (RQS):

- What is a modular approach to the passive treatment of nutrients, organic contaminants, and pathogens of concern or brine concentration? Modular design should effectively address varying water quality and quantity and should specify the appropriate plant and microbial species, hydraulic residence time, directed flow, and soil/substrate to remove specific constituents that are associated with the nontraditional water sources. The cost target for passive systems is an order of magnitude lower than engineered systems if land area is significantly larger.
- How can sensors, actuators, and technological interventions (e.g., modification of substrates or flow paths) be used to augment or intensify treatment in nature-based systems?
- What is the life cycle cost-effectiveness of modified brine evaporation pond designs to reduce the amount of land needed to dewater desalination brines? How do fluctuating water quality and weather influence this cost-effectiveness?

78. Ag.R5. Develop low-energy natural systems (e.g., resilient engineered wetlands) enabling effective response to varying water quality and quantity. These wetlands should be optimized for removal of nutrients, organic contaminants, and pathogens. Implement recovery of metals such as selenium by hyper-accumulating plants or novel sorbents.

4.7 Circular Water Economy

Systems level research to gain insight into factors affecting technology adoption and progress toward pipe-parity.



During the analysis of the A-PRIME AOIs, it became evident that additional research was needed to assess the implications of advances in desalination and advanced water treatment at the systems level. For a systems-level analysis of progress toward pipe-parity, analysis conducted as part of ongoing research projects will provide estimates of their impacts on a specific unit process (e.g., it is possible to estimate reductions in energy consumption or operating costs from a more efficient desalination process). When the outcomes of several research projects affecting a representative treatment train are combined, the overall impact on the performance of the treatment system can be estimated and compared to baseline performance of existing treatment processes to assess progress towards pipe-parity. However, not all analyses of progress towards pipe-parity are this straightforward. Changes to one unit process might affect the performance of the rest of the treatment system. In addition, new treatment technologies and treatment trains can alter multiple aspects of system performance (e.g., a new technology that increases the resilience of a water supply might consume more energy or result in the production of a residual stream that in some situations is more difficult to manage).

Adoption of new types of small-scale desalination and advanced water treatment systems also must be evaluated at the systems level because their impact extends well beyond the treatment system itself. For example, in the municipal sector, a building-scale water recycling system might still require a connection to an external water supply (i.e., for drought periods) and a sewer (i.e., for disposal of residuals). When a small fraction of the buildings in a community are equipped with such systems, it may be appropriate for the building practicing recycling to receive the benefit of reliable water supply and waste disposal for a relatively low cost because they are helping the utility avoid the need to expand their water supply (i.e., the marginal cost of water is high so there is an incentive for construction of recycling systems). However, when many buildings are equipped with recycling systems, the price of water and sewer provision might have to increase to enable system operations and maintenance (i.e., the cost of providing municipal water and sewer services is only weakly tied to the volume of water and sewage that the building uses and discharges). To gain insight into these kinds of issues and their impact on efforts to achieve pipe-parity, innovations like building-scale recycling systems need to be evaluated at the systems level.

Another clear outcome of the roadmapping and baseline effort was the importance of location to technology adoption. The clearest example of this is the effect of water scarcity on the LCOW. In places where water is already scarce, the marginal cost of water is high and many of the available water sources are less reliable (i.e., they may be curtailed during droughts). Certain regions of the country also are likely to experience greater stress to their water supplies due to climate change (e.g., regions that rely upon snowmelt as part of their surface water storage will be faced with bigger challenges than those regions where most precipitation already falls as rain). Therefore, pipe-parity is more likely to be achieved when desalination or water recycling is competing with conventional sources in these parts of the country. Thus, when evaluating pipe-parity at a national level, understanding regional variations in cost is important in determining the scale of the impact of a new technology. Beyond water scarcity, location also affects options for residual management (e.g., access to the ocean or a deep saline groundwater formation can reduce the costs of brine management), costs of transporting materials, opportunities to valorize wastes, and the relative importance of water quality and regulatory concerns. In water resources management, insight into the importance of geographic setting can be obtained through case studies of key opportunities in different regions. From these analyses, insights may be gained into the likelihood of technology diffusion in different parts of the country as well as analytical frameworks and tools that can be applied in the planning process.

4.7.1 Summary of Priority Areas of Interest

1. **Quantifying the benefits of APRIME for distributed and centralized systems:** Determine the impacts of location, treatment train, and technology deployment modes of desalination and water recycling systems that employ A-PRIME advancements.

4.7.2 Targets

1. **Develop decision-support tools** accessible to each water user sector that facilitate the quantitative evaluation of nontraditional water sources within the context of a secure and resilient water supply portfolio.
2. **Evaluate trade-offs among different elements** of system performance for new types of distributed and centralized treatment processes.
3. **Assess the barriers to adoption** and remaining technological issues necessary to assure widespread implementation of next-generation desalination and fit-for-purpose water treatment technologies.

AOI C-1: Quantifying the benefits and costs of APRIME for distributed and centralized systems

Prior to deployment at scale, it is difficult to accurately assess the benefits and costs of new types of desalination and advanced water treatment technologies. In part, this is due to the challenge of projecting the decreases in costs and improvements in performance that are likely to occur through experience in manufacturing and application of the technologies. In addition, designers, operators, and regulators of water systems do not have experience with these types of systems because few have yet been deployed. To enable the diffusion of new technologies, NAWI seeks research that supports the decision-making process by projecting the performance of APRIME-enabled treatment technologies for distributed and centralized systems. Research that identifies water user sectors and specific applications that have a high potential for adoption at scale are particularly encouraged. NAWI envisions place-based research conducted in collaboration with key stakeholders will be used to provide an understanding of the factors affecting technology uptake and that the outcomes of these studies are used to create decision-support tools or identify lessons that can be applied in other applications and locations.

AOI C-1.
RESEARCH QUESTIONS (RQS):

- In what sectors and geographies would distributed desalination and advanced water treatment technologies achieve pipe-parity with existing centralized systems? What are the critical aspects of treatment performance that need to be improved to make these systems more attractive to decision makers?
- How can decision-support tools represent the costs and benefits of distributed treatment systems and their potential for adoption over timescales of relevance for water system planning?
- What are the existing water reuse and treatment regulations, policies, and institutional practices that are having the largest impacts on the deployment of desalination and fit-for-purpose water treatment systems?
- How can desalination and advanced water treatment systems leverage multiple aspects of A-PRIME to improve performance and hasten progress toward pipe-parity?

4.8 Cumulative Impacts of NAWI Master Roadmap Priorities

NAWI's goal is to facilitate the adoption of use and reuse of nontraditional water sources through technical advances that cumulatively achieve pipe-parity. The research program is designed to identify and build upon synergies across the A-PRIME Challenge Areas that are consistent with the Circular Water Economy objectives. Because no one single investment or technology breakthrough can solve the multitude of challenges facing water treatment R&D described in Section 3, we are focused on the cumulative impacts of NAWI investments across multiple A-PRIME priorities that enable distributed systems to achieve pipe-parity (Figure 13). Innovations are needed across many different unit processes, with each advancement contributing to the cost reductions or performance improvements needed to achieve pipe-parity and foster localized water reuse and/or the use of nontraditional water sources.

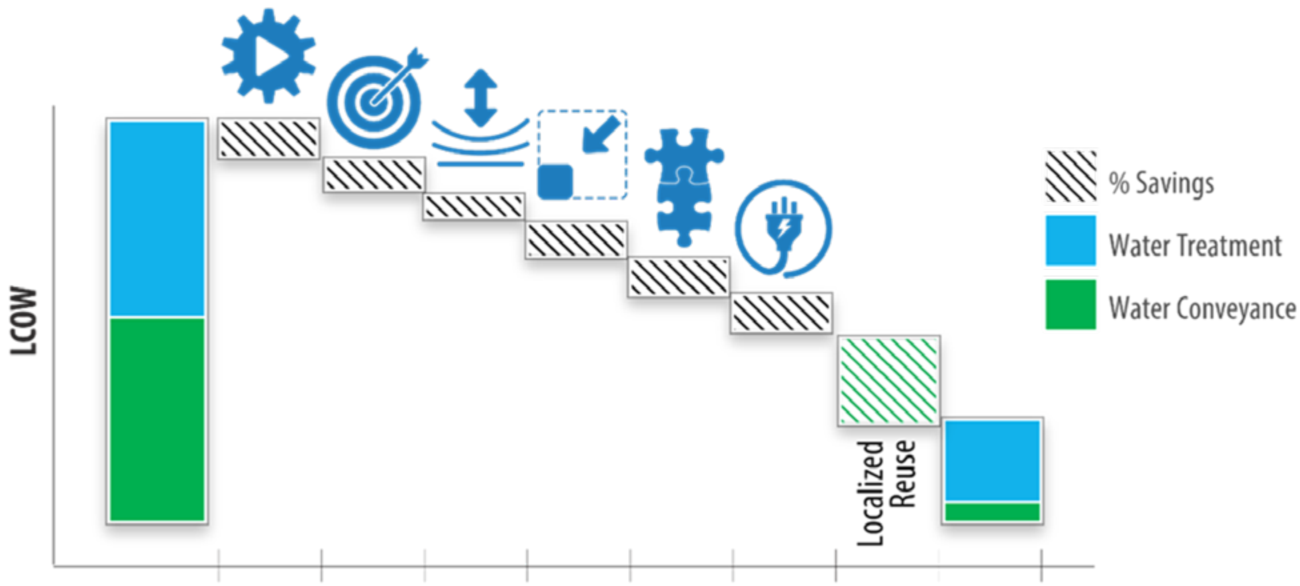


Figure 13. Cumulative Impacts of NAWI Challenge Area Investments on Pipe Parity

Analyzing the cumulative impacts of early-stage research on LCOW and other performance metrics is complicated by the diversity of operations across different water sectors. As described in previous sections, the needs of each of the PRIMA water user sectors and variations in treatment due to influent water quality, local regulations, and geographic factors make it difficult to make broad generalizations about research impacts. It may be possible to estimate the cumulative effects of A-PRIME innovations at specific facilities where baseline data are available, but there will be considerable uncertainty in efforts to use these data to make nationwide projections.

Furthermore, the assignment of benefits associated with advancements associated with a specific AOI is challenging because there is considerable overlap among the A-PRIME AOIs described in Section 4 when they address different aspects of the same water treatment challenges. In some cases, several innovations will need to be implemented together to realize substantial cost reductions and performance improvements. As an example, to address challenges of fouling and scaling, an autonomously operated system (A3) could detect anomalies on a resilient membrane designed to operate under conditions of variable water quality (R1); data collected by sensors could provide a means of continuously adjusting the operation of an electrified pretreatment technology (E1, M2) to counteract the fouling and scaling. Each of these innovative components (A3, R1, E1, M2) requires advancements in others to achieve the most impactful result of minimizing the potential negative consequences of fouling and scaling.

For some treatment trains, advancements in one or more AOIs could obviate the need for other process improvements. For example, a new modular and electrified pretreatment process (E1, M2) could be utilized to selectively remove a contaminant of concern (P1). This treatment may negate the need for a more bulk separation membrane treatment process that would have required a brine management system (I3) to comply with discharge regulations. In this case, advancements in the E, M, and P Challenge Areas would render the brine management system (the focus of the I Challenge Area) unnecessary. NAWI will continue to evaluate where such opportunities exist and what cost and performance tradeoffs may be most impactful under diverse conditions as part of its Circular Water Economy challenge area.

Some Challenge Areas and AOIs are focused on technology and process improvements for well-defined unit processes (e.g., more mature technologies for which extensive baseline data are available). For example, it is relatively straightforward to assess the impacts of improving the performance of brine concentration technologies or sorbents used for selective separations on the costs of operating centralized brackish water desalination facilities. Other Challenge Areas and their associated AOIs focus on advancements that enable NAWI's vision of autonomous, decentralized treatment systems; these types of advancements can be more challenging to quantify because there are very few operational facilities for which baseline data are available (Figure 14). NAWI prioritizes investments in both technology and process improvements as well as enabling decentralized systems to fully capture the synergies described above across the A-PRIME Challenge Areas.

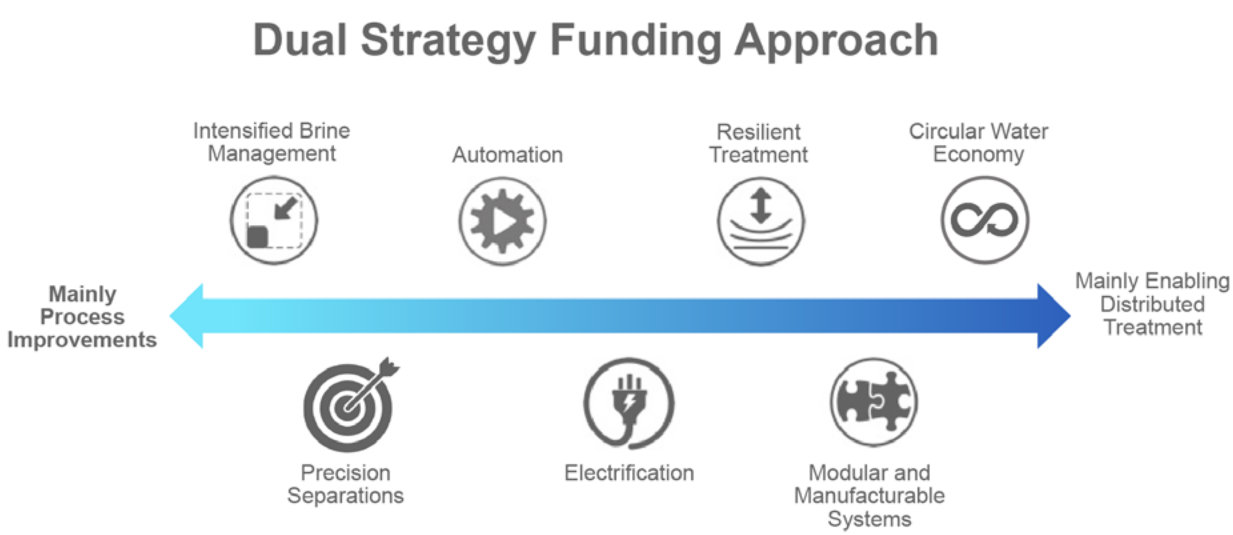


Figure 14. Continuum of NAWI challenge areas and investment type

The connections and synergies across A-PRIME Challenge Areas, in addition to understanding how some are enabling capabilities and others are technology and process improvements, are more explicitly highlighted in the descriptions below.

AUTONOMOUS

Autonomous operations advancements can serve as an enabling feature for new forms of distributed desalination and water recycling systems. It also can reduce operational costs for existing, centralized facilities. The magnitude and type of impact will depend upon the unit processes, treatment objectives and influent water quality. Many treatment systems are designed with redundancies that provide a safety factor for operations (e.g., in ZLD systems). Some of the added costs of such systems could be decreased if processes were better automated and controlled, leading to reductions in the capital costs of new facilities as well as lower operating costs. Furthermore, most existing desalination and water recycling plants do not take advantage of variations in electricity prices, even when doing so would not impact their ability to meet end-use quality requirements. This offers another opportunity for realizing savings through autonomous operations. For treatment systems in which extensive automation already exists and labor accounts for a smaller fraction of the LCOW, the effects of autonomous operations are likely to be relatively modest compared to those that are possible for small-scale distributed systems, where influent water quality and quantity may vary temporally and labor costs are increased due to the need for technicians to travel to remote locations to service equipment. Autonomous operations also may have other benefits: nearly every plant could benefit from reductions in planned and unexpected downtime (A3), increased labor efficiencies (A3), and improved performance from the utilization of data being collected (A1–A4). These advancements in turn enable greater impacts from other A-PRIME priorities, including reductions in energy and chemicals consumption (E2), and improved operational efficiency of pretreatment (M2), precision separation (P1), and brine management (I3) technologies.

PRECISION

To achieve water quality objectives, desalination and water reuse treatment trains are sometimes configured around the need to remove specific, trace contaminants. When bulk separations technologies (e.g., RO membranes) are employed for removing trace contaminants, capital costs, operating costs and energy consumption can be quite high. Replacing bulk separations technologies with precision technologies to address trace contaminants has the potential to drastically reduce energy consumption and costs, in part because it could reduce the production of brine for which management technologies (I3) are required. Precision separation technologies could be enabled by related advancements in technology manufacturing (M1); their performance could be improved through cost reductions and electrification of pretreatment technologies (M2, E2); O&M costs could be reduced through lengthening lifetime of process components (R1). Precision separations advancements may also create new opportunities to valorize valuable materials.

RESILIENT

Resilience improvements that dramatically increase the service life of treatment system components and expand operation in diverse conditions (R1) can reduce operational costs of water treatment systems. However, the greatest benefits of resilience may be realized in decentralized desalination and water recycling systems, which are subject to variable water quality and quantity, conditions that are more likely to cause fouling and scaling. These conditions may prevent investment in some decentralized systems. In centralized desalination facilities (e.g., seawater RO plants), membrane biofouling during algal blooms can increase energy consumption (E2), increase downtime (A3), and/or shorten the life of the membranes (M1) while overloading pretreatment systems that cannot handle higher biomass loading (M2). Advancement related to resilience can improve facility performance by counteracting some of these impacts. Resilience of materials and processes is a critical enabling factor for implementation of decentralized systems under variable conditions, especially those requiring advanced brine management (I3), electrified pretreatment technologies (M2), or conducting precision separations (P1). Autonomous innovations (A3) can also enable systems to adapt to changing conditions and support operational strategies that reduce fouling and scaling issues.

INTENSIFIED

The costs of brine management depend on the source water and available brine disposal options. In some cases, the absence of an inexpensive means of brine disposal (e.g., seawater disposal or deep well injection) is a barrier to desalination and water reuse (I3). Reducing the costs of brine management that facilities currently experience would be valuable. Substantial cost reductions are also needed to enable both centralized and distributed facilities to be economically viable. In the absence of inexpensive disposal options, ZLD or near-ZLD technologies will require substantial cost reductions and performance improvements if desalination is to achieve pipe-parity. Beyond economic considerations, higher recovery rates in brine management approaches could expand available water resources for beneficial use in some specific contexts, while also avoiding some environmental challenges from deep well injection. Advancements in precision separations (P1) could lead to further opportunities associated with brine management if constituents of brines can be valorized. To achieve capital cost reductions, brine management technologies will benefit from advancements in technology manufacturing (M1); electrified pretreatment and other brine management technologies (M2, E1); O&M costs could be reduced through lengthening lifetime of process components and making them more resilient to fouling and scaling (R1). Finally, advances in automation could reduce costs of brine management technologies through greater control of process performance and creating the ability to take advantage of fluctuating electricity prices.

MODULAR

Innovations in technology modularity and manufacturing approaches will affect technology capital costs (M1); pretreatment needs (M2); and regulatory, construction, and long-term operational contingencies (M2) of advanced water treatment trains. These advancements will also enable more tailored treatment configurations that can reduce operational costs through reductions in energy needs (E2) and the facilitation of robust operations under variable water quality and quantity (R1). Reducing capital costs and associated project contingencies will be essential for distributed desalination systems to achieve pipe-parity. In particular, manufacturing advancements can help reduce the costs of precision separations (P1) and brine management technologies (I3), while electrified pre-treatment advancements (E1) can enable these technologies to achieve higher performance and recovery.

ELECTRIFIED

Electrified processes can reduce energy costs and carbon footprints by eliminating expensive and carbon/energy-intense commodity chemical production (E1); by reducing transport and storage of chemicals by implementing onsite, in situ electro-chemical production (E1); and by adapting operations in response to variable pricing of grid electricity (E2). Although electrification of processes could lead to higher energy demands, these potential increased costs could be mitigated by the reduction of expenditures on chemicals and through flexible operations that take advantage of lower cost electricity. The greatest benefits could be experienced by smaller and remote treatment systems, where the need for external sources of chemicals can lead to higher costs for purchasing, higher transport costs, greater susceptibility to supply chain disruptions, the need for onsite storage infrastructure, and increased health and safety concerns over managing hazardous chemicals. Electrified processes could benefit pretreatment technologies (M2); precision separations technologies (P1); and brine management technologies (I3). Electrified processes would also better integrate with autonomous systems (A3) in the context of flexible operations and in responding to early detection of fouling and scaling.

5. NEXT STEPS

This comprehensive and dynamic roadmap for low-TRL desalination and water treatment technologies is intended to guide future NAWI R&D investments throughout the duration of the research program. NAWI's Master Roadmap has compiled high-value, crosscutting themes across end-use water roadmaps and is categorized under the A-PRIME areas. In 2021, NAWI will begin implementing the crosscutting research priorities outlined in the Master Roadmap via requests for projects (RFPs) and a project selection process designed to align member needs with the Alliance's research and development efforts. The funded projects will represent the most impactful development opportunities that will ultimately motivate subsequent industry investments required to further enable the use of nontraditional waters sources in a cost-effective manner.

Because the roadmap is a forward-looking document meant to guide NAWI throughout its existence, the Alliance will update its roadmap periodically. NAWI encourages and facilitates additional feedback from stakeholders on the Master Roadmap via the NAWI website.[12] Regular updates will also be critical to ensure that NAWI's roadmap evolves with the changing landscape of U.S. water treatment technologies, including the advancement in materials R&D, new processes, novel modeling and simulation tools, and expanded integrated data and analysis capabilities. Each aspect of the A-PRIME hypothesis, as well as the identified research priorities, will be regularly vetted with water treatment professionals from each PRIMA industry sector to ensure that it is a relevant pathway to advancing desalination and water treatment capabilities with nontraditional source waters. In successive roadmap iterations, the feedback will be used to assess the relevance of each research priority to the roadmap and evaluate progress toward achieving its goal of enabling a water circular economy while considering all relevant pipe-parity metrics. NAWI will adjust its priorities and expand its available resources to maximize the impacts of its efforts. The technology advancements developed by the NAWI research program are geared to help domestic suppliers of water desalination systems to design and manufacture critical equipment, components, and small-modular and large-scale systems.

Appendix A: Acronyms

A-PRIME	Autonomous, Precise, Resilient, Intensified, Modular, and Electrified – NAWI R&D focus area
AOI	Areas of interest
AOP	Advanced oxidation process
CEC	Contaminants of emerging concern
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
EPRI	Electric Power Research Institute
GAC	Granular activated carbon
g/L	Grams per liter
IoT	Internet of things
LCOE	Levelized cost of electricity
LCOW	Levelized cost of water
LED	Light emitting diode
m^3	cubic meters
mg/L	Milligrams per liter
MVC	Mechanical vapor compression
NAWI	National Alliance for Water Innovation Hub
O&M	Operations and maintenance
PARAFAC	Parallel factor analysis
PLC	Programmable Logic Controller
ppm	Parts per million
PRIMA	Power, Resource Extraction, Industry, Municipal, Agriculture End-Use sector focus for NAWI
RAC	Research advisory council
R&D	Research and development
RFP	Request for projects

RO	Reverse osmosis
SAR	Sodium absorption ratio
SCADA	Supervisory control and data acquisition
TDS	Total dissolved solids
TRL	Technology readiness level
USBR	U.S. Bureau of Reclamation
USDA	U.S. Department of Agriculture
UV	Ultraviolet
WRF	Water Research Foundation

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