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Advanced Materials, Technologies, and Complex Systems Analyses: Emerging Opportunities to Enhance Urban Water Security

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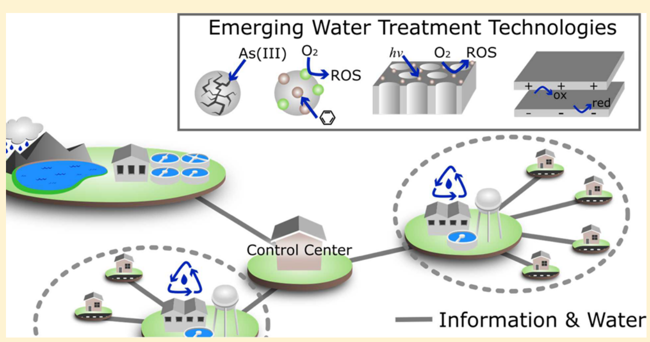
ABSTRACT: Innovation in urban water systems is required to address the increasing demand for clean water due to population growth and aggravated water stress caused by water pollution, aging infrastructure, and climate change. Advances in materials science, modular water treatment technologies, and complex systems analyses, coupled with the drive to minimize the energy and environmental footprints of cities, provide new opportunities to ensure a resilient and safe water supply. We present a vision for enhancing efficiency and resiliency of urban water systems and discuss approaches and research needs for overcoming associated implementation challenges.



INTRODUCTION

Economic and population growth are stressing urban systems worldwide. In many regions, insufficient access to water of suitable quality to meet domestic, thermoelectric, industrial, and landscape irrigation needs may also be aggravated by climate change.[1,2] The growing gap between water demand and supply, exacerbated by water pollution and underinvestment in water infrastructure, has led to a reconsideration of the centralized water treatment and distribution paradigm that is at the heart of many modern water systems.[3,4]

One emerging paradigm for enhancing urban water security involves decentralized treatment and reuse of municipal wastewater and stormwater to supplement the conventional water supply.[5,6] This approach offers several advantages. First, the additional water supply from reclaimed wastewater and/or stormwater, and the distributed locations of the reuse facilities improve water infrastructure resiliency (i.e., the ability to quickly recover from damage or disruption, such as drought or equipment failure). Decentralization generally increases system resiliency because damage of one component (e.g., loss of function of one decentralized treatment facility) would only affect a small number of users. Second, enhanced wastewater and stormwater treatment reduces contaminant discharge into the environment and protects downstream ecosystems. Finally, integrating decentralized treatment and reuse facilities that match the treated water quality to the intended use can enhance the capacity and cost-effectiveness of both existing and future centralized water infrastructure. Such fit-for-purpose treatment facilities would be integrated into an existing urban water network at locations closer to the end users (Figure 1), which would reduce the distance and associated energy requirements to transport water.[7,8] Water supply costs would

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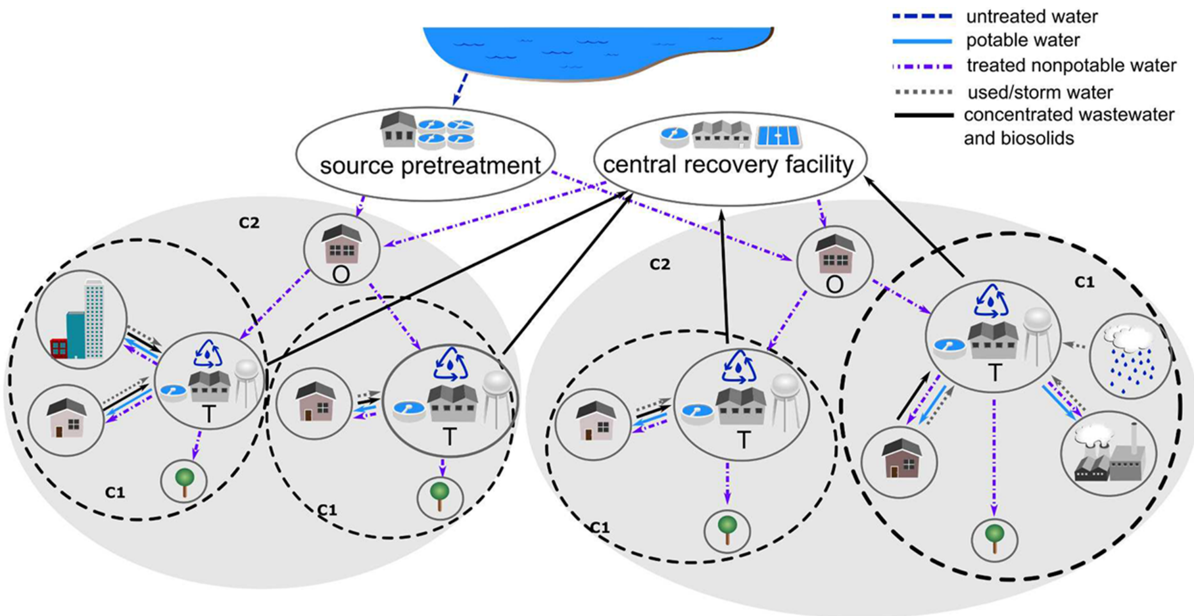

Figure 1. Hierarchical network representation of a hybrid centralized/distributed treatment system. Each distributed treatment and reuse facility ("T") provides water separately for both potable and nonpotable uses. Local operation and distribution centers ("O") oversee these "T" facilities and coordinate distribution of pretreated surface water and collection and transport of concentrated wastewater and biosolids to central recovery facilities. The adaptive-scale model can represent the system at varying resolution. At the finest resolution, all system components are represented as individual nodes, including all end users—commercial users (tall buildings), residential users (houses), and urban greenspace (trees), water sources, centralized and distributed treatment facilities, and operation centers. A lower resolution model may group users and their local treatment facility into one node, shown as level-1 clusters ("C1") in the dashed black circles. Even coarser resolution may be used by grouping several level-1 clusters and their local operation center into one node; for example, level-2 clusters ("C2") represented by the filled gray circles.

also be reduced by avoiding treating water intended for nonpotable use (e.g., landscape irrigation) to potable standards.

However, this approach faces significant technological and institutional challenges, including utilities' risk aversion and potential regulatory, political, and social barriers.[9] Nevertheless, these challenges are now upstaged in many urban areas by the financial burden of maintaining and upgrading aging water infrastructure.[3,8] Furthermore, new advances in materials science, novel treatment processes, and network science[10,11] create opportunities for reexamining and improving the efficiency and resiliency of urban water infrastructure.[3,12]

Hybrid centralized/distributed water systems and fit-for-purpose treatment facilities require comprehensive system design and optimization, and enabling technologies suitable for the widely varying scales and treatment goals of decentralized systems. Potential autonomous operation is also desirable. Innovations in advanced materials, modular treatment processes, sensing and monitoring technologies, multiple-resolution network analysis and design methods, and cyberinfrastructure provide opportunities to redesign, retrofit, and repurpose urban water infrastructure while upgrading performance and capacity. Herein, we discuss how these advances enable the system-level analysis, design, and operation of the hybrid systems, as well as decision-making to select and deploy enabling technologies. We also identify research and innovation opportunities for overcoming associated hurdles.

RESHAPING URBAN WATER MANAGEMENT

Current urban water infrastructure was designed for separate centralized water and wastewater treatment systems. These legacy systems treat freshwater to potable quality prior to distribution for all uses, and collect and treat wastewater for subsequent discharge to receiving waters. They take advantage of economies of scale and are cost-effective given a relatively clean, plentiful water source, a well-maintained distribution network, and large, healthy surface water bodies to receive treated wastewater. However, the existing centralized infrastructure faces high energy demand and water quality deterioration associated with transporting potable water across an extensive, often leaky pipe network, which is exacerbated by insufficient investment in system maintenance and expansion.

Although freshwater scarcity and environmental stewardship have been key drivers for water conservation and reuse,[13] considerations such as pollution mitigation and flood control have become increasingly important in the design of urban water infrastructure.[14,15] In this context, supplementing water supply with locally reclaimed municipal wastewater and stormwater promotes efficient use of urban water resources and reduces reliance on conventional water supplies while minimizing both energy consumption to transport water and downstream contamination by reducing effluent discharge and stormwater runoff. Therefore, future innovations should not only improve treatment technologies to ensure water safety, but also optimize system configuration to enhance overall water and energy efficiency and infrastructure resiliency. Such innovations are necessary because aging water infrastructure threatens public health,[16] and the unreliable supply, high cost of water, or the energy needed to treat and deliver it may significantly hamper economic development and quality of life.[17]

We envision expanding urban areas adopting a fit-for-purpose water treatment and (local) resources recovery and reuse approach that accommodates both centralized and distributed treatment components. Adding distributed facilities at carefully chosen locations could be an economical and practical solution to increasing water demand, especially in

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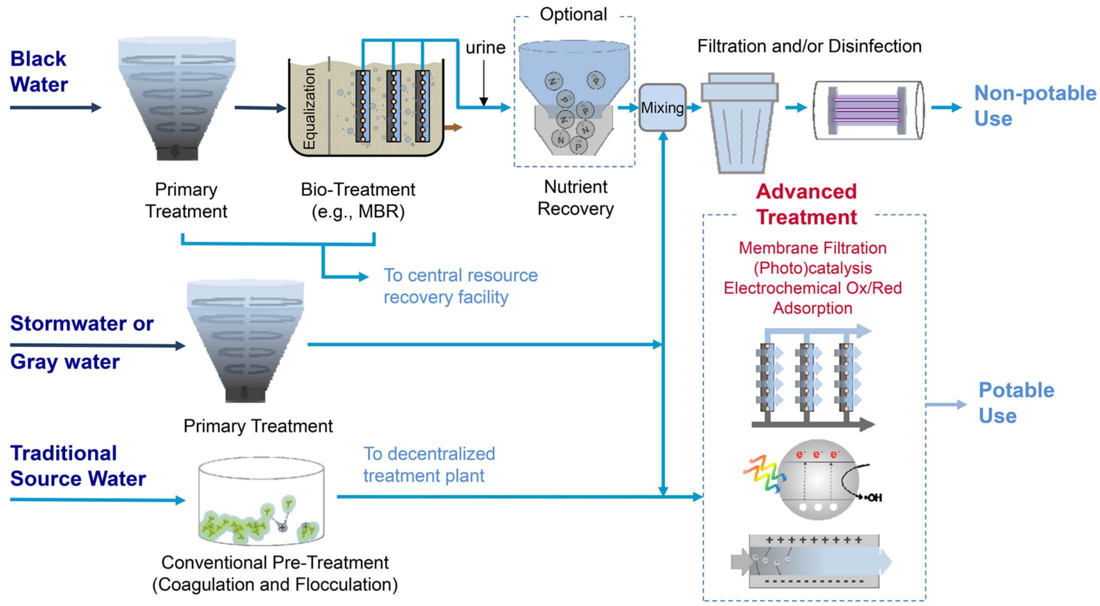

Figure 2. Conceptual modular treatment system at distributed treatment centers. Municipal wastewater effluent supplements traditional fresh water sources and/or pretreated stormwater for nonpotable uses, while traditional fresh water sources are mainly used for potable or ultrapure industrial water supply. The system would utilize the existing stormwater infrastructure (e.g., retention ponds) for harvesting and storage of stormwater.

sprawling urban areas with a number of high demand centers. Hybrid centralized/distributed systems may treat conventional water sources to adequate quality for nonpotable applications in existing centralized facilities using traditional unit processes.[18] This water would be transported to distributed treatment facilities through existing transmission pipelines, where part of it may be mixed with adequately treated wastewater and stormwater from local sources to meet nonpotable water demands through a designated distribution network (Figure 1). The remaining pretreated source water would be further treated by advanced technologies for specific uses like drinking or ultrapure industrial water, in point-of-use (POU) (e.g., faucet scale) or point-of-entry (POE) (e.g., building or small community scale) treatment systems (Figure 2).

Local operation centers would oversee distributed treatment facilities (Figure 1) and coordinate with the centralized facilities to meet fluctuating water needs while considering the availability of local wastewater and stormwater. Wastewater and stormwater would be collected from a small area, treated, and disinfected at the same distributed treatment facility, according to the local nonpotable water requirements. This differs from the current fit-for-purpose treatment approach, where various influent streams are collected and treated by different systems usually at multiple locations, which requires more infrastructure for both treatment and distribution.[19] Additionally, in the proposed scheme, energy and nutrients can be recovered from the wastewater and used to power some distributed treatment systems and fertilize greenspaces, respectively. Alternatively, the concentrated waste streams and biosolids from distributed treatment facilities could be sent to existing centralized sewage treatment plants, which could be retrofitted to recover energy, nutrients, and water.

A key aspect of the envisioned urban water systems is the ability to differentially treat multiple water sources with vastly different qualities and varying flow rates in one system at each distributed treatment facility. For example, a distributed treatment system could receive domestic sewage (potentially separated into black water and urine), stormwater, gray water, and pretreated surface water (Figure 2). These sources would be treated and disinfected according to local water quality needs for potable or nonpotable use. Considering the large difference and temporal variation in flow rates and characteristics of these waters, a modular treatment approach is desirable to provide the needed versatility, flexibility, and adaptability. Different water sources would be introduced into the treatment train at different points, where the feedwater quality matches the effluent quality from the upstream treatment module (Figure 2). A modular approach also facilitates flow reconfiguration, system expansion or downsizing, and inclusion of advanced processes for efficient removal of toxic and recalcitrant contaminants.

Because these systems would be located in urban areas with limited space, they also must be compact. Conventional tank/reactor-based treatment processes (e.g., coagulation/flocculation and sedimentation) are challenged on these fronts. They are not suitable for small systems as they require long hydraulic residence times and hence large reactors, cannot handle large variations in flow rate, and rely heavily on economies of scale. This underscores the need for new technologies to enable distributed fit-for-purpose treatment.

■ ADVANCED MATERIALS AND ENABLING TECHNOLOGIES

We envision compact, modular adsorbent-, membrane-, or electrode-based reactors and catalytic processes as key technologies for fit-for-purpose water treatment and reuse. These technologies can accommodate increases in demand by increasing the number of parallel modules and adapt to changes in source water or desired treated water quality by incorporating appropriate modules (e.g., reverse osmosis, RO, for potable reuse) into the treatment train. Multifunctional materials with enhanced selectivity, efficiency, and reliability, as well as innovative treatment processes that utilize renewable or low-grade energy are critical to meet these needs. These materials and the technologies they enable would enhance the

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cost-effectiveness of water treatment, and are hence relevant to both centralized and distributed treatment systems.

Multifunctional and Selective Adsorbents. Adsorption processes are well suited for removal of priority pollutants that are present at low concentrations and/or cannot be easily converted to innocuous compounds through chemical reactions (e.g., arsenic). Adsorption can also remove viruses, inorganics, and recalcitrant organic pollutants, and recover nutrients from wastewater. It is already widely used in POU and POE treatment devices, including faucet filters and building-scale treatment systems.

Central to the efficiency and longevity of adsorption processes are rapid kinetics, selectivity toward target pollutants in the presence of interfering species (e.g., hardness, silica), high sorption capacity, minimal chemical addition or waste stream generation, and an ability to regenerate the adsorbents (Figure 3A). A major challenge in adsorbent materials

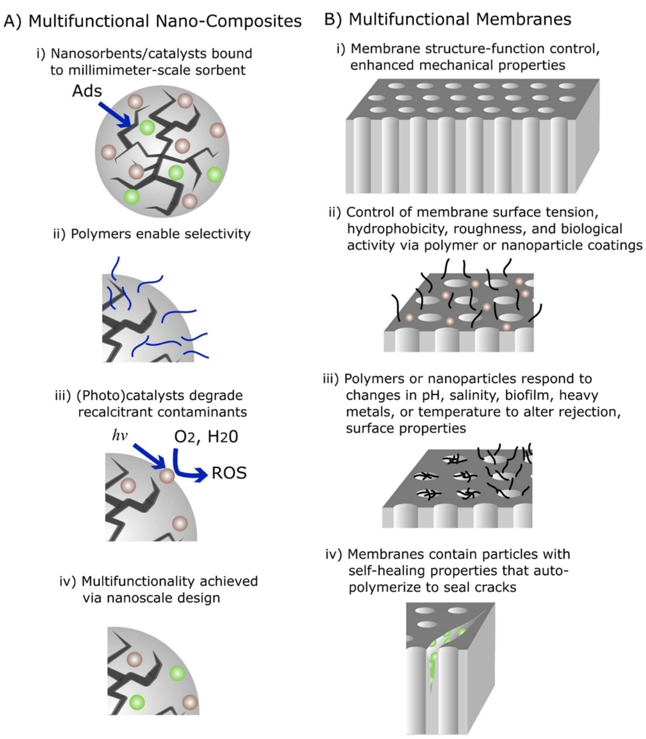

Figure 3. Design of novel enabling water treatment technologies. (A) Multifunctional nanomaterial adsorbents and catalysts covalently bound to larger adsorbent materials and (B) multifunctional membrane-based platforms. (Ads = adsorption; ROS = reactive oxygen species).

development is the trade-off between selectivity and regenerability. High selectivity is achieved through precise control of surface chemistry and—for polymeric sorbents—polymer chain length.[20−22] However, high selectivity can lead to specific, irreversible interactions between target contaminants and reactive surface sites, hindering regeneration. Conversely, lower-selectivity adsorbents (e.g., metal oxides and activated carbon) can be regenerated, but adsorption of target contaminants is susceptible to competing species, such as natural organic matter and silica that are usually present at high concentrations in reclaimed wastewater.[23,24]

Research is needed to develop selective adsorbents with improved regeneration capabilities. One approach involves the use of porous and reactive nanocomposites.[10] These nanocomposite adsorbents could be designed to facilitate in situ regeneration without chemicals (e.g., use of microwaves to superheat carbon nanomaterials and oxidize organic pollutants[25]). Novel adsorbents include aptamer-functionalized, chemo-mechanically modulated, and thermoresponsive materials that trigger adsorption upon interaction with target pollutants.[26−28] Another research need is developing sensors that "self-sense" when the adsorption capacity is depleted (e.g., color changing adsorbents with optical sensors).[29]

Enhanced Membrane Processes. Membranes are well suited for distributed treatment systems due to their compact modular design, high throughput removal of a wide range of contaminants, and their ability to meet multiple water quality objectives such as particle removal, disinfection, softening, and desalination. Several membrane processes—including microfiltration, ultrafiltration, nanofiltration (NF), and RO—are commercially available and capable of removing contaminants of different sizes from bacteria to salt ions. However, existing membrane materials lack sufficient selectivity for target pollutants in water reuse applications. Consequently, removal of low molecular weight, neutrally charged chemical contaminants requires RO membranes, which consume large amounts of energy and produce a concentrated brine that is expensive to manage. Moreover, membrane surfaces are prone to foul by inorganic and organic compounds and biofilms. The maintenance needed to combat membrane fouling and damage caused by cleaning hinders autonomous operation of systems. Consequently, innovation in materials that minimize fouling and improve the selectivity and reliability of membranes is a high research priority, especially for RO membranes. For feedwater with low salt concentrations (e.g., municipal wastewater), further increasing water permeability (i.e., rate of water production per unit membrane area per unit pressure) may offer more benefit in membrane flux than for brackish or seawater desalination.[30,31] However, the higher flux expected from the higher water permeability would also result in more severe fouling and concentration polarization (i.e., accumulation of solutes on the feed side of the membrane surface), which decrease the net driving force and hence the membrane flux. Therefore, development of fouling resistant membrane materials is a greater priority than high permeability membranes.

Advances in bottom-up, molecular-level design and scalable synthesis of membranes provide opportunities to more accurately manipulate membrane pore size/structure, charge, hydrophobicity/oleophobicity and surface morphology[32] to tailor membranes for treatment goals and combat fouling (Figure 3B).[11,33] For example, small molecular building blocks can be used to construct NF membranes with uniform pore sizes and structures for contaminant rejection,[11] while incorporating nanomaterials in polymeric membranes could impart hydrophilicity, biofouling resistance, or photocatalytic activity (Figure 3B).[34−36] Several methods can render the membrane surface or pore wall resistant to organic fouling without significantly changing the manufacturing process or hindering performance.[11,33]

Robust and reliable membrane materials and systems are particularly important for distributed modular treatment systems to accommodate the wide flow rates and hence pressure variation the systems may encounter. Real-time membrane damage detection and self-healing capabilities are important research needs.[37] Smart membrane materials (Figure

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3B) may ensure membrane integrity, reliability, and flexibility in fit-for-purpose systems.

Catalytic and Advanced Oxidation/Reduction Processes. Because transport, storage, and accurate dosing of water treatment chemicals and sludge disposal may be challenging for distributed treatment systems located in areas requiring autonomous operation, processes that minimize chemical consumption and associated sludge generation are particularly attractive. Advanced oxidation processes (AOPs) enable degradation of recalcitrant compounds and inactivation of pathogens by producing reactive oxygen species (ROS), including •OH from in situ ozone production and exposure to UV light, semiconductor photocatalytic processes, or electrochemical processes (Figure 3A).[10,38] Conversely, reductive treatment using hydrogen or cathodic processes[39] can treat oxidized pollutants (e.g., nitrate, chromate, perchlorate, and trichloroethylene) with minimal chemical use. Electrochemical and photocatalytic oxidation or reduction processes are particularly well-suited as a polishing step to remove residual recalcitrant compounds and reduce the need for waste management and chemical delivery.[40−42]

Key research needs include enhancing process selectivity to remove target pollutants, photoreactors that more efficiently deliver light, and mitigating catalyst or electrode fouling by common water constituents such as iron or manganese. Better selectivity could be achieved by enhancing interactions between the target pollutants and the catalyst surface (e.g., electrostatic or hydrophobic attraction), attaching catalysts to selective sorbents or scaffolds, or utilizing permselective barriers (e.g., ion exchange polymer coatings that exclude nontarget ions). Further development of these technologies should utilize inexpensive materials (or small amounts of expensive materials) and consider renewable energy (e.g., from sunlight, photovoltaic devices, or microbial fuel cells) to lower treatment costs.

Harnessing Variable, Low-Grade Energy. Distributed treatment systems should be as energy efficient at their applicable scales as conventional technologies. Although some advanced treatment technologies (e.g., RO and AOPs) require more energy per volume of water treated than conventional treatment processes, they are reserved for a very small fraction of the water supply (e.g., potable reuse).[8,17] Water treatment and transport can benefit from a growing trend of distributed energy production from primarily renewable sources (e.g., solar, wind, and biogas). Increasing renewable energy use and decreasing embedded energy in water systems will lower reliance on grid energy, potentially lessening operation costs and increasing overall system resiliency. This is especially important for regions where grid electricity is not reliable or is susceptible to natural disasters.

Advanced solar technologies, such as photocatalytic, photoluminescent, and photothermal materials that convert sunlight to chemical potential or thermal energy, can be used directly for water treatment,[43−45] reducing electric energy use and reliance on the power grid. Commercial application of these materials, however, requires research that addresses the low quantum efficiency, low light penetration into reactors, large land use for sunlight harvesting, intermittent availability of sunlight, retention and reuse of the photoactive materials, and integration with distributed power systems.

Organic matter in wastewater is an energy source already harvested in some centralized systems.[46] Concentrating organic matter by separating gray and black waters at the source could increase the efficiency of energy capture via anaerobic digestion or microbial fuel cells. Emerging anaerobic treatment technologies such as anaerobic membrane bioreactors can enhance biofuel production.[46,47] Alternatively, microbial fuel cells (MFCs) can directly produce electricity from organic matter in wastewater, avoiding methane as an intermediate.[46,48]

Energy may also be harnessed from low-grade heat in wastewater using emerging thermal energy recovery technologies like the hybrid pressure retarded osmosis-membrane distillation (PRO-MD) process[49] or thermo-osmotic energy conversion (TOEC) process.[50]

Recovering Nutrients. Nutrient recovery could be a means to compensate for the cost associated with treating wastewater and stormwater for reuse. Current regulatory guidelines and practice focus on removing nitrogen (N) and phosphorus (P) from wastewater to prevent eutrophication of receiving water bodies. The main obstacles for economically recovering nutrients from wastewater are low concentrations of N, P, and potassium (K), and large volumes of wastewater. Because 80, 50, and 70% of the total N, P, and K, respectively, in wastewater come from urine, which contributes to ∼1% of the wastewater volume,[51] ongoing research focuses on nutrient recovery from urine streams separated at the toilet.[52,53] Because many trace organic contaminants of emerging concern (e.g., endocrine disrupting compounds, pharmaceuticals, and personal care products) are also concentrated in urine, source separation of urine also provides an opportunity for removing these contaminants from a relatively small volume of wastewater.[54] However, this approach faces multiple implementation challenges in dense urban areas in developed countries, including product collection and formulation for direct application as fertilizer and uncertain market demand in urban locations where local demand for agricultural nutrients is low. Early success is more likely at locations with significant farming at urban outskirts, where local demand for nutrients is high.

Sensing and Monitoring. Cyber-Physical Systems (CPS) are integrations of computation, networking, and physical processes.[55] In our envisioned CPS for urban water supply, sensors and data analytics will operate in near real-time to meet potable and nonpotable water demands from multiple water sources. Multiparameter online water quality monitoring devices, as well as smart water meters that provide near real-time flow measurements to houses, businesses, and industry[56] will be necessary. These monitoring devices exist,[57−60] but capital costs, calibration and maintenance costs, and reliability must improve if they are to be used for stormwater or reclaimed wastewater due to the large number of entry points into the water network. Opportunities and challenges of a data-driven urban water management system were recently reviewed from the viewpoint of runoff and outdoor waterways.[61] Safe, efficient operation of hybrid systems will require secure two-way data access between sensors and utilities and cost-effective monitoring to enable efficient decision making by utilities.

■ COMPLEX SYSTEM ANALYSES

The design and implementation of the proposed hybrid water systems should consider water sources, user locations, temporal and spatial distribution of potable and nonpotable water demand, cost, and availability of suitable treatment technologies. Thus, this design involves interactions across multiple temporal and spatial scales. This represents a complex nonlinear optimization with several, often conflicting, objectives[62] (e.g., system reliability, water safety, energy use, and

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downstream ecosystems health). Modeling such complex systems under multiple physical, operational, regulatory, environmental, technological, and equity constraints remains a challenge, although such models are starting to emerge for analyzing and optimizing urban water systems and broader infrastructure networks.[63−66]

Complex network models represent urban water systems as networks consisting of (1) nodes, including water sources, central and distributed operation centers and treatment facilities, and points of use; (2) pathways of materials (e.g., water and wastewater) and information exchange, such as pipes and communication between treatment facilities, operation centers and users; and (3) transformations (e.g., wastewater treatment and resource recovery) (Figure 1). These network models are much less computationally intensive than conventional hydraulics-based models. Thus, they are suitable for iterative design, technology selection, uncertainty and sensitivity analyses, and CPS data integration.[60,65,67]

Complex network models offer the flexibility to cluster system components (based on geographical location or shared operational time-scales) to create a hierarchy of subnetworks, each with a different scale and resolution. This enables adaptation of the network scale and resolution to generate information at the level of detail necessary to support decision-making (e.g., high-resolution models for short-term operation, and coarse representations for long-term planning), making it computationally feasible to examine the large number of alternative system designs for multiple objectives.

Interdependent and adaptive-scale network models have been used to represent power and transportation systems at different levels of resolution and could be applied to water systems.[65,68] At large scale, they could be used to analyze the overall performance (e.g., demand satisfaction, water quality, and pressure compliance) of alternative water system architectures, providing data for multicriteria decision-making tools[69] to determine the benefits and costs of a system design such as the number, capacity, and location of distributed treatment and reuse facilities as well as number and location of operation centers that oversee subnetworks (Figure 1). At smaller scale, these network models could be coupled with physics-based process models to guide the selection of treatment technologies at the distributed facilities. The benefit of this adaptive-network-scale approach was demonstrated in recent studies using both clustering methods and hydraulic models to study emerging challenges in water distribution networks, including contaminant detection, sensor placements, and system reliability.[70,71]

As more CPS data on system operation and use become available, and interdependencies across infrastructure systems become better understood, continuing advances in hierarchical adaptive network modeling will help balance the multiple objectives of urban water systems through computation supported, systematic planning, design and operation of the proposed hybrid systems.

■ OVERCOMING NON-TECHNICAL HURDLES AND OUTLOOK

Urban water system management is influenced by many nontechnical factors including water pricing and policy. Whereas a policy discussion is beyond our scope, we recognize that significant logistical, legal, and bureaucratic obstacles exist for implementation of the proposed water systems. Furthermore, the price of water might provide incentives or disincentives for such change. There is broad consensus that freshwater is generally undervalued,[72,73] and many have proposed a price differential for water based on its source, quality, and/or use.[74,75] Thus, water from distributed reuse facilities may be discounted or incentivized to encourage freshwater reuse and conservation. Ultimately, these measures may avoid costs associated with new water supply projects.

Overall, the integration of advanced materials and decentralized fit-for-purpose water treatment and reuse technologies—informed by complex systems analyses and modeling—should contribute to a more efficient and resilient urban water supply that minimizes the associated energy and environmental footprints of cities.

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Notes

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