

Responding to the Water-Energy Nexus Challenge: NETL's Comprehensive, Integrated Research & Development (R&D) Program

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Abstract

The Department of Energy/Office of Fossil Energy's National Energy Technology Laboratory has long recognized the critical link between sustainable water and energy. Since 2002, NETL has been engaged in integrated, comprehensive research and development (R&D) to advance our understanding of fossil energy exploration, extraction, development, and use on freshwater availability and quality with the goal of improving the security and resiliency of our fossil-energy investments. Research on water is being carried out in a synergistic manner across the Lab's programs in thermoelectric power generation, oil and gas development, carbon capture and storage, value product recovery, coal combustion products, university coal research, life cycle analysis, and systems modeling and analysis. More recently NETL is now part of the DOE's National Alliance for Water Innovation Desalination Hub that is directed at advancing technologies and processes to achieve "pipe parity" in the treatment and utilization of saline and other non-traditional water sources. Future activities may include the application of machine learning and artificial intelligence to critical water-energy challenges. Collectively, these projects support the DOE's Water Security Grand Challenge, a White House initiated, DOE-led effort to advance transformational technology and innovation to meet the global need for safe, secure, and affordable water. This paper presents a summary of NETL's water-energy research projects and related activities.

Introduction

Only 2.5% of the world's water is fresh. Of that freshwater, over 98% is tied up in glacier and polar ice, locked deep underground, or contaminated and not suitable for use. That leaves a little more than 1% available for human consumptionⁱ. About two thirds of freshwater comes from surface sources (lakes, rivers) with groundwater providing roughly a third of supply. Over 7.7 billion people worldwide are dependent upon this limited resource for drinking, bathing, and other basic

human needs. According to United Nations, about 1.9 billion people live in severely water-scare areas and nearly 2.1 billion people lack access to safe drinking water services. It has been suggested that almost one in four countries have extremely high ratio of withdrawal to supply including much of the Middle East, Central Asia, and Indiaⁱⁱ. Further, the U.N. reports that global demand for water has been increasing at a rate of about 1 % per year over the past decade and is projected to continue to grow due to increasing population, economic

development, and changing consumptive patternsⁱⁱⁱ.

While agriculture is the largest use sector for water, representing about 70% of freshwater demand, the U.N. expects industrial use to see a significant demand growth globally, particularly in countries with developing or emerging economies such as China and other Asian and African countries. Water use for industry accounts for roughly 20% of total global demand and is dominated by energy production and electricity generation.

Throughout the world, water is essential to virtually all phases of energy production. From the mining of coal and uranium and the drilling for oil and gas to the upgrading, processing and transport of fuels to the generation of electricity and the control and management of power plant emissions including carbon dioxide. According to the International Energy Agency's World Energy Outlook (2018) the energy sector accounts for roughly 10% of global water withdrawals and about 3% of worldwide water consumption mainly for cooling of thermoelectric power plants^{iv}. It is expected that water withdrawals for the energy sector will rise by nearly 2% to reach over 400 billion cubic meters (about 106 trillion gallons) by 2040. However, the amount of water consumed increases by almost 60% to over 75 billion cubic meters (19.8 trillion gallons) during that same period. This is due in part to the deployment of additional recirculating cooling technology that withdraws less water but consumes more¹. Further, an increase in biofuels demand pushes up water use and greater deployment of

¹ *Water withdrawal* refers to water removed from the ground or diverted from a surface water source

nuclear power increases both withdrawal and consumption levels.

Global challenges to adequate supplies of water for energy are both natural and man-made. Shifting climate or altered precipitation patterns can create or exacerbate periods of excessive heat and drought. Over the past several summers this has led to the temporary shutdown of nuclear reactors in France^v and Spain^{vi} due to exceedance in cooling water discharge temperatures and the disruption of barge transport of oil in Germany to power stations because of low river levels^{vii}. Competing demands for water from other use sectors such as domestic and agricultural can also limit the water available for primary energy and power generation. Geographical disparities within countries between water supply and demand centers can also create water chokepoints. For example, three quarters of China's renewable water resources are in the south, but two of its largest water use sectors – agriculture and coal mining – are primarily located in northern China^{viii}. Considering this, water scarcity could become a constraining factor for coal development in China^{ix}. Finally, regulatory policies can preclude access for certain use sectors to water that is otherwise available or prevent or make it technically or economically prohibitive to withdraw or discharge water.

Water and energy are reciprocally linked. Not only is water critical in energy production, energy – especially electricity -- is needed to source, extract, treat, pump, and distribute water. Water is extremely heavy at 8.35 pounds per gallon, so it

for use. *Water consumption* is the fraction of the water withdrawn that is not returned to the source.

requires a significant amount of energy to lift. As population grows in water deficient regions such as the arid western U.S., conveying water to those locations and treating it to drinking water quality becomes more energy intensive. In 2002, the Electric Power Research Institute (EPRI) estimated that nearly 4 percent of U.S. electricity goes towards water treatment and conveyance^x. A 2009 study by the University of Texas estimated that energy associated with public water supply is 6.1 percent of national electricity consumption^{xi}. From an economic perspective, the 2002 EPRI study suggests that 80 percent of the cost of treating and distributing potable water is for electricity, while a 2017 Congressional Research Service states that energy represents the second highest budget item for drinking water and wastewater treatment facilities in the U.S. after labor costs^{xii}.

Water-for-Energy Nexus in the United States

In the United States there are many water-energy challenges that are complicated by factors such as population growth in water deficient regions, shifting precipitation patterns, and competing demands for water. The siting of new thermoelectric power plants and the continued operation of existing plants must address multiple water-related issues including securing adequate water supply, particularly in regions where there are constraints on the availability of fresh water like the arid west and southwest. According to the U.S. Geological Survey (USGS), in 2015 thermoelectric power generation accounted for 34 percent or about 96 billion gallons per day of the total of 281 billion gallons of fresh water withdrawn daily^{xiii}.

This water was used primarily for cooling the nation's fossil-energy and nuclear power plants. In places where freshwater is not available, thermoelectric power plants have turned to alternative sources of water. For example, the Palo Verde Nuclear Generating Station in Phoenix, Arizona receives its cooling water from a local wastewater treatment plant. In another example, the Exelon Limerick Nuclear Plant in Limerick, Pennsylvania has used mine water from a flooded anthracite mine to supplement water drawn from the Schuylkill River to cool its reactors. In addition to the Limerick station, several small coal-based power plants in northeastern Pennsylvania have used mine water as makeup water for cooling^{xiv}.

While power plants were responsible for the second largest withdrawal of freshwater after irrigation, they consume only about 3 percent of the water they withdrawal. It is also interesting to note that withdrawals for thermoelectric power were at the lowest level for this sector since 1970^{ix}. This is likely attributed to two main factors. First, a significant percentage of coal-based power plants, many of them older, less efficient plants equipped with once-through cooling have been retired over the past decade. Since its peak in 2005, coal-based electricity generation had decreased by 40 percent in 2017^{xv}. Second, much of the retired coal capacity has been replaced with more efficient natural gas generation units that require less water to operate and employ recirculating cooling systems and, in some cases, dry cooling.

From a regulatory standpoint power plants are faced with a myriad of Federal, state, and local water-related requirements. Thermoelectric generation – from coal, oil,

natural gas, and nuclear – must comply with the Clean Water Act’s 316(a) and 316(b) provisions that regulate the discharge and intake of cooling water, respectively^{xvi}. State and local regulations can also restrict the intake of cooling water even when there are adequate supplies available, particularly in western and southeastern states where power plants often must compete for limited freshwater supplies with other water-use sectors including agriculture, domestic, and industry. In addition, the U.S. Environmental Protection Agency (EPA) promulgated revised effluent guidelines and standards for steam electric power generating units in 2019 that impact how flue gas desulfurization (FGD) wastewater and bottom ash transport water are treated and discharged^{xvii}. EPA is also in the process of revising rules governing the safe management and disposal of coal combustion residuals (CCR) such as fly ash to prevent impacts to ground and surface waters^{xviii}. The permitting, construction, and operation of coal-based power generation will need to comply with these as well as future water-oriented regulations and requirements.

Substantial volumes of water are also used in oil and gas exploration and production in the U.S., particularly for unconventional supplies such as shale gas. Hydraulic fracturing represents the most common unconventional oil and gas extraction technology in use today. This technology is very water intensive. However, the USGS *Estimated Use of Water in the United States in 2015* report referenced above does not account for unconventional oil and gas water use separately but rather includes it as a component of mining water use. The report estimates that the mining industry (including oil and gas) accounted for less

than 1 percent of total U.S. water withdrawals (both fresh and saline) in 2015, of which about 47 percent or about 1.8 billion gallons per day was from a freshwater source^{ix}. Groundwater supplied almost fifty-four percent of the freshwater withdrawals for the mining sector. While representing a relatively small fraction of freshwater withdrawals on a national level, oil and gas development often occurs in water-scarce regions such as Texas, New Mexico, Wyoming, Oklahoma, and California.

Recognizing that hydraulic fracturing is a water-intensive process that can be particularly challenging in water-stressed states, the USGS has initiated the Oil and Gas Waters Project to provide more detailed information on the volume, quality, impacts, and possible uses of water produced during generation and development of energy resources, particularly hydrocarbons^{xix}. As part of this effort it estimates that between 2000 and 2014 nearly 264,000 oil and gas wells were hydraulically fractured in the U.S. and each well used an annual average of about 4 million and 5.1 million gallons of water respectively^{xx}. Further, the study shows that the amount of water injected per well for hydraulic fracturing varies across the United States depending upon distinctions in well borehole configuration, hydrocarbon type, target oil or gas reservoir characteristics, and the completion year of the well. Therefore, the USGS notes that assumptions and generalizations regarding water use in hydraulic fracturing operations should be made with caution.

Oil and gas wells also produce large volumes of water along with hydrocarbons. This water is commonly referred to as

“produced water” (PW) and can contain elevated concentrations of dissolved salt, petroleum and other organic compounds, suspended solids, trace elements, bacteria, naturally occurring radioactive materials, and anything injected into the well^{xxi}. It has been estimated that each day approximately two billion gallons of water are produced during oil and natural gas production operations that must be treated for reuse or disposed of via injection into deep disposal wells in oil and gas producing regions^{xxii}. Over the past decade, the increase in hydraulic fracturing in the U.S. has led to a dramatic increase in the volumes of PW requiring treatment and disposal, particularly in Texas, Oklahoma, and Appalachia.

The production of coal can also have direct impacts on water quality. Acid mine drainage (AMD) from both active and legacy coal mining activities remains a serious water issue for Appalachian and other hard rock and coal mining areas of the United States with thousands of miles of streams impacted in the mid-Atlantic region alone. AMD is the formation and movement of highly acidic water rich in metals. This acidic water forms through the chemical reaction of surface water (rainwater, snowmelt, stream water) and shallow subsurface water with coal that contains sulfur-bearing minerals such as pyritic sulfur, resulting in sulfuric acid. Metals and other elements such as rare earth elements can be leached from rocks and mineral matter associated with coal that contact the acid^{xxiii}. The resulting AMD if untreated can have harmful effects on drinking water, aquatic organisms, and infrastructure such as bridges^{xxiv}. Considerable Federal and state resources continue to be directed at the

control and remediation of AMD and impacted waterways.

NETL is carrying out an integrated R&D program to provide science and technology solutions to many of the water-energy challenges described above.

A Long History of Water-Energy R&D

The Department of Energy’s National Energy Technology Laboratory (NETL) has been carrying out a comprehensive, integrated R&D program directed at nexus between water and energy for nearly two decades^{xxv, xxvi}. Recognizing the intimate link between water and energy, NETL sponsored the first public workshop on electric utilities and water in July 2002. The issues and research needs identified and discussed at this workshop served as the starting point for the Laboratory’s water-for-energy R&D initiative within the Innovations for Existing Plants (IEP) Program. The initial focus of NETL’s water-energy program was on water-related issues impacting the resiliency of the existing fleet of coal-fired boilers including advanced cooling systems, advanced water treatment technologies, water recovery and reuse, and use of non-traditional waters such as mine water, treated wastewater, and brackish water for plant operations^{xxvii}.

Additionally, the Lab conducted research in the late 1990s to mid-2000 directed at the potential environmental impacts of coal combustion products (e.g., fly ash, FGD materials) on the environment including ground and surface water quality^{xxviii}, with a focus on the fate of mercury in fly ash and FGD solids^{xxix}. Also, NETL adsorbed much of the former Bureau of Mines expertise in active and passive AMD treatment when the agency closed in 1996^{xxx}. This expertise

is now being applied to the Lab's efforts in the recovery of value products from mine drainage.

Today, NETL's water program has expanded to include the Lab's water efforts in oil and gas development, carbon capture and storage, modelling and systems analysis, coal combustion byproducts utilization and management, life cycle analysis, and recovery of valued products from coal residuals such as rare earth elements (REE). Most recently, NETL is now part of the DOE's National Alliance for Water Innovation Desalination Hub that is directed at advancing technologies and processes to achieve "pipe parity" in the treatment and utilization of saline and other non-traditional water sources.

With its focus on enabling the discovery, development, and deployment of early-stage technology solutions that enhance the nation's energy foundation and protect the environment for future generations, NETL is well situated to lead an integrated research program directed at advancing our understanding of the critical link between water and fossil energy. Leveraging its core capabilities, competencies, and authorities, NETL partners with DOE's other national laboratories, academia, non-government organizations, and industry, to develop and bring to commercial readiness the technology needed to continue the environmentally sound and sustainable use of our domestic fossil energy resources.

NETL has established a robust portfolio of both intramural (in-house) and extramural water-related research projects and initiatives needed to ensure the environmentally sound and sustainable use of our fossil energy resources essential to

support increased domestic manufacturing, improve infrastructure, enhance global competitiveness, revitalize the workforce, and free the United States from dependence on foreign oil. Today, NETL has more than 45 active projects valued at over \$100 million dedicated to research directed at water and energy.

Below is a summary of water-energy projects and activities being carried out by NETL across its thermoelectric generation, oil and gas development, carbon capture and storage, value product recovery, university coal research, desalination Hub, and systems modeling and analysis programs. Collectively, these projects support the DOE's Water Security Grand Challenge, a White House initiated, DOE-led effort to advance transformational technology and innovation to meet the global need for safe, secure, and affordable water.

Thermoelectric Power Generation Water R&D

The International Energy Agency describes water use by coal-fired thermoelectric power plants as a critical global issue within the water-energy nexus^{xxxi}. NETL's thermoelectric power generation water research was started in 2002 under the IEP Program and is now currently managed out of the Lab's Crosscutting and Advanced Energy System Programs. These programs are directed at both water availability and water quality issues impacting thermoelectric power generation taking into consideration plant capital costs, operating costs, and system integration. More specifically, research is focused in three primary areas: (1) increase power plant water-use efficiency through advances in cooling technology and

condenser performance and advanced sensors and controls; (2) treatment of plant effluents and reuse of alternative (non-traditional) sources of water; and (3) modeling and analysis of water-energy systems. In addition, the Crosscutting Program manages the Lab's University Coal Research (UCR) water-related projects that include research on managing effluents from coal combustion residuals such as fly ash. The UCR program is designed to increase the competitiveness of universities in fossil energy research and discoveries^{xxxii}.

The results of the water-related research focused on the existing fleet of coal-based power systems carried out under NETL's IEP program have been highlighted in several papers.^{xxxiii, xxxiv} The following are summary-level descriptions of the current water-energy research managed under the Crosscutting Program^{xxxv}.

- *Water Treatment and Water-Vapor Recovery Using Advanced Thermally Robust Membranes.* Los Alamos National Laboratory is developing a thermally robust membrane separation technology for use in challenging corrosive flue gas and high-salinity brine environments for clean water production.
- *Development of a High-Efficiency Membrane-Based Wastewater Management System for Thermal Power Plants.* SRI International is developing innovative effluent water management practices at coal-fired energy plants using polybenzimidazole hollow-fiber membrane technology for removing selenium from FGD wastewater.
- *Flue Gas Desulfurization Wastewater Treatment, Recovery, and Reuse.* The University of New Mexico is developing a computer model of both the unit processes and overall treatment system to concentrate divalent ions from high salinity FGD wastewater of varying chemistry and precipitate gypsum and magnesium hydroxide from concentrated ion-exchange brines.
- *Energy Efficient Waste Heat Coupled Forward Osmosis for Effluent Water Management at Coal-Fired Power Plants.* The University of Illinois will evaluate a transformational low waste heat coupled forward osmosis-based water treatment system called Aquapod© to recover at least 50 percent of the water from highly degraded water sources without extensive pretreatment in a cost-effective manner.
- *Intensified Flue Gas Desulfurization Water Treatment for Reuse, Solidification, and Discharge.* The University of Kentucky Research Foundation is developing a novel electrocoagulation coupled with air-dissolved flotation and nanofiltration process to treat and reuse FGD scrubbing effluents.
- *Integrated Sensors for Water Quality.* Sporian Microsystems is developing an integrated water sensor package that is low-cost, rapidly deployable, wireless, and self-powered and can relay real time relevant in-situ water measurements.

- *Water Atlas Extension.* Sandia National Laboratory will update its Water Atlas to include: (1) water data for Alaska and Hawaii; (2) data on power plant water ownership; particularly, details on where each power plant gets its water and any potential constraints on water deliveries in times of drought; and (3) adding a metadata layer that contains specifics concerning the origins of the water availability, cost, and future use data (including past and present data entries). The current Water Atlas supports energy sector planning and includes estimates of water availability at the watershed level for the lower 48 states.
- *Developing Cost Effective Biological Removal Technology for Selenium & Nitrate from Flue Gas Desulfurization Wastewater from Existing Power Generating Facility.* West Virginia State University is investigating a technically feasible and cost-effective process for designing photosynthetic organisms capable of sequestering selenium and nitrates from FGD wastewater.
- *Demonstration of Holistic Lower Cost/Energy Effluent Water Management Approaches for Coal-fired Energy.* EPRI is evaluating a set of effluent water management technologies and strategies that yield lower-cost clean water and reduced energy consumption compared to conventional systems used in coal-fired energy plants, and additionally generate salts and solids byproducts that can be reused or disposed as non-hazardous waste materials in landfills.
- *Exploring Energy-Water Issues in the United States.* In a separate project Sandia National Laboratory is developing a data set to help better understand the linkage between thermoelectric power generation and water as part of its efforts to update the Water Atlas. Data from this effort will be used to refine NETL's Water-Energy Model (NWEM) discussed later in this paper.
- *Flue-Gas Desulfurization Effluent Management Using an Innovative Low-Energy Biosorption Treatment System to Remove Key Contaminants.* ES Engineering Services is demonstrating an innovative, energy-efficient water treatment system for FGD wastewater treatment. The proposed treatment system uses hybrid biosorption, which is an adsorption process enhanced by biological activity to remove selenium, arsenic, nitrate, and potentially other contaminants from FGD wastewater.
- *Develop and Optimize an Electrical Plume Collection System.* Infinite Cooling will build and optimize an electrical plume collection system and test it in a high-fidelity lab setting and in actual field conditions on an industrial cooling tower.
- *Wastewater Recycling Using a Hygroscopic Cooling System.* The University of North Dakota will develop a hygroscopic cooling technology to eliminate power plant wastewater by recycling the water fraction to augment the plant's cooling load and collecting the remainder as a solid by-product for reuse or disposal. Benefits to coal-fired

power plant are to improve the plant's overall water-use efficiency while allowing the plant to conform with zero-liquid-discharge requirements.

The Lab's Advanced Energy Systems/Transformative Power Generation (AES/TPG) Program is also supporting water-related research with application to thermoelectric power generation, unconventional resource development, and carbon storage^{xxxvi}. Projects funded by the AES/TPG Program are highlighted below:

- *Advanced Anti-Fouling Coatings to Improve Coal-Fired Condenser Efficiency.* Oceanit Laboratories is developing an advanced coating material called HeatX™ to reduce fouling, corrosion, and film-wise condensation of the heat-transfer surfaces of condensers. HeatX™ is a composite coating material that has demonstrated adhesion and abrasion resistance even at thin applied thicknesses that may enable its use on heat conducting surfaces without impacting heat transfer.
- *Development and Field Testing Novel Natural Gas Surface Process Equipment for Replacement of Water as Primary Hydraulic Fracturing Fluid.* Southwest Research Institute is investigating whether natural gas can be used as the primary fluid in hydraulic fracturing processes. The project focused on developing and demonstrating affordable non-water-based and non-CO₂-based stimulation technologies. Such technologies can serve as alternatives to, or be combined with, water-based hydraulic fracturing fluids

to reduce water consumption and the volume of flowback fluids.

- *Investigation of Technologies to Improve Condenser Heat Transfer and Performance in a Relevant Coal-Fired Power Plant* – EPRI will evaluate the application of various surface modification technologies on coal-fired power plant condenser tubes to enhance their heat transfer properties and increase overall plant performance. EPRI will identify surface modification technologies (i.e., coatings, etching) and apply them to tubing components to study the potential for improved heat transfer by either reducing surface fouling or by altering the physical steam condensation process.
- *Anti-Biofouling Surface Treatment for Improved Condenser Performance for Coal-Based Power Plants* – Research Triangle Institute will design and engineer novel surface treatments and secondarily applied remediation components to mitigate biofilm growth on condenser tube surfaces in coal-fueled power plants with the goal of developing a strategy to mitigate biofilm growth by at least 50 percent.

In late 2019, the Crosscutting Program issued a Financial Opportunity Announcement (FOA) for the cost-shared R&D for advanced dry cooling for coal- and natural-gas fired power plants recognizing the cost and performance challenges associated with this technology particularly under hot climatic conditions^{xxxvii}. It is anticipated that selections under this FOA will be announced by the second quarter of 2020.

Below is a summary-level description of the water projects funded under the University Coal Research Program^{xxxviii}. These projects include water-related research directed at the utilization and management of the byproducts of coal combustion such as fly ash, bottom ash, and FGD materials to prevent potential impacts on surface and groundwater. The projects have direct relevance to EPA's CCR rulemaking and power plant effluent guidelines discussed above.

- *Characterization of Arsenic and Selenium in Coal Fly Ash to Improve Evaluations for Disposal and Reuse Potential.* Duke University is investigating the chemical forms of arsenic and selenium in coal fly ash and improve methods of characterization. This project will establish high-throughput characterization methods for arsenic and selenium species in coal fly ash and enhance understanding of how coal combustion parameters influence leachable arsenic and selenium contents from fly ash.
- *Elucidating Arsenic and Selenium Speciation in Coal Fly Ashes.* Georgia Tech Research Corp. is characterizing arsenic and selenium speciation within coal fly ashes, using synchrotron X-ray spectroscopic and microscopic techniques to develop a comprehensive correlation and searchable database for coal source/type, generation condition and arsenic/selenium speciation and mobility.
- *Trace Element Sampling and Partitioning Modeling to Estimate Wastewater Composition and Treatment Efficacy at Coal Generator.*

The University of Alabama Birmingham is developing an integrated water-sensor package capable of measuring multiple contaminants and common water quality indicators, such as pH, oxidation-reduction potential, and temperature. A proof-of-concept prototype will be integrated with a commercial, off-the-shelf trace-metal-concentration measurement device to accurately detect trace metal concentrations on a real-time, continuous basis.

- *Applying Anodic Stripping Voltammetry to Complex Wastewater Streams for Rapid Metal Detection.* The University of California Los Angeles is developing a lab-on-a-chip electrochemical sensor capable of accurately measuring heavy metal concentrations, including lead, cadmium, and arsenic, in complex aqueous streams such as wastewater.
- *Trace Element Sampling and Partitioning Modeling to Estimate Wastewater Composition and Treatment Efficacy at Coal Generator.* Carnegie Mellon University is sampling pulverized-coal-fired power plants (CFPPs) owned and operated by Louisville Gas & Electricity–Kentucky Utilities (LGE-KU) to build a predictive model that will enable utility decision makers, academic researchers, and policymakers to simulate trace element emissions from CFPPs.
- *Coal-Fired Power Plant Configuration and Operation Impact on Plant Effluent Contaminants and Conditions.* Lehigh University Lehigh University, working with Western Kentucky University, will

characterize coal contaminants in power plant wastewater as a function of coal type, plant type, plant operational profile, environmental controls, water treatment technology, and effluent species. Effluent samples will be analyzed for mercury, arsenic, selenium, nitrate/nitrite, and bromide as well as proximate and ultimate analysis.

- *Produced Water and Waste Heat-Aided Blowdown Water Treatment Using Chemical and Energy Synergisms for Value* – West Virginia University will develop and test an innovative treatment process that utilizes PW to create chemical and energy synergisms in blowdown water treatment with the goals of maximizing generation of a product stream low in fouling potential for reuse and a concentrated stream of commercial value (i.e., 10-lb Brine) while reducing chemical and energy costs for the treatment.

Value Product Recovery from Water/Wastewater Treatment

NETL is actively investigating the recovery of valued products such as rare earth elements (REE) from raw coal, coal preparation refuse, and the byproducts from coal combustion. The recovery of REE and other value products from the treatment of AMD is emerging area of interest^{xxxix}, and one that the Laboratory is also pursuing. AMD continues to be an issue in the coal mining regions of Appalachia as well as the coal and hard rock mining areas of the West with thousands of miles of rivers and streams affected. The Laboratory's efforts in this area provide the opportunity not only to recover valuable materials from coal mining waste streams

but also to mitigate an environmental impact associated with mining.

Under funding from NETL, West Virginia University (WVU) has been conducting research on AMD treatment and REE recovery since 2016. The AMD treatment being developed by WVU concentrates the rare earths leached out of the waste rock from coal mining into a sludge that can be then refined into marketable products. It is anticipated that the recovery of a value product from acid discharges will help to stimulate AMD treatment at abandoned mines and allow operators to offset treatment costs. WVU has evaluated the reserves at 140 acid mine drainage treatment sites throughout West Virginia, Pennsylvania, and Ohio and are developing commercially viable refining methods. If successful, the project could lead to economic diversification, new economic development opportunities, and improved environmental quality in the Appalachian region and other regions of the United States and the world impacted by AMD^{xl}.

Research Triangle Institute is also investigating value product recovery under the project *Low-Cost REE Recovery from Acid Mine Drainage Sludge*. This project aims to develop a membrane-based, bench-scale system to extract strategic minerals such as REE, and other critical minerals, from AMD sludge generated as part of coal mining activities in the United States. The proposed effort will use a staged, membrane-based treatment approach to separate, concentrate, and ultimately recover REEs from AMD.

Ohio State University's *Concentrating REE in Acid Mine Drainage Using Coal Combustion Products through Abandoned Mine Land Reclamation* project will develop an

integrated process that first uses stabilized FGD materials to recover REE from AMD and a sequential extraction procedure to produce a rare earth feedstock with above 2 wt.% REE. The objectives are to (1) validate the effectiveness and feasibility of the integrated REE recovery/concentrating process, (2) determine mechanisms controlling the rare earth recovery process, (3) quantify the associated economic and environmental benefits, and (4) evaluate the full-scale application of the process.

The Lab's Research Innovation Center (RIC) is also investigating the potential to recover REE and other transition metals (e.g., cobalt, nickel, and zinc) from AMD. Working with Hedin Environmental, Inc. and the University of Pittsburgh, RIC researchers are collecting chemically diverse AMD treatment solids from passive AMD treatment systems such as limestone beds, settling ponds, and vertical flow ponds in the western Pennsylvania region^{xli}. Based on solid characterization and extraction tests, RIC researchers effectively recovered value products containing approximately 10% REE, as well as 50% transition metals (Co, Ni and Zn) from AMD solids. This project aims at developing a low-cost mild acid extraction system to extract REE and other critical minerals from AMD solids generated from various passive remediation systems in Pennsylvania.

Carbon Capture, Utilization, and Storage Water Research

It is expected that the installation of carbon capture and storage (CCS) systems on fossil-fuel-fired power plants will impose additional stress on the sustainability of freshwater resources^{xlii}. Water is required by the chemical and physical processes that capture and separate CO₂. Moreover, the operation of these CO₂ capture and compression systems can have a significant

parasitic power demand and therefore increase process and cooling water requirements. The Lab's carbon capture research is directed at improving the efficiency of CO₂ capture and compression, thereby reducing costs, parasitic power demand, and associated water-use requirements. Information on the Lab's CO₂ capture projects can be found on NETL's website^{xliii}.

In 2019 NETL announced the selection of nine projects to conduct front-end engineering design (FEED) studies for installing CO₂ capture systems on coal and natural gas power plants^{xliiv}. The FEED studies will include an assessment of water impacts including sourcing, treatment, and reuse of water.

The Lab's Carbon Storage Program is also engaged in water-related research. The program seeks to develop technologies for commercial readiness beginning in 2025 that ensure safe, secure, efficient, and affordable CO₂ injection and containment in diverse geologic settings. Commercial scale geologic storage of CO₂ will require storage formations to handle significant amounts of CO₂ over many years. CO₂ injection into saline formations will result in increased pressure throughout portions of the subsurface and depending on the operating conditions and nature of the storage formation could result in fluid displacement or geomechanical phenomena such as ground deformation.

Active CO₂ plume management through utilization of brine extraction is one approach for managing formation pressure, effective stress, and plume movement through a saline storage reservoir. While brine extraction can be used to manage a formation's pressure, a required next step is

the disposition of the produced brine. These brines can have total dissolved solids (TDS) concentrations up to 320,000 parts per million, or almost ten times higher than seawater, and can contain metals and other contaminants^{xlv}. Therefore, treatment of these brines once they are brought to the surface will be necessary in order to be beneficially reused or discharged into surface or to recharge groundwater.

To address formation pressure and stress management through brine extraction, the carbon storage program initiated the Brine Extraction Storage Test (BEST) project in 2018. BEST facilities in North Dakota and Florida will focus on managing formation pressure as well as measuring and monitoring the movement of the differential pressure and CO₂ plumes in the subsurface for future saline CO₂ storage projects. Further, pilot testing of cost-effective technologies for treating high TDS waters extracted at the two BEST sites will be performed in order to beneficially recycle the brines for industrial and domestic use and to produce saleable byproducts. The BEST located in the oil and gas fields of western North Dakota managed by the Energy and Environmental Research Center is currently operating^{xlvi}. The BEST in Florida located at Gulf Power's Plant Smith is still under construction.

The Florida BEST is an outgrowth of the Carbon Storage Program's *Field Demonstration at Plant Smith Generating Station Assessment of Opportunities for Optimal Reservoir Pressure Control Plume Management and Produced Water Strategies* project being carried out by EPRI. This project involves a techno-economic analysis and field testing of optimal water injection and extraction strategies to

control subsurface pressures and plume movement in a demonstration reservoir at Plant Smith^{xlvii}.

In addition to the BEST brine management and treatment, NETL has funded eight recently completed projects under the Crosscutting Program in support of the Carbon Storage Program to beneficially use brines collected from CO₂ sequestration or to minimize the cost of treating these brines. A brief description of these projects is presented below.

- *Treatment of Produced Water from Carbon Sequestration Sites for Water Reuse, Mineral Recovery and Carbon Utilization.* Southern Research Institute investigated integrating a membrane separation with a thermal evaporation system followed by a solidification and stabilization step to immobilize contaminants. The membrane and evaporation system will build on concepts tested for oil and gas produced water.
- *Model-Based Extracted Water Desalination System for Carbon Sequestration.* GE Global Research leveraged a new, pilot-ready pretreatment and desalination technologies to develop a cost-effective desalination system for extracted water from deep saline formations.
- *Water Desalination Using Multi-Phase Turbo-Expander.* GE Global Research carried out another project that investigated freezing brine to separate water from salt. Ice crystals will then be separated from salt crystals to yield pure water after the ice is melted. The approach is to cool the brine by

expansion of a compressed air/brine stream in a turbo-expander.

- *An Integrated Supercritical System for Efficient Produced Water Treatment and Power Generation.* The University of Illinois carried out a project that used methane or coal as an energy source to drive a system that generates both electricity and pure water via supercritical precipitation.
- *Advanced Integrated Technologies for Treatment and Reutilization of Impaired Water in Fossil Fuel-based Power Plant Systems.* Ohio University developed a method based on a multi-stage treatment process that utilizes commercial solids filtering, ultra violet light, a low-cost natural zeolite, electrochemical stripping, selective sulfation, and a new supercritical water unit design to remove major constituents and hydrocarbons.
- *Fouling-Resistant Membranes for Treating Concentrated Brines for Water Reuse in Advanced Energy Systems.* Research Triangle Institute worked on a project in which electrically conductive membrane distillation was demonstrated for the reuse of water contained in concentrated brines.
- *Development of Membrane Distillation Technology Utilizing Waste Heat for Treatment of High Salinity Wastewaters.* The University of Pittsburgh evaluated the feasibility of using membrane distillation technology to treat high salinity wastewaters utilizing waste heat that is available in thermoelectric power plants or compressor stations.

- *Low-Energy Water Recovery from Subsurface Brines.* Research Triangle Institute investigated a low-energy treatment method using non-aqueous solvent extraction to recover water from high TDS aquifer brine.

From a water perspective, the Carbon Storage Program is also leading a multi-laboratory effort that leverages broad technical capabilities across the DOE complex to develop the integrated science base that can be applied to risk assessment for long-term storage of CO₂^{xlviii}. The National Risk Assessment Partnership (NRAP) involves five DOE national laboratories: NETL, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and Pacific Northwest National Laboratory. The goal of NRAP is to build methods and tools and improve the science base to quantify key environmental risks at geologic carbon storage sites including the potential release of CO₂ or brine from the storage reservoir and its impacts on surface and groundwater.

In support of the commercialization and deployment of CCS, NETL created the Regional Carbon Sequestration Partnerships (RCSP) in 2003 to characterize the large-scale carbon storage potential of geological formations in seven regions of the U.S. In 2009, the Water Working Group (WWG) was formed within the RCSP to investigate the potential interaction between CCS and local and regional water resources^{xlix}. Under the WWG, NETL and its partners are conducting fundamental and applied research to quantify the security of freshwater during subsurface CO₂ injection. The research combined with the results of other research initiatives will help to define

“best practices” that can be applied at the pre-injection, active, and post-closure stages of CO₂ geologic storage operations to prevent impingement of freshwater resources.

Regarding water and CO₂/carbon reuse, NETL’s Carbon Utilization Program is sponsoring a project with the University of Illinois entitled *Improving the Economic Viability of Biological Utilization of Coal Power Plant CO₂ by Improved Algae Productivity and Integration with Wastewater*. The project will generate algal biomass products to market as liquid fuel and livestock feed using captured CO₂ and concentrated wastewater nutrients as a growth medium^l.

Oil & Gas Program Produced Water Management Research

Significant amounts of water are used in oil and gas exploration and production in the U.S., particularly for unconventional supplies such as shale gas. The USGS estimates that between 2000 and 2014 nearly 264,000 oil and gas wells were hydraulically fractured and each well used an annual average of about 4 million and 5.1 million gallons of water respectively^{xvi}. Conversely, oil and gas wells also produce large volumes of water along with hydrocarbons. This PW from oil and gas development can contain elevated concentrations of dissolved salt, petroleum and other organic compounds, suspended solids, trace elements, bacteria, naturally occurring radioactive materials. It has been estimated that each day approximately two billion gallons of water are produced during oil and natural gas production operations that must be treated for reuse or disposed of via injection into deep disposal wells in

oil and gas producing regions of the United States^{xviii}.

From 2007 to 2016 NETL managed the Research Partnership to Secure Energy for America (RPSEA), a non-profit consortium that conducted research in three oil and gas development areas: (1) ultra-deepwater production; (2) unconventional natural gas and other petroleum resources; and (3) technology challenges for small producers^{li,lii}. RPSEA-sponsored research included over thirty projects focused on the management, treatment, and reuse of PW from the Barnett, Utica, Marcellus and other unconventional oil and gas fields^{liii}. A complete listing and description of each of the water-related reports under RPSEA can be found in NETL’s Research Portfolio Accomplishment Report^{liv}

More recently the Oil and Gas Program’s Unconventional Oil and Gas Research Area announced four new PW management projects under an FOA entitled *Low Cost, Efficient Treatment Technologies for Produced Water*^{lv}. These projects will accelerate the development and commercialization of pre-treatment (upstream of TDS removal) technologies for wastewater associated with oil and gas production by significantly reducing the volume of water requiring deep well disposal and by creating a supply of fresh water for regional users. A brief summary of these projects is provided below.

- *A New Membrane-Based Treatment Process for Reclaiming and Reutilization of Produced Water*. TDA Research, Inc. with Matheson and Gas Technology Institute will develop a new membrane-based filtration system for removing organic compounds from PW. The

proposed membrane treatment process integrates the new filter with a series of well-established water treatment technologies, such as mechanical filtration and RO filters to remove all suspended and dissolved solids, organic molecules, bacteria and radioactive particles from the PW generated in oil and gas production received from Niobrara Basin (and potentially from other fields).

- *Non-Fouling, Low Cost Electrolytic Coagulation and Disinfection for Treating Flowback and Produced Water for Reuse.* The University of Arizona with WaterTectonics will develop and test a new method for delivering a Fe³⁺ coagulant and disinfectant for treating flowback and produced water (FPW) so that it can be reused for fracking and water-flooding at a cost savings of at least 50% compared to current practices. The treatment system will remove suspended solids, dispersed oil, H₂S, microorganisms and scale-forming cations from FPW. Test the treatment system at three oil and gas production locations in Colorado, Texas and/or New Mexico.
- *Resource Recovery and Environmental Protection in Wyoming's Greater Green River Basin Using Selective Nanostructured Membranes.* A team led by the University of Wyoming will develop a working prototype of a two-part affinity-based membrane separation process for recovering hydrocarbons and separating organics from PW. This effort is focused on PW originating from the Greater Green River Basin (GGRB) in Wyoming. The

University of Wyoming will synthesize, and document the performance of, optimized super-hydrophilic/superhydrophobic membranes based on their existing designs and made using the electrospinning/spraying technique. Performance data will include water/benzene, toluene, ethylbenzene, and xylene/oil fluxes, selectivity for the permeating phases, solids rejection, and performance degradation (fouling). Data will be reported using both synthetic PW and PW samples collected from the GGRB.

- *Fouling-Resistant, Chlorine-tolerant Zwitterionic Membranes for the Selective Removal of oil, Organics, and Heavy Metals from Produced Water in the Permian Basin.* A team led by ZwitterCo, Inc. will develop a novel membrane technology based on zwitterionic copolymers that can reject key constituents from PW in the Permian Basin while maintaining unprecedented immunity to detrimental and irreversible membrane fouling. These membranes can remove nanoscale oils, greases, colloidal material, heavy metals and dissolved organic molecules without removing salts and dissolved solids, making filtration of challenging, highly saline waste streams practical and cost-effective.

Under the Oil and Gas Program, NETL is also supporting the Risk Based Data Management System (RBDMS) being developed by the Ground Water Protection Council (GWPC)^{vi}. The RBDMS is a tool used in twenty-two oil and natural gas producing states to manage oil and gas

activities and evaluate the risk to source water posed by operations. Along with RBDMS, GWPC and the Interstate Oil and Gas Compact Commission maintain *FracFocus*^{lvii}, a disclosure and education website for public and industry to communicate and relay information on the chemicals used during the process of hydraulic fracturing. GWPC is also developing a Web-based GIS model to assess water management options using existing and enhanced RBDMS analytical capabilities.

Desalination Hub Research/RIC Water Activities

NETL is part of the winning team announced on September 23, 2019 under the DOE Advanced Manufacturing Office's \$100 million Desalination Hub solicitation^{lviii}. Led by the Lawrence Berkeley National Laboratory, the National Alliance for Water Innovation (NAWI) will focus on desalination and related-water treatment R&D to allow for "non-traditional" water sources to be used to replace or supplemental freshwater in various municipal, industrial, and agricultural applications^{lix}. The NAWI team will assess non-traditional waters including ocean water, brackish groundwater, municipal wastewater, agricultural wastewater, mining wastewater, industrial wastewater, thermoelectric generation/cooling water discharge, and oil and gas produced water. The treatment and recycling of several of these non-traditional waters is currently part of NETL's water-energy program as described elsewhere in this paper.

The overall goal of NAWI is to achieve "pipe parity" between non-traditional or impaired

waters and freshwater on a levelized cost of water basis. The concept of pipe parity will take into consideration quantitative measures such as the energy intensity of pumping, treating, and distributing alternative sources of water and more qualitative factors such as water system resiliency and security. To achieve this goal the NAWI team will conduct innovation R&D across four technical areas: (1) materials research and development; (2) new processes research and development; (3) modeling and simulation tools; and (4) integrated data and analysis.

NETL's RIC will be responsible for coordinating the Lab's participation in the Desalination Hub. RIC's efforts will be directed at modeling and simulation tools development and will focus on water treatment systems using the Lab's Institute for the Design of Advanced Energy Systems (IDAES) framework. IDAES is a next generation modeling and optimization platform used to develop multiscale, simulation-based computational tools and models in support of the Lab's efforts in advanced technologies like chemical looping, carbon capture, and advanced combustion systems. The outcome of NETL's support of NAWI will be an open-source, predictive suite of models for steady-state and dynamic optimization of integrated water systems and treatment trains called Proteus.

The initial implementation of Proteus will focus on building the steady-state unit and property models and system level capabilities to provide an initial version of a water desalination system simulator using the IDAES framework. The developed suite of models will add to the existing library of IDAES models to specifically incorporate those unit operations needed to fully

represent a desalination process and track ions, mass, and energy flows throughout the system. The project scope will also include the development of a roadmap to determine additional capabilities needed to fully represent the advanced precision separation techniques identified in this proposal.

In addition to the research directly supported by the NAWI, RIC is also investigating two different options for treating the heavy metal laden effluent streams from coal-fired power plants: (1) selective removal using novel sorbents, and (2) concentrating these waste streams during zero-liquid discharge processing. It is expected that these research efforts will significantly lower the cost of treating FGD and other effluents from the operation of coal-based power generation^x. The development of novel sorbents will focus on removal of the six heavy metal species currently regulated by EPA that includes lead, arsenic, mercury, selenium, chromium, and cadmium.

In the second approach, a novel swept-reverse-osmosis membrane capable of selectively removing water from effluent streams is being developed that will effectively concentrate the heavy metals within a brine that can be injected in salt water disposal wells or can be further treated. A subset of the RIC research will model advanced cooling options and investigate the possible use of alternative or non-traditional water for thermoelectric power plants. Current water-energy models focus on longer-term water stresses often based on climate change scenarios. Newly developed models will explore the various acute, shorter-term impacts of water stresses on power plant operations such as changes in electricity price,

environmental regulations, and supply and demand.

NETL's RIC is also developing a novel method for imbedding polyamines within inexpensive, porous silica particles to remove organic-based colorants and other pollutants from a variety of water sources including drinking water supplies, ponds, rivers, lakes, seawater, groundwater, textile waste water streams, food processing waste water streams, and coffee bean waste waters. NETL researchers have also recently developed an amine-based sorbent that has shown promise for removing radioactive contaminants from wastewater. This technology is available for licensing and further collaborative development^{lxi}.

As discussed above, RIC researchers are also investigating the recovery of REE from passive AMD treatment processes.

Water Related Modeling and Analysis

NETL's System Engineering and Analyses group has developed several modeling and analysis tools directed at the link between fossil energy and water. One of the landmark analyses carried out by the Lab is entitled "*Estimating Freshwater Needs to Meet Future Thermoelectric Generation Requirements*" that projected future freshwater withdrawal and consumption for thermoelectric power generation under five different scenarios related to plant retirements and additions, cooling water source, and cooling technology (once-through, recirculating, dry, and hybrid systems)^{lxii}. The report was updated annually from 2006 to 2013 using the latest EIA Annual Energy Outlook (AEO) regional projections for capacity additions and retirements for power generation.

The group's Life Cycle Analysis (LCA) team has constructed a set of tools that can be used to assess the environmental, economic, and social attributes of energy systems including water^{lxiii}. For example, the LCA toolbox has been applied to evaluating the impact of installing CCS on water withdrawal and consumption for various power technologies including integrated gasification combined cycle, natural gas combined cycle, and subcritical and supercritical pulverized coal. LCA modeling has also been carried out on water use in natural gas production^{lxiv} and regional impacts of coal mining on water consumption^{lxv}.

NETL has also developed the first prototype water-energy model as part of a larger effort to comprehensively model water-energy interactions^{lxvi}. The NETL Water-Energy Model (NWEM) passively couples a variety of data on water supply, water availability, and power plant water use with the National Energy Modeling System (NEMS) power generation forecasts. NWEM operates at a watershed level and its efficacy in resolving local water supply and water-use trade-offs was demonstrated using data from Sandia National Laboratory along with a water supply scenario projected by the World Resources Institute. The prototype model only passively utilized a forecast of power generation from an existing forecast; the model's choices were limited to purchases or retrofitting to meet future water supply constraints. NETL is continuing to integrate the water sub-module into the NEMS framework, which will allow active interaction between the water market and power markets, extending the industry's ability to project the amount of water available for power generation, to project water demand for

future power generation based on a NEMS forecast, to identify regions that experience potential water shortfalls, and to estimate the cost of meeting water demand where water shortfalls exist for each water availability scenario.

International Water Activities

Water is essential throughout the world in all phases of energy production and use^{lxvii}. It can be particularly challenging for countries such as China to balance demands for water needed for energy and water needed for other critical sectors like agriculture and domestic use. NETL has been supporting DOE's effort under the U.S./China Clean Energy Research Center for Water-Energy Technologies (CERC-WET) to facilitate R&D between the U.S. and China that builds and transfers knowledge and technology on the relationship between energy and water^{lxviii}. As noted above, China is faced with significant geographical disparity between the country's freshwater resources in the south and agricultural and energy demands for water in the north. The WET effort is part of a larger CERC agreement signed in November 2009 and extend for five years in 2015 that addresses five areas of collaboration including water. Water-related research is being conducted in five topic areas: (1) water use reduction in the energy sector, (2) water treatment and management of non-traditional waters, (3) sustainable hydropower design and operations, (4) climate impacts for energy-water systems, and (5) planning and policy processes. NETL has also carried out an assessment of the water-energy nexus in China.^{lxix}

Maximizing Water-Energy Program Synergies

While water-related research is being conducted across several program areas – e.g., Crosscutting, Advanced Energy Systems, CCS, Unconventional Oil and Gas, REE Recovery -- the Lab recognizes the critical synergies between the various projects and activities and manages the portfolio of research in an integrated, coordinated manner. Examples of the synergies between program areas include the R&D on brine treatment and reuse being carried out under the Oil and Gas, Carbon Storage, and Crosscutting Programs. The recently selected oil and gas PW desalination pretreatment technology projects will be closely coordinated with brine extraction, treatment and reuse efforts under the carbon storage BEST and Crosscutting activities. Similarly, value product recovery under BEST will be leveraged against similar work looking at the recovery of REE from AMD and research on value product recovery supported by NAWI. Likewise, advances in dry cooling supported by the Crosscutting Program will be coordinated with the Carbon Capture Program's FEED studies. Further, the Lab's overall water-energy program will closely align with the goals of the AMO Desalination Hub and future research sponsored through DOE's Water Security Grand Challenge.

NETL Water Program Success Stories

Over the past two decades, NETL and its partners have developed a suite of advanced tools and technologies applicable to the recovery, treatment, and reuse of water for fossil energy production and power generation. Below are several

examples of NETL's water-energy nexus success stories.

- *Recovering Water from Power Plant Cooling Plumes*

The ClearSky® Plume-Abatement System developed by SPX in partnership with NETL is a commercial technology to minimize cooling plumes and reduce evaporative water loss. The ClearSky® moisture capture technology recovers an average of 18 percent of the water evaporated from a cooling tower, offering an economical and environmentally friendly solution for reducing the amount of water used by fossil fuel-fired power plants. The technology is being marketed worldwide with a recent order placed for the system on a coal liquefaction facility in China.

- *Water Treatment System Cleans Marcellus Shale Produced Water*

Altela Inc. successfully tested its AltelaRain® 4000 water desalination system on produced water at BLX, Inc.'s Sleppy hydraulic fracturing well site in Indiana County, Pennsylvania. During nine continuous months of operation, the unit treated 77 percent of the water produced by the well. As of March 1, 2011, over 275,000 gallons of Marcellus Shale frack flowback water were treated and purified at the well-site resulting in the production of more than 182,000 gallons of clean, distilled water. The treated water was shown to be suitable for re-use by well operators and could also be discharged to surface waterways without the need for further treatment, thus reducing the economic and environmental impacts of the well.

- *Acid Mine Drainage Treatment Process for Source Water*

With cost-share funding from NETL Battelle conducted the first field demonstration of the Flotation Liquid-Liquid Extraction water treatment system at Fawn Mine in Sarver, Pennsylvania. Currently offered commercially by Winner Water Services as HydroFlex™, the technology treats AMD contaminated water so that it can be used for hydraulic fracturing operations. HydroFlex™ was shown to reduce sulfate concentrations in AMD by up to 90 percent—a significant improvement over competing technologies.

- *Drying and Refining Coal for Increased Value and Reduced Emissions*

The DryFining™ process was developed by Great River Energy in partnership with NETL to use excess heat from electricity generation to dry coal prior to combustion. In addition to using less cooling water to produce electricity, drying coal prior to combustion is more efficient and results in more electricity with less coal usage and air emissions. Although coal drying is well known, the DryFining process is commercially viable due to the process using waste heat as the energy source.

- *Advanced Systems Modeling and Simulation-Based Engineering*

NETL is leading a multi-lab initiative called the Institute for the Design of Advanced Energy Systems (IDAES) to develop and employ process systems engineering models and computational tools to analyze advanced energy

systems. IDAES will be a very valuable tool in supporting NETL's water-energy research. Models are currently being developed to track the partitioning of contaminants in various power plant wastewater streams. In addition, IDAES can be used to optimize water use within an entire power plant.

- *Data-Driven Tool for Science-Based Decision Making*

NETL's Energy Data eXchange (EDX) is a platform for data sharing and collaborative research and includes an NETL-developed suite of tools for data visualization and analyses, such as the Variable Grid Method (VGM). NETL's VGM allows for better communication of uncertainties by combining flexibility of input with visual spatial data output to facilitate understanding of the results and has been used to quantify and limit uncertainty in subsurface groundwater distribution.

- *Water-Energy Model for National Energy Modeling System*

NETL has developed a prototype model for the National Energy Modeling System (NEMS) that can be used to estimate the impact of fossil energy technologies on water resources. The model currently operates at a Hydraulic Unit Code 8 (HUC 8) sub-basin watershed level and has been beta tested under HUC 8 water demand-supply scenarios using data compiled by Sandia National Laboratory (partially funded by NETL) and the World Resources Institute.

- *A Unique, Split Laser System for Environmental Monitoring*

Regulatory agencies, state and local governments, energy resource developers, research organizations, and others have a need for real-time, high-quality water data. Unfortunately, water quality monitoring solutions available today are expensive and labor intensive. NETL researchers are developing a more affordable, in-situ monitoring tool based on laser induced breakdown spectroscopy (LIBS) by measuring the elemental concentrations in simulated brines. LIBS technology provides rapid elemental analysis without extensive sample collection or preparation. NETL has designed a simple, easy-to-fabricate, handheld LIBS system fully adaptable to field use and capable of measurements even in harsh environments.

- *Wireless Network Sensors and Integrated Sensors for Water Quality*

Under a Phase II Small Business Innovative Research grant, Sporian Microsystems Inc. is developing a low-cost, rapidly deployable, wireless, self-powered, real-time, in-situ water quality monitoring technology. The device will measure key parameters associated with power plant water use including temperature, turbidity, pH, total dissolved solids, scale forming minerals, and heavy metals. The detection system is based on Sporian's patented detection element comprised of molecularly imprinted polymers and ion imprinted polymers. Another company, NanoSonic, Inc., is developing wireless sensors for use in

analyzing heavy metal chemistry for power generation facilities and, more broadly, for commercial use. The company will develop wireless networked sensors using conformal nanomembrane-based chemical field effect transistors (ChemFETs) to detect heavy metals in water, enabling efficient monitoring of heavy metals in water for environmental surveillance, location of pollution sources, and detection and mapping of chemical concentrations that are potentially harmful to people and/or destructive to agriculture.

Summary and Conclusion

The sustainability of our limited freshwater resources underpins the nation's health, economy, and quality of life. The balance between water and energy is being challenged by several factors including population growth in historically water deficient regions, demands from competing end-use sectors, and shifting precipitation patterns. NETL has been engaged in integrated, comprehensive research and development (R&D) to advance our understanding of fossil energy exploration, extraction, development, and use on freshwater availability and quality since 2002. With the goal of enhancing the security and resiliency of our fossil energy investments, research on water treatment, recovery, and reuse is being carried out across the Lab's programs in thermoelectric power generation, oil and gas development, coal combustion byproduct utilization and management, carbon capture and storage, value product recovery, university coal research, life-cycle analysis, and systems modeling and analysis.

NETL will continue to assess the need and opportunity to engage in further water-energy research. For example, future work may apply the Lab's machine learning and artificial intelligence capabilities to critical water-energy issues including the development of cost-effective treatments and reuse options for PW, brines, and other effluents from energy production. The program may also expand efforts to recover other value products from various fossil energy wastewater streams including zero liquid discharge brines, advance options for managing CCR disposal and reuse, and

improve water sensor and detection technologies. In responding to these water-energy challenges, the Lab will continue to leverage its participation in NAWI as well as its partnerships with DOE's other national laboratories, academia, non-government organizations, and industry, to develop and bring to commercial readiness the technology needed to continue the environmentally sound and sustainable use of our domestic fossil energy resources.

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