Modular, Adaptive, and Low-Carbon Water Treatment and Desalination

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Abstract
The proposed research will design and develop a novel modular system for simultaneous water treatment and desalination that can adapt to different water/wastewater sources and be treated in a low-carbon process driven by renewable energy such as solar. There is a high demand for decentralized water treatment and desalination technology to satisfy the water needs in rural or remote areas lacking infrastructure or for on-site treatment at point sources. The proposed novel modular system integrates two processes, solar evaporation and electrochemical degradation of contaminants, to produce clean or potable water and treat contaminated water simultaneously. The proposed research will maximize the synergies between the two concurrent processes through numerical simulation and experimental validation. The system is primarily solar powered and thus, has low carbon footprint. The outcome of the research is a systems design that can adapt to different water sources especially unconventional water such as brackish water, seawater, industrial wastewater, and water containing emerging contaminants (e.g., PFAS) by operating at different systems parameters. A prototype of the system will be fabricated and validated. The proposed research addresses two of the TWRI priority areas: (1) innovative strategy of desalination and water reuse and (2) addressing hazardous contaminants including contaminants of emerging concern.

Two proposals are planned to submit to National Science Foundation (NSF):

1. Environmental Engineering Program; Funding level: \$350,000 ~\$450,000 over three years
   Planned submission date: March 2024 (proposal accepted any time throughout the year)
   URL: https://beta.nsf.gov/funding/opportunities/environmental-engineering-1
   Note: This is a regular NSF program that supports research on pollution prevention and remediation. The PI will submit as single PI proposal or collaborate with one co-PI for this opportunity.

2. Environmental Convergence Opportunities in Chemical, Bioengineering, Environmental, and Transport Systems (ECO-CBET); Funding level: \$1,700,000 over four years
   Planned submission date: Preproposal: September 18, 2024; Full proposal: January 31, 2025
   URL: https://beta.nsf.gov/funding/opportunities/environmental-convergence-opportunities-chemical
   Note: This is a special NSF program that supports highly interdisciplinary research that will enable the design of new materials, processes, and systems to address environmental engineering and sustainability problems. The PI will collaborate with two to three co-PIs for this opportunity.

Proposed Research

Statement of critical regional or state water problem

Decentralized water treatment (DWT) is beneficial for small communities, remote locations, or areas where it is not practical or cost-effective to build a large, centralized treatment facility.[1] Common DWT technologies includes membrane filtration, lagoons, coagulation, and aerobic treatments that can remove phosphorus, nitrogen, chemical oxygen demand (COD), and/or suspend solids.[1] However, as the increasing complexity of chemical components found in wastewater and contaminated surface or groundwater, the current DWT processes are unable to meet the growing demand for contaminants removal. The emergence of new pollutants, such as PFAS, bring new challenges to DWT design and operation.[2] Also, it is desirable to reuse the treated water after contaminants removal for various purposes such as irrigation or fracking, especially for water scarce regions like Texas. Furthermore, inadequate access to freshwater is another challenge in the rural areas, poverty areas, and developing regions.[3] Therefore, there is a high demand for cost-effective and sustainable solution to address the water treatment/reuse and clean water production in Texas and southwest regions. Solar evaporation and desalination is an emerging, sustainable technology for clean water production that has attracted increasing amounts of research effort. Compared with conventional desalination technologies such as RO and multistage flash distillation that require high energy input or high-cost infrastructures,[4, 5] solar desalination is less energy- and capital-intensive, providing decentralized and affordable water solutions.[6, 7] It is also worth noting that Texas and southwest regions have abundant solar resources. Solar thermal energy can be used to desalinate water while solar electricity can power electrochemical degradation of water contaminants, another emerging water technology.

Nature, scope and objectives of the research

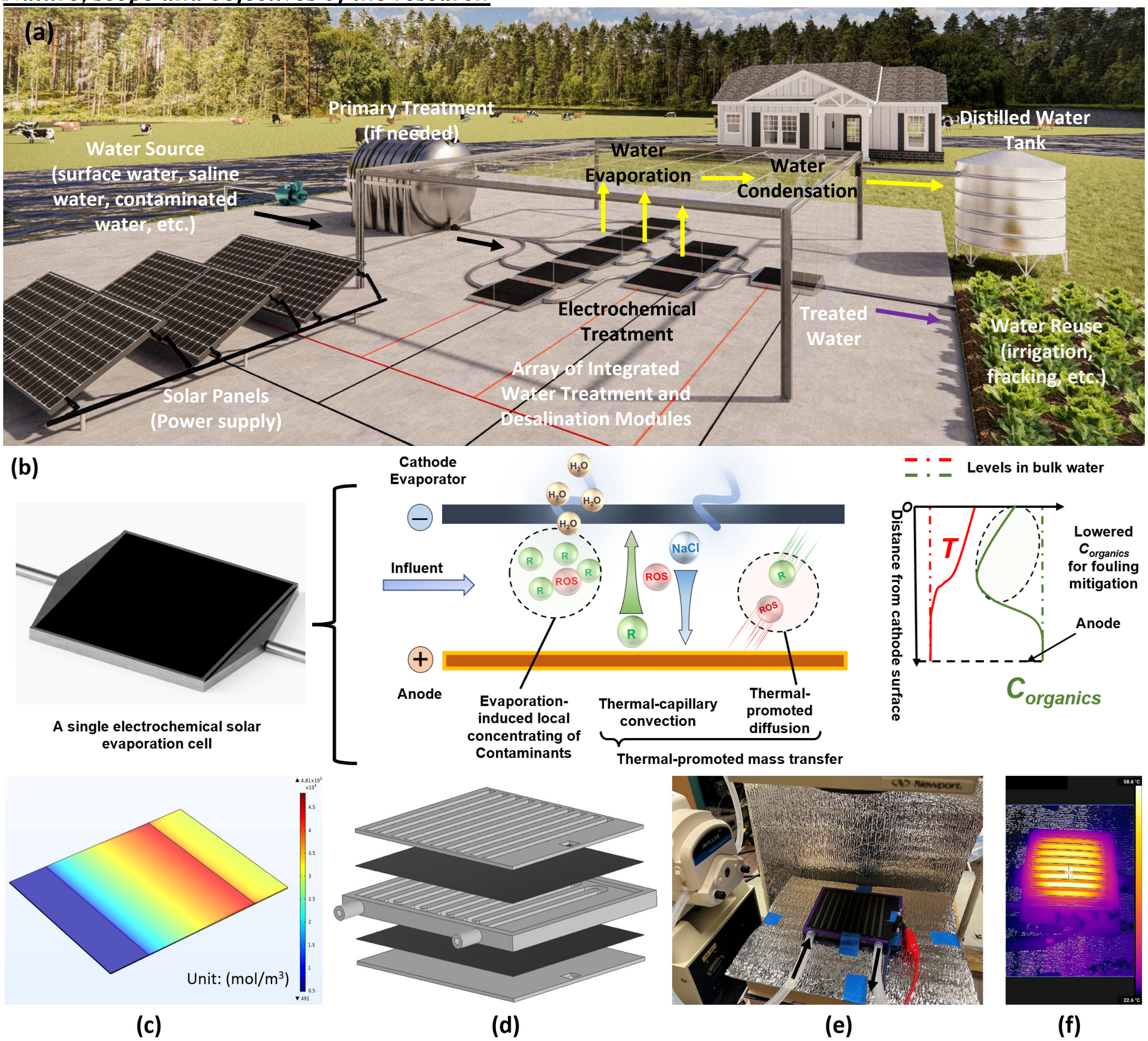

Figure 1. (a) A conceptual illustration of the proposed system and application in rural areas; (b) hypothesized synergies between solar evaporation and electrochemical decontamination. ROS: reactive oxygen species; R: Contaminants; (c) salt concentration distribution by numerical simulation; (d) design of 3D-printed treatment module; (e) laboratory testing apparatus; (f) thermal image of the module under simulated sunlight.

The **objective** of the proposal is to design and validate a modular, adaptive, and low-carbon electrochemical treatment and solar evaporation system as a cost-effective and sustainable DWT technology suitable for rural and remote areas in southwest regions (concept illustrated in **Figure 1a)**. This is a novel system design that integrates treatment and desalination both powered by solar energy. The unique features of the proposed system are as follows. First, it is a **modular** system that can be easily operated in an array or network, depending on the capacity requirement. Second, the system can be **adaptive** to different water sources (contaminated surface water, groundwater, or industrial wastewater with varied type or level of contaminants) by varying the system dimensions and operation parameters (e.g., water flow rate, cell voltage). Finally, it is a **low-carbon** technology because it is driven by solar energy.

In this proposal, fundamental research will be conducted to test the **hypothesis** that synergies exist between electrochemical treatment and solar evaporation **(Figure 1b)**, and as a result, the integrated system is more effective and energy efficient. First, solar evaporation will result in the concentration of water contaminants near the electrodes, enhancing contaminants removal (**Synergy 1**). Second, the photothermal effect (i.e. local heating) will induce higher temperatures near the electrode, favoring electrochemical degradation due to enhanced diffusion and decreased kinematic viscosity of the solution[8, 9] (**Synergy 2**). Meanwhile, the temperature difference between the water near the solar absorber interface and the bulk water initiates thermal-capillary convection,[10] that can not only enhance the mass transfer of water contaminants and reactive species and thereby promote electrochemical removal but also facilitate the diffusion of salt to the bulk water, preventing salt precipitation on the solar absorber[11] (**Synergy 3**). Finally, the electrochemical process will eliminate volatile organic compounds (VOCs) in water, if any, preventing VOCs from migrating to distilled water through solar evaporation (**Synergy 4**). The proposal will also emphasize on the demonstration of the adaptive feature by treating different types of water contaminants (e.g., PFAS, humic acid, BPA). Electrochemical approaches, including anodic oxidation and electrochemical adsorption, have been proved as feasible methods to eliminate PFAS and other refractory organic matters in wastewater.[12-14] The anodic oxidation degrades organics by direct electron transfer or through hydroxyl radicals.[15-20] Electrochemical adsorption is an add-on benefit in which charged contaminants are attracted to and accumulate on the surface of electrodes. It is anticipated that the combined electrochemical adsorption and degradation processes will promote the removal of refractory water pollutants like PFAS.

Methods, procedures and facilities.

A combined numerical simulation and experimental investigation will be pursued. Numerical simulation will study the solar evaporation process (**Figure 1c**), the mass transport of contaminants and salts, and the electrochemical reactions in the modular system under operation conditions. *COMSOL* software will be applied to simulate the system and a few modules will be utilized such as *heat transfer module*, *fluid flow module*, *chemical engineering module*, and others. The simulation results will be used to guide the geometric design and operating parameters of the system to adapt to treatment requirements. A few lab-scale prototypes of continuous water treatment will be fabricated and validated (example shown in **Figure 1e-f**). Results in terms of solar evaporation rate, contaminants degradation rate, and energy efficiency will be obtained. The synergies between solar evaporation and electrochemical treatment will be understood. Assessment of water quality and reuse in agriculture will be conducted. The PI has extensive experience in wastewater treatment,[21-27] oi/water separation,[28, 29] and desalination.[30-32] The PI's lab is equipment with advanced facilities such as TOC, HPLC, FTIR and fabrication platforms that can be used for this research.

Timeline of activities of a 4-yr project *(for 3-yr project the # of contaminants in case studies can be reduced)*

Task	Year 1	Year 2	Year 3	Year 4
Numerical simulation and modular system design	■		■	
Prototype fabrication and experiment preparation	■		■	
Case study: PFAS, humic acid, BPA + solar evaporation	■	■	■	
Mechanistic understanding of synergies and water chemistry		■	■	■
Real water/wastewater testing and reuse assessment in agriculture				■

Statement of expected results or benefits

The expect results from this research include the fundamental understanding of synergies between electrochemical water treatment and solar desalination as well as engineering design and prototyping of a modular, adaptive, low-carbon treatment system. This research will accelerate the development of DWT technologies and benefit Texas and southwest U.S. by addressing critical water treatment and reuse issues.

List of Potential Collaborators and/or Partners

Shankar Chellam, Civil and Environmental Engineering, TAMU: membranes; produced water treatment
Kung-Hui (Bella) Chu, Civil and Environmental Engineering, TAMU: biological wastewater, PFAS
Jake Mowrer, Soil and Crop Sciences, TAMU: soil nutrient and water resource management
Will also seek industrial partners or collaborators, for example, from oil/gas and agriculture sectors

References

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Education

University of Florida, Gainesville, FL, Environmental Engineering Sciences, Ph.D. 2007
Lehigh University, Bethlehem, PA, Mechanical Engineering, M.S. 2004
Zhejiang University, Hangzhou, China, Thermal Engineering, M.E. 2002
Zhejiang University, Hangzhou, China, Thermal Engineering, B.E. 1999

Professional Appointments

- 2020 – present, Professor, J. Mike Walker '66 Department of Mechanical Engineering, Texas A&M University, College Station, TX.
- 2018 – 2020, Director of Graduate Programs, J. Mike Walker '66 Department of Mechanical Engineering, Texas A&M University, College Station, TX.
- 2014 – 2020, Associate Professor, J. Mike Walker '66 Department of Mechanical Engineering, Texas A&M University, College Station, TX.
- 2009 – 2014, Assistant Professor, Mechanical Engineering Department, University of Wisconsin-Milwaukee, Milwaukee, WI.
- 2007 – 2009, Postdoc Researcher, Washington University in St. Louis, St. Louis, MO,

Research Areas

- Solar Energy, Carbon Capture and Utilization, Nanomaterials, Catalysis, Photocatalysis, Electrocatalysis, Energy Storage, Sensors, Wastewater Treatment and Reuse, Desalination, Emissions Control, Aerosol Technology

Selected Honors and Awards

- Fellow, Royal Society of Chemistry, 2022.
- Southeast Conference (SEC) Faculty Travel Award, 2021.
- ACS-PRF New Directions Award, 2017; ACS-PRF Doctoral New Investigator Award, 2011.
- Pioneer Natural Resources Faculty Fellow, Texas A&M University, 2014 – 2023.
- NSF CAREER Award, 2013.

Google Scholar Profile https://scholar.google.com/citations?hl=en&user=85bcOkYAAAAJ
Total Citations > 9400; H-index = 51 (as of January 2023)

Selected Publications Most Closely Related to the Proposal (in water treatment and desalination)

1. Fan, T., Deng, W., Feng, X., Lan, S., Pellessier, J., **Li, Y.*** Integrating solar steam generation with electrochemical with electrocatalysis to achieve simultaneous fouling-resistant desalination and accelerated organics degradation. *Desalination*. **2022**, 532, 115763.
2. Deng, W., Fan, T., **Li, Y.*** Water Wave Vibration-Promoted Solar Evaporation with Super High Productivity, *Nano Energy*, **2022,** 92, 106745.
3. Deng, W. Fan, T., **Li, Y.*** In Situ Biomineralization-Constructed Superhydrophilic and Underwater Superoleophobic PVDF-TiO_2 Membranes for Superior Antifouling Separation of Oil-in-Water Emulsions. *Journal of Membrane Science*, **2021**, 622, 119030.

4. Deng, W., **Li, Y.*** Novel Superhydrophilic Antifouling PVDF-BiOCl Nanocomposite Membranes Fabricated via A Modified Blending-Phase Inversion Method, *Separation and Purification Technology*. **2021**, 254, 117656.
5. Xiang, X., Pan, F., Du, Z., Feng, X., Gao, C., **Li, Y. *** MgAl-layered double hydroxide flower arrays grown on carbon paper for efficient electrochemical sensing of nitrite, *Journal of Electroanalytical Chemistry*. **2019**, 855, 113632.
6. Li, C., Deng, W., Gao, C., Xiang, X., Feng, X., Batchelor, B., **Li, Y. *** Membrane Distillation Coupled with a Novel Two-Stage Pretreatment Process for Petrochemical Wastewater Treatment and Reuse, *Separation and Purification Technology.* **2019**, 224, 23-32.
7. Deng, W., Pan, F., Batchelor, B., Jung, B., Zhang, P., Abdel-Wahab, A., Zhou, H-C, **Li, Y.*** Mesoporous TiO_2-BiOBr Microspheres for Photodegradation of Organic Water Pollutants: Probing Adsorption-Photocatalysis Synergy by Combining Experiments and Kinetic Modeling, *Environmental Science: Water Research & Technology*. **2019**, 5, 769-781.
8. Deng, W., Li, C., Pan, F., **Li, Y. *** Efficient Oil/Water Separation by a Durable Underwater Superoleophobic Mesh Membrane with TiO_2 Coating via Biomineralization, *Separation and Purification Technology*, **2019**, 222, 35-44.
9. Scott, T., Zhao, H., Deng, W., Feng, X., **Li, Y.*** Photocatalytic degradation of phenol in water by an ultrathin MgO coated Ag/TiO_2 nanocomposite, *Chemosphere*, **2019**, 216, 1-8.
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12. Rao, G., **Li, Y.***, Feasibility Study of Flowback/Produced Water Treatment Using Direct-Contact Membrane Distillation, *Desalination and Water Treatment,* **2016**, 57, 21314-21327.

Selected Research Grants (related to water treatment and desalination)

1. Solar-driven Advanced Reduction Processes for Destroying Persistent Contaminants in Water. Qatar National Research Fund, $809,607, 03/16 - 2/19 (co-PI).
2. Nature-inspired solar steam generator design through additive manufacturing, $30,000, Texas A&M Mechanical Engineering Seed Grant, 09/2020 – 08/2021 (co-PI).
3. Nanotechnology Based Selective Heavy Metal and Hydrocarbon Removal from Wastewaters Generated in Energy Production Processes, TEES/TAMUK, $50,000, 02/2016 – 02/2017 (PI).
4. Toward Commercialization of Novel Nanofiber Membranes with Anti-Fouling Ability, UW-Milwaukee Freshwater Science Water Catalyst Grant Program, $120,000, 03/14 - 05/15 (PI).
5. Novel Nanofiber Membrane and Hybrid-Composite Cartridge for Concurrent Filtration and Removal of Multi-Pollutants in Water, NSF Industry/University Cooperative Research Center (I/UCRC) for Water Equipment &Policy, $92,372, 07/12 - 06/14 (PI).
6. Development of a Novel Water Softening Process. A.O. Smith Corporation, $158,899, 09/10 - 08/15 (PI).

Selected Professional Services and Activities

- Co-Editor-in-Chief, *ES Materials and Manufacturing*, 2020 – present
- Co-Editor-in-Chief, *ES Energy and Environment*, 2020 – present
- Associate Editor, *Engineered Science*, 2018 – present
- Editorial Board, *Advanced Composites and Hybrid Materials*, Springer, 2017 – present
- Reviewer for more than 40 international journals
- Organizer, Symposium on Remediation of Wastewater from Energy Usage, at 255th American Chemical Society (ACS) National Meeting, New Orleans, LA, 2018