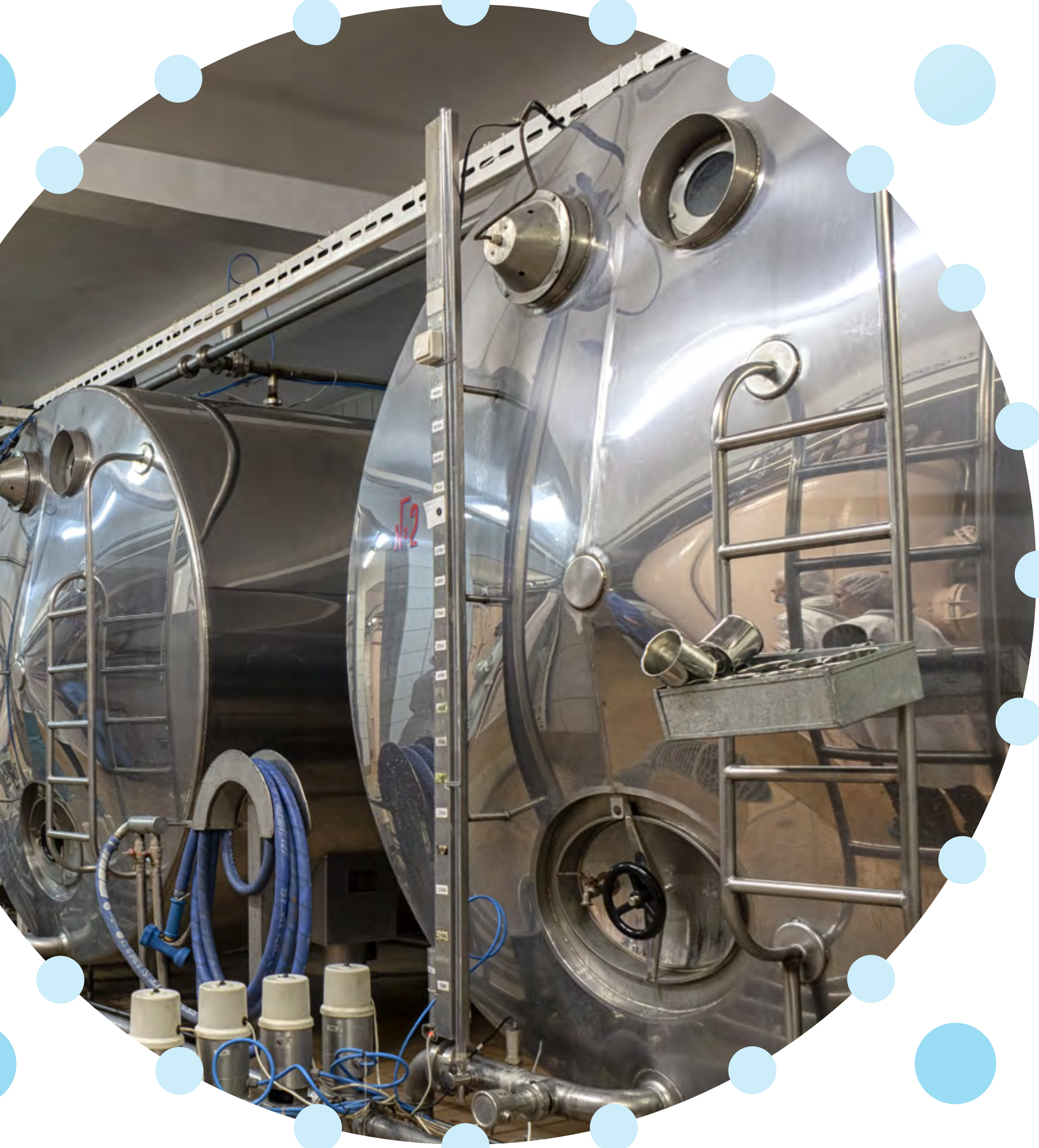
National Alliance for Water Innovation

INDUSTRIAL SECTOR

TECHNOLOGY ROADMAP



Tzahi Cath
Colorado School of Mines

Shankar Chellam
Texas A&M University

Lynn Katz
University of Texas-Austin

Jaehong Kim
Yale University

Richard Breckenridge
Electric Power Research Institute

Jordan Macknick
National Renewable Energy Laboratory

Aidan Meese
Yale University

Jason Monnell
Electric Power Research Institute

Trenton Rogers
Electric Power Research Institute

David Sedlak
University of California-Berkeley

Sridhar Seetharaman
Arizona State University

Jennifer Stokes-Draut
Lawrence Berkeley National Laboratory

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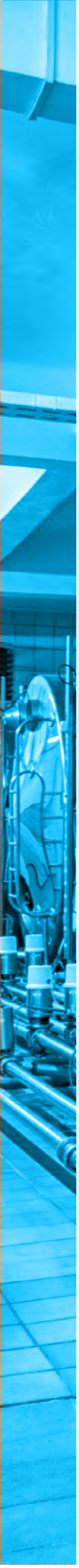
- Add Acknowledgements section
- Correct numerical errors in Table 3
- Correct grammatical errors
- Added new and deleted unused acronyms (Appendix A)
- Renumbered end note citations in sequential order throughout document



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INDUSTRIAL SECTOR

TECHNOLOGY ROADMAP

1. EXECUTIVE SUMMARY

1.1 Introduction to NAWI and the NAWI Roadmap

The National Alliance for Water Innovation (NAWI) is a research consortium formed to accelerate transformative research in desalination and treatment to lower the cost and energy required to produce clean water from nontraditional water sources and realize a circular water economy.

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.***

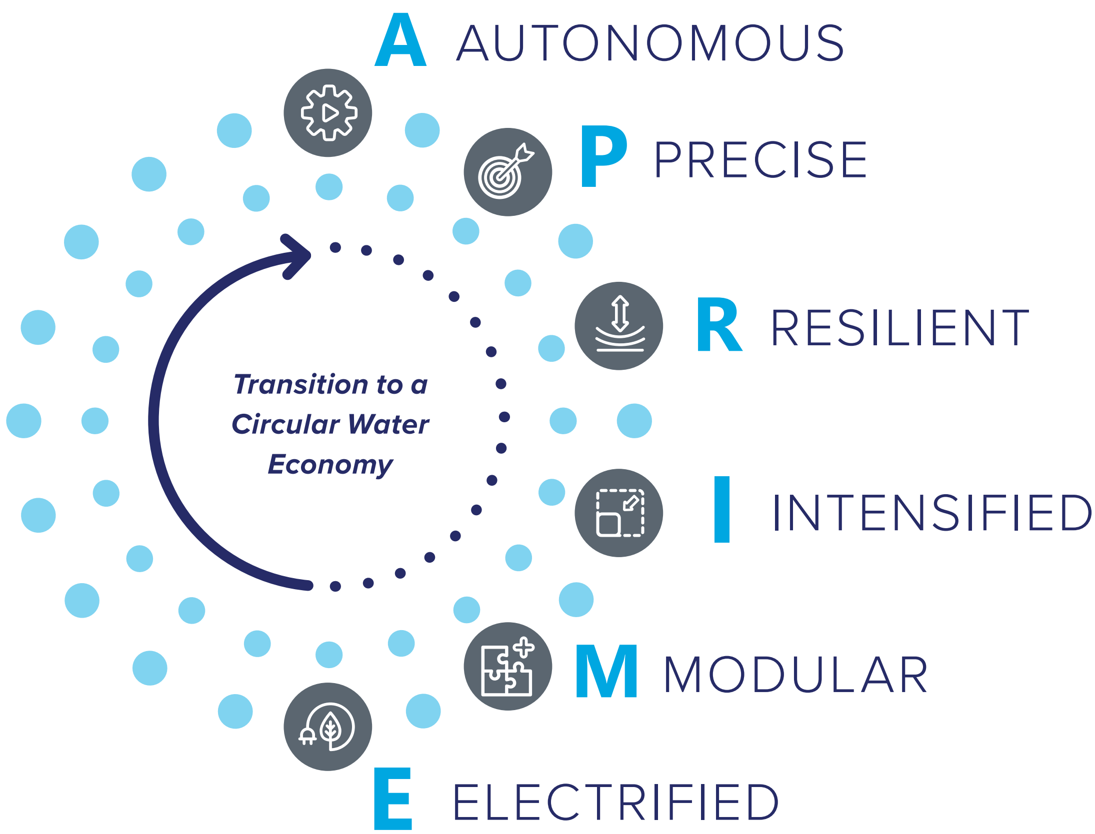
The nontraditional source waters of interest include brackish water; seawater; produced and extracted water; and power, mining, industrial, municipal, and agricultural waste waters. When these desalination and treatment technologies are fully developed and utilized, they will be able to contribute to the water needs of many existing end-use sectors. **NAWI has identified five end-use sectors that are critical to the U.S. economy for further exploration: Power, Resource Extraction, Industry, Municipal, and Agriculture (PRIMA).**

Power | **Resource Extraction** | **Industry** | **Municipal** | **Agriculture**

This **Industrial Sector** roadmap aims to advance desalination and treatment of nontraditional source waters for beneficial use in public water supplies by identifying research and development (R&D) opportunities that help overcome existing treatment challenges.

Under NAWI's vision, the transition from a linear to a **circular water economy** with nontraditional source waters will be achieved by advancing desalination and reuse technologies in six key areas: Autonomous, Precise, Resilient, Intensified, Modular, and Electrified, collectively known as the **A-PRIME** challenge areas.

Technological advances in these different areas will enable nontraditional source waters to achieve pipe parity with traditional supplies.



Pipe parity is defined as the combination of technological solutions and capabilities (e.g., resiliency enablers and strategies leading to long-term supply reliability) and non-technological solutions that make impaired water sources competitive with traditional water resources for various end-use applications.

To effectively assess technology advances and capabilities, NAWI will use pipe parity metrics relevant for the Industrial End-Use Sector. These metrics can be quantitative or qualitative, depending on how an end user would evaluate different potential water sources and whether they could be integrated into their supply mix.

1.2 Water User Sector Overview

The Industrial Sector Roadmap includes water use in the Oil Refineries, Pulp and Paper, Primary Metals, Chemicals, and Food and Beverage industries as well as Data Centers and Large Campuses. Total withdrawals for the Industrial Sector are about 68.5 million m^3 per day (18.1 billion gallons per day).[1,2,3] The primary sources of water for the Industrial Sector are from self-supplied water (either surface or ground water). This sector makes use of both fresh and brackish water sources, depending on location, availability, and application. Municipal water is the first alternative source because it is available in most industrial locations, is of consistent quality, and is relatively inexpensive. After self-supply and municipal sourcing, industries are also examining and investing in internal water recycling and reuse of reclaimed water from other industries' waste streams. While there is an increasing need for industries to consider such alternative nontraditional water sources, especially in water-stressed regions, financial, regulatory, and other challenges affect the sector's ability to use them cost-effectively. As the U.S. population grows, industry expands, and climate change impacts water supplies, current sources will be placed under greater stress, and nontraditional/impaired source waters will need to play a bigger role in meeting water supply needs.

1.3 Water Treatment and Management Challenges

Broad industry challenges and key gaps that need to be addressed to enable the Industrial Sector to efficiently use nontraditional source waters are summarized in Table 1. These barriers have been identified through workshops and discussions with subject matter experts, as part of a structured roadmapping process. The barriers are too large and far-reaching for any one organization to solve on its own. NAWI intends to invest in promising technology readiness levels (TRL) 2–4 concepts that are crosscutting across the PRIMA areas and that address some technical limitations discussed below, and welcome complementary efforts by other research organizations.

Table 1. Synopsis of technical and non-technical challenges to utilizing nontraditional water sources for the Industrial Sector

TECHNICAL

Constituent Detection, Analysis Challenges, and Process Monitoring and Control

- The industry needs improved means for real-time data collection, characterization, and quantification of constituents of concern in source, process, and wastewaters.
- Accurate modeling and analysis of water quality data generated within complex source water matrices and treatment systems are needed to optimize industrial treatment system operations, promote reuse and recycling within an industry, and ensure consistent process and effluent water quality.

TECHNICAL

Design and Manufacturing Challenges

- The industry needs new water treatment and reuse technologies and equipment designed to seamlessly integrate into existing treatment trains and industrial processing systems.
- The design, manufacturing, and control of new water treatment technologies need to be scalable and resilient to meet evolving industry needs.
- The industry needs efficient, cost-effective, and modular water treatment systems that can be applied to various industries.

Supply Limitation Challenges

- Identifying, sourcing, and ensuring a reliable supply of nontraditional water will be a continued challenge for the sector.

Quality Limitation Challenges

- Varying source water quality can impact industrial operations, risking product quality and creating downstream and environmental impacts.

NON-TECHNICAL

- Due to a variety of factors, water is undervalued in many industries and the motivation for investment is often lacking.
- Water and wastewater treatment and disposal regulations and requirements vary by jurisdiction (federal, state, local, and tribal) and location.
- Data collection and sharing are limited by the lack of standards, liability concerns, and limited understanding of business and operational benefits.
- The Industrial End-Use Sector is adverse to assuming risks related to the use of nontraditional water sources and the implementation of new technologies that have not been proven by other industries.
- There are a number of environmental risks stemming from the increased use of nontraditional waters.
- Nontraditional water use introduces challenges relating to the education and skills of the sector’s workforce.
- Technologies for nontraditional water use—including internal reuse and wastewater reuse outside of the industrial sector—could develop faster than related regulations or could spur additional, challenging regulations.

NON-TECHNICAL

- Even if developments in nontraditional water use succeed technically and meet regulatory requirements, public acceptance may prove to be another challenge for some industries (e.g., food and beverage industry).
- Familiarizing technicians, engineers, and decision makers with capabilities and limitations as well as installation, operation, and maintenance of new technologies is critical to its proper implementation and acceptance by the community.

1.4 Research Priorities

To overcome these industry challenges, strive towards meeting pipe parity, and achieve NAWI's mission of expanding the use of nontraditional source waters for the Industrial Sector, this roadmap lays out several research priorities that were identified through structured roadmapping processes with subject matter experts. These R&D Areas of Interest (AOIs) are grouped under the individual A-PRIME challenge areas discussed earlier. Specific research gaps—technologies or problems that have not been sufficiently answered by existing studies—are also included with each development area. At the end of this summary of topics, a short discussion on the benefits of new technoeconomic analysis (TEA) and life cycle analysis (LCA) research is also provided.

The Autonomous area entails developing robust sensor networks coupled with sophisticated analytics and secure controls systems. Specific prioritized research areas include:

- **Automate decision-making and control of water treatment processes –** autonomous system operation tools, artificial intelligence (AI)/machine learning (ML) algorithms, and digital twins supported by big data to provide monitoring, prediction, and management of water treatment processes. The solutions need to be easy to implement and cyber-secure.
- **Use advanced sensors for the online monitoring of water quality –** innovative materials, material architecture, and integrated devices to detect target water constituents with high sensitivity and selectivity under a wide range of complex industrial water conditions. They need to be low-cost, durable, easy to calibrate, and capable of real-time detection and communication with control systems. They need to be supported by an understanding of the complex interactions of water constituents, water treatment steps, process steps, and equipment.

The Precise area focuses on a targeted treatment approach with precise removal or transformation of treatment-limiting constituents and trace contaminants. Specific research areas include:

- **Develop materials and processes for the selective separation or destruction of recalcitrant organic pollutants in industrial wastewater –** materials and processes that enable precision separations or destruction and that are sustainable, durable, and maintain high efficiency over long term use. These devices should be integrated into treatment processes for synergistic removal of recalcitrant pollutants.

- **Develop materials and processes for selective separation and recovery of metal ions and nutrients from waste and brine streams –** materials and processes with precise control of properties to enable selective transport, binding, and removal of target solutes. These materials should be supported by a fundamental understanding of the behavior of colloid, molecule, and ion interactions and transport. These materials and material-based processes would also support selective reduction, resource recovery, and onsite chemical synthesis.

- **Develop and optimize pretreatment of bulk constituents to enhance and protect downstream treatment processes –** develop materials and treatment processes, either non-chemical or non-biological approaches, that enable highly efficient oil-water separation, provide fouling and scaling control under a broad range of conditions, and treat high-strength wastewater containing high levels of organics.

The Resilient area looks to enable adaptable treatment processes and strengthen water supply networks. Specific research areas include:

- **Enhance chemical and biological resiliency of materials and process components in water treatment –** develop materials and process components, including membrane materials, composite membrane structures, ion exchange resins, and adsorbent materials that are durable in harsh operating conditions, can control microbial growth and biofilm formation, can control fouling and scaling, and can maintain high selectivity and permeability. These materials and approaches can be supported by advanced materials modeling and characterization methods which accurately relate materials' properties to their overall performance.

The Intensified area focuses on innovative technologies and process intensification for brine concentration and crystallization and the management and valorization of residuals. Specific research areas include:

- **Develop cost-effective waste/brine management and solidification –** develop innovative process configurations, process designs, stabilizing mixtures, zero liquid discharge (ZLD) and minimum liquid discharge (MLD) strategies that combine processes and technologies that reduce leaching of difficult-to-solidify trace elements. Support these developments with TEAs to identify the appropriate strategies for implementation and with improved theoretical understanding of conditions and governing processes.

- **Improve prediction and chemical modeling of concentrated waste and brine streams and verify with experiments –** develop and verify predictive models describing chemical and physical properties of potential resources and hazardous constituents and their interactions, and models describing nucleation and crystalline phase growth to simulate scaling formation and crystallization in complex systems.

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. Specific research areas include:

- **Define the level of wastewater treatment necessary to protect downstream processes and develop economically scalable, modular pre- and post-treatment processes with reduced weight and footprints that can be flexibly integrated with various treatment processes –** develop robust, high-rate, modular pretreatment processes for suspended solids and organics removal. Reduce weight, footprint, and overall complexity of pre- and post-treatment technologies and systems. Support these developments with material and/or treatment process changes to increase process throughput and operational flexibility, improve valorization, and increase water recovery and performance.

- **Improve module design and fabrication techniques for various treatment technologies to optimize integrated system performance, flexibility, and scalability, and to develop cost-effective modular treatment systems –** develop flexible treatment trains to adapt to industry-specific needs, supported by innovate manufacturing designs that allow for customization and modifications. Develop mechanistic and/or stochastic models and control algorithms for the variety of process and operating configurations.

The Electrified area aims to replace chemically intensive processes with electrified processes that are more amenable to variable or fluctuating operating conditions. Specific research areas include:

- **Chemical-supply-free electrocatalytic processes for pollutant destruction –** develop innovative electrode materials and cell designs for production of treatment chemicals, selective cathodic reduction of oxyanions, and selective anodic oxidation of recalcitrant organic pollutants. Support with an improved understanding of surface and electrochemical phenomena of electrodes and strategies to promote faster technology development and transfer to industry.

- **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 –** create treatment modules and operating systems that are able to efficiently ramp capacity up and down based on energy cost and/or availability and are designed to integrate with renewable energy and optimized for flow equalization. Support these technologies by developing intensified treatment options and by combining process steps into single modules to improve implementation.

1.5. Next Steps

NAWI's comprehensive and dynamic roadmap for desalination and water treatment technologies for the Industrial End-Use Sector is intended to guide future R&D investments throughout the duration of the research program. Because this roadmap forecasts into the future and is meant to guide NAWI throughout its existence, it should be considered a living document that is periodically re-evaluated and revised to ensure its continued relevancy. With ongoing input from industry stakeholders and support from academia, water utilities, water professionals, and other NAWI partners, the Alliance will update this roadmap to ensure it evolves to capture progress of high-priority objectives as well as the emergence of new technologies.

1.6. Appendices

The appendices include a list of relevant acronyms for this document (Appendix A); an expanded description of the NAWI A-PRIME hypothesis (Appendix B); Department of Energy (DOE) Water Hub development background (Appendix C); roadmap teaming structure (Appendix D); in-depth examination of the roadmap development process (Appendix E); technology roadmap contributors (Appendix F); and relevant references (Appendix G).

2. INTRODUCTION

2.1. Growing Challenges with Water

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.[4] Water managers in 40 states expect water shortages in some portion of their state in the next several years.[5] As water insecurity grows in severity across the United States and populations increase in regions with limited conventional sources, using water supplies traditionally ignored or avoided due to treatment challenges are being reconsidered.

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.[6] As an added benefit, **these water supplies could contain valuable constituents that could be reclaimed to further a circular economy.**

2.2. Establishing an Energy-Water Desalination Hub

In 2019, DOE established an Energy-Water Desalination Hub (part of a family of Energy Innovation Hubs)[7] to address water security issues in the United States. NAWI was funded to address this critical component of DOE's broader Water Security Grand Challenge 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 (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 strategic roadmap was developed for the Industrial Sector to identify R&D opportunities that help address their particular challenges of treating nontraditional water sources. Recognizing the important sector-specific variations in water availability and water technology needs, NAWI has also published four other end-use water roadmaps each with specific R&D and modeling opportunities (power, resource extraction, industry, and agriculture). Each roadmap has been published as a standalone document that can inform future NAWI investments as well as provide insight into priorities for other research funding partners.

2.3. 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 operations 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 contaminants 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, the ability to incorporate variable input water quantity flows, the ability to produce variable output water quality, and the ability to 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 calculation of potential ranges of improvement.

Specific baseline information required includes:

a) information on the type, concentration, availability, and variability of impurities in the source water;
b) identification of key unit processes and representative treatment trains treating the source water and their associated cost, removal efficiency, energy use, robustness, etc.;
c) ranges of performance metrics for treatment of the source water for applicable end-uses; and
d) definitions of pipe parity for the source water type and water use.

2.4. Nontraditional Waters of Interest

2.4.1. Sources of Nontraditional Waters

NAWI has identified eight nontraditional water supplies of interest for further study (Figure 1):

Seawater and Ocean Water	Water from the ocean or from bodies strongly influenced by ocean water, including bays and estuaries, with a typical salinity around 30,000 parts per million (ppm)
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 g/L total dissolved solids (TDS).
Industrial Wastewater	Water from various industrial processes that can be 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

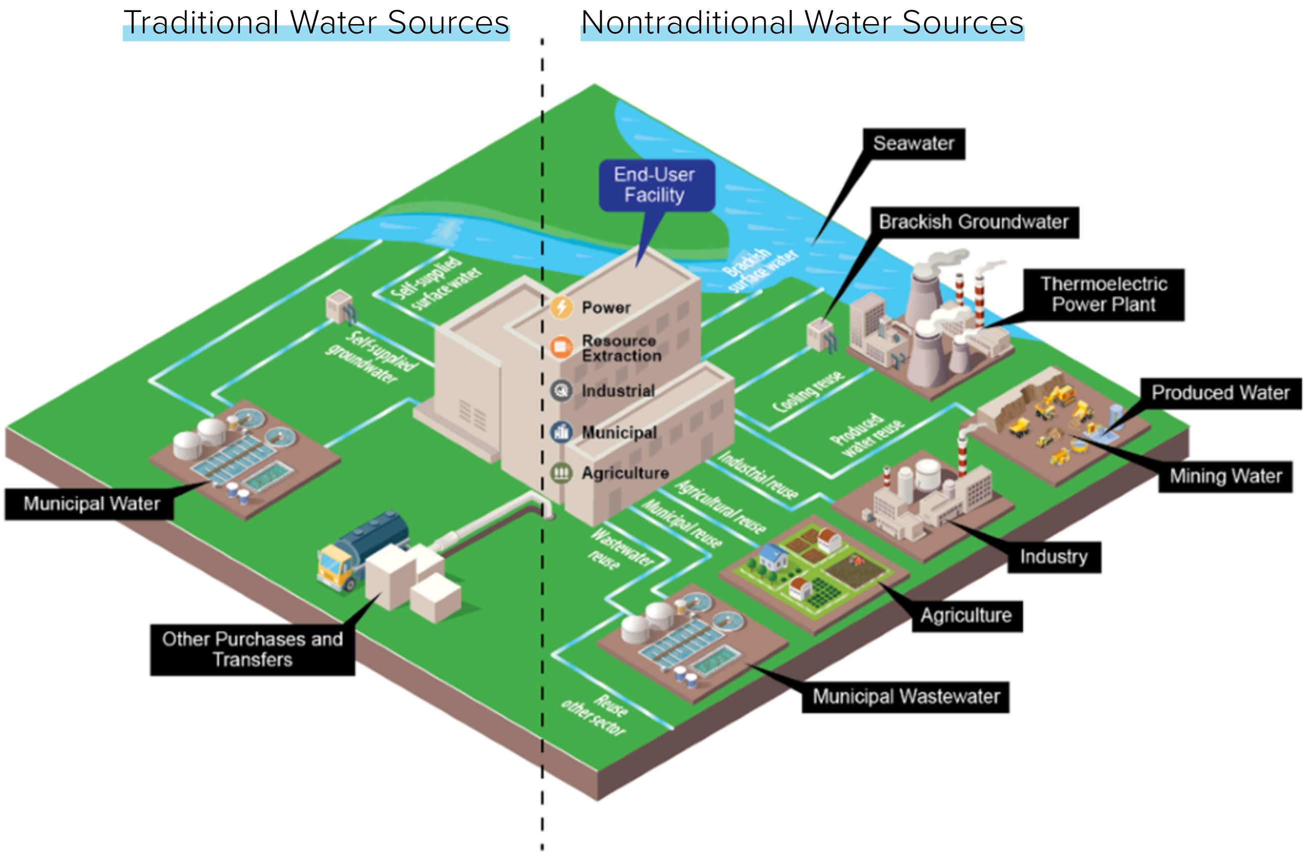


Figure 1. Schematic of traditional and nontraditional sources of waters, as defined by NAWI
(Graphic courtesy of John Frenzl, NREL)

These water sources range widely in salinity (100 ppm – 800,000 ppm total dissolved solids) as well as the type and concentrations of contaminants (e.g., nutrients, hydrocarbons, organic compounds, metals). **These different supplies require varying degrees of treatment to reach reusable quality.**

2.4.2. End-Use Areas Using Treated Nontraditional Source Waters

When these 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 2 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 2. PRIMA and the industries covered in each area

2.5 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.[6] 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.

* 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.

The NAWI A-PRIME hypothesis outlines the following six major challenge areas needing improvement for water treatment to reach pipe parity for nontraditional waters. An A-PRIME synopsis is provided below; a more in-depth discussion on the A-PRIME challenge areas can be found in Appendix B.

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.

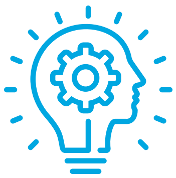
M The **Modular** area looks to improve materials and manufacturing processes and scalability to expand the range of cost-competitive treatment components and eliminate intensive pre/post-treatment.

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

2.6. Desalination Hub Topic Areas

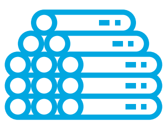
There are key technology areas of R&D, modeling, and analysis that cut across the water sources and sectors in the NAWI Hub.

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



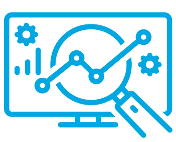
Process Innovation and Intensification R&D

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.



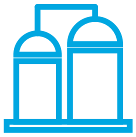
Data, Modeling, and Analysis

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.

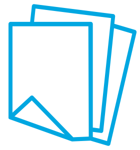
3. INDUSTRIAL WATER USER SECTOR OVERVIEW

This overview of the Industrial Sector provides a high-level synopsis of the industry and rationale for this roadmap's focus—expanding the availability and reliability of nontraditional water sources for industrial operations.

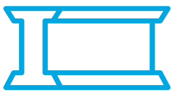
As introduced in Chapter 2, the Industrial End-User Roadmap includes the following industrial subsectors:



Oil Refineries

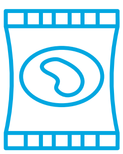


Pulp and Paper



Primary Metals

Chemicals



Food and Beverage

Data Centers and Large Campuses

Many sectors have potential overlap with NAWI Roadmaps, in particular the Resource Extraction and Power End-User Sector Roadmaps. Oil Refineries are the downstream portion of the Oil and Gas (O&G) Sector, while the Chemical Sector also processes O&G products. The Primary Metals Sector processes Mining industry products. All industrial sectors have significant electrical use and onsite cooling that overlap with the products and technologies researched in the Power End-User sector. **This Industrial End-User roadmap focuses on the direct water uses in these sectors, including source water quality and treatment needs, water reuse opportunities, and water and wastewater disposal.** This does not include upstream or downstream uses like off-site electric power generation or supply chain uses.

This roadmap has a focus on these industries within the United States, but due to the international nature of the companies involved and the universality of the challenges and opportunities for the industry and NAWI, worldwide trends and challenges are also included.

3.1. Overall Water Stress

As a result of factors such as population growth, expansion of industry, and climate change impacts, many regions of the United States are facing increased risks of water shortages. Figure 3 illustrates the predicted overall water stress in the United States in 2050 as a projection of current trends in population growth, power generation demand, and climate change.[8] Figure 4 shows the locations of manufacturing jobs in metropolitan areas (as of 2010 and in areas with populations greater than 55,000).[9] Viewing Figures 3 and 4 together illustrates that many industrial sites are already located in or will be in future areas of water stress.

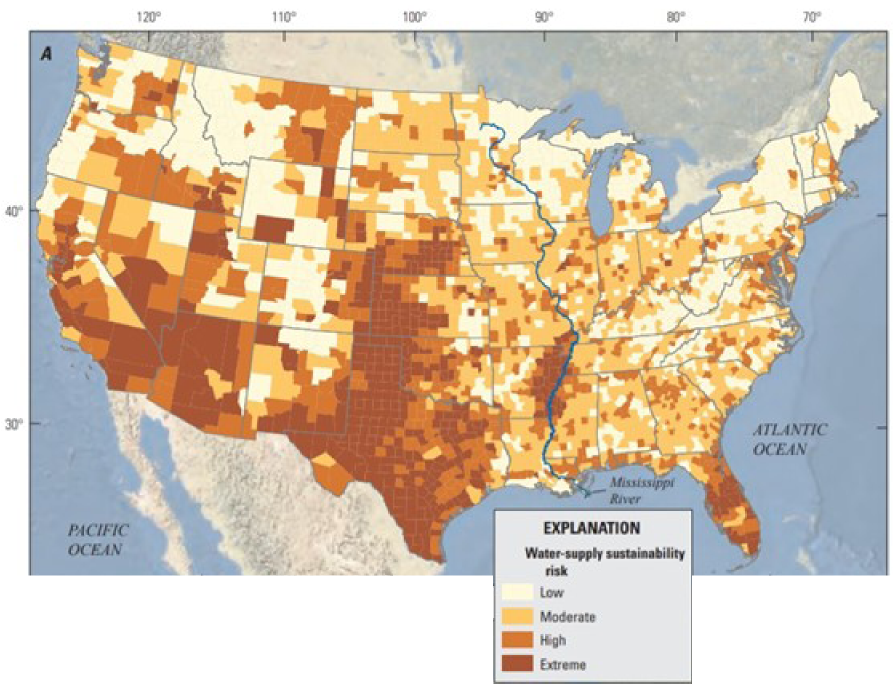


Figure 3. Water-supply sustainability risk index for the conterminous United States in 2050 linking water demand to population growth, increases in power generation, and climate change[8]
(Source: USGS)

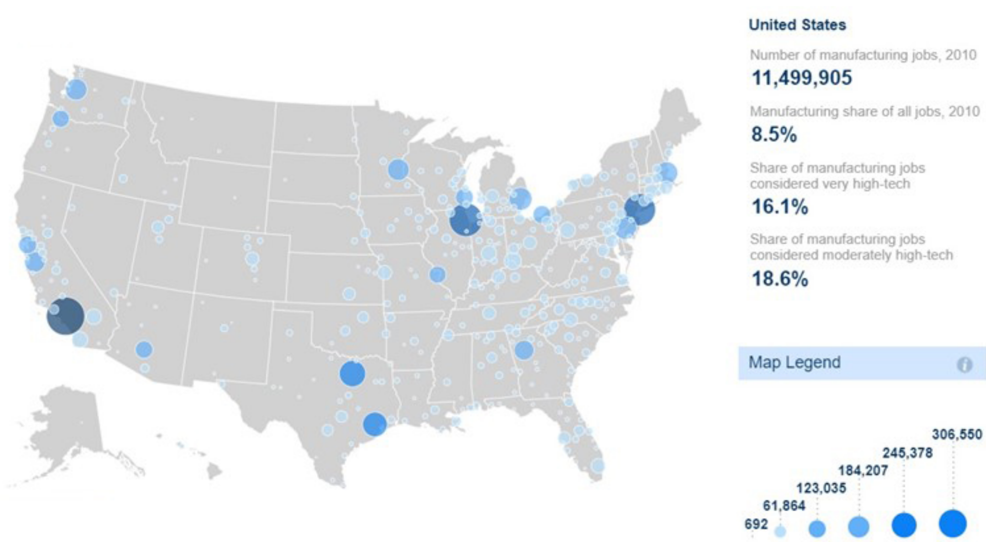


Figure 4. Manufacturing Jobs by metro center of population larger than 55,000 in 2010[9]
(Source: *Locating American Manufacturing*, Howard Wial: Brookings Institution, 2012)

3.2. Major Uses of Water in the Industrial Sector

3.2.1. Overall Industry Water Uses

The Pulp and Paper, Primary Metals, and Chemical (petrochemical and allied chemical, hereby referred to as Chemical) industries are the most significant direct users of water within the Industrial Sector.[1] The technologies and operations implemented by each subsector vary based on a wide range of factors: the finished products, local water and power sources, and discharge options all affect how water is used. Such an extensive variability in influencing factors makes it difficult to characterize applications to industry's water use and water technology implementation. Table 2 illustrates the distribution of water uses, by category, in several major industrial subsectors.

	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**%

*Data Center onsite water use is primarily for cooling purposes, while Large Campus water use varies widely—see Section 3.1.8.

Table 2. Fraction of water used within each industrial subsector for cooling water, boiler feedwater, process water uses, and other uses.[9]

Two high-demand needs for water are cooling and boiler feed. Cooling is required for nearly all industries with purposes ranging from heating, air conditioning, and refrigeration to direct and indirect cooling of molten metal.[10] Cooling processes and the water used for cooling share common features which characterize them as one of three categories: once-through, open-recirculating, or closed-recirculating cooling systems.[11] Boilers are widely employed across industries and require higher-quality water (and associated treatment) compared to other water-intensive processes within the industry.[12]

Table 3 provides estimates of total water withdrawals (not necessarily consumed) by the industrial subsectors in 2017. These values represent total water use, which may include both self-supplied water and water from public supplies.

INDUSTRY SUBSECTOR	ALL WITHDRAWALS m^3/day (MGD)
Oil Refineries[13]	**9,100,000** ***(2,400)***
Chemicals[4]	**15,000,000** ***(3,900)***
Primary Metals[4]	**19,000,000** ***(4,900)***
Food and Beverage[4]	**4,200,00** ***(1,100)***
Pulp and Paper[4]	**21,000,000** ***(5,600)***
Data Centers (NAICS 518210 only)[14,15]	**1,700,000** ***(450)***
Total Withdrawals (self-supply and water purchases)	**70,000,000** ***(18,000)***
Self-Supplied Withdrawals (self-supply estimate only, 2015)[16]	**56,000,000** ***(14,800)***

Table 3. Estimated annual water withdrawals for industry subsectors, 2017

3.2.2. Oil Refinery

The Oil Refining Industry's variability and complexity makes it difficult to identify the biggest process water uses. The amount of water used varies with the refinery's technologies, products, and raw materials composition. Some of the low-volume process water uses include crude water desalting (water mixed with crude to remove salts and ions), diluting waste streams, and desulfurization (removing sulfur dioxide and other sulfur compounds).[17] Other uses include equipment washing and utility water.

3.2.3. Pulp and Paper

Pulp and paper mills withdraw approximately 31 percent of the water identified herein as industrial (Table 3), making this subsector the largest industrial user of water in terms of withdrawals. Almost all phases of pulp and paper manufacturing require water—the largest of which are the bleaching process and the chemical solution for pulp making.[18] Another major use is for steam generation—for both onsite electricity production and for process use.[10]

3.2.4. Primary Metals

The major use of water in primary metals production is cooling and support for large equipment, including direct contact with both raw and processed steel and other metals.[12] Process water uses (and quality requirements) may depend on the material/product (e.g., ferrous and non-ferrous; alloys), whether the product is a finished one or a raw material for further modification, and the degree and level of finishing (e.g., coatings), but typically include material conditioning, equipment cleaning, air pollution control, and/or lubrication of rolling processes.[12,19] The water used in primary metals manufacturing is largely returned to its source after meeting the sites permit requirements (e.g., up to 90 percent in steelmaking).[20] Water is also used in air compressor systems for steam generation or for cooling. For those plants with onsite power generation, water is used in cooling towers.

3.2.5. Chemicals

Similar to the primary metals industry, the majority of water in the chemical industry is used for cooling and boiler processes.[10] Other uses include cleaning of equipment and supporting systems, hydraulic conveyance, and use as part of the finished product.[12] Much of the process water used in the manufacture of chemicals undergoes significant pretreatment to prevent equipment failure and ensure high quality end-products.

3.2.6. Food and Beverage Processing

Water used in the food and beverage sector is highly concentrated for sanitation and processing procedures—including raw materials washing (as much as 50 percent of total water use in, for example, fruits and vegetables handling and processing),[21] bottle washing (as high as 50 percent in soft drinks),[11] pasteurization, and condensation. Much like in the pulp and paper industry, the majority of water used in food and beverages manufacturing is for process uses, rather than for cooling and boiler feedwater.

3.2.7. Data Centers and Large Campuses

Data Centers

Data centers' onsite water is primarily used for cooling the electronics[22] (off-site water use is primarily from electric power generation and is covered in the Power End-User Roadmap). For example, the Lawrence Berkeley National Laboratory estimates Data Centers use 1.7 m^3 per MWh (460 gal per MWh) of electricity in their operations.[9] While this is currently a relatively low volume of water compared to other industrial uses (Table 3), it is a rapidly growing sector of the economy. Moreover, data centers tend to be located in close proximity to urban centers, which are often areas of relatively high water stress.[23]

Large Campuses

A large industrial campus's water uses and quality considerations are complex and can have many site-specific variations.[24] Large campuses can contain a variety of industrial and commercial operations including retail operations, manufacturing, and food and beverage processing, as well as other industrial applications like cooling towers and refrigeration, heating and boilers, electricity generation, and water used for research in academic institutions.[25,26,27] Water uses at such campuses also consist of domestic purposes including potable water, washing, and sanitization. In retail operations within large campuses, the primary uses are for direct consumption, sanitation processes, irrigation, and fire suppression.

3.3. Water Sourcing

3.3.1. Overall Industry Water Sourcing

The primary sources of water for industry are withdrawn from surface or groundwater; other sources include municipal water and/or treatment effluent (secondary or tertiary), followed by seawater.[28,29] This is largely driven by cost and generalized water quality requirements that surface waters often meet and include:

- chloride concentration limitations
- temperature (generally less than 75-85 degrees F)
- neutral pH (6.8-7.0)
- low hardness (<50 milligrams per liter [mg/L]), low suspended matter (<25 mg/L), and low organic matter content
- low dissolved metals[30]

Costs of water withdrawals are generally limited to infrastructure, pretreatment, and permitting and management costs, since in many cases there is currently no direct purchase price for the water. Municipal water usually is the first alternative source because it is available at most industry locations, is of consistent and high quality, and is relatively inexpensive: costs are negotiated by contract (typically on a sliding scale based on use rate) and can range from \$0.50 per m^3 to \$3 per m^3 for industrial purchasers.[31] Municipal sourcing (meeting federal drinking water standards) can sometimes mean lower total costs for water supply. This is because municipal water requires less additional pretreatment before industrial use as compared to water withdrawn from a surface or well source, due to prior treatment by the municipal provider. This may not be the case in secondary or tertiary treatment, where the requirements for pretreatment varies significantly based on the source and regulatory standards.

After self-supply and municipal sourcing, the industrial segment is evaluating technologies and investing in internal water recycle and potential for direct water reuse from their own and/or other industries' waste streams. These are the second alternative source options because, within the tolerances of daily process variances, the water quality and contaminants are known and are likely able to be treated with known or existing industrial water treatment operations. Moreover, in numerous industries, wastewater effluent being discharged is already of high enough quality for on-site reuse.

In current practice, seawater is generally a last resort as a source for many industrial non-cooling applications because it requires a higher investment in treatment technology (desalination in particular) and access is geographically limited due to infrastructure and transportation costs required to convey seawater inland any considerable distance.

Overall, the trend in water sourcing for new industrial demands is shifting from high quality (e.g., aquifers) to low quality (e.g., surface water or reused industry wastewater) to minimize water footprints and because of increasing stress on existing water supplies. Drivers for this trend are economic (withdrawal fees are being imposed), regulatory (where statutes limit quantity withdrawn and quality discharged), and social (environmental impact statements and negative publicity). Additionally, industry is experiencing sourcing challenges from climate change impacts, population growth, regulatory and public pressure to use nontraditional sources, saltwater intrusion into coastal freshwater sources, and general competition from agricultural and other non-industrial water uses.

3.3.2. Oil Refineries

Many of the largest refineries in terms of capacity are located in overall water-strained states, namely Texas and California,[32] though water stress varies by location within those states. They source their water by a variety of means dependent on usage within the facility. This can include municipal sources for domestic use (e.g., office, sanitary, drinking), seawater and municipal wastewater (for cooling), and a mixture of all sources for process waters.

3.3.3. Pulp and Paper

Pulp and paper mills are located where wood is abundant, along rivers, or close to rail and seaports that allow transit of raw and recycled feedstock. Thus, primary water sources for pulp and paper are from surface waters (e.g., oceans, lakes, rivers) or groundwater (e.g., wells). Some pulp and paper mills use municipal source water.

Pulp and paper mills are in varying geographical areas, and even though they access the same general types of water sources, the quality and constituents can vary significantly from site to site. Additionally, some mills using water from wells are pulling groundwater from aquifers that are under severe stress from various sources (e.g., drought, climate change, excessive withdrawals from the aquifer). The water requirements for pulp and paper vary by process requirements: boiler, evaporator and steam operations may require high purity, whereas washes, cooling and other processes may require lower quality water.

3.3.4. Primary Metals

Source water (and therefore treatment needs) for the Primary Metals Industry stem from internal requirements such as use in boiler feedwater or effects on product quality (e.g., contaminants affecting surface finish), as well as external requirements including blowdown water discharge requirements and other permit requirements. Many metal refineries are located near large bodies of water to ensure high intake demand is met with a source of low-cost, plentiful surface water.[12] Since a large fraction of the industry's water use is for cooling, there is a general requirement on source temperature to be significantly below the prevailing air temperature.

3.3.5. Chemicals

Much of the U.S. chemical industry and manufacturing is located along the Gulf of Mexico Coast[33] and other areas near surface water. The industry supplements its needs from well water, municipal sources, and recycled water from internal production. The volume and quality of the water varies by process; cooling processes may require high volumes of relatively low-quality water, while smaller volumes of ultrapure water are required for use as an ingredient in end products.

3.3.6. Food and Beverage Processing

Food and beverage processing industries generally use municipally sourced water, though some plants use other freshwater sources if the quality is sufficient, supplemented by onsite treatment. Food and beverage processing plants depend heavily on feed water quality, but different uses will require different qualities.

Water used as a product ingredient has some of the strictest quality guidelines, but water used for cooling and washing is similar to other industries. Meat handling plants utilizing municipal water generally require little to no additional treatment, while beverage plants sometimes implement additional treatment to help address equipment startup challenges or ensure that the water doesn't affect the resulting beverage taste or cause health concerns.

3.3.7. Data Centers and Large Campuses

Data centers generally obtain their water supplies from municipal sources, though they do also source directly from groundwater (aquifers) when their demand is high enough and where aquifer water is available.[34,35] Many campuses are supplied by municipal sources (one industrial entity reported 98 percent of their campuses were supplied from municipal sources with the remaining locations using wells with onsite treatment). Individual location requirements are often met with application-dependent water treatment systems

3.4. Water Reuse

3.4.1. Overall Industrial Reuse

Several industry subsectors (e.g., refining and primary metals) use mostly once-through or one-pass systems in their operations because of the generally high availability of water and its relatively low cost. Once-through systems are mostly for non-contact cooling applications. Implementing higher levels of recycling requires additional treatment and piping and thus higher costs compared with sourcing fresh water. Additionally, the introduction of nontraditional water sources—with potentially lower water quality or more and different constituents—could cause problems in closed systems, especially when concentrated (e.g., chlorides could lead to corrosion and higher total suspended solids [TSS] could lead to fouling).

Industries or applications that do not need high-quality water for operations will be more likely to look at effluent recycling to reduce stress and ensure availability of their existing water supplies. Common industrial systems, like cooling towers and condensate recovery,[20,36] implement reuse. Cooling loops generally require minimal pretreatment and can handle intake from many different processes simultaneously. However, water in these operations can only be recycled a limited number of times before contaminant levels exceed precipitation, corrosion, or discharge limits. Although dry cooling systems exist, which rely solely on air to operate, they tend to be highly energy intensive and costly to install and maintain.

Most of the water treatment and reuse solutions available now are geared toward higher-water-use industries, and where the systems can be designed and optimized for individual applications. Such customization generally is a very expensive and labor-intensive process. Some industry applications or locations have a large variety of low-volume waste streams with different treatment requirements. Comprehensive treatment systems (including pretreatment, operations, and disposal) that work efficiently at a smaller scale, handle the variety of contaminants, and require minimal labor/operational support are not yet generally commercially available.

3.4.2. Oil Refineries

Interviews conducted with industry representatives indicate that there is awareness of the potential cost savings and supply assurance benefits that come from reuse, and some refinery operators have been able to capture up to 50 percent of their wastewater for reuse.[‡]

3.4.3. Pulp and Paper

The Pulp and Paper Industry is a large water consumer, but it is also very efficient with water—88 percent of water is returned to the water source;[37] of the remaining, 11 percent is lost to evaporation and 1 percent incorporated in products. Because most mills are located in areas that are not particularly water-stressed,[4] there are currently few incentives to implement much additional reuse. However, due to increasing environmental concerns and regulations, the industry is implementing more reuse. Capturing and reusing biomass and important processing chemicals is another major benefit. Technology exists to completely close-loop the mill processes and recycle all water with minor losses, but it is very expensive and can cause additional operational issues.[§]

3.4.4. Primary Metals

One option for reuse within the Primary Metal Industry is other plants' waste streams, but mill sites are not often co-located, making it difficult and costly to transport one site's waste stream to other sites. For co-located facilities, and for internal reuse, additional treatment prior to reuse is required to remove toxic metals, salts, and oils which contaminate water that comes in direct contact with the metal product or intermediates.[19]

3.4.5. Chemicals

With the introduction of advanced treatment and the rapid reduction in cost for such technologies (e.g., membranes), the worldwide chemical industry made significant investments in water reuse projects. Between 2000 and 2012, more than large 20 ultrafiltration (UF) or UF/reverse osmosis (RO) systems were installed at chemical facilities, with many more in development.[38]

‡ From interview with Oil Refining Industry representative.

§ From interview with Pulp and Paper Industry representative

The industry also utilizes advanced oxidation, adsorption, and biological treatment technologies as well as combined or hybrid systems. The industry faces considerable challenges from fouling by oil and organics, scaling by metals, high-temperature effects on membrane and bonding materials, and expensive membrane replacement requirements—all of which make the development of alternative treatment solutions a priority.

3.4.6. Food and Beverage Processing

Many large food and beverage companies, including Kraft, Nestle, and Coca-Cola, have plans to reduce their water footprints (largely to meet their Environmental, Social, and Governance [ESG] goals), although much of this is achieved through water conservation rather than reuse.[39,40,41] Because a large share of the industry is owned by only a few companies, there is a high potential for replication of water reuse strategies and thus high potential for impact on the industry's water use.

3.4.7. Data Centers and Large Campuses

Data Centers

Data centers can increase their water recycling to reduce makeup water requirements. The major recycling requirements are to control pH and chloride ion concentrations,[42] but additional treatment considerations depend on the initial feed water quality.

Large Campuses

The variety of water uses on a campus means there are a wide array of water treatment requirements as well various contaminants and other wastewater challenges, which make it difficult to efficiently treat all the waste streams onsite for reuse. Currently, the most cost-effective solution is to send wastewater to a local municipal treatment facility designed to handle large volumes of wastewater from a variety of sources and for a variety of uses.

3.5. Water Disposal

State-level regulations and permits (e.g., National Pollutant Discharge Elimination System [NPDES]) outline water quality requirements and limit for industry discharge of effluent water. These permits generally have concentration-based limits which can be reached or exceeded with the incorporation of nontraditional source waters with different constituents, the use of traditional sources with lower quality, or the implementation of greater internal reuse. Additionally, the discharge limits can be affected by the conditions of the body of water into which the discharge is flowing. If this source/discharge location is a river, for example, there are times during the year when the river's temperature might be limiting industrial thermal discharges. The plant would have to find alternative solutions like costly additional (cooling) treatment or holding their discharge water in retention ponds—with the associated monitoring challenges.

For industrial wastewater treatment with the generally high levels of salinity and other contaminants, the associated brine management, solids handling, and disposal needs can become major cost considerations. **Brine disposal costs in some sectors and geographical areas can be much higher the costs of the water treatment operations.**

3.6. Regional Variations

The main regional variation of importance to industry is access to sufficient water sources (Figures 5, 6, 7a, b, e). For those industries that require large amounts of water for processing or cooling (Chemicals, Primary Metals, or Pulp and Paper), access to river or lake water is a key advantage. As industry expands, and new facilities are built—often located closer to demand centers or raw materials but sometimes further from water sources (as in the American West)—they face greater sourcing and disposal challenges and a higher water cost.

For those industries that are tied into municipal water supplies (Refining, Food and Beverages, Data Centers and Large Campuses), the greater concern is overall water supply (and water supply sustainability) and competition from other demands, like population and irrigation. As these industries transition to more reuse and greater reliance on nontraditional water sources, they will increasingly face challenges of utilizing lower-quality source water, such as water with increased salinity.

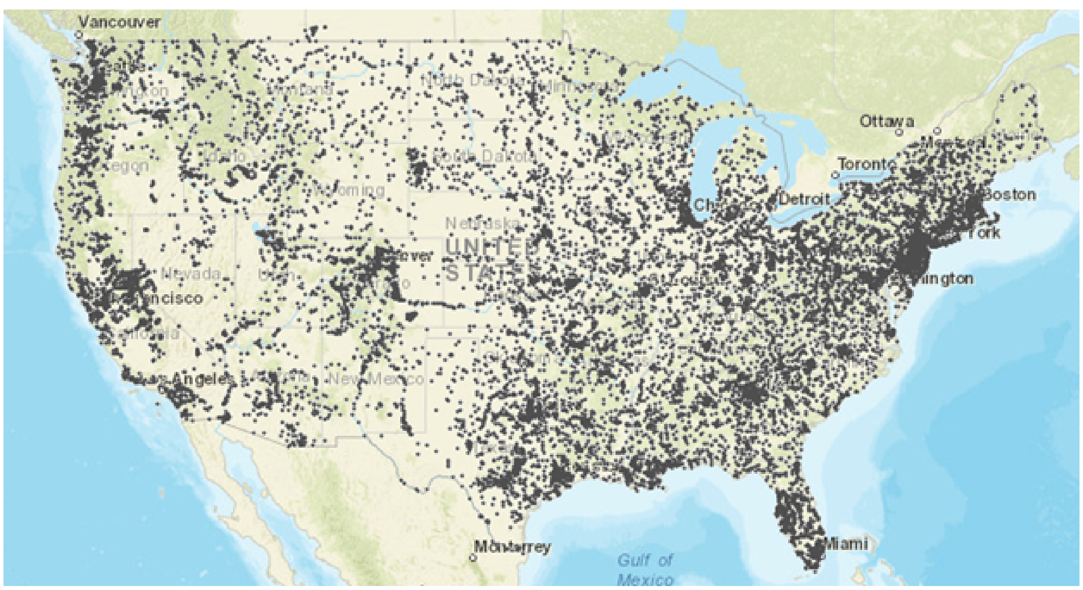


Figure 5. Fresh water withdrawal sites[43]
(Source: USGS)

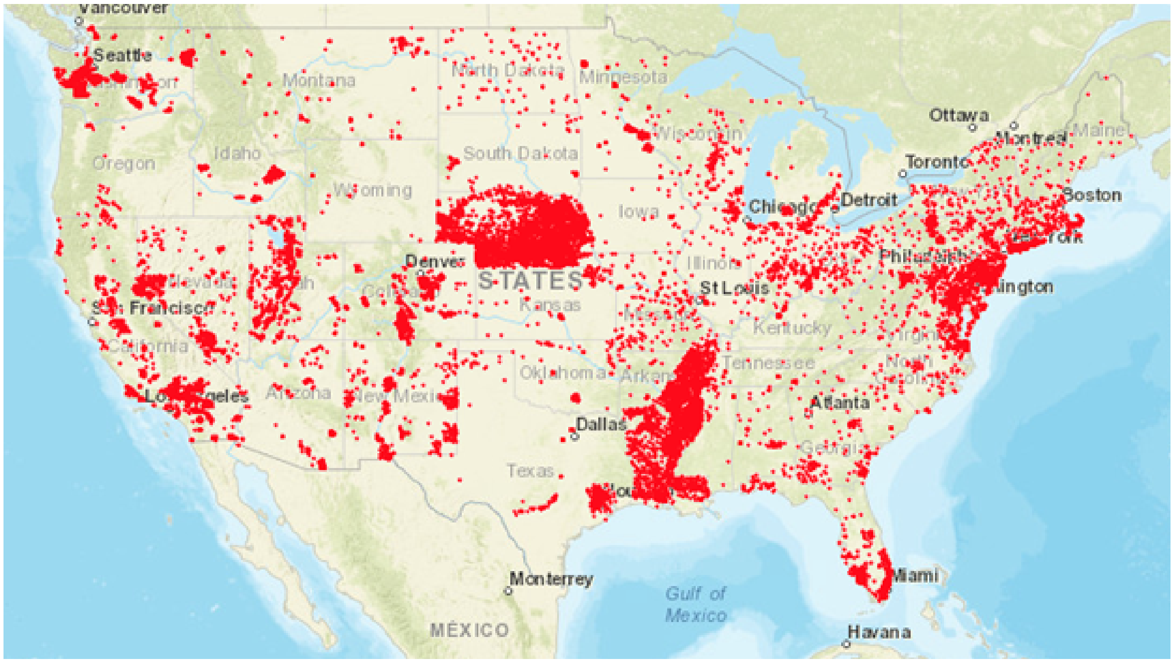


Figure 6. Groundwater withdrawal sites[44]
(Source: USGS)

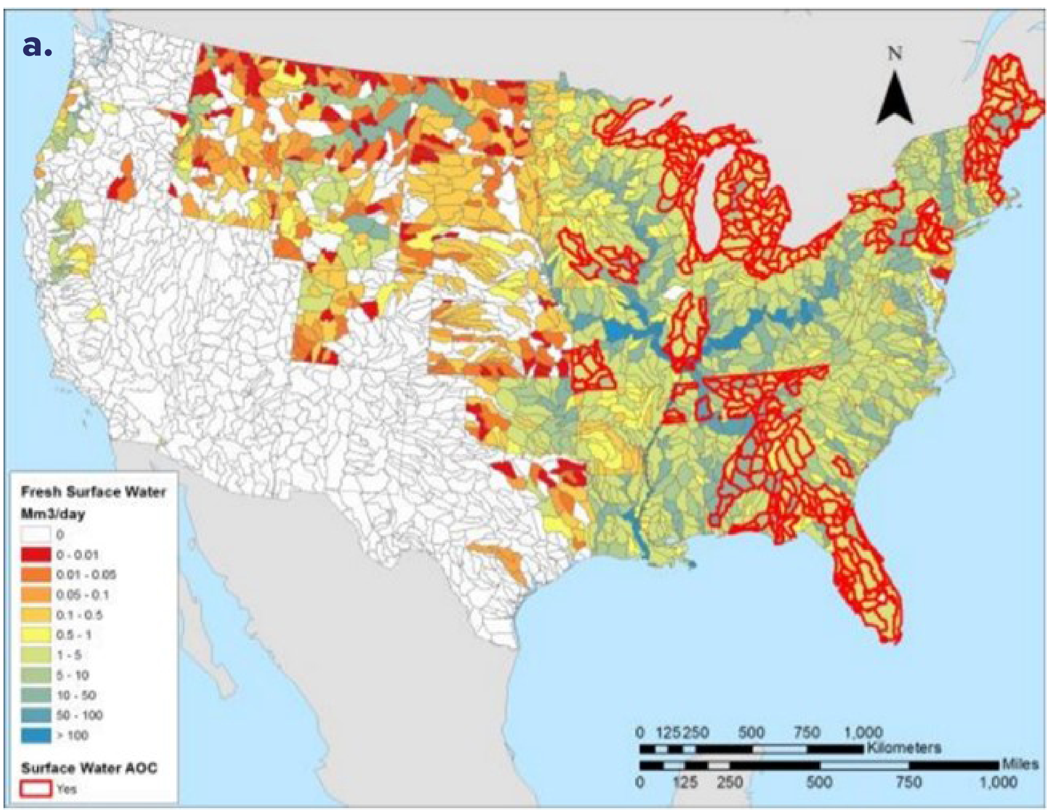


Figure 7a.

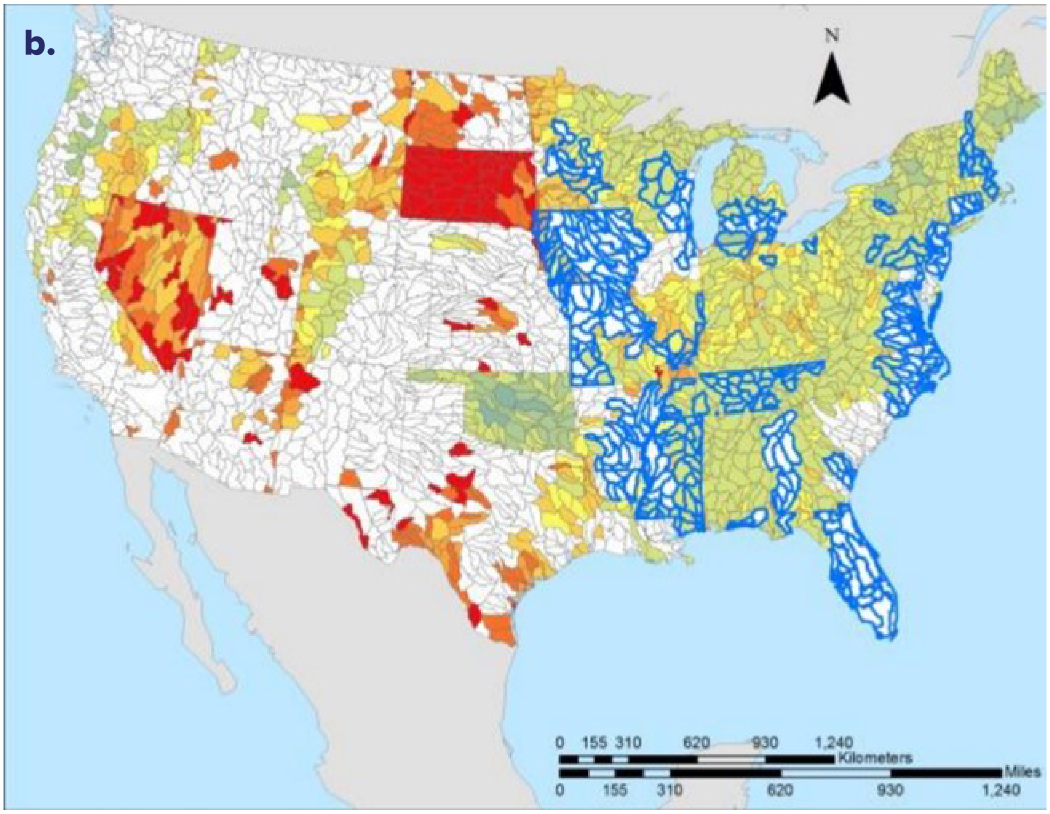


Figure 7b.

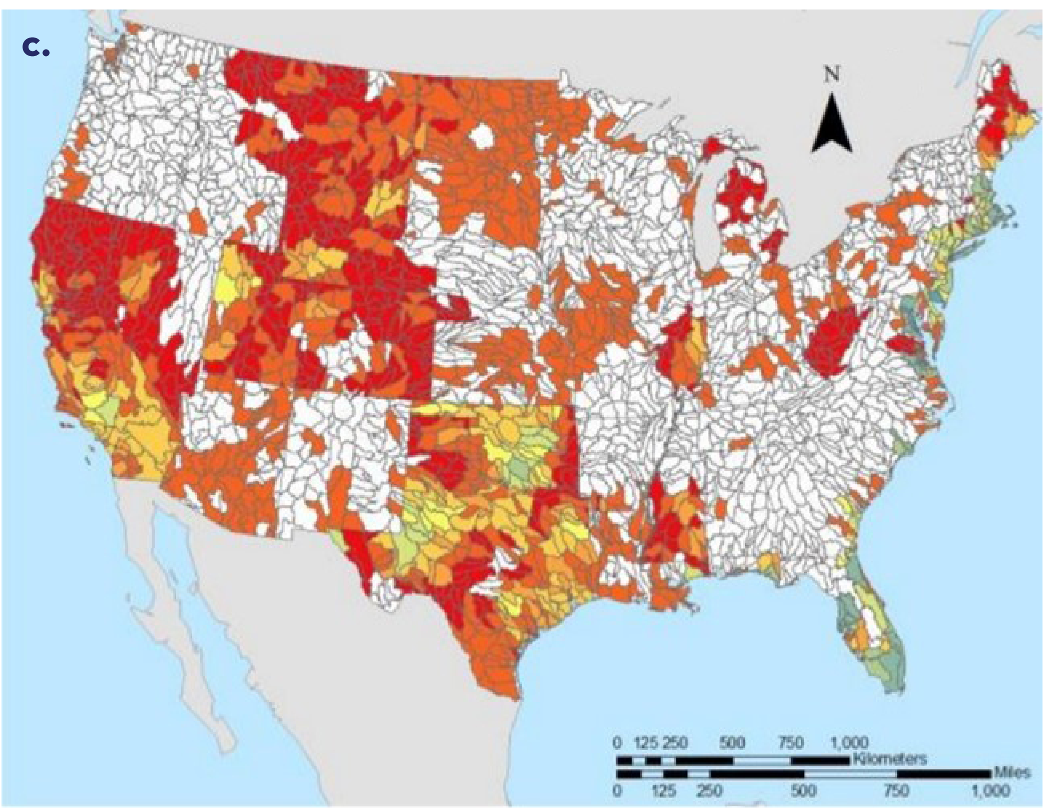


Figure 7c.

Figure 7 a,b,c. Water Availability in the United States: a) fresh surface water availability, b) fresh groundwater availability, and c) brackish groundwater availability[45]

(Source: Sandia National Laboratories)

3.7. Pipe Parity in Industry Sectors

The United States is home to a diverse set of industries exemplified by the Bureau of Labor Statistics recognizing 21 separate manufacturing industries in the North American Industry Classification System (NAICS) three-digit code for manufacturing alone. Additionally, the United States Geological Survey (USGS) considers these 21 manufacturing industries plus Construction when reporting on industrial water withdrawals.[45] Superimposed on this is the vast heterogeneity in manufacturing processes employed even in a specific industry class (e.g., different products in food and beverage industry) that is coupled to significant regional variations in water resources. Therefore, it is impractical to consider "industry" as a single unified water-use sector and propose a consolidated set of pipe-parity measures in a single overarching roadmap. Rather, the pipe-parity definition should be specific to the type of industry of interest and the set of manufacturing processes inherent to the particular NAICS code.

This makes NAWI's approach to achieve pipe-parity across the entire industrial sector difficult to quantify—but not necessarily impossible to achieve. It is critical to expand the types of industries covered in future case studies to encompass a wide range of activities, so that similar industries and manufacturing plants can be cross-compared based on a variety of measures such as cost, energy and resource consumption, process adaptability, impact on manufactured products, and other non-technical constraints such as regulation, sustainability, health implications, and public acceptance. The manufacturing industries are particularly driven by cost competitiveness, which can potentially be quantified based on levelized cost of water.

3.8. Current Trends in Nontraditional Water Sourcing and Use

Industry has already implemented reuse of the "easiest" or least contaminated water streams (e.g., recovery of steam condensate) in many facilities. Reuse of their own industrial wastewater will continue to be a good potential option but costly because of additional piping and treatment requirements.

Municipal wastewater will continue to be a heavily utilized source of nontraditional source water due to reliability of supply and quality (for example, 18 percent of refinery water use is from municipalities[46])—though quality is being stressed by demand and source water quality drops. Expanding the use of municipal water supplies to new facilities is potentially costly because new piping and conveyance is needed. However, the utilization of this water strongly depends on long-term contracts and pricing that, when expired, can often create sourcing issues.

Co-location with other industrial sites with similar operations or similar wastewater (e.g., refineries near carbon black or asphalt plants) will make reuse of other industrial waste streams an option—but this involves necessary associated planning, infrastructure, and operational challenges. Centralized collection, treatment, and reuse of wastewater in highly industrial areas—from either multiple co-located industrial sites or from multiple streams within a single industrial complex—may become viable as more waste streams are characterized and treatment technologies improve.

As efficiency and internal water reuse volumes increase, concentration/brine management and disposal will be a further challenge given current concentration-based discharge regulations.

When sectors (chemicals manufacturing and pharmaceuticals in particular) move away from traditional manufacturing methods (synthesis) to more "green" methods (e.g., biopharmaceutical production), they could use less water and generate fewer synthetic materials, which could ease waste treatment and disposal.

3.9. Current Trends in Traditional Water Sourcing and Use

Provided that no significant changes are made in water sourcing, treatment, and disposal technologies, these trends are likely to continue to affect industry:

- **Water supplies, especially in the west and in arid locations, will continue to be stressed** and will become more limited.
- **More competition from agriculture and other municipal and industrial demands will decrease water availability** in currently water-abundant locations.
- **Industry will continue to take advantage of other benefits (labor access/ costs, raw materials availability, etc.),** which sometimes correspond to dryer locations, thus putting more stress on already stressed water supplies.
- **Quantity requirements will continue to increase**, but more slowly than productivity or gross domestic product.

3.10. Major Future Water Use Scenarios

The following are some potential scenarios that will affect water costs and supplies for these industries:

- **Conflict Increases over Water Ownership or Water Access Rights –** Ownership and access rights to already stressed water resources impact sourcing costs, water use, industrial expansion, and disposal and recycle considerations, among other concerns. It is expected that water resources will be more stressed in the future, causing additional conflicts over these rights, driving up costs, and reducing availability or quality of available water. Additionally, laws governing water ownership and access rights might be changed to accommodate better water management practices or to accommodate changing supply and demand. Water conflict is already an influential consideration in the Western United States.
- **Greater Value Is Placed on Energy Intensity and Carbon Footprint –** It is possible that as impacts from climate change worsen, the United States and other nations will place greater costs (through direct regulations or market mechanisms) on the energy and carbon intensity of water use and treatment—which will directly affect industry costs. Companies will also likely respond to customer and

general public sentiment on these issues, based on their assessment of the public relations significance of environmentally sustainable water use.

- **Risk/Liability Assessments Become a More Significant Consideration –** More companies will likely need to include risk and liability assessments in their water sourcing, treatment, use, and disposal decision-making. This could include developing and implementing risk/liability and cost-equivalent metrics for water sourcing/use, anticipating regulatory delays relating to risk assessments.

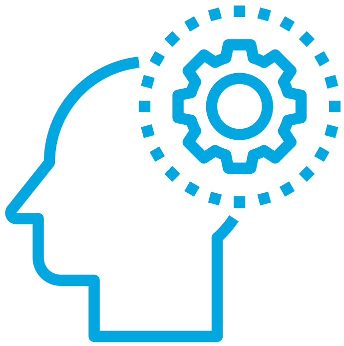
- **Industrial and Population Expansion, Co-Location, and Discharge Exacerbate Stress on Current Water Resources –** As more industry is co-located and as more disposal affects shared water sources, those shared water sources will continue to decrease in quality. The sources will contain more evolving constituents of concern, including recalcitrant organics, pharmaceuticals, and halogenated compounds. This contamination will increase all of industry's water treatment requirements including source water, reuse, and wastewater treatment.

- **Climate Change Impacts Worsen –** Climate change impacts will exacerbate or drive many of the other scenarios listed, increasing costs and reducing the availability or reliability of traditional water supplies. These cost increases will likely make traditional water supplies more expensive. But climate change will likely influence nontraditional supplies as well—either as pass-through costs for reused water, decreased water quality (higher salinity, etc.), or increased demand from other sectors for those nontraditional resources. These effects could be both positive (e.g., new revenue streams) and negative (e.g., higher water costs) for industry.

4. TECHNICAL CHALLENGES
And Associated Knowledge Gaps

The overarching challenge for water and wastewater treatment in Industry is the variability across all industrial sites. A wide range of conditions and factors affect the operations of a site, including the products, source waters, processing technologies, ambient conditions, operator errors, and many other factors.

This makes the implementation of water treatment technologies expensive, requiring customization or more difficult operations. It also makes widespread adoption and implementation of treatment technologies and systems more challenging, impacting the efficiency of manufacturing as well.



This section identifies broad industry challenges and gaps (technical and non-technical) that limit integration of nontraditional water sources with existing supplies for this sector. These barriers have been identified through workshops and discussions with subject matter experts, as part of a structured roadmapping process. They are too large and far-reaching for any one organization to devote all the resources needed to develop suitable solutions. ***NAWI intends to invest in promising technologies that are cross-cutting across the PRIMA areas*** and that address some of the technical limitations discussed below.

4.1. Technical Challenges

4.1.1. Constituent Detection, Analysis, and Process Monitoring and Control

The industry needs improved means for real-time data collection, characterization, and quantification of constituents of concern in source, process, and wastewaters. Online, real-time sensors to collect water quality data are available for a range of bulk surrogate parameters (e.g., conductivity, chemical oxygen demand, total organic compound, total chlorine [Cl_2], turbidity) and specific water constituents (e.g., ammonia, nitrate, orthophosphate, pH, oxygen, chloride, sulfate, silica). However, many of these sensors are limited because they are not truly real-time; have insufficient capability for automated quality assurance and quality control, error detection, and re-calibration; are subject to Interferences with other constituents; cannot detect concentrations within or across the ranges needed; or lack durability under the harsh conditions of industrial waters and wastewaters. Sensors are needed both for compliance and process control. Feedback control needs to be reliable and highly sensitive to some constituents of concern, including families of chemicals or proxies for some hard-to-detect species. The sensors need high durability as well as the ability to function under a wide range of harsh industrial operating conditions (e.g., high temperature, high-pressure, or corrosive environments). And the systems need to provide real-time or near real-time detection of constituents and monitoring of conditions.

Accurate modeling and analysis of water quality data generated within complex source water matrices and treatment systems are needed to optimize industrial treatment system operations, promote reuse and recycling within an industry, and ensure consistent process and effluent water quality. Analysis and modeling should take advantage of improved water quality data collection to enable predictions of process performance and impacts of constituents (and their interactions) on processing equipment and materials (e.g., corrosion, fouling, scaling). These models should guide treatment operations and predict potential process failure. These predictions will improve efficiency and effectiveness of water and wastewater treatment operations, particularly with nontraditional water sources and internal water reuse.

4.1.2. Design and Manufacturing Challenges

The industry needs new treatment and reuse technologies and equipment designed to seamlessly integrate into existing treatment trains and industrial processing systems. New treatment technologies, as well as existing technologies with new capabilities for handling nontraditional water sources, will be easiest to deploy by industry if they are physically and technically compatible with existing plant and system designs. Physical components must be capable of fitting within existing spatial, power piping, and storage limitations. Technical compatibility requires treatment efficiency and resiliency, especially as it impacts downstream water quality requirements, chemical addition needs, and heating/cooling requirements. New water treatment technologies must be designed to handle the industrial process flow rate ranges employed at the site and be operated as, or more efficiently than, the treatment processes they are replacing. They will need to be designed to minimize operator learning curves and should include as much automation as possible to ensure resilient, robust, and reliable treated water quality.

The design, manufacturing, and control of new water treatment technologies need to be scalable and resilient to meet evolving industry needs. Industry subsectors with high water demands (i.e., high water throughput) need efficient and improved separation technologies (and other treatment operations) capable of treating the high flow rates required. Many traditional high-throughput processes utilize technologies that employ relatively long residence times, requiring a large footprint. In other industries, water demand is not as high, but the same traditional processes are often employed (e.g., coagulation/flocculation/sedimentation). New technologies are needed that can support smaller-scale modular water treatment needs and opportunities but with the potential to scale up to larger demands (e.g., through seamless integration of modular systems). This will require supporting systems designed to operate at the scale appropriate to the industrial site (e.g., occasions with few workers available to operate systems, or workers with limited training on the water treatment systems).

The industry needs efficient, cost-effective, and modular water treatment systems that can be applied to various industries. The industry needs to understand where larger-scale systems that could treat waste streams of an entire plant or from multiple industrial sites would be more effective than treating individual waste streams. Large-scale systems often exchange the effectiveness of treating individual constituents for the cost-effective treatment of the larger volume of wastewater, but there is potential to leverage both. Industry would benefit from the ability to identify which waste streams and which constituents of concern are more effectively treated at the individual stream level (e.g., extracting treatment chemicals for better chemical and water reuse) and which are more efficient at the larger scale. Where it is more effective, industries could pool waste streams—from facilities with similar waste streams—to gain efficiencies from treating at large scale and minimizing duplication of treatment systems and equipment. This could include determining how best to incorporate these modular systems into industrial facilities that already have dedicated water treatment systems or utilizing them for integration with greenfield industrial development.

4.1.3. Supply Limitations

Identifying, sourcing, and ensuring a reliable supply of nontraditional water will be a continued challenge for the sector. Reliable water supply is a major requirement for industry, and supply variability and inconsistency can impact both operations and profitability of many sites. Water location, cost, and availability are and will be increasingly factored into site selection for many industries (e.g., Pulp and Paper, Food and Beverage Processing, Primary Metals). It is anticipated that there will be increased competition for nontraditional source waters (e.g., municipal effluent, brackish water) in water-limited or water-stressed areas (e.g., dense urban areas, coastal areas, or arid areas). Industries will have to anticipate potentially reduced access to source water due to changes in water and land rights or the application of law in that area. There will also be continued variations in supply due to decreased water levels from drought or climate change, increased salt levels due to stress on aquifers or infiltration from brackish water or seawater, and the continued impact of annual and seasonal variations on water levels. A converse challenge in currently non-water-stressed environments is the relative lack of incentive for investing in nontraditional water sources.

4.1.4. Quality Limitations Challenges

Varying source water quality can impact industrial operations, risking product quality, and creating downstream and environmental impacts. Source water quality can decrease due to increasing salinity and contamination, increased competition for standard water sources, and decreased quality from municipal effluent supplies due to flow-through effects. Additionally, there is a lack of reliable, robust monitoring technologies that would allow flexibility in process operations for changing water quality. Moreover, industrial treatment technologies often have limited flexibility to handle unexpected changes in water quality; they are often designed and optimized for treatment of high-quality source water using standard operating conditions. These limitations mean current treatment technologies might be unable to handle increasing water quality variations, leading to negative impacts on industrial processes and their products.

4.2. Non-Technical Challenges

The list below identifies those non-technical challenges associated with enabling nontraditional water sources to be utilized for the Industrial End-Use Sector. These concepts are included here for thoroughness in identifying other gaps that could limit the use of nontraditional waters, but, with the exception of cost, they are generally out of NAWI's scope.

4.2.1. Cost

Due to a variety of factors, water is undervalued in many industries, and the motivation for investment is often lacking. Water needs to be valued correctly—capturing the full value of water, not just the direct monetary costs (e.g., cost of purchasing municipal water)—and that value needs to be communicated to industry personnel, regulatory or legislative entities, and the public. The value needs to include the full lifecycle costs including sourcing, treatment, storage, and disposal. In addition, long-term impact management vs. the costs of third-party water supply and residual handling must be included in the valuation. The costs of incorporating nontraditional water sources and new treatment technologies and systems into existing plants and operations, or even into greenfield sites where they might affect proven operations, are often seen as prohibitive when the current water costs are undervalued.

4.2.2. Standards Development

Water and wastewater treatment and disposal regulations and requirements vary by jurisdiction (federal, state, local, and tribal) and location. These variances can make the implementation of alternative treatment technologies or water/wastewater management options either too costly to implement in a given location or can simply bar their use. Varying standards can also have effects on transportation costs, energy costs and regulatory compliance costs.

The variances can also affect disposal, storage, and waste/wastewater shipment options. This non-uniformity/non-universality requires customization of solutions to meet local regulations and limits technology development to the most common or highest volume/highest margin treatment opportunities. It also limits manufacturing efficiency, economies of scale, and the development and broad implementation of effective treatment solutions. Thus, standards are needed that can be implemented universally, independent of local conditions (e.g., geohydrology land use) which impact source and discharge limitations, water quality requirements (e.g., total maximum daily load discharge requirements), constituents of concern, and industry processes involved.

Data collection and sharing are limited by the lack of standards, liability concerns, and limited understanding of business and operational benefits. The sharing and use of data across the entire Industrial Sector is challenging due to considerations associated with the release of potentially proprietary business data, spurring increased regulation or increasing legal liability. The benefits of data sharing would include supporting improved process modeling and operational decisions, reducing environmental impacts, and informing product and technology developers to support better design. The development of data collection, anonymization, and sharing agreements and standards is needed.

4.2.3. Liability and Risk

The Industrial End-Use Sector is adverse to assuming risks related to the use of nontraditional water sources and the implementation of new technologies that have not been proven by other industries. These risks include coordinating with other industries on nontraditional water supplies, integrating nontraditional waters and new technologies into current operations, and increasing supply stress from climate change and pressure on current water sources. The industry also faces liabilities related to greater regulation of contaminants of emerging concern (CECs) and industrial wastewater reuse in other sectors (i.e., impacts on water consumers including people, agriculture, and animals).

4.2.4. Environmental

There are a number of environmental risks stemming from the increased use of nontraditional waters. Nontraditional water use, including greater internal reuse, often results in increasing the concentration of bulk constituents such as TDS and contaminants of concern. The risks involved in storing, transporting, and disposing of more concentrated waters and residuals include the potential for spills, leaks, and leachate entering the local environment

4.2.5. Workforce and Training

Nontraditional water use also includes challenges relating to the education and skills of the workforce. Staff at all levels need additional education and training related to their organization's water demand and potential production impacts and opportunities. Often businesses are not aware of their own water dependencies and the potential impacts of supply changes or treatment technology changes. These water considerations need to be integrated into every level of decision-making. Additionally, the implementation, maintenance, and operation of new water treatment technologies or changes to existing processes and systems will require training for the onsite workforce. Industry faces the challenge of having knowledgeable and trained workers at multiple facilities empowered and capable of managing water treatment processes and their impacts on industrial production and normal operations.

4.2.6. Regulations and Public Acceptance

Technologies for nontraditional water use including—internal reuse and wastewater reuse outside of industry—could develop faster than related regulations or could spur additional challenging regulations. These developments could result in stranded resources if regulations move in a different direction or in the case of significant additional compliance costs. **Even if developments in nontraditional water use succeed technically and meet regulatory requirements, there can be additional challenges from public acceptance.** Public buy-in—particularly for infrastructure/transportation issues, especially pipelines and trucking—will be a challenge. This challenge can be exacerbated by a lack of transparency regarding the composition and potential toxicity of the source waters and effluents which will make water reuse outside of the Industrial Sector itself more challenging despite safety steps taken.

Familiarizing technicians, engineers, and decision makers with capabilities and limitations as well as installation, operation, and maintenance of new technologies is critical to its proper implementation and acceptance by the community.

5. RESEARCH PRIORITIES

Areas of Interest for Industrial End-Use Roadmap

To overcome the challenges presented in Section 4, this roadmap identifies the following set of research priorities needed to expand the use of nontraditional sources waters for the Industrial Sector.

To overcome the challenges presented in Section 4, this roadmap identifies the following set of research priorities needed to expand the use of nontraditional source waters for the Industrial Sector. 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, a suite of next-generation desalination technologies that autonomously adapt to variable water chemistry, precisely and efficiently remove trace constituents 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 are needed. Investing R&D resources in the following priorities will lead to a revolution in desalination and treatment processes for the Industrial Sector.

The identified AOI is followed by a short discussion on the current research challenges (a technology or problem that has not been sufficiently answered by existing studies) and continues with specific TRL 2–4 research needs. Advances in these technologies and capabilities aim to reduce the cost of treating nontraditional source waters to the same range as marginal water sources, thereby achieving pipe parity. Where possible, quantitative estimates of potential impacts are given.

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.

5.1 Autonomous

Sensors and Adaptive Process Controls for Efficient, Resilient, and Secure Systems

A1. **Develop automated decision-making and control of water treatment processes based on big data and using machine learning algorithms.**

Challenges

Industrial water treatment processes are often designed and operated with a safety factor to ensure regulatory compliance for waste streams and quality requirements for recycle/reuse streams; this redundancy intrinsically means that more resources and energy than necessary are spent. Many small- and medium-sized facilities do not have automated controllers for their treatment operations, but rely only on inefficient on/off systems, often managed by human operators and pragmatic decisions. Therefore, decision-making in response to perturbations in source water quality, process upsets, and other unpredictable events is dependent on institutional memory, which may or may not exist. Predictive process models based on fundamental transport phenomena, thermodynamics, and kinetics (e.g., process models for biological wastewater treatment, membrane processes, and oxidation processes) often fail in practice due to inaccurate representations of complex physical, chemical, and biochemical phenomena occurring at varying spatial and temporal scales. NAWI recognizes that there is a large amount of water quality and operating parameter data that are not effectively utilized for treatment process design and optimization, especially in planning for future challenges associated with broader issues facing industry such as climate change, resource depletion, and increasingly stringent regulations. Collectively, these limitations make it difficult for industries to develop cost-effective, robust, and resilient process control strategies that would lead to positive returns on investment in water reuse or alternative water sources.

Impacts

All manufacturing industry subsectors can benefit from the development of automated decision-making and control tools. Many existing large facilities in oil refinery, chemical, and food and beverage industry already use various automated controls, which can benefit from further big data collection and machine learning-based process control. Many small- and medium-sized facilities do not have automated controllers for their treatment operations, but rely only on inefficient on/off systems, often managed by human operators and pragmatic decisions, presenting a large opportunity with this technological advancement.

There is a large amount of water quality and operating parameter data that are already available and being collected. This information could be effectively utilized for treatment process design and optimization, especially in planning for future challenges associated with broader issues facing industries such as climate change, resource depletion, and increasingly stringent regulations, especially in regions with high water stress.

A1.

RESEARCH NEEDS:

- **Develop** autonomous system operation tools that can a) collect and process a large amount of water quality and process control data, b) enable real-time, self-adaptive control of processes, c) predict process performance without requiring a priori modeling assumptions, and d) improve the prediction accuracy of existing mechanistic models that are based on physical, chemical, and biological fundamentals (TRL 4 and greater).
- **Identify** algorithms, among a large number of machine learning/deep learning algorithms, that are most effective for optimization and prediction of water treatment unit operations such as membrane, electrochemical, oxidation, adsorption, and biological processes; alternatively, develop water treatment process-specific, sophisticated machine learning algorithms that utilize big data and/or deep learning algorithms that perform unsupervised learning based on existing unstructured data (TRL 2–3).
- **Develop** approaches to enable seamless, cyber-secure integration between data collection, machine learning algorithms, and process control devices.
- **Develop** a digital twin system of an existing water treatment system for large data collection, parallel comparison, supervised learning of algorithms, and calibration of mechanistic models (TRL 3 and greater).

A2. Develop and use advanced sensors for the online monitoring of water quality.

Challenges

The capability to monitor the status of an operative treatment system and the quality of water prior to and after treatment is a prerequisite for collection of large quantities of operational data that would enable the development of autonomous processes. Monitoring needs to be in real time in order for real-time process control. At the core of monitoring capabilities are robust sensors that measure various water quality parameters in the harsh environments of many industrial processes (e.g., high temperature, high salinity, and high pressure). Despite decades of research in developing water quality monitoring sensors, current technologies have not yet advanced beyond gross measurement of basic water quality parameters such as pH, dissolved oxygen (DO), total organic carbon (TOC), turbidity, TDS/conductivity, and some readily measurable ionic species, and even these have limited reliability under extreme conditions. Technologies to measure specific organic compounds such as per- and polyfluoroalkyl substances (PFAS) and challenging water constituents such as oil and grease, heavy metals, oxyanions, and silica, to name a few, are not yet available in a configuration (e.g., online), capability (e.g., a complex water matrix), or a price range that are appealing to industrial end users. Sensors developed under laboratory environments often fail to function accurately in complex water matrices; there is a need to overcome challenges associated with high cost, short lifetime, and lack of durability.

Impacts

Nearly all industrial subsectors could benefit from this AOI. Sensors for constituents such as oil and grease, heavy metals, and toxic organics are needed by multiple industry subsectors from chemical to oil refinery, food and beverage, and primary metals. Some sensors on specific compounds such as phenolic compounds, hydrocarbons, and pathogens could also be impactful.

A2.

RESEARCH NEEDS:

- **Improve** the understanding of the fundamental science that governs the pollutant-substrate interaction in molecular and atomic scales. Such understanding is essential to develop precision separation and treatment that one of NAWI's A-PRIME research goals pursues. The development of sensors that provide precision detection is likely to rely on the same fundamental principles and plays a critical role in the development of 'precision separation' technology (TRL 2–4).

- **Develop** innovative materials, material architecture, and integrated devices that a) enable binding and detection of target water constituents with high sensitivity and selectivity under a wide range of complex industrial wastewater matrices; b) are low cost (and therefore disposable in select applications); c) are easy to calibrate and maintain; d) exhibit durability against environmental stress and long lifetime; and e) are capable of signaling sensing-system failure (TRL 2–4).

- **Develop** online, real-time sensors that measure pollutants such as hydrocarbons, phenolic compounds, halogenated compounds (e.g., PFAS), oil and grease, and various oxyanions and heavy metals as well as species that interfere with treatment processes, such as silica and microorganisms (TRL 4 and greater).

- **Develop** system strategies (e.g., incorporation of proper pretreatment prior to sensing or in operando separation as a part of sensing system) to avoid interference and complication by background matter. in complex media (TRL 4 and greater)

5.2. Precise

Targeted Removal of Trace Solutes for Enhanced Water Recovery, Resource Valorization, and Regulatory Compliance

P1. **Selectively separate and destroy recalcitrant organic pollutants in industrial wastewater.**

Challenges

Conventional water treatment processes that target the removal of organics and surrogate measures, such as biological or chemical oxygen demand (BOD and COD, respectively) and TOC, for regulatory compliance often fail to remove recalcitrant organic pollutants that are either generated within the industry or associated with the source water. The occurrence of recalcitrant organic compounds such as PFAS, lignin-derived compounds, dyes, adsorbable organic halides (AOX), artificial food additives, and pharmaceutical and personal care products (PPCP) complicates water reuse/recycling as well as discharge for industries such as Food and Beverage Processing, Pulp and Paper, and Oil Refineries. Analysis of the Camas Pulp and Paper Plant in the Water Technoeconomic Assessment Pipe-Parity Platform (Water-TAP3) tool reveals that aeration treatment steps account for more than 80 percent of the cost for electricity used in water treatment and that electricity costs were 46 percent of the levelized cost of water (LCOW) at the facility. Technologies to selectively remove these pollutants are in critical need to maximize water reuse opportunities.

Impacts

Nearly every industrial water treatment facility needs to remove organics. Removing recalcitrant organic compounds such as PFAS, lignin-derived compounds, dyes, AOX, artificial food additives, and PPCPs are particularly challenging for industries such as Food and Beverage Processing, Pulp and Paper, Oil Refineries, Chemical, and Primary Metals.

P1.

RESEARCH NEEDS:

- **Develop** materials and devices that: a) enable precision separation (e.g., membrane, adsorption, ion exchange) or destruction (e.g., catalytic, electrochemical, and advanced oxidation) of recalcitrant organics with high efficiency under complex industrial wastewater matrices; and b) can be cost-effectively regenerated, resistant to environmental stress, and maintain high efficiency over long term use (TRL 2–4).
- **Develop** integrated, sequential treatment strategies that synergistically remove recalcitrant pollutants (e.g., pretreatment to convert recalcitrant organics into products that are easily biologically degradable in a subsequent step) (TRL 4 and greater).

P2.

Investigate selective separation and recovery of metal ions and nutrients from waste and brine streams.

Challenges

Technologies to selectively remove specific inorganic constituents (e.g., metals, oxyanions, nutrients, silica) with high efficiency in complex water matrices are lacking. These specific constituents may inhibit downstream processes and ultimately limit available reuse, end-use, and disposal options for industrial wastewaters. Enhanced precision separation technologies that exploit underlying separation mechanisms and chemical speciation may be able to address these issues when incorporated into integrated treatment trains. Further, the development of enhanced separation technologies may allow for recovery and valorization of specific minerals. In many cases, recovery of valuable resources from industrial waste and brine streams can be more effective because the concentrations are elevated. However, current separation technologies are often overly costly, operationally demanding, and energy intensive.

Impacts

The Pulp and Paper Industry is the largest consumer of freshwater in the United States (28 percent) among all manufacturing industries. It produces a massive amount of wastewater containing wood-driven biomass that can be valorized for fuel. The Food and Beverage Processing Industry is the fourth-largest water-consuming industry in the United States and also produces a large amount of wastewater that contains biomass which can be valorized for energy production and carbon sources. The slag produced from the Primary Metals Industry is an overlooked opportunity for valorization. They have mechanical and thermodynamic characteristics for concrete construction, wastewater treatment, thermal energy storage, carbon sequestration, and energy recovery sectors.

P2.

RESEARCH NEEDS:

- **Develop** porous materials and membranes with precise control of morphology, pore dimension, and surface chemistry that enable selective transport of target solutes. Establish fundamental understanding of the behavior of colloids, molecules, and ions under nanoscale confinement and specific surface interaction that govern differential transport (TRL 2–4).
- **Develop** materials and surface modification methods that enable selective binding with metals and ionic species and develop processes that enable selective removal (e.g., ammonia, cyanide, silica, metals, mercury, radioactive materials, and selenium) or recovery (e.g., lithium) under complex industrial wastewater matrices over long term use (TRL 2–4).
- **Develop** catalytic and electrocatalytic materials and processes that selectively bind with and reduce constituents such as oxyanions under complex industrial wastewater matrices over long term use (TRL 2–4).
- **Develop** brine management systems that combine resource recovery (e.g., metals, water) with onsite chemical synthesis (e.g., chlorine [Cl]) (TRL 2–4).

P3.

Develop and optimize pretreatment of bulk constituents (e.g., insoluble organics, TSS, TDS) to enhance and protect downstream treatment processes.

Challenges

Precision separations are often hampered by inadequate removal of bulk constituents that either interfere with separation, compete for selectivity, or reduce process efficiency (e.g., fouling and scaling). Current pretreatment strategies often require large footprints, high-energy, high-chemical usage that limit the ability for particular water sources to achieve pipe parity. There is a need for resilient, modular, high-rate pretreatment processes that are integrated with downstream precision separations processes to reduce complications in downstream treatment processes. These processes include pretreatment and recovery of hydrocarbons, petroleum, grease, and oil from waste streams, sludge, or waste solids to improve phase separations prior to downstream treatment or integrated within treatment systems. There is also a need for enhanced, resilient methods of handling complex industrial wastewaters with TSS and/or TDS to increase the efficiency of precision separations for the reuse and disposal of waste streams.

Impacts

Most industrial water treatment employ primary treatment to remove organics. Pretreatment in industries such as primary metals, oil refinery, and chemical targets removal of oil and grease and TOC/COD. Pretreatment of TDS is essential for cooling and boiler-feed water that is used across almost all industry subsectors.

P3.

RESEARCH NEEDS:

- **Develop** materials and treatment processes that enable highly efficient oil-water separation. Innovate conventional approaches such as gravity separations and centrifugal separations to be more efficient, modular, compact, and fit-for-purpose (FfP) (TRL 3 and greater).

- **Develop** non-chemical approaches for fouling and scaling control on membranes, heat exchanger surfaces, pipelines, and other water treatment devices. Establish the mechanisms and evaluate factors affecting the efficiency of these technologies for a broad range of water quality and chemistry (TRL 2–4).

- **Develop** non-biological pretreatment processes (e.g., adsorption and electrochemical) that treat high-strength wastewater (e.g., high TOC and high oil-and-grease content wastewater found in select industries such as oil refineries, chemical industries, and metal processing industries) containing high levels of recalcitrant organics that cannot be readily treated by biological processes (TRL 3 and greater).

5.3. Resilient

Reliable Treatment and Distribution Systems that Adapt to Variable Water Quality and Are Robust to Corrosive Conditions

R1. Enhance chemical and biological resiliency of materials and process components in water treatment.

Challenges

The performance of desalination membranes declines over time due to organic, inorganic, biological, and colloidal fouling, thereby increasing operation and maintenance costs and downtime for chemical cleaning. Current polyamide membranes exhibit high permeability and can operate in a wide range of pH but have poor chemical resistance to Cl used to control microbial growth. On the other hand, cellulose acetate membranes can tolerate Cl, but have low permeability to water and a low range of operating pH. The range of temperature and pressure that current membranes can tolerate is also relatively narrow, limiting the adoption of membrane processes such as RO and nanofiltration (NF) to a wider range of industrial water treatment applications. Many other materials used for separation processes, including ion exchange resins and various adsorbents, are also not resistance to Cl and oxidants, and easily compromised by common industrial and natural constituents (e.g., iron, manganese, calcium [Ca], magnesium [Mg], silica). However, materials with improved chemical tolerance often experience losses of other beneficial properties (e.g., membrane permeability and surface hydrophilicity).

Industrial water treatment processes, in particular high pressure membrane processes and thermal processes, are energy intensive. Renewable energy can replace existing sources of energy, especially in remote locations, thus reducing the lifecycle cost and environmental impact of water treatment systems. Yet, sources of renewable energy may be intermittent and therefore require that the treatment systems be more resilient and keep efficient operations under intermittent operating conditions. The treatment system can be designed to be more resilient, more cost-effective, and more carbon-neutral by also adopting strategies to recover energy from waste heat and fuels (e.g., biomass and methane) such that their reliance on the electrical grid is reduced. State-of-art practices are limited to recovery of methane from anaerobic digestion, which is not widely practiced in small-scale systems. Strategies and technologies that enable energy recovery in smaller, distributed water treatment systems are lacking.

Impacts

Materials and strategies to control microbial growth, biofilm formation, and scale formation, and to process water with wider pH and temperature range can be useful for various components of industrial water treatment systems beyond membranes (e.g., cooling water, heat exchanger surfaces, pipelines, and other water treatment devices) across nearly all industries, particularly due to the prevalent use of cooling and boiler-feed water at most industrial facilities.

R1.

RESEARCH NEEDS:

- **Develop** innovative membrane materials, composite membrane structure (e.g., ceramic and mixed matrix), and surface modification strategies that substantially improve tolerance to Cl, oxidants, wider pH and temperature range, and corrosive environments, while maintaining high selectivity and permeability (TRL 2–4).
- **Develop** ion exchange resins (e.g., for recovery of iodide, lithium, pure silica, rare earth elements) and adsorbent materials (e.g., for removal/recovery of hydrocarbons) with improved resistance to oxidants and corrosive environment (TRL 2–4).
- **Develop** materials, strategies, and alternative disinfectants to control microbial growth and biofilm formation in various components of industrial water treatment systems beyond membranes (e.g., cooling water, industrial production lines) (TRL 2–4).
- **Develop** membranes and components of membranes and membrane modules (e.g., support, sealant, spacers) that can withstand high temperatures and pressures (TRL 2–4).
- **Develop** innovative advanced characterization methods from first principles (both in operando and offline) to accurately relate materials' properties to their overall performance, especially with respect to their resiliency to environmental stress (TRL 2–4).
- **Develop** non-chemical approaches for fouling and scaling control on membranes, heat exchanger surfaces, pipelines, and other water treatment devices. Establish the mechanisms and evaluate factors affecting the efficiency of these technologies for a broad range of water quality and chemistry (TRL 2–4).

5.4. Intensified

Systems and Process Optimization to Maximize Brine Reuse, Improve Brine Concentration and Crystallization, and Manage Residuals

I1. Establish cost-effective waste/brine management and solidification.

Challenges

In many industries, the major challenge associated with water use is the disposal and management of concentrated brines and residuals. Residual streams are often aqueous based but are high in total organic content, hazardous metals, recalcitrant organics, TDS, TSS, and/or microorganisms. As industrial water reuse increases and/or desalination processes reduce residual volume, these wastes can become more concentrated. ZLD strategies that couple brine concentrator and downstream solidification have been proposed for several industries. However, MLD systems may prove to be more cost-effective and have greater potential to achieve pipe parity because of easier waste disposal. Regardless, sustainable disposal of residuals must be addressed as an integral part of all treatment trains. Solidification and stabilization processes for industrial brines require an understanding of the physical and chemical processes that control the equilibria and rates of stable phase formation.

Impacts

This AOI has particular relevance for oil refinery, chemical, and primary metal industries, which produce waste streams that contain high concentrations of oil and grease, recalcitrant organics, and solids. It is also relevant for the Food and Beverage Processing and Pulp and Paper industries, which produce waste streams that contain high concentrations of biodegradable organics and biomass.

I1.

RESEARCH NEEDS:

- **Intensify** water recovery and minimize discharge volume through innovative process configurations (e.g., osmotically assisted RO and humidification/dehumidification processes), operating modes (e.g., non-steady-state operation), and process design (e.g., removing organics before resource recovery operations) (TRL 4 and greater).
- **Develop** innovative stabilizing mixtures for solid extraction to improve stabilization techniques for highly saline streams and to optimize salinity ranges for both extracting water and encapsulating leachate in order to facilitate hazardous waste handling (TRL 3 and greater).
- **Develop** innovative ZLD and MLD strategies that combine processes (e.g., waste and brine intensification) (TRL 4 and greater).
- **Conduct** TEA of these technologies to identify the appropriate strategy for various industries, regions, and influent, waste, and brine streams (TRL 4 and greater).
- **Develop** technologies that reduce leaching of difficult-to-solidify trace elements (e.g., selenium), improve theoretical understanding of solid-state diffusion, and implement lab simulation methods to capture realistic/complex field-relevant leaching conditions (TRL 2–4).

12.

Improve prediction and chemical modeling of concentrated waste and brine streams and verify with experiments.

Challenges

Industrial brines have widely varied compositions depending on the types of source waters and processes used upstream. As such, management of resource recovery and disposal is challenging because there are no one-size-fits-all methods possible. In order to optimize brine treatments, including waste disposal, it is important to involve modeling to predict phase formation during solidification and encapsulation or adsorption of contaminants in the solidified phases. Such modeling reduces costly and time-consuming iterative testing. However, chemical modeling of concentrated waste and brine streams is difficult due to limited characterization of resource constituents and limited use of activity correction models that are appropriate for high ionic strengths.

Impacts

This AOI has particular relevance for oil refinery, chemical, and primary metal industries, which produce waste streams that contain high concentrations of oil and grease, recalcitrant organics, and solids. It is also relevant for the Food and Beverage Processing and Pulp and Paper industries produce waste streams that contain high concentration of biodegradable organics and biomass.

12.

RESEARCH NEEDS:

- **Develop** and verify predictive models to accurately describe chemical and physical properties of potential resources and hazardous constituents and their interactions in extremely high ionic strength conditions (TRL 3 and greater).
- **Develop** a robust model to predict nucleation and crystalline phase growth to simulate scaling formation and crystallization in complex mixtures as it applies to technological systems (e.g., osmotically assisted RO) (TRL 2).

5.5. Modular

Materials, Manufacturing, and Operational Innovations to Expand the Range of Cost-Competitive Treatment Components and Eliminate Intensive Pre/Post-Treatment

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.**

Challenges

Available treatment options for improving the quality of alternative water for use in industry vary across industries and even within industries. High-quality water (e.g., conductivity values lower than that in typical municipal drinking waters) requires treatment trains including RO or NF, whereas in other cases, chemical-based softening, coagulation/flocculation, adsorption, and ion exchange processes are employed for the removal of hardness, specific ions and/or turbidity. In cases where organic removal is required for use of an alternative water, either biological treatment or advanced oxidation processes (AOPs) are typical. In many cases, these systems are designed as stand-alone processes targeting a specific objective rather than designed to address multiple objectives either simultaneously or in sequential integrated steps. While some of these processes are modular by nature (e.g., membranes), others require forethought to conceptualize them into a modular design that increases overall system flexibility and allows for distributed application. In addition, many of these processes require pretreatment to ensure that they are not hindered by the presence of non-targeted species (e.g., silica, suspended solids and organics to reduce fouling, solids removal prior to biological treatment). For these systems, current pre- and post-treatment processes are often heavy, spatially inefficient, relatively slow, and may have a prohibitively high total installation cost (due to extensive onsite engineering and integration during installation), although they have the advantage of providing industries with a proven technology, an advantage that is highly valued within industry.

Challenges, continued

One example is provided by an analysis of the Ultra-Pure Water at Spansion FAB25 Facility in Austin, TX produced using the Water-TAP3 tool. The primary treatment trains use UF and RO in combination with other pre- and post-treatment steps, and those primary filtration steps make up at least 85 to 95 percent of the LCOW (depending on the treatment train). Optimizing the pre- and post-treatment technologies with the treatment steps will have a significant impact on costs and operations. Limitations in these supporting processes can be a major challenge to alternative water use, especially if those water sources are temporally or spatially variable.

Impacts

This AOI is particularly useful for many medium- or small-scale manufacturers across all industry subsectors, where there is a need for modular approach that can be integrated easily in various existing processes.

M1.

RESEARCH NEEDS:

- **Develop** and optimize robust, high-rate, modular pretreatment processes for suspended solids and organics removal and integrate them with desalination systems. Examples of possible pretreatment technologies include chemical mixing, settling, flotation, and filtration units for treatment of industrial wastewater with high organic and suspended solids contents, as is typical for both the Food and Beverage Processing and Pulp and Paper industrial sectors (TRL 4 and greater).
- **Reduce** the weight, footprint, and overall complexity of pretreatment and post-treatment for desalination processes to promote portability and simple integration into systems at existing facilities. Pre- and post-treatment processes should also be robust and capable of handling feed disturbances. Examples include decreasing the size required for coagulation/flocculation and sedimentation and decreasing the costs of operation of dissolved air flotation and precipitation (TRL 4 and greater).
- **Identify** material and/or treatment process changes necessary to increase process throughput and operational flexibility (e.g., varied throughput and water quality) for application across all scales. Examples include materials that could be used within existing equipment and integrated into novel design approaches to increase throughput (TRL 4 and greater).
- **Develop** valorization techniques for wastewater generated in pretreatment simultaneously with techniques to increase water recovery and desalination performance (TRL 2–4).

M2.

Improve membrane module design and fabrication techniques to optimize integrated system performance, flexibility, and scalability, and develop cost-effective modular treatment systems.

Challenges

When adopting new technologies, engineers evaluate the ease of installation, long-term maintenance requirements, and capital and operating costs, as well as operational simplicity and flexibility. Novel treatment technologies and modular systems often lack sufficient information to support performance guarantees, limiting their implementation within industries that are slow to adopt technologies that do not have a long track record. Technology adoption is hindered by both perceived and actual problems. Building centralized, non-modular treatment facilities has been the more traditional approach, especially for industries that utilize large volumes of water such as Pulp and Paper, Chemicals, and Oil Refineries. For many of these existing plants, conversion to modular treatment facilities should consider the integration of current practices and current facilities to provide increased flexibility for alternative water qualities, the potential for blending water, and increased throughput without excessive infrastructure costs. Packaged plants are also appealing to industry as coordination of system construction and operation is simplified by working with a single vendor. However, if industry is to adopt a package plant mentality, the components need to be flexible (and reliable) enough for the range of source water conditions expected and the variable demands of a particular industry. Site-specific custom solutions are needed based on unique water quality considerations (both influent and effluent) and require objective third-party pilot-testing to ensure reliable and optimal performance under facility-specific conditions. Rigorous, peer-reviewed onsite evaluations of new treatment technologies are necessary to generate reliable operational information and increase level of comfort of engineers and regulators to increase the pace of adoption.

Impacts

This AOI is particularly useful for many medium- or small-scale manufacturers across all industry subsectors, where there is a need for modular approach that can be integrated easily in various existing processes.

M2.

RESEARCH NEEDS:

- **Develop** flexible treatment trains that quickly and efficiently adapt to site-specific needs. Potential research includes the identification of specific feed water quality parameters to adjust which parameters favor selected removal of one constituent over another, as dictated by irregular site conditions (e.g., constituent concentration, capacity, temperature), through modular treatment systems (e.g., membranes) (TRL 4 and greater).

- **Develop** mechanistic and/or stochastic models and control algorithms for modular processes, capturing various possible process and operating configurations. Improving our fundamental understanding of modular processes will allow better operation and design of modular processes, making them more cost-effective. This will generate more interest from industry and also reduce regulatory hurdles (see Section A as well) (TRL 2–4).

- **Develop** innovate manufacturing design (e.g., 3D printing of filter media) for fabrication of flexible modular treatment systems that allow for customization and modifications during the entire life of the facility to adapt to influent water quality variations, changing effluent water quality requirements, and increases/decreases in system capacity. Successful modular systems will decouple energy consumption from treatment flow rate and constituent removal so as to maintain energy efficiency even for high-capacity and high-salinity systems. They will also incorporate scalable components that can be configured to increase throughput, allowing for high-capacity modular systems with small footprints (TRL 2–4).

5.6. Electrified

Electrifying Water Treatment Processes and Facilitating Clean Grid Integration

E1.

Develop chemical-supply-free electrocatalytic processes for pollutant destruction.

Challenges

Electrochemical reductive and oxidative processes have significant potential to drastically improve the performance of pollutant removal and destruction schemes required by various manufacturing industries. Appealing attributes include a small footprint, modular nature, in-parallel and in-series connectivity for facile adjustment of process capacity and efficiency, minimal waste production, autonomous and responsive operation, and the potential for selective pollutant destruction. Electrochemical processes that generate oxidants such as ozone, hydrogen peroxide (H_2O_2), and hydroxyl radical from water and ambient oxygen obviate the need for the continuous supply of chemicals and can lead to replacement of chemically based CI systems. Energy- and cost-effective oxidative processes are expected to be particularly useful for the production of low-TOC, high-purity process water, washing water, and boiler feed water required in food and beverage, pulp and paper, textile, semiconductor, and various consumer goods manufacturing industries. With large-quantity production of oxidants and effective oxidant activation strategies (i.e., to enable advanced oxidation), recalcitrant pollutant destruction and TOC reduction can be pursued for the treatment of wastewaters from the Chemical, Oil Refineries, and Primary Metals industries. Analysis of the Iron and Steel Plant in Ohio in the Water-TAP3 tool showed that chemicals and catalysts costs made up 11 percent of the LCOW at the facility—the percentages ranged from 9 percent for oil wastewater treatment to 14 percent for steel wastewater treatment. Alternatively, direct reductive removal of oxyanions such as nitrate and oxidative destruction of organic pollutants such as PFAS can be an appealing treatment option that can replace existing chemical and biochemical pollutant destruction processes in various industries.

Challenges, cont.

Despite significant advances in commercial electrochemical systems in energy sectors such as batteries and fuel cells, Faradaic electrochemical processes are not yet widely employed in water treatment. Various electrodes and cell designs that have been successfully implemented in energy applications are not considered ideal in oxidant production and water treatment scenarios where water contains foulants such as reducible metals, organics, and particulate matter but often with low electrolytes for sufficient conductivity. Few electrode materials and architecture have targeted the properties required for selective destruction of pollutants at the electrode surface. There is a dearth of fundamental understanding of the mechanisms of electrode performance deterioration over long-term operation due to scaling, catalyst leaching, aging, electro-corrosion, and surface fouling.

Impacts

This AOI is relevant for many medium- or small-scale manufacturers across all industry subsectors for oxidation treatment, in situ chemical production, and/or Faradaic oxidation/reduction of pollutants. It is also relevant for TOC reduction after tertiary treatment in many industries, including petrochemical, oil refinery, and metal processing. This is particularly useful in industries where high-quality water is required (i.e., by AOPs) such as the food and beverage, pharmaceutical, and semiconductor industries.

E1.

RESEARCH NEEDS:

- **Develop** innovative electrode materials and cell designs that can achieve a) cost-effective production of treatment chemicals such as H_2O_2 without precursor supply, b) selective cathodic reduction of oxyanions such as nitrate, and c) selective anodic oxidation of recalcitrant organic pollutants such as PFAS under complex, realistic water matrices (TRL 2–4).
- **Develop** a fundamental understanding of surface and electrochemical phenomena of electrodes that lead to the performance deterioration in water treatment scenarios, with the ultimate goal of utilizing this knowledge to develop strategies to minimize these phenomena through material advances, surface coating, and innovative cell design (TRL 2–4).
- **Develop** strategies for fast screening of a wide range of materials and cell designs in order to promote faster technology development and transfer to the industry. These strategies can be pursued by a) mechanistic understanding of material behavior, b) development of a library of new catalysts such as cost-effective single atom (alloy) catalysts that enable selective electrode reaction, c) novel accelerated cell life testing protocols, and d) robust computational capability (TRL 2–4).

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.

Challenges

Although water is critical to several industrial processes, water treatment is often viewed as only being secondary to the primary products generated and simply the means to provide the FfP use for their own economic needs and/or to meet regulatory discharge requirements. Currently, industrial processes are often centralized and designed to operate continuously (i.e., in a steady state) to maintain performance efficiency and ease of operation, and reduce waste, emissions, and downtime. Water is a critical component in many industrial systems (e.g., cooling, process operation, and material transport). Given water's critical role and the preferred continuous operation of industrial processes, treatment systems must provide a high degree of reliability, both with regards to water quality and operation. Electrified treatment processes have the potential to reduce, or in some cases even eliminate, external chemical addition. A reliable energy source is paramount to ensuring uninterrupted operation of critical electrified water treatment processes. Temporal variations in energy costs related to periods of high demand from the grid may limit the economic viability of transitioning to completely electrified treatment processes. An ideal electrified process would smoothly respond to real-time electrical demands and restrict operation to periods of low electricity costs, which is inconsistent with a steady water source required by industrial applications. Hence, equalization basins to store treated or raw wastewater would be necessary to facilitate intermittent operation, which contradicts NAWI's modularity theme. Industries may decide to switch to renewable energy to increase their sustainability and also improve public relations. One constraint of renewable energy sources is the inherent intermittency of energy generation. Hence, a move towards renewable energy would be accompanied by reliable access to the electrical grid and/or onsite energy storage for backup power. In order for industry to adopt electrified treatment processes, the dual challenges of access to constant and reliable sources of energy and influent/treated water must be resolved.

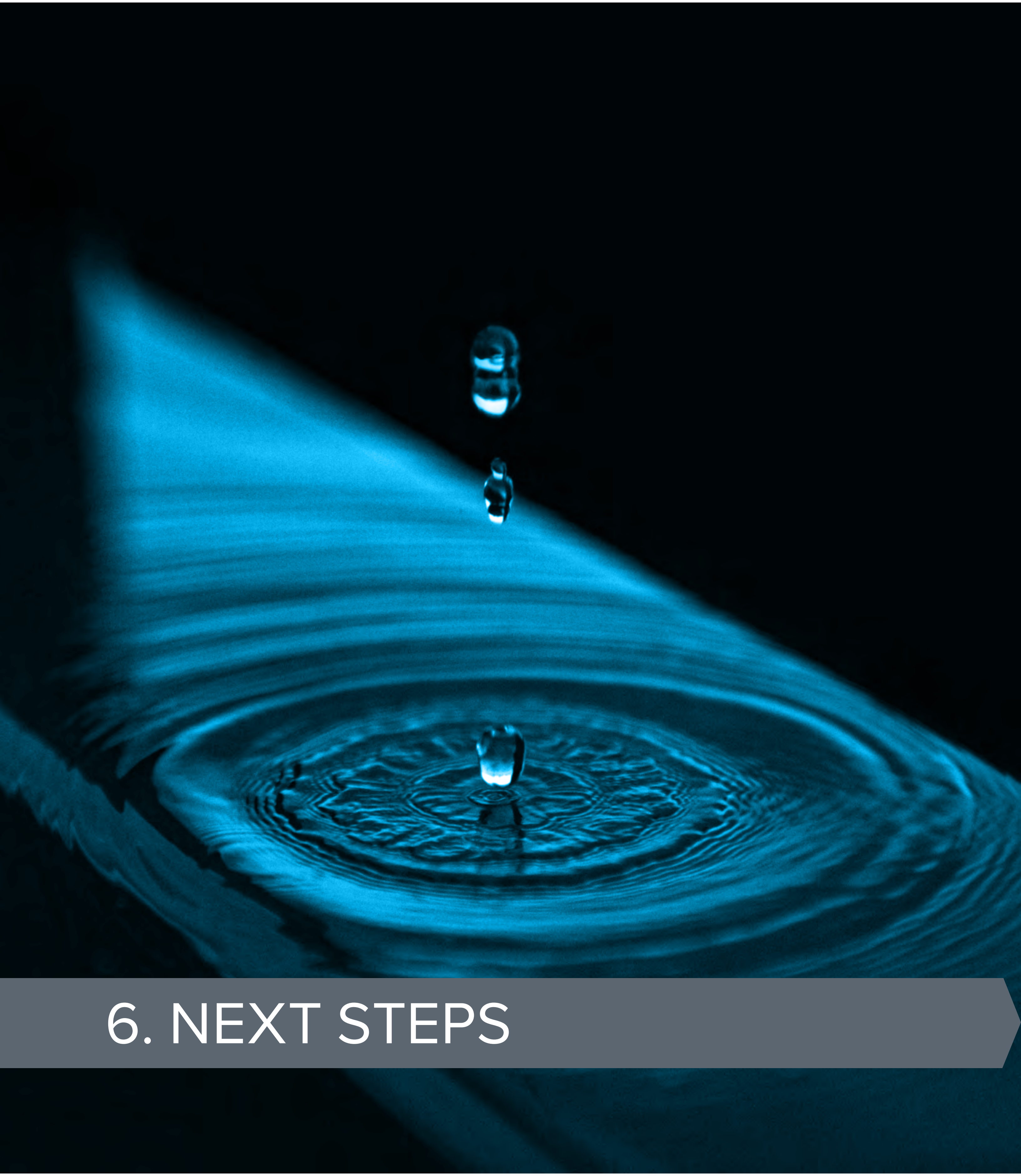
Impacts

This AOI is relevant for many medium- or small-scale manufacturers across all industry subsectors for oxidation treatment, in situ chemical production, and/or Faradaic oxidation/reduction of pollutants. It is also relevant for TOC reduction after tertiary treatment in many industries, including chemical, oil refinery, and metal processing. This is particularly useful in industries where high-quality water is required (i.e., by AOPs) such as the food and beverage, pharmaceutical, and semiconductor industries.

E2.

RESEARCH NEEDS:

- **Develop** water treatment modules that are able to 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, and environmental emissions (TRL 4 and greater).
- **Reduce** energy costs associated with electrified water treatment systems and enable intermittent operation by integrating renewable energy and flow equalization (relatively constant throughput and process efficiency) to enable operation during non-peak hours (TRL 4 and greater).
- **Pursue** the possibility of reducing the number of conventional unit processes through intensified treatment (e.g., combining pretreatment and treatment within a single module) to facilitate easier adoption by industry (TRL 4 and greater).



6. NEXT STEPS

This comprehensive and dynamic roadmap for low-TRL desalination and water treatment technologies for the Industrial End-Use Sector is intended to guide future R&D investments throughout the duration of the research program. NAWI's Master Roadmap will compile high-value, crosscutting themes across all PRIMA end-use water roadmaps, including this one, and will be 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 it annually. Annual 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 circular water economy for the Industrial Sector following the A-PRIME technology development hypothesis 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 design and manufacture critical equipment, components, and small-modular and large-scale systems.

Innovations from the NAWI Energy-Water Desalination Hub will promote energy-efficient, cost-effective water purification, ensuring a secure supply of clean water for the nation and the world.

Appendix A: Acronyms

3D	Three-dimensional
A-PRIME	Autonomous operations, Precision separations, Resilient treatment and transport, Intensified brine management, Modular (membrane) systems, and Electrified treatment systems – NAWI R&D focus area
AOI	Areas of Interest
AOP	Advanced oxidation processes
AOX	Adsorbable organic halides
AI	Artificial intelligence
BOD	Biological oxygen demand
Ca	Calcium
CEC	Contaminants of emerging concern
Cl	Chlorine
COD	Chemical oxygen demand
Cr	Chromium
DO	Dissolved oxygen
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
ESG	Environmental, Social, and Governance
FfP	Fit-for-purpose
H_2O_2	Hydrogen peroxide
IoT	Internet of Things
LCA	Life cycle analysis
LCOE	Levelized cost of electricity
LCOW	Levelized cost of water
mg/L	Milligrams per liter

Mg	Magnesium
MGD	Million gallons per day
ML	Machine learning
MLD	Minimum liquid discharge
NAICS	North American Industry Classification System
NAWI	National Alliance for Water Innovation Hub
NF	Nanofiltration
NPDES	National Pollutant Discharge Elimination System
O&G	Oil and gas
O&M	Operations and maintenance
O_3	Ozone
OCWD	Orange County Water District
PFAS	Per- and polyfluoroalkyl substances
pH	Potential of hydrogen to specify the acid or base strengths
PPCPs	Pharmaceutical and personal care products
ppm	Parts per million
PRIMA	Power, Resource Extraction, Industry, Municipal, Agriculture End-use sector focus for NAWI
R&D	Research and Development
RAC	Research advisory council
RFP	Requests for projects
RO	Reverse osmosis
TDS	Total Dissolved Solids
TEA	Technoeconomic analysis
TOC	Total organic carbon
TRL	Technology readiness level

TSS	Total suspended solids
USGS	United States Geological Survey
UF	Ultrafiltration
Water-TAP3	Water Technoeconomic Assessment Pipe-Parity Platform
ZLD	Zero-liquid discharge

Appendix B: NAWI A-PRIME Expanded Descriptions

Autonomous

Current water treatment systems are designed to operate at nominally steady-state conditions, relying on human intervention to adapt to variations in water quality and correct failures in process performance. Simple, robust sensor networks coupled with sophisticated analytics and controls systems could enhance performance efficiency and process reliability. These more adaptable, smart systems could also minimize the need for on-site, manual interventions. Together, these innovations would significantly lower the cost of distributed, FfP desalination systems.

Early-stage applied research can improve Internet of Things (IoT) infrastructure to meet the need for water treatment that is generalizable, secure, and resilient when managing sparse data and calibration errors. System identification and physics-based approaches can be used to develop reduced-order models and adaptive methods for closed-loop feedback control and optimization of interdependent water treatment processes. The developed controls approaches can be augmented with statistical and machine-learning-informed process monitoring techniques to diagnose system inefficiencies and faults. Data needs for process control and monitoring include temporal, nonlinear, stochastic, and uncertainty aspects of process parameters.

Precise

Current water treatment systems often rely on inefficient bulk separation processes to remove solutes that occur at trace levels. A more targeted treatment approach for trace contaminant removal can reduce the cost and energy intensity of treatment processes, while offering major reductions in system complexity and waste disposal costs. Precise separation or transformation of constituents also enhances the likelihood of profitable recovery and valorization of waste streams, offsetting the overall costs of desalination systems.

Early-stage applied research can improve the selectivity of materials and the efficiency of removal technologies for hard-to-treat or valuable-to-extract compounds (e.g., boron, hexavalent chromium [Cr], lead, nitrate, perchlorate, selenium, uranium, lithium, iodide). Simulation platforms can exploit molecular recognition principles in the design of highly selective materials. There is a need to synthesize and characterize these materials in high-throughput experimentation platforms. There is also a need to use process modeling and optimization tools to ensure that the high selectivity and affinity for target species, fast uptake kinetics, and efficient regeneration are fully exploited in continuous and intensified process designs. Such materials may become more cost effective if they can tap into recent additive, gradient, and roll-to-roll manufacturing advances that lower production costs.

Resilient

Current municipal water infrastructure relies on aging centralized water treatment, storage, and distribution systems that are energy-intensive, corroding, leaking, and costly to replace. In addition, key U.S. industries face complex logistics constraints in storing water and residuals and transporting them between remote locations, often via truck. While distributed treatment can reduce conveyance issues, these systems must function under conditions in which water quality, temperature, or water residence times undergo large fluctuations. Resilient water supply networks, adaptable treatment processes, and robust materials are needed if we are to realize the benefits of distributed, FfP desalination systems.

Early-stage applied research to advance resilient water treatment and distribution systems will span molecular-scale to systems-scale research. Robust optimization techniques for materials and process design are needed to ensure compatibility with a wide variety of solution chemistries and accelerated materials. Aging platforms coupled with state-of-the-art in operando characterization tools can be used to test materials that resist corrosion and fouling in distributed desalination and conveyance systems. Step changes in treatment system reliability and resiliency can be enabled by the design of optimal sensor networks and analytics approaches that inform adaptive control techniques and allow processes to robustly operate over a wide range of feedwater quality levels. At the distribution system level, computationally efficient multiscale modeling and multi-objective optimization platforms are needed for water network designs that maximize reuse and minimize cost.

Intensified

Current thermally driven brine management technologies are energy intensive, complex, and poorly suited for the modest flows of small-scale desalination systems. At the same time, there is an ongoing revolution in unconventional oil and gas development; expanded exploitation of inland brackish water resources; new regulatory requirements for effluent discharge at power generation, mining, and manufacturing facilities; and planning for future carbon storage in saline reservoirs, which are creating new demands for more efficient brine and concentrate management. Innovative technologies for brine concentration and crystallization would eliminate the need for brine conveyance, reduce dependence on finite injection well capacity, enhance water recovery from nontraditional sources, and lower energy intensity and cost of desalination facilities.

Early-stage applied research can focus on developing process alternatives to traditional, thermally driven brine management technologies, and materials innovations to improve the efficiency of existing processes. To concentrate brines between 75,000 and 200,000 ppm TDS, there is a need for materials and manufacturing platforms that extend the pressure tolerance of RO membrane modules, process configurations that combine multiple driving forces, and systems that couple brine treatment with metals recovery and chemical synthesis. For higher-salinity brines treated by thermal processes, topology optimization and precision manufacturing methods can be paired to improve heat transfer in thermal processes, enabling efficient system integration with waste heat sources. Models of nucleation and crystalline phase growth that open new avenues for controlling scaling and promoting crystallization in energy-saving, small-scale units are also needed.

Modular

Current seawater desalination systems use energy-efficient, modular, and mass-manufactured RO membrane systems. When these same types of modules are used to desalinate organic and mineral-rich waters with higher fouling and scaling potential, energy consumption and maintenance costs increase. Furthermore, commercially available membranes are unable to separate ions of the same valence or remove low-molecular-weight neutral compounds from water. Finally, membranes are manufactured via poorly understood, highly nonequilibrium processes that limit property control and customization for specific feedwater compositions. Innovations in both membrane materials and manufacturing processes could vastly expand the range of water chemistries over which modular membrane systems are cost-competitive and potentially eliminate the need for intensive pretreatment and post-treatment (e.g., multi-stage RO for boron removal). Further modularizing pretreatment and post-treatment processes would increase reliability and reduce the costs of operating moderate-scale, distributed desalination systems.

Early-stage research is needed to advance the next generation of membrane materials and processes. These advances include the development of techniques that enable control of membrane properties during manufacturing, in operando materials characterization techniques that facilitate understanding of membrane performance under varying solute conditions, and manufacturing innovations that enable the scalable deployment of novel membrane materials in cost-competitive modules. It will also require process optimization models that explore the full range of process configurations, operating schema, and treatment train configurations for minimizing fouling and scaling while maximizing recovery. Advances in computational methods for materials design and selection, modeling platforms for accurately describing coupled mass transport and reactivity in porous media, materials processing approaches (e.g., additive, roll-to-roll, spray coating), and multiscale simulation tools for process optimization are needed to enable the necessary improvements in membrane flexibility and performance.

Electrified

Current water treatment trains use large volumes of commodity chemicals that are high in embedded energy, expensive, and difficult to implement in distributed treatment systems. These processes are typically designed for steady-state operation, reducing their ability to ramp in response to fluctuations in water quality and the price of electricity. Replacing chemically intensive, steady-state processes with electrified and intermittently operated processes will reduce operating costs and provide a means of exploiting renewable energy resources and temporal variations in the cost of electricity. It will also promote small-scale, distributed water treatment by reducing the need for chemical supply and minimizing the complexity of water desalination operations.

Early-stage research to extend material and component longevity during intermittent process operation will reduce wear associated with rapid or frequent ramping. Process simulation models can be used to identify low-wear component designs and advanced manufacturing processes to realize them cost-effectively. To expand the number of electrified processes that might be ramped, there is a need to develop high-fidelity simulation models of electrochemical processes that include chemical, flow, faradaic, and non-faradaic effects in a variety of complex fluid compositions. These models can be applied in pretreatment, treatment, and post-treatment processes to design materials and processes that improve performance consistency, eliminate chemical use, or generate chemicals (e.g., caustic, Cl) in situ. There is a need for *in situ* methods for characterizing poorly understood process conditions, such as precipitation kinetics, flocculation dynamics, and ion distribution in boundary layers. Maximizing the potential of electrified treatment processes will also require the development of integrated energy-water economic models to quantify the synergies between these two systems as well as system improvements in stability, reliability, and flexibility.

Appendix C: DOE Water Hub Development Background

DOE's Water Security Grand Challenge is a White House-initiated, DOE-led framework to advance transformational technology and innovation to meet the needs for safe and affordable water and help secure the nation's water supplies. Using a coordinated suite of prizes, competitions, early-stage research and development funding opportunities, critical partnerships, and other programs, the Water Security Grand Challenge sets the following goals for the United States to reach by 2030:[47]

- Launch desalination technologies that deliver cost-competitive clean water
- Transform the energy sector's produced water from a waste to a resource
- Achieve near-zero water impact for new thermoelectric power plants and significantly lower freshwater use intensity within the existing fleet
- Double resource recovery from municipal wastewater
- Develop small, modular energy-water systems for urban, rural, tribal, national security, and disaster response settings

The Energy-Water Desalination Hub, or NAWI Hub, will support the goals of the Water Security Grand Challenge.[48] Specifically, the NAWI Hub will:

- Address water security needs for a broad range of stakeholders, including utilities, oil and gas production, manufacturing, agriculture, and states and municipalities;
- Focus on early-stage R&D for energy-efficient and low-cost desalination technologies, including manufacturing challenges, for treating nontraditional water sources for beneficial end-use applications and achieve the goal of pipe parity;
- Establish a significant, consistent, and multidisciplinary effort (i.e., using a broad set of engineering and scientific disciplines) to identify water treatment challenges and opportunities;
- Enhance the economic, environmental, and energy security of the United States; and
- Lead to fundamental new knowledge to drive energy-efficient and low-cost technological innovations to the point that industry will further develop and enable U.S. manufacturing of these new technologies to be deployed into the global marketplace.

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.

Appendix D: Roadmap Teams

Cartography Team

Each PRIMA end-use sector was led by a small group of academic experts (3–4 people). This group is collectively known as the cartography team (total of 10 researchers) and identified challenges and research needs associated with the recovery and reuse of nontraditional waters. They are the primary authors for their end-use sector roadmap. The Master and Deputy Master cartographers synthesized high-value, crosscutting themes across multiple end-use water roadmaps for the Master Roadmap.

Core NAWI Teams

Each PRIMA end-use cartography team was supported by a small group of subject matter experts (3–5 people) from industry, national labs, government, and academia; they contributed regularly to NAWI's water user roadmapping effort to help identify and establish future research priorities for NAWI, focusing particularly on the needs and opportunities of one assigned group of water users (municipal, agriculture, power, industrial, or resource extraction). Their activities included:

1. **Participating in roadmapping meetings**: Meeting twice a month to provide input, shape the direction of roadmapping activities, discuss recent developments, and review materials.
2. **Identifying key experts and practitioners to participate in roadmapping activities**: Recommending participants for interviews, workshops, and/or surveys as part of the roadmapping data collection process to obtain a wide array of industry insights.
3. **Providing insight on current and future needs for water treatment technologies**: Participating in meetings, (virtual and/or in-person) workshops, interviews, and/or surveys.
4. **Providing insights into quantitative data to support industry analysis, when possible**: Connecting NAWI researchers to sources of data that would facilitate baseline assessments.

Broader Teams

Each end-use cartography team was supported by a broader, more diverse group of subject matter experts (10–20 people); they contributed periodically to NAWI's water user road-mapping effort to help identify and establish future research priorities for NAWI, focusing particularly on the needs and opportunities of one assigned group of water users (municipal, agricultural irrigation, power, industrial, or resource extraction). Their activities included:

1. **Participating in roadmapping meetings**: Meeting monthly to provide input, shape direction of roadmapping activities, discuss recent developments, and review materials.
2. **Identifying other key experts and practitioners to participate in roadmapping activities**: Contributing to discussion of identifying participants for interviews, workshops, and/or surveys as part of the roadmapping data collection process.
3. **Providing insights on current and future needs for water treatment technologies**: Participating in meetings, (virtual and/or in-person) workshops, interviews, and/or surveys.
4. **Providing insights into quantitative data to support industry analysis, when possible**: Connecting NAWI researchers to sources of data that would facilitate baseline assessments.

Appendix E: Development of the NAWI Industrial Sector Technology Roadmap

Data Collection Process

The NAWI End-Use Sector Roadmaps were developed using a multi-step process coordinated by the NAWI end-use cartography teams. The key component of this process was a two-day virtual Technology Roadmapping Workshop—held in August 2020 and facilitated by Nexight Group—that included participants from industry, academia, national laboratories, and associations. Surveys and interviews with water and industry professionals were conducted in the months leading up to the workshop. Outputs from the surveys and interviews—including a comprehensive list of challenges and potential research solutions—were used to provide direction to the workshop sessions.

The result of these workshops was a refined list of industry-specific challenges and associated research solutions for each area of A-PRIME. These solutions were coupled with ongoing inputs from surveys, subject matter expert interviews and discussions, and other relevant documents to create the recommended list of research priorities in the End-Use Roadmaps. At several points during the roadmapping process, workshop participants, NAWI technical teams, and the DOE Advanced Manufacturing Office (AMO) reviewed the preliminary findings, intermediate, and final roadmap drafts prepared by NAWI and Nexight Group to further refine the content.

Activities Prior to the Technology Roadmapping Workshop

Online Survey

The NAWI teams and Nexight Group distributed an online survey to: 1) share a general understanding of water use and critical needs by sector; 2) identify critical barriers for nontraditional water treatment and reuse; and 3) identify early-stage applied research needs and opportunities (TRL 2–4) that will improve access and performance of nontraditional water desalination and treatment processes.

Between June and August 2020, the survey was sent to a diverse group of industry stakeholders covering all five of the end-use sectors. In the survey, participants were asked to provide their assessment and notional solutions to address these challenges. Additional optional questions were asked to gather targeted input based on the participant's sector (i.e., academia, industry, or government). The optional questions touched on the following areas: 1) decision criteria for using nontraditional water sources, 2) future water technology trends, 3) treatment system operations/design, and 4) regulatory conditions. The challenges and notional solutions identified from the survey findings were discussed and scrutinized during the technical workshops. Other findings were supplied to NAWI to further inform technical strategy and operations.

Subject Matter Expert Interviews

From June to August 2020, Nexight Group conducted more than 95 one-hour technical interviews with subject matter experts covering each of the 5 end-use sectors. These individuals were recommended by NAWI team members. These interviews were designed to engage stakeholders to 1) establish a baseline understanding of water use and minimum water quality for industry or business needs, 2) identify critical barriers for nontraditional water treatment and reuse, and 3) identify early-stage applied research needs that will improve access to and performance of nontraditional water desalination and treatment processes (e.g., by lowering the cost, decreasing energy use, increasing reliability, minimizing environmental impacts, maximizing resource recovery, removing contaminants). The challenges and notional solutions identified from the interview findings were discussed and scrutinized during the technical workshops. Other findings were supplied to NAWI to further inform technical strategy and operations.

Core and Broader Team Brainstorming

The end-use sector broader teams were engaged in an online brainstorming activity. They identified critical barriers for nontraditional water treatment and reuse and the research needs that will improve access to and performance of nontraditional water desalination and treatment processes. The challenges and notional solutions identified from these brainstorming sessions were discussed and scrutinized during the technical workshops. Other findings were supplied to NAWI to further inform technical strategy and operations.

Technology Roadmapping Workshop

Workshop Purpose

The NAWI roadmapping workshop was designed to identify potential research topics needed to address industry's water challenges and achieve the NAWI vision and pipe parity goals. Each of the five NAWI end-use sectors had its own two-part, virtual roadmap workshop. Each workshop was built on the input collected from nearly 300 NAWI stakeholders via surveys, interviews, and working meetings conducted from June to October 2020.

Workshop Format

During the weeks of August 10 and 17, 2020, Nexight Group conducted 2 two-hour virtual sessions (using Zoom Video Communications) of up to 25 participants, with a homework assignment in between sessions. A minimum of 24 hours between the virtual sessions was provided to allow the completion of homework assignments. Prior to the workshop, participants reviewed a preliminary set of findings from previously collected input.

During the first of the two workshops, participants shared ideas through facilitated sessions. Structured brainstorming and critical analysis were used to refine the proposed list of NAWI research topics and identify additional research topics. After the first workshop for each end use, participants' homework consisted of ranking all potential research topics by a) probability of technical success, b) potential impact on NAWI goals, and c) timeframe for completion. These rankings were reviewed during the second workshop, and the research priorities were refined further based on feedback. After the second workshop, the raw data from the session was analyzed by Nexight and the cartography teams to arrive at a preliminary list of TRL 2–4 research priorities for each end-use sector. These topics were further reviewed, amended, and augmented by industry and expert engagement before being finalized in the five roadmap documents.

Workshop Outputs

The workshops were designed to deliver specific outputs necessary for the NAWI roadmapping process, including:

- Categorized sets of potential research topics for addressing water user challenges
- Ratings of each research topic in terms of probability of technical success and potential for impact on pipe parity metrics
- Notional research timelines (near, mid, and long term)

Preparation of the NAWI Technology Roadmaps

Research priorities in this roadmap are categorized under the six NAWI Challenge Areas (A-PRIME), which have been identified as critical to achieving a circular water economy. Using the information collected during the workshop and synthesized by the cartography team, these preliminary findings were reviewed in September and October 2020 by the Core and Broader teams, NAWI Technical Teams, and DOE AMO staff. Concurrently, the Nexight Group and cartography teams compiled an initial draft (NAWI Internal Use Only) of the five roadmaps, which was reviewed by NAWI Technical Teams, Core and Broader Teams, and key DOE AMO staff in November and December 2020. Based on feedback from these sources, additional roadmap versions were developed and iterated on. A final public draft of the five NAWI roadmaps was then published.

Appendix F: **Contributors**

NAWI Executive and Technology Team

Deb Agarwal
Lawrence Berkeley National Laboratory

Peter Fiske
Lawrence Berkeley National Laboratory

Steve Hammond
National Renewable Energy Laboratory (NREL)

Eric Hoek
University of California-Los Angeles

Robert Kostecki
Lawrence Berkeley National Laboratory

Jordan Macknick
National Renewable Energy Laboratory (NREL)

Meagan Mauter
Stanford University

Jeffrey McCutcheon
University of Connecticut

Yarom Polsky
Oak Ridge National Laboratory

David Sedlak
University of California-Berkeley

Sridar Seetharaman
Arizona State University

Renae Speck
Oak Ridge National Laboratory

Jennifer Stokes-Draut
Lawrence Berkeley National Laboratory

Carol Valladao
Lawrence Berkeley National Laboratory

Michelle Wong
Lawrence Berkeley National Laboratory

NAWI Research Advisory Council

Pedro Alvarez
Rice University

John Crittenden
Georgia Institute of Technology

Menachem Elimelech
Yale University

Benny Freeman
University of Texas at Austin

Lisa Henthorne
Water Standard

Thomas Kurfess
Oak Ridge National Laboratory

John Lienhard
Massachusetts Institute of Technology

Bruce Moyer
Oak Ridge National Laboratory

David Sedlak
University of California-Berkeley

David Sholl
Georgia Institute of Technology

NAWI Core Industrial Team

Jason Monnell
Electric Power Research Institute

Sharon Nolen
Eastman Chemical

Paul O'Callaghan
Bluetech

Prakash Rao
Lawrence Berkeley National Laboratory

NAWI Additional Contributors

Carolyn Cooper
University of Texas-Austin

Sourav Das
Texas A&M University

Cameron McKay
University of Texas-Austin

Aidan Meese
Yale University

Kaleisha Miller
Texas A&M University

Kyungho Kim
Texas A&M University

NAWI Broader Industrial Team

Fernando Almada Calvo
Chevron

Sébastien Bessenet
Veolia Water Technologies

Bill de Waal
TrojanUV

Margaret Donoghue
Commonwealth Scientific and Industrial Research Organisation (CSIRO) - Global Office

Grant Douglas
Commonwealth Scientific and Industrial Research Organisation (CSIRO)

Susana Garcia Gonzalez
Oak Ridge National Laboratory

Christopher Gasson
Global Water Intelligence

Laurie Gilmore
The Coca-Cola Company

Anna Kaksonen
Commonwealth Scientific and Industrial Research Organisation (CSIRO)

Michael Kavanaugh
Geosyntec

Jason Kirby
Commonwealth Scientific and Industrial Research Organisation (CSIRO)

John Koon
Georgia Institute of Technology

Matt Mallory
Bluetech

David Marrs
Valero Energy Corp.

Jason Monnell
Electric Power Research Institute

Sankar Nair
Georgia Institute of Technology

Sachin Nimbalkar
Oak Ridge National Laboratory

Julie Noblitt
CSIRO - Global Office

Sharon Nolen
Eastman Chemical

Paul O'Callaghan
Bluetech

Tom Pankratz
Global Water Intelligence

Prakash Rao
Lawrence Berkeley National Laboratory

Brad Smith
BHP

Kiran Thirumaran
Oak Ridge National Laboratory

Rhodes Trussell
Trussell Tech

Greta Zornes
CDM Smith

NAWI Industrial Workshop Participants

Brent Alspach
Arcadis

Sebastien Bessenet
Veolia Water Technologies

Sarah Condon
BlueTech

Jordan Cox
National Renewable Energy Laboratory

Bill de Waal
Trojan/Consultant

Susana Garcia
Oak Ridge National Laboratory

Laurie Gilmore
The Coca-Cola Company

David Ingram
National Renewable Energy Laboratory

Jeff Guild
BlueTech

David Ingram
Phillips 66

David Kim
Yale University

John Koon
Georgia Institute of Technology

Kenneth Kort
U.S. Department of Energy

Darin Kuida
Amgen

Linh Le
Yale University

Matthew Mallory
BlueTech

James McCall
National Renewable Energy Laboratory

Jeffrey McCutcheon
University of Connecticut

Aidan Meese
University of Delaware

Jason Monnell
Electric Power Research Institute

Cade Napier
Yale University

Sachin Nimbalkar
Oak Ridge National Laboratory

Sharon Nolen
Eastman

Paul O'Callagan
BlueTech

Tom Pankratz
GWI

Toni Pezzetti
California Department of Water Resources

Yarom Polsky
Oak Ridge National Laboratory

Prakash Rao
Lawrence Berkeley National Laboratory

Mike Rinker
Pacific Northwest National Laboratory

James Rosenblum
Colorado School of Mines

Nate Rothe
Colorado School of Mines

John Rydzewski
Nike

Kiran Thirumaran
Oak Ridge National Laboratory

David Turpin
Alliance for Pulp & Paper Technology Innovation (APPTI)

NAWI Agricultural Interview Participants

Rishabh Bahel
ArcelorMittal

Sébastien Bessenet
Veolia Water Technologies

Fernando Almada Calvo
Chevron

Brad Crocker
Airgas

G Anders Hallsby
Mazarine Ventures

David Ingram
Phillips 66

Raj Kailasam
Phillips 66

Grant Douglas, Anna Kaksonen
Commonwealth Scientific and Industrial Research Organisation (CSIRO)

Douglas Kepler
Seneca Resources

John Koon
Georgia Institute of Technology

Darin Kuida
Amgen

Toni McCrory
Wal-Mart

Sankar Nair
Georgia Institute of Technology

Tom Pankratz
Global Water Intelligence

John Rydzewski
Nike

Richard Stover
Gradiant Membrane Systems

David Turpin
Alliance for Pulp and Paper Technology Innovation (APPTI)

Bill de Waal
TrojanUV

Tony Wachinski
Wisewater Global LLC

Katherine Yarberry
Wal-Mart

Greta Zornes
CDM Smith

Joe Zuback
Global Water Advisors

NAWI Survey Participants

Miguel Acevedo
University of North Texas

Andrea Achilli
University of Arizona

Anne Aiken
Tennessee Valley Authority

Hannah Ake
Metropolitan Water District of Southern California (MWD)

Fernando Almada Calvo
Chevron

Brent Alspach
Arcadis

Pedro Alvarez
Rice University

Gary Amy
Clemson University

Laura Arias Chavez
Tennessee Tech University

Lisa Axe
New Jersey Institute of Technology

Rick Bacon
Aqua Metrology Systems

Richard Belt
Xcel Energy

Ignacio Beneyto
ACCIONA Agua

Sebastien Bessenet
Veolia Water Technologies

Ramesh Bhave
Oak Ridge National Laboratory

Kevin Boudreaux
ChemTreat

Steven Buchberger
University of Cincinnati

Donald Bull
Hess Corporation

Don Cameron
Terranova Ranch

Mik Carbajales-Dale
Clemson

David Cercone
DOE National Energy Technology Laboratory (NETL)

Barbara Chappell
City of Goodyear

Shankar Chellam
Texas A&M University

Yongsheng Chen
Georgia Institute of Technology

Zaid Chowdhury
Garver

Jared Ciferno
National Energy Technology Laboratory (NETL)

Nicholas Charles Clarke
Imtech Pty Ltd

Edward Clerico
Natural Systems Utilities

Yoram Cohen
University of California—Los Angela

Terrence Collins
Carnegie Mellon University

Regis Conrad
U.S. Department of Energy (DOE)

Vince Conrad
RJ Lee Group

Glen Daigger
University of Michigan

Gary Darling
Darling H2O Consulting

Seth Darling
Argonne National Laboratory

William de Waal
Trojan Technology—Retired

Allison Deines
Alexandria Renew Enterprises

Ashwin Dhanasekar
The Water Research Foundation

Michael DiFilippo
DiFilippo Consulting

Kim Dirks
Tyson Foods

Mark Donovan
GHD

Grant Douglas
Commonwealth Scientific and Industrial Research Organisation (CSIRO)—Australia's National Science Research Agency

Patrick Drew
Pioneer Water Management

Christopher Drover
ZwitterCo

Matthieu Dubarry
University of Hawaii at Manoa / Hawaii Natural Energy Institute (HNEI)

Clark Easter
Global Water Innovations

Arian Edalat
Pacifica Water Solutions

Thomas Feeley
U.S. Department of Energy (DOE)/ National Energy Technology Laboratory

Val Frenkel
Greeley and Hansen

Neil Fromer
Caltech

Edward Furlong
U.S. Geological Survey

Carlos Galdeano
ExxonMobil

Christopher Gasson
Global Water Intelligence

Laurie Gilmore
The Coca-Cola Company

James Golden
Poseidon Water

Rowlan Greaves
Southwestern Energy

Sargeant Green
California Water Institute

Emily Grubert
Georgia Institute of Technology

Djuna Gulliver
National Energy Technology Laboratory (NETL)

Sally Gutierrez
U.S. Environmental Protection Agency (EPA)

NAWI Survey Participants

Alexandra Hakala
National Energy Technology Laboratory (NETL)

Brent Halldorson
RedOx Systems, LLC

Evan Hatakeyama
Chevron

Lisa Henthorne
Produced Water Society

Amanda Hering
Baylor University

Roxana Herrera
BP America Production

Eric Hoek
University of California—Los Angeles (UCLA) Samueli Engineering School

Tim Hogan
TWB Environmental Research and Consulting

Megan Holcomb
State of Colorado, CO Water Conservation Board

Juliet Homer
U.S. Department of Energy (DOE)

Chuanxue Hong
Virginia Tech

Jan Hopmans
University of California (UC)—Davis

Robert Huizenga
Cimarex Energy Co.

Christopher Impellitteri
U.S. Environmental Protection Agency (EPA)

David Ingram
Phillips 66

Joe Jacangelo
Stantec

David Jassby
University of California—Los Angeles (UCLA)

Logan Jenkins
Pheneovate

Graham Juby
Carolla Engineers

Asha Kailasam
Chevron

Tetsuya Kenneth Kaneko
Forward Greens

Stephen Katz
SUEZ Water Technologies & Solutions

Paula Kehoe
San Francisco Public Utilities Commission (SFPUC)

Dan Keppen
Family Farm Alliance

Kyoung-Yeol Kim
State University of New York at Albany (SUNY)

Ryan Kingsbury
Lawrence Berkeley National Laboratory / Membrion

Isaya Kisekka
University of California (UC)—Davis

John Koon
Georgia Institute of Technology

Jane Kucera
Nalco Water, and Ecolab Company

Ted Kuepper
Pacific Research Group

Darin Kuida
Amgen

Kuldip Kumar
Metropolitan Water Reclamation District of Greater Chicago (MWRD)

David Ladner
Clemson University

Qilin Li
Rice University

Sun Liang
Metropolitan Water District of Southern California (MWD)

Xiao-Min Lin
Argonne National Laboratory

Yupo Lin
Argonne National Laboratory

Glenn Lipscomb
University of Toledo

Adrienne Little

Frank Loeffler
Oak Ridge National Laboratory and University of Tennessee

Sue Longo
Goolder Associates

Nancy Love
University of Michigan

Stan Luek
RODI Systems Corp.

Cissy Ma
U.S. Environmental Protection Agency (EPA)

Yanbao Ma
University of California (UC)—Merced

John MacHarg
Ocean Pacific Technologies

Dave MacNevin
CDM Smith

Ivan Mantilla
Chevron

Mike Markus
Orange County Water District (OCWD)

David Marrs
Valero Energy Corporation

Mike Mathis
Continental Resources

Scott Mauger
National Renewable Energy Laboratory

Brandon McAdams
National Energy Technology Laboratory (NETL)

Mark Meyer
Flow-Tech Systems

Michael Mickley
Mickley & Associates

NAWI Survey Participants

Thomas Missimer
Florida Gulf Coast University—Emergent Technologies Institute (ETI)

Matthew Montz
Southern Company

Adrien Moreau
SUEZ Water Technologies & Solutions

Sankar Nair
Georgia Institute of Technology

Sachin Nimbalkar
Oak Ridge National Laboratory

Richard Noble
University of Colorado—Boulder

Sharon Nolen
Eastman Chemical Company

Aleksandr Noy
Lawrence Livermore National Lab (LLNL)

John Ocana
California Resources Corporation

Declan Page
Commonwealth and Scientific and Industrial Research Organisation (CSIRO)

Bill Parmentier
DUCTOR

Mehul Patel
Orange County Water District (OCWD)

Toni Pezzetti, CA Dept of Water Resources

Megan Plumlee
Orange County Water District (OCWD)

Clarence Prestwich
U.S. Department of Agriculture (USDA)—Natural Resources Conservation Service

Kevin Price
AWTT

Tanya Prozorov
Ames Lab

Amy Pruden
Virginia Tech

Jing Qi
Unviersity of Hawaii at Manoa/ Hawaii Natural Energy Institute

Jason Ren
Princeton University

Debora Rodrigues
University of Houston

Arup SenGupta
Lehigh University

Godwin Severa
University of Hawaii/Hawaii Natural Energy Institute

Vesselin Shanov
University of Cincinnati

Wu-Sheng Shih
Brewer Science

Nicholas Siefert
U.S. Department of Energy (DOE)/ National Energy Technology Laboratory (NETL)

Jack Simes
U.S. Bureau of Reclamation (USBR)

A.J. Simon
Lawrence Livermore National Lab (LLNL)

Medi Sinaki
Valley Water

Kamalesh Sirkar
New Jersey Institute of Technology

Igor Slowing
U.S. Department of Energy (DOE) Ames Laboratory/Iowa State Universtiy

Brad Smith
BHP

Ben Sparrow
Saltworks Technologies, Inc.

Pete Spicer
ConocoPhillips

Bryan Staley
Environmental Research & Education Foundation

Dean Stanphill
NOVA

Edward Steele
Ambiunt Environmental and Regulatory Consulting

Mihaela Stefan
Trojan Technologies

Ashlynn Stillwell
University of Illinois at Urbana-Champaign

Mark Stoermann
Newtrient

Jean St-Pierre
Unviersity of Hawaii at Manoa/ Hawaii Natural Energy Institute

Matthew Stuber
University of Connecticut

Mengling Stuckman
U.S. Department of Energy (DOE)/ National Energy Technology Laboratory (NETL)

Chinmayee Subban
Pacific Northwest National Lab

Arun Subramani
Chesapeake Energy Corporation

Randal Thomas
LRST-Battelle (National Energy Technology Laboratory (NETL) contractor)

Vincent Tidwell
Sandia National Laboratories

Cliff Tsay
Quick's Net Consulting

Costas Tsouris
Oak Ridge National Laboratory

Jason Turgeon
U.S. Environmental Protection Agency (EPA)

Alan Van Reet
Pioneer Natural Resources

Hendrik Verweij
The Ohio State University

Radisav Vidic
University of Pittsburgh

Edward Von Bargen
Bottom Up Enterprises

NAWI Survey Participants

Nikolay Voutchkov
Water Globe Consultants

Jeff Wall
Eastern Municipal Water District

Hailei Wang
Utah State University

Ben Warden
Diamondback Energy

Briggs White
National Energy Technology Laboratory (NETL)

Clinton Williams
U.S. Department of Agriculture (USDA)—Agricultural Research Service

David Williams
Texas Commission on Environmental Quality

Ronald Wyss
Lake Erie Foundation

Ngai Yin Yip
Columbia University

Yunfeng Zhai
University of Hawaii at Manoa

Nexight Group Roadmapping Team

Beza Bisrat

Ross Brindle

Joan Kohorst

Anand Raghunathan

Morgan Smith

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19. Çağin, V.; Yetiş, U. I., Water Reuse Strategies: Iron and Steel Industry Case Study. In Security of Industrial Water Supply and Management, Dordrecht : Springer Netherlands: 2011; pp 141-158. https://doi.org/10.1007/978-94-007-1805-0_10.

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25. Iverson, Jacob O. "Analysis of Potable Water Use at Yale University." Yale University. May 18, 2010. https://sustainability.yale.edu/sites/default/files/files/research-publications/AnalysisPotableWaterUse_YaleUniversity.pdf.

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