Sandia National Laboratories Response to Request for Information on lab capabilities relevant to the Solar Desalination Prize

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Purpose

Sandia National Laboratories (Sandia) seeks to inform the American Made Challenge: Solar Desalination Prize Teams on our labs capabilities and expertise that are available to support their submissions to the next phase of the Solar Desalination Prize. We have reviewed the teams that were selected to move to the "Teaming" Phase of the competition and look forward to partnering with the teams to refine their concepts and provide them with technical assistance. Sandia's Energy-Water and Concentrating Solar Technologies programs have various capabilities to support thermal desalination technologies. These technologies can be used to provide new water supplies through the treatment of non-traditional water sources to ensure the resiliency of the nation's energy-water infrastructure systems. Please feel free to contact us for further information.

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Advising and Providing Subject Matter Expertise

- Expertise in optics and test methods for applying solar flux.

-Performance modeling and evaluation of ZLD systems for power plants.

-Performance modeling and evaluation of membrane distillation and vacuum multi-effect membrane distillation systems.

-Performance modeling and systems improvement recommendations for the use of warm lime softening technologies in the oil and gas industry.

System Design and Materials Selection

Systems Design and Evaluation

-Design, pilot demonstration and performance evaluation of systems for the treatment of cooling tower blowdown water.

-Design, operation and performance evaluation of bench scale and pilot scale demonstrations of produced water treatment.

-Pilot demonstrations utilizing high recovery RO/capacitive deionization on brackish water with concomitant high purity salt recovery

Materials Design and Development

-Atomistic to molecular modeling to inform novel membrane design and performance.

-Development and performance evaluation of novel inorganic and polymeric membranes including graphene oxide membranes, biomimetic membranes and acid-base stable bipolar membranes.

-Design, development and deployment of patented materials for selective ion and contaminant removal from high TDS waters.

Modeling Support for Thermal Solar Systems

- Modeling of systems that include solar thermal collectors.

Solar Collector Material and Coatings Selection

- Design of solar collectors and coating materials for collectors.

Prototyping Capabilities

Building on Sandia's heritage of silicon-based microfabrication of integrated devices and sensors, embodied by the MESA facility, Sandia is rapidly advancing low-cost, solution-based printing routes to integrated electrical, electrochemical and electro-mechanical devices. At Sandia's Advanced Materials Laboratory (AML), materials science, process science and functional prototyping are uniquely integrated to provide a rapid device fabrication development environment. Conductive inks deposited by any printing method vary in composition and may include nanoparticle dispersions as well as molecular precursor inks. As deposited, devices formed from inks often require thermal post-processing to impart useful functionality. The sintering processes are often performed at temperatures that are incompatible with polymer substrates. We develop, in-house, new formulations of molecular and nanoparticle precursors to meet the challenges of low sintering temperatures and fine detail printing. New materials precursors and non-traditional, rapid or flash post-processing methods can yield device structures unobtainable by current technologies.

Sandia's AML is advancing state-of-the-art coating printing technology that greatly increases throughput of printed devices with routes that are adaptable to roll-to-roll manufacturing. These new capabilities include slot-die/flexographic coating and micro-gravure printing that can print/coat multiple, registered layers at overlay precision less than 10 microns and print feature sizes down to two microns, thus greatly improving printed electronics efficiencies. We will explore the use of these new capabilities to develop manufacturing methods for devices amenable for roll-to-roll processing

Our scientists and engineers have contributed to the development of discrete sensors for measurements of pressure, temperature, pH and chemicals (e.g., organophosphates). We have engineered thin and thick film batteries, thermoelectric conversion devices, photonic, and radiation detecting devices using conventional technologies. We seek to demonstrate the additive manufacturing of these devices by combining writeable metals, semiconductors, dielectrics, electrolytes, catalysts and enzymes. Printable bio-immunoassays with electrochemical or optical detection technology are also possible. We wish to explore printing of the devices on a variety of substrates and tailored to needs of customer-specific applications.

Other Expertise Related to Solar-thermal Desalination

High Flux On-Sun and Off-Sun Testing

The National Solar Thermal Test Facility (NSTTF) has the capability to perform high-flux solar testing in a controlled environment. The Solar Furnace provides up to 16kW optical/thermal power with a peak flux of 6000 kW/m^2 with controllable solar input. The solar furnace concentrates sunlight from a 120 m² heliostat into a stationary parabolic dish. An adjustable test platform moves the target into the focal point of approximately 5 cm (3 in) can be developed to accommodate a wide variety of test specimens and set-up configurations. The solar furnace is configured with open channels to handle up to 32 thermocouples, 12 analog input and output channels of analog voltage and current, high-speed/high-resolution video cameras with light filtering, and developing gas and particulate capture techniques for material analysis.

The solar tower provides up to 6.2 MW of optical/thermal power with up to 3500 suns of peak concentration. Unlike the solar furnace with a fixed focal point, the solar field can provide temporal and spatial flux profile control. The solar tower has extensive bandwidth for data streaming. High-speed shutters, wind tunnels, and mechanical fixtures are available.

The High-Flux Solar Simulator with Automated Sample Handling and Exposure System (ASHES) is an off-sun tester which uses halogen lamps to provide up to 1.3 MW/m² peak irradiance over a 2.54 cm diameter spot size. ASHES is programmable with a robotic sample holder that can provide multi-sample testing 24/7.

Oak Ridge National Laboratory (Yarom Polsky)

Please find below a number of brief descriptions of ORNL capabilities that could potentially assist Prize contestants.

- Prototyping of parts using Additive Manufacturing
- Prototyping capabilities for thermal desalination technologies
- Desalination equipment and system characterization (evaporator, condenser, humidifiers, dehumidifiers, crystallizers)
- System integration approaches (standalone/hybrid systems)
- Waste heat recovery systems for desalination
- Solar desalination simulator (1000-1500 X solar irradiation)
- HPC simulation of fluid flow, heat transfer and reactive transport for evaporative desalination systems
 - Fundamental thermodynamics and process modeling
 - Modeling high pressure and temperature boiling systems (unique methods and codes validated up to 15 MPa).
- Expertise related to UF, NF, RO membrane selection, implementation and characterization
- Material selection and characterization:
 - Surface characterization/material selection (hydrophobic, anti-fouling/ anti-scaling)
 - In situ microscale/nanoscale characterization of desalination system material surfaces using neutron scattering techniques (to enable in situ characterization)
 - High temp materials for CSP
 - Molten salt expertise for CSP
 - Molten salt test loop for CSP

National Renewable Energy Lab (Sam Gage)

I would be able to offer materials selection and testing expertise. As an experimentalist, I could provide high temperature and corrosion testing of materials and system components. In addition this may be coupled with materials characterization and failure analysis. The SIMPA facility at NREL's mesa top laboratory is equipped to handle an on-sun demonstration of a prototype concentrator, which could be made available to prize winners.

My colleagues at NREL could offer different expertise including analysis of manufacturing costs, market potential, and thermal efficiency (Contacts: Parthiv Kurup and Chad Augustine), as well as optical properties characterization (Contact: Guangdong Zhu).

×	s Response to American-Made Solar Desalination Prize
Category	Solar thermal-driven desalination
Capability	Photothermal materials for solar steam generation
Laboratory	Argonne National Laboratory
Capability experts	Seth Darling (<u>darling@anl.gov</u>)
Description	Darling's group has developed a suite of materials that meet the design criteria and collectively offer flexibility in material choice when implementing a solar steam generation system. For example, carbon-based materials can be very effective at localizing thermal energy at the evaporation interface. The water evaporation rate is more than <i>doubled</i> relative to water without a photothermal material. Another set of photothermal materials is based on ferric tannate complexes, which can absorb nearly 100% of incoming solar photons across visible and near-infrared regions and can be readily coated onto many different supports. Among the simplest options developed to date from a potential manufacturing standpoint, porphyrin organic frameworks (POFs) can be synthesized directly on porous substrates in a single step. The POF-based photothermal materials have been successfully demonstrated to deliver ~80% <i>light-to-steam conversion efficiency</i> .
Citations/references	 HC. Yang, Z. Chen, Y. Xie, J. Wang, J. W. Elam, W. Li, and S. B. Darling. Chinese ink: A powerful photothermal material for solar steam generation. <i>Advanced Materials Interfaces</i> 6, 1801252 (2019). C. Zhang, Z. W. Chen, Z. J. Xia, R. Z. Waldman, S. L. Wu, H. C. Yang, and S. B. Darling. Ferric tannate photothermal material for efficient water distillation. <i>Environ. SciWat.</i> <i>Res. Technol.</i> 6, 911 (2020). Z. X. Wang, M. C. Han, F. He, S. Q. Peng, S. B. Darling, and Y. X. Li. Versatile coating with multifunctional performance for solar steam generation. <i>Nano Energy</i> 74, 11 (2020). Z. J. Xia, H. C. Yang, R. Z. Waldman, S. N. Patel, and S. B. Darling et al. Porphyrin covalent organic framework (POF)- based interface engineering for solar steam generation. <i>Advanced Materials Interfaces</i> 6, 6 (2019).
Category	Produced water (primarily from oil and gas operations) desalination
Capability	Materials for fouling prevention/mitigation
Laboratory	Argonne National Laboratory

Capability experts	Seth Darling (<u>darling@anl.gov</u>) and Jeff Elam (<u>jelam@anl.gov</u>)
Description	Argonne has created membranes that degrade foulants and organic pollutants when exposed to light, including sunlight. ALD was used to deposit onto a hydrophobic membrane a thin, conformal layer of hydrophilic TiO ₂ doped with nitrogen; SIS can also be used. The nitrogen dopant shifts the optical absorption of TiO ₂ from UV into the visible wavelengths => photocatalytic activity can be activated by sunlight.
Citations/references	 U.S. Patent Application 15/002,102, filed January 20, 2016 Lee et al., <i>Adv. Sust. Syst.</i> 1 (1–2), 1600041 (2017).
Category	Brackish/groundwater desalination
Capability	Resin wafer electrodeionization
Laboratory	Argonne National Laboratory
Capability experts	YuPo Lin (<u>yplin@anl.gov</u>)
Description	Electrodeionization (EDI) is a commercial technology to produce ultra-pure water for the semiconductor and pharmaceutical industries. It contains ion-exchange resin beads as an adsorbent to capture very dilute ions from water and electrochemically extract the ions into a separate ions brine. An innovative re-engineered material created by Argonne, resin wafer (RW), immobilizes ion-exchange resin beads inside the EDI into a porous structure. RW-EDI enables a low-maintenance and robust water treatment technology that can be applied to develop cost-effective industrial applications by tuning or adding new adsorbents of the RW material. Large-scale, field operation of RW-EDI applications on chemical, biorefinery, and produced water separation have been demonstrated, as has reduction of processing cost (>50%) by replacing ion-exchange column technology in a biorefinery. Our TRL 6-8 technology platform can be leveraged to investigate adsorption performance and assess technical and economic viability of innovative adsorbents at low TRL under continuous operation.

Citations/references	 A platform technology for separations and reactions that won 2002 & 2006 R&D 100 Award Synder, S., et al., 2003. Advanced Electrodeionization Technology for Product Purification, Waste Recovery, and Water Recycling, AICHE, 2003 Spring annual meeting, New Orleans, Louisiana. Lin, Y.J., Hestekin, J.A., Sather, N., 2016. Bioprocessing of Cost-Competitive Biobased Organic Acids, in <i>Commercializing Biobased Products: Opportunities, Challenges, Benefits, and Risks, The Royal Society of Chemistry</i>, Green Chemistry series No. 43, Chapter 9.
Category	System design and materials selection
Capability	Life-cycle analysis (LCA); water impact analysis
Laboratory	Argonne National Laboratory
Capability experts	Hui Xu (<u>hui.xu@anl.gov</u>), Troy Hawkins (<u>thawkins@anl.gov</u>)
Description	Life-cycle analysis (LCA) explores key sustainability metrics critical to ensure that an underlying integrated process will be an environmentally-beneficial design, which is the desired outcome when pursuing innovative solar desalination technologies. The Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET®) model can be used to quantify the life cycle emissions, energy use, and water consumption for technologies considered in Solar Desalination Prize. Also, the effects of water use and savings are spatially dependent. Argonne's AWARE-US life cycle water-stress impact assessment method can help with benchmark new technology against existing systems and quantify water-stress benefits of desalination across regions.
Unique aspects	The GREET model provides an objective, rigorous, and consistent transparent platform for life cycle analysis of conventional and alternative technologies, based on publicly-available datasets. It includes pathways for energy, materials, and chemical inputs required along the supply chains. GREET is publicly available and free of charge since its original release in 1995. The model is regularly updated and expanded with new versions released on an annual basis. Through collaboration with industrial and academic partners, a new module dedicated to LCA of desalination and wastewater treatment technologies is being added to GREET, as part of a US-Israel consortium called the Collaborative Water-Energy Research Center (CoWERC). Users of GREET are able to leverage datasets built up through years of its development through DOE

	 sponsorship. GREET allows life cycle analyses to be performed consistently across DOE technology areas supporting fair, apples-to-apples comparisons. AWARE-US supports seasonal, location-specific water stress impact characterization by month and by county. It can quantify how utilization of unconventional water resources may help address water-stress issues, reflecting both regional and seasonal variations in water supply and demand across conterminous United States.
Availability	The analysis team is available for consultation with industry and academic partners.
Citations/references	Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) model. (<u>https://greet.es.anl.gov</u>) Available Water Remaining for the United States (AWARE-US) Model. (<u>https://greet.es.anl.gov/aware</u>)
Category	Prototyping capabilities
Capability	Process engineering and scale-up associated with the Materials Engineering Research Facility (MERF)
Laboratory	Argonne National Laboratory
Capability experts	Greg Krumdick (<u>gkrumdick@anl.gov</u>), Krzysztof Pupek (<u>kpupek@anl.gov</u>)
Description	The MERF is an integral part of the laboratory's Manufacturing Science and Engineering program. The MERF's capabilities include:
	 Development of analytical methods and quality control procedures for new material specifications Scale-up of the manufacturing processes for newly discovered materials and chemicals Analysis and refinement of processes for materials and chemicals synthesis Providing kilogram quantities of novel materials to industry for testing Evaluation of emerging manufacturing technologies Workforce development on process R&D, scale up,
	 advanced characterization, modeling and simulation, and advanced materials manufacturing The MERF is open to outside organizations, including other national laboratories, universities and industry for process R&D and scale-up of new materials and validation of emerging manufacturing processes. By bridging the gap between small-scale laboratory research and high-volume manufacturing, research at the MERF

	promotes the development, de-riskng, validation and ultimate commercialization of advanced materials and chemistries.
Citations/references	https://www.anl.gov/amd/materials-engineering-research-facility