NETL
Science & Technology
ACCOMPLISHMENTS
2020

DRIVING TECHNOLOGY INNOVATION AND DELIVERING SOLUTIONS FOR CLEAN ENERGY

U.S. DEPARTMENT OF ENERGY | **NETL** NATIONAL ENERGY TECHNOLOGY LABORATORY

MESSAGE
FROM THE DIRECTOR

I am pleased to present the National Energy Technology Laboratory's (NETL) **FY 2020 Science & Technology Accomplishments**. These demonstrated accomplishments, which represent an outstanding selection of our researchers' achievements, characterize NETL's six Core Competencies—*Computational Science and Engineering, Energy Conversion Engineering, Geological and Environmental Sciences, Materials Engineering and Manufacturing, Program Execution and Integration, and Systems Engineering and Analysis.*

A significant portion of the NETL research portfolio includes research and development (R&D) conducted through partnerships, cooperative research and development agreements, financial assistance, and contractual arrangements with universities, research organizations, the private sector, and other national laboratories. Together, coupled with our own research, these efforts serve to focus the national wealth of scientific and engineering talent to create commercially viable solutions to help solve national and global energy and environmental problems.

NETL's demonstrated competencies and portfolio of successes constitute a robust national asset that is poised to directly address the nation's energy and environmental priorities.

Sincerely,

Brian J. Anderson, Ph.D., Director
National Energy Technology Laboratory

CONTENTS

CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING (CSE)

CSE develops science-based simulation models, mathematical methods and algorithms, and software tools required to address the technical barriers to the development of next-generation technologies. CSE works together with others at NETL to generate information and understanding beyond the reach of experiments alone. Through the integration of experimental information and computational sciences, scientists and engineers can simulate variations more efficiently while saving time, money, and materials.

MATERIALS ENGINEERING and MANUFACTURING (MEM)

NETL is internationally recognized for its leadership in designing, developing, and deploying advanced materials for use in energy applications and extreme service environments. Of particular note is NETL's ability to design, engineer, and evaluate materials at size and time regimes ranging from atomistic to pilot-plant scales. To accomplish this, NETL utilizes a one-of-a-kind suite of computational and experimental methods for translating new material science concepts into practical technologies.

ENERGY CONVERSION ENGINEERING (ECE)

Using fundamental and applied modeling tools coupled with experimental testing, NETL researchers accelerate development of technologies by reducing the time, cost, and technical risk associated with bringing advanced technologies from concept to market. Capabilities related to this competency include Clean Energy Systems, Multiphase Flow Science, Combustion Sciences, Innovative Energy Concepts, Reaction Engineering and Diagnostics and Controls.

PROGRAM EXECUTION and INTEGRATION (PEI)

PEI functions are powered by highly trained management experts that are effective technical managers, communicators, and quality assurance analysts able to assess technical risks, assist with technical problem solving, and evaluate and manage project risk. Through integrated technical and business teams, NETL defines, solicits, negotiates, awards, manages, and delivers federally sponsored research and development benefits to the nation.

GEOLOGICAL and ENVIRONMENTAL SCIENCES (GES)

CSE develops science-based simulation models, mathematical methods and algorithms, and software tools required to address the technical barriers to the development of next-generation technologies. CSE works together with others at NETL to generate information and understanding beyond the reach of experiments alone. Through the integration of experimental information and computational sciences, scientists and engineers can simulate variations more efficiently while saving time, money, and materials.

SYSTEMS ENGINEERING and ANALYSIS (SEA)

NETL researchers develop and use advanced models coupled with optimization and uncertainty quantification to support decision-making. Methodologies based in the fundamental disciplines of mathematics, economics, finance, operations research, chemical engineering, and computer science are complemented by experimental capabilities in chemistry, physics, and biology, as well as pilot-scale evaluation. Integration of computational and applied research provides insights to new technology; identifies new energy concepts; and analyzes energy system interaction at plant, regional, national, and global scales.

DOE-NETL'S REE-CM PROGRAM ACCELERATES MINERAL EXTRACTION FROM DOMESTIC COAL-BASED RESOURCES

Mineral extraction technologies using domestic coal enable our Nation's independence for Critical Minerals and Rare Earth Elements.

THREE FIRST-OF-A-KIND RARE EARTH ELEMENT (REE) AND CRITICAL MINERAL (CM) PILOT-SCALE FACILITIES MOVE TECHNOLOGY CLOSER TO FULL-SCALE COMMERCIALIZATION

Domestic pilot-scale REE-CM extraction-separation-recovery facilities have generated high purity, mixed rare earth oxide (MREO) concentrates of 80–99 wt.% purity from diverse coal-based materials, including coal refuse, acid mine drainage, and power generation ash. These first-of-a-kind pilot-scale facilities enable rapid development and evaluation for fully integrated systems that are the next step in technology commercialization.

Courtesy of Prakash Joshi & David Gamliel, Physical Sciences Inc.

Courtesy of Rick Honaker, University of Kentucky

Courtesy of Paul Ziemkiewicz, West Virginia University

Roe-Hoan Yoon, Virginia Tech

REE SEPARATION PROCESS ACHIEVES PRODUCTION OF HIGH PURITY, SINGLE RARE EARTH OXIDE (REO)

Battelle Memorial Institute and Rare Earth Salts are utilizing acid digestion and a novel electrowinning separation and purification process to produce a ~90% pure single individually separated REO. The high purity of the REO product and the techno-economic analysis of the process support technical feasibility and economic viability of REE extraction from coal-based resources.

REEs are used in many advanced energy, defense, and high-tech applications and industries, Courtesy of NETL REE-CM Website

LEVERAGING NATIONAL LABORATORY EXPERTISE

National laboratories, including National Energy Technology Laboratory (NETL), Los Alamos National Laboratory (LANL), Idaho National Laboratory (INL), Lawrence Livermore National Laboratory (LLNL), and Pacific Northwest National Laboratory (PNNL), are enhancing REE-CM technology development in materials characterization, sensor development, and separation processes.

NETL LIBS Sensor

Mars Land Rover to Use LANL LIBS Sensor, *Courtesy of LANL*

LANL LIBS-Raman Sensor, *Courtesy of LANL*

NETL Fiber Optic Sensor

- LANL utilizes laser-induced breakdown spectroscopy (LIBS) technology developed for the Mars Land Rover to produce a lightweight backpack LIBS to advance rapid characterization of promising coal-based REE resources, significantly reducing characterization costs and time.
- LANL demonstrates actinide separation technology transfer to lanthanide (REE) extraction from coal-based resources.
- NETL's Research & Innovation Center's REE Sedimentary Resource Assessment Method is a first-of-its-kind, big-data, machine learning (ML)-enabled, geoscience approach to improve prediction and identification of domestic coal-based resources and deposit locations with high REE and CM concentrations.

These achievements in 2020 lay the foundation for accelerated RD&D to produce 1–3 tonnes MREO/day in engineering prototype facilities to enable future REE-CM commercialization.

PARTNERS

West Virginia University · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Virginia Tech · Idaho National Laboratory · Battelle · Pacific Northwest National Laboratory · Physical Sciences Inc. · Winner Water Services · UND University of North Dakota · Rare Earth Salts · University of Kentucky

COAL FIRST COMPLETED SEVEN PRE-FEED STUDIES, INITIATED CRITICAL COMPONENTS R&D, AND SELECTED PILOT TEST ENGINEERING STUDIES

Next generation coal-fired power plants will be cleaner, more efficient, stable, and adaptive to meet the nation's future electricity needs.

COAL FIRST (FLEXIBLE, INNOVATIVE, RESILIENT, SMALL, TRANSFORMATIVE) INITIATIVE – DEVELOPING THE COAL POWER PLANT OF THE FUTURE

Flexible
Innovative
Resilient
Small
Transformative

Coal FIRST will integrate critical R&D on power plant components with currently available technologies into a first-of-a-kind system to make electricity and hydrogen energy plants more adaptive to the modern electrical grid.

Plants would be small and modular, cost less to build, have near-zero emissions, and located strategically to provide extra stability to the grid. The smaller power plant of the future would provide highly efficient, cleaner, stable power to meet the needs of an everchanging electricity grid.

PRE-FRONT END ENGINEERING DESIGN (PRE-FEED) STUDIES ESTABLISH BENCHMARKS FOR THE COAL PLANT OF THE FUTURE

Under the Coal FIRST Initiative, technology developers, architect engineers, and researchers have completed seven pre-FEED studies, a significant step for the Coal FIRST initiative.

The analysis and conclusions in these studies provided a critical starting point to advance Coal FIRST plant concepts to FEED studies for pilot testing and R&D on critical components. Final Pre-FEED studies on the Coal FIRST plant concepts can be found at: *https://netl.doe.gov/coal/tpg/coalfirst/concept-reports*.

CRITICAL COMPONENTS RESEARCH LEADS THE WAY TO NEXT GENERATION OF COAL-FIRED POWER PLANTS

NETL awarded seven projects to undertake critical R&D on power plant components that can be integrated with currently available technologies into a first-of-a-kind system to make coal-fired power plants more adaptive to the modern electrical grid.

FOA-0002057 - Critical Components Projects

FOUR PLANT CONCEPTS SELECTED FOR EVALUATION OF COAL FIRST PILOTS

NETL selected four projects to complete FEED studies and prepare these systems for pilot testing or commercial deployment. These projects are developing 21st century electricity and hydrogen energy plants that have net-zero carbon emissions and will be fueled by coal, natural gas, biomass, and waste plastics and incorporate carbon capture, utilization and storage (CCUS) technologies.

FOA-0002180 - FEED Study Projects

PROJECT BUDGET
DOE FUNDING

$125.9M

- FEED STUDIES............ est. $82,100,000
- CRITICAL COMPS $36,228,976
- PRE-FEED STUDIES............. $7,589,275

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VENKAT VENKATARAMAN

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

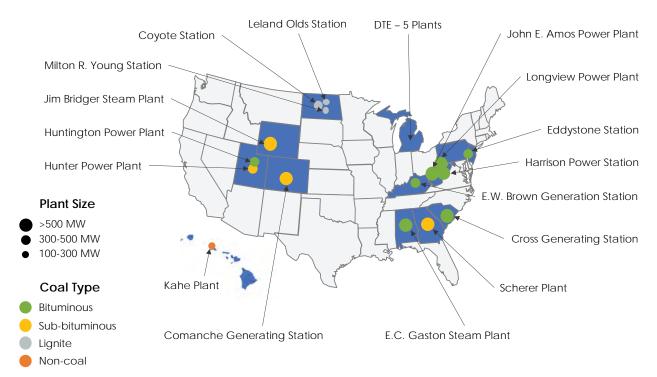PROGRAM EXECUTION and INTEGRATION

SYSTEMS ENGINEERING and ANALYSIS

WIDESPREAD INDUSTRY TESTING DRIVING CRITICAL R&D ON EXISTING COAL-FIRED FLEET TECHNOLOGIES

Partnering with utility providers to advance technologies for improved performance and reduced cost – boosting fleet efficiency, longevity, and competitiveness of coal-fired power plants across the U.S.

DEVELOPING TECHNOLOGIES WITH INDUSTRY TO IMPROVE FLEXIBILITY, RELIABILITY, AND EFFICIENCY OF COAL-FIRED POWER PLANTS

Researchers in industry, NETL, and academia have partnered with 19 utilities to perform testing and research at 21 power plants across the U.S. to improve the flexibility, reliability, and efficiency of existing and new coal-fired power plants. These field tests are focused on advanced sensors for temperature, corrosion, ash deposition, and online coal analysis; improved load-following capability, energy storage, efficiency improvements, intelligent controls, condition-based monitoring, component performance improvement, advanced component and system modeling; and technologies using artificial intelligence, machine learning, and data analytics.

Leland Olds Station
Coyote Station
DTE – 5 Plants
John E. Amos Power Plant
Milton R. Young Station
Longview Power Plant
Jim Bridger Steam Plant
Huntington Power Plant
Eddystone Station
Hunter Power Plant
Harrison Power Station
E.W. Brown Generation Station
Cross Generating Station
Kahe Plant
Scherer Plant
Comanche Generating Station
E.C. Gaston Steam Plant

Plant Size
- ● >500 MW
- ● 300-500 MW
- ● 100-300 MW

Coal Type
- ● Bituminous
- ● Sub-bituminous
- ● Lignite
- ● Non-coal

Advanced technologies are being tested at existing coal-fired power plants ranging in size from 135 MW to 952 MW. These tests include a wide range of coals (bituminous, sub-bituminous, and lignite), boiler types (cyclone-fired, opposed-wall fired, and tangential-fired configurations), and steam conditions (sub-critical, supercritical, and ultra-supercritical).

UTILITY PARTNERS

IMPROVING THE EXISTING COAL FLEET

The Improvements for Existing Plants R&D initiative includes over $65M of federal funding totaling over $80M of cost shared R&D. Across 31 projects, recent achievements include:

- ✓ Installation of an extended low-load boiler system
- ✓ Testing of an online coal tracker with combustion system performance prediction
- ✓ Testing of wireless temperature and corrosion sensors
- ✓ Testing of ultrasonic sensors for real-time temperature profiles
- ✓ Detecting and diagnosing premature equipment failure using machine learning
- ✓ Testing improved condenser coating technology

PROJECT PERFORMERS

Industry's widespread involvement in this R&D establishes the relevance and importance of the technologies to the existing U.S. coal-fired power generation fleet and to the Coal FIRST Initiative.

RESEARCH PARTNERS

AWARD NUMBERS
DE-FOA-0001989
DE-FOA-0001728
DE-FOA-0001686

PROJECT BUDGET
TOTAL AWARD VALUE
$80.3M
DOE FUNDING
$66.7M

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VENKAT VENKATARAMAN

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

PROGRAM EXECUTION and INTEGRATION

SYSTEMS ENGINEERING and ANALYSIS

TESTING CONFIRMS LONG-TERM VIABILITY OF INNOVATIVE SOLID OXIDE FUEL CELL (SOFC) SYSTEMS

Innovative research and prototype testing to develop a combustion-free method of power generation

INTEGRATED PROTOTYPE SYSTEMS ADVANCE SOFC TECHNOLOGY TOWARDS COMMERCIAL READINESS FOR NATURAL GAS-FUELED DISTRIBUTED GENERATION POWER

This prototype testing is an important intermediate step toward viable SOFC technology for large-scale coal and natural gas fueled power applications.

SOLID OXIDE FUEL CELLS PROVIDE EFFICIENT, LOW-COST ENERGY

Solid oxide fuel cells are electrochemical devices that directly convert the chemical energy in fuels into electrical energy—eliminating steps required for conventional energy conversion systems.

Solid oxide fuel cell systems are capable of operating with natural gas or coal-based fuel, and do not require combustion of the fuel to produce heat and the associated thermal and mechanical steps to produce electrical power.

FUELCELL ENERGY COMPLETES TARGET 5,000 HOURS OF TESTING

The fully integrated SOFC prototype system was built, installed, and has completed long-term testing to prove multiple performance parameters.

The prototype 200 kWe SOFC power system incorporates current technologies and operates under a range of conditions, assessing system durability, performance, and operating costs toward commercial readiness. The grid-connected system was tested on natural gas.

BENEFITS OF SOLID OXIDE FUEL CELLS

» **Higher efficiency**

» **Fuel flexibility**

» **Low water use**

» **Ease of CO_2 capture**

» **Lower emissions**

» **Modularity**

CUMMINS/CERES POWER COMPLETE TARGET 1,000 HOURS OPERATION ON 10 kWe INTEGRATED SYSTEM

Proving an Innovative Fuel Cell Concept

- Larger active cell area to achieve integrated, compact, low-cost stack

- Modular stack platform readily scalable

- Data Center compatible

Testing Campaign Shows Long-Term SOFC System Performance

PARTNERS

FuelCell Energy

Pacific Northwest NATIONAL LABORATORY

UCONN UNIVERSITY OF CONNECTICUT

Cummins

CeresPower®

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

PROGRAM EXECUTION and INTEGRATION

NETL RESEARCH INNOVATION CENTER (RIC) OPERATES A FIRST-OF-ITS-KIND WATER-COOLED H$_2$/AIR ROTATING DETONATION ENGINE (RDE) COUPLED WITH MACHINE LEARNING
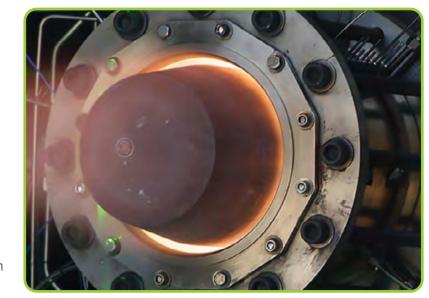
New rotating detonation combustion rig puts NETL at the forefront of pressure gain combustion research with extended duration testing.

EFFICIENCIES SURPASS CONVENTIONAL ENGINES

Reducing losses with RDEs

Performance improvements from integrating pressure gain combustion with combustion gas turbines can be further increased by incorporating RDEs, achieving a combined cycle efficiency equal to or greater than the DOE target of 65%.

The rapid detonation of RDEs initiate a steady, self-sustaining detonation wave that uses fuel more efficiently and improves scalability and turn-down performance. It also eliminates the need for purge and fill events as well as complicated valving, which contribute to process inefficiencies.
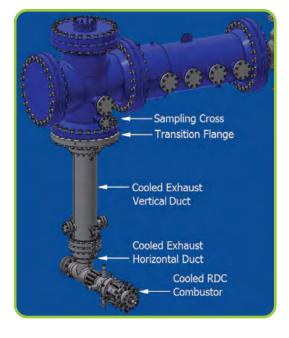
FIRST-OF-A-KIND ROTATING DETONATION RIG

NETL operated a rig that allows for extended duration testing

- Increased thermal stability allows for study of steady and transient state operation.
- Unique equipment positions NETL to better understand detonation wave stability and transitioning between operational conditions and fuel compositions.

Sampling Cross
Transition Flange
Cooled Exhaust Vertical Duct
Cooled Exhaust Horizontal Duct
Cooled RDC Combustor

RDE OVERCOMES RESEARCH LIMITATIONS

Stable performance provides crucial data

- Current RDE combustors operate at atmospheric pressure, and only for a few seconds, due to the excessive heat that is generated.
- Longer performance research is critical to transition this technology from research to a marketable product.
- Early in FY20, NETL researchers began to operate a first-of-its-kind water-cooled H$_2$/Air RDE that can be operated at elevated pressures and have adequate time to reach a stable operating temperature.

TOOLS TO LOWER COSTS IN PRACTICAL APPLICATIONS

Advanced tools used for real-time diagnostics

NETL RIC researchers have also developed a new method to extract detonation wave mode characteristics utilizing machine vision / deep learning algorithms. This will lead to a first-of-its-kind, real-time diagnostic for RDE to help to advance RDE technology into practical applications.

In stationary gas turbine combined cycle applications, there is the potential to realize a 2–4% increase in efficiency as well as a reduction in cost of electricity.

Coolant Injection Hole

PARTNERS

University of Central Florida

UNIVERSITY OF MICHIGAN

PURDUE UNIVERSITY

AUTOMATED OPTIMIZATION OF sCO₂ POWER PLANT DESIGNS MINIMIZES COST OF ELECTRICITY

Systems analyses at NETL's Research and Innovation Center determine optimized plant designs for increased efficiency and reduced energy costs using supercritical carbon dioxide power cycles.

NETL AT FOREFRONT OF sCO₂ POWER CYCLE DEVELOPMENT AND ANALYSIS
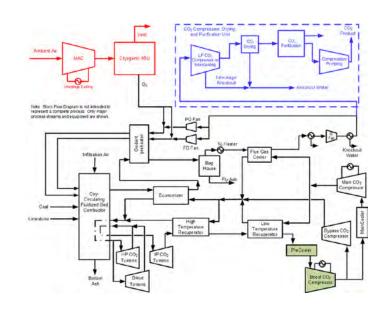
NETL's Systems Engineering & Analysis group is leading efforts to perform technoeconomic analyses on various configurations of super-critical carbon dioxide (sCO_2)-based power plants to quantify the benefits of this novel technology compared to current technologies and optimize designs of plants to minimize levelized cost of electricity (LCOE).
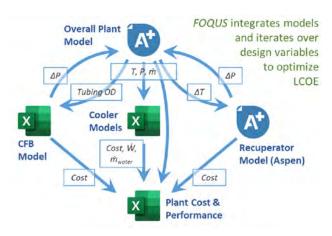
sCO₂ POWER CYCLES OFFER POTENTIAL FOR LOWER COST POWER GENERATION WITH IMPROVED EFFICIENCIES

» **Higher efficiency** » **Lower LCOE** » **Enables cost-effective carbon capture** » **Reduced water use**

First of a kind study using automated optimization solvers to minimize LCOE for sCO₂ power plants *using 12-17 global plant design variables*

Optimized coal-fired indirect sCO₂ power plant designs identified

Developed truly optimized indirect sCO_2 coal-fired power plant designs with respect to LCOE. The models were integrated using the Framework for Optimization and Quantification of Uncertainty (FOQUS), from the Carbon Capture Simulation Initiative Toolset, to perform automated sCO_2 plant design optimization.

Integrated the detailed component cost and performance models and lessons learned from prior studies to conduct a global plant optimization
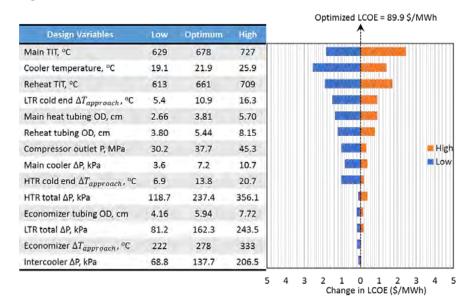
This sophisticated LCOE optimization modeling work also developed performance and cost modeling tools for various components of sCO_2 power cycles, including recuperators, coal-fired circulating fluidized bed primary heaters, and sCO_2 cycle coolers.

KEY STUDIES IMPROVE ECONOMICS AND COMMERCIALIZATION POTENTIAL FOR sCO₂ POWER CYCLES
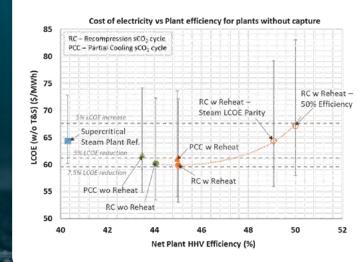
Coal-Fired sCO₂ Power Plant Designs Exceed Performance Of Reference Pulverized Coal Supercritical Steam Plant:

1 WITH CARBON CAPTURE AND STORAGE (CCS)
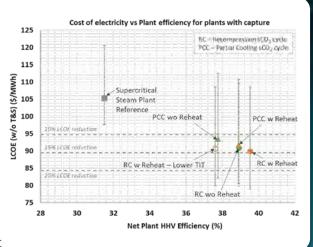
- The best-performing sCO_2 plant with CCS has a higher heating value (HHV) efficiency of 39.5% and an LCOE of $89.9/MWh, about 15% lower than the reference supercritical steam plant with CCS (case Rev4 B12B).
- Optimal turbine inlet temperatures for reheat cases are 650-685 °C with IN740H heater tubing material. Non-reheat cases are ~30 °C higher.

2 WITHOUT CARBON CAPTURE AND STORAGE

The sCO_2 plant without CCS has an HHV efficiency of 45% and an LCOE of $59.9/MWh, 7% lower than the reference supercritical steam cycle case (Rev4 B12A).
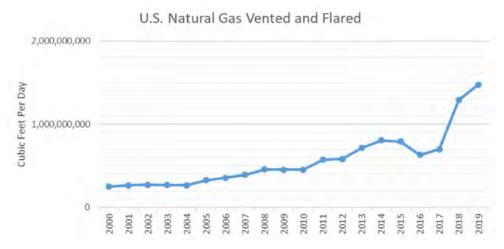
NETL'S NEW NATURAL GAS UPCYCLING PROGRAM ACCELERATES PROFITABLE UTILIZATION OF FLARED NATURAL GAS

Transformative natural gas conversion technologies allow for operators to fully leverage our domestic resources.

FROM WASTED RESOURCE TO BENEFICIAL USE
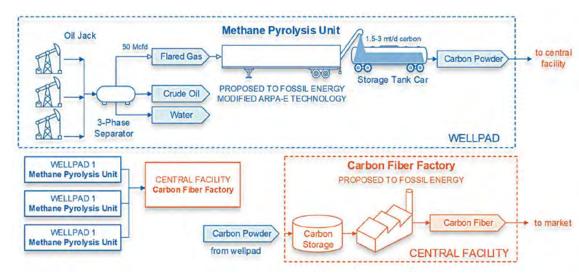
Lack of infrastructure and a high oil-to-gas price ratio can drive operators across the United States to discard natural gas by combusting it in flares. The unprocessed gas is flared or vented at a rate of over a billion cubic feet each day, unfavorably affecting the environment while wasting the heat content of our cleanest burning natural resource. The U.S. Department of Energy (DOE) and NETL's new Natural Gas Upcycling Program aims to find technology-based solutions to convert this wasted resource into beneficial products with high economic value.

U.S. Energy Information Administration Natural Gas Gross Withdrawals and Production – Vented and Flared 2000–2019

RESEARCH AND DEVELOPMENT FOCUSED ON FINDING TECHNOLOGY-BASED SOLUTIONS TO ASSOCIATED NATURAL GAS FLARING

DOE is developing new materials, equipment, and processes to enable conversion of natural gas into valuable products that can be economically transported to market. These advancements will be integrated into small-scale modular systems that can be moved from one well location to the next, allowing operators to monetize the gas rather than wasting it.

Proposed Process by Palo Alto Research Center Inc., *Courtesy Dr. Jessy Rivest*

PROCESS INTENSIFICATION AND CATALYST DESIGN FOR MODULAR GAS-TO-LIQUIDS PROCESSES
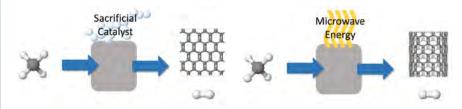
Projects led by Clemson, Stanford, NC State, Notre Dame, the University of Maryland, the University of South Carolina, and NETL are developing new reactor designs for efficient conversion of natural gas into liquid products like benzene, toluene, xylene, and methanol, and key precursors like ethylene and propylene. Nano-engineered catalyst structures and precisely integrated process steps enable modular chemical conversions powered by revolutionary processes that can produce electricity or hydrogen, are self-driven by generating their own heat energy, use highly-tuned plasma to precisely target chemical bonds, and can even use normal sunlight to drive their reactions.

Autothermal benzene synthesis proposed by NC State University and photocatalytic methanol synthesis proposed by Stanford University

ENHANCED MODULAR PRODUCTION OF SOLID CARBON PRODUCTS FROM NATURAL GAS

Scale-up of pyrolysis-based processes to create solid carbon nanoproducts from natural gas is underway at West Virginia University (WVU), the University of Colorado, Palo Alto Research Center (PARC), and NETL. The processes produce products such as low-cost, automotive-grade carbon fiber and high-quality carbon fiber structural additives and can target specific nanotube structures. The remote reactors leverage advanced aerogel-based catalysts and molten-phase metallic seeding, and benefit through new mechanisms of carbon structure assembly and through the elimination or redesign of catalyst separation steps.

Carbon fiber chemical vapor deposition process proposed by University of Colorado and plasma catalytic process for nanotube creation by WVU

PARTNERS

PROJECT BUDGET

TOTAL AWARD FUNDING

$35.9M

● DOE	$16,064,805
● WVU	$3,791,212
● CU	$3,750,000
● PARC	$3,362,361
● NETL RIC	$1,375,000
● UMD	$1,292,515
● UofSC	$1,261,624
● NCSU	$1,256,191
● STANFORD	$1,250,000
● CLEMSON	$1,250,000
● ND	$1,249,998

FY20 FUNDING
$7.5M

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CORE COMPETENCIES

 ENERGY CONVERSION ENGINEERING

 PROGRAM EXECUTION and INTEGRATION

NETL'S SMART INITIATIVE IMPROVES RECOVERY EFFICIENCY FROM UNCONVENTIONAL NATURAL GAS RESERVOIRS

Science-informed machine learning unlocks real-time information, leading to dramatic improvements in subsurface visualization, dynamic forecasting, and autonomous control.

ADVANCED DATA CONCEPTS UNLOCK OUR ABILITY TO CHARACTERIZE AND MANAGE UNCONVENTIONAL RESOURCES

The **Science-informed Machine Learning for Accelerating Real-Time** Decisions in Subsurface Applications (SMART) Initiative is a ten-year, multi-organizational effort that is transforming understanding of the subsurface through real-time visualization, forecasting, and virtual learning.

The SMART Initiative is funded (in part) by the Department of Energy's Upstream Oil & Gas Programs to transform how people interact with subsurface data, improving the efficiency and effectiveness of exploration and production operations by application of science-based machine learning and data analytics.

Real-Time Visualization
"CT" for the Subsurface

Enable dramatic improvements in the visualization of key subsurface features and flows by exploiting machine learning to improve speed and enhance detail.
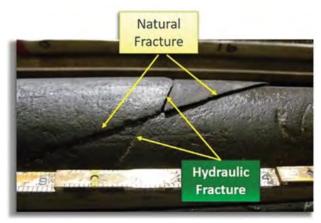
Real-Time Forecasting
"Advanced Control Room"

Develop a computer-based experiential learning environment to improve field development and monitoring strategies.

VISUALIZING FAULTS AND FRACTURE NETWORKS: A VITAL TOOL FOR IMPROVING WELL COMPLETIONS

Better understanding the nature and dynamics of fractures within unconventional reservoirs is a critical factor in optimizing well completion design and improving recovery efficiency. A fundamental element to better understand these fractures will be to leverage data, physics-based modeling, and machine learning to visualize fracture networks and fluid flow within these reservoirs.

Natural Fracture

Hydraulic Fracture

Core section showing natural and hydraulic fractures from the Hydraulic Fracture Test Site

The project team is focused on:
- Testing physics-based modeling platforms as a mechanism for fracture stimulation and subsurface signal generation
- Testing and implementing machine learning technologies to accelerate and optimize fracture visualization
- Testing and implementing history matching elements for fluid flow visualization
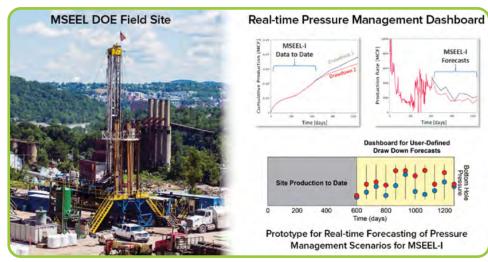
LEVERAGING HISTORY MATCHING AND DATA ANALYTICS TO FORECAST UNCONVENTIONAL RESERVOIR PERFORMANCE

Pressure management is an important process for maintaining production in unconventional reservoirs but is not well understood, as reservoir dynamics are fracture driven. The SMART team seeks to improve production efficiency from unconventional reservoirs by building a toolset to help answer the following questions:

- Are there potential pathways to "real-time" forecasting of reservoir performance in a fractured reservoir?
- Can synthetic data from conventional reservoir and discrete fracture simulators be used to train machine learning algorithms to forecast production parameters?
- Can science-informed machine learning be used to interpret distributed temperature system data to provide stage-specific production data? Can these data be used in history matching reservoir properties?

These workflows will be developed and tested using data from the DOE-funded field laboratories, starting with the Marcellus Shale Energy and Environment Laboratory (MSEEL) near Morgantown, West Virginia.

MSEEL DOE Field Site | Real-time Pressure Management Dashboard

Prototype for Real-time Forecasting of Pressure Management Scenarios for MSEEL-I

Prototype Dashboard for Real-time Pressure Management at MSEEL

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CORE COMPETENCIES

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

SYSTEMS ENGINEERING and ANALYSIS

PARTNERS

Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY

A&M

West Virginia University

BERKELEY LAB

EERC

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F A C T

UTILIZED SUPPLY CHAIN ASSESSMENTS TO ESTABLISH HIGH-TECH WORKFORCE JOB TRAINING IN THE APPALACHIAN REGION

Implementing supply chain analyses to identify domestic market opportunities and partner with the Appalachian Regional Commission on their procurement strategy

DEVELOPING HIGH-TEMPERATURE MATERIALS ASSESSMENTS TO IDENTIFY OPPORTUNITIES

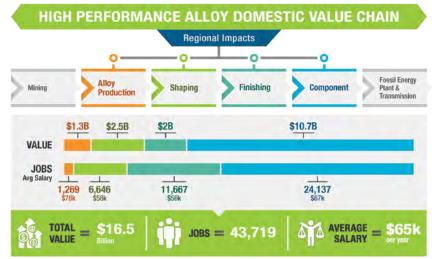NETL's High Performance Materials (HPM) program created numerous assessments on the high-temperature materials ecosystem including supply chain function, entities, jobs, Gross Domestic Product contributions, non-FE domestic markets, and location. These assessments highlighted:

- The economic value created at each step of the supply chain
- The domestic market opportunities for high-temperature alloys outside of fossil energy (FE) applications, which can provide guidance and insight to the program outside of a coal focus

High-Temperature Materials Supply Chain Assessment

LEVERAGING HIGH-TEMPERATURE MATERIALS KNOWLEDGE TO CREATE WORKFORCE DEVELOPMENT OPPORTUNITY

Using the findings from the high-temperature materials assessments as well as stakeholder engagement, the HPM program conducted a deep dive into workforce development program opportunities for welding to determine what gaps existed in training for the welders in the power industry.

ADVANCING WELDING SKILLS TO CREATE A WORKFORCE FOR THE FUTURE

Utilizing the knowledge from the workforce development program deep dive and the high-temperature materials assessments, NETL released a Request for Information (RFI) on workforce development needs within the high-performance materials supply chain which, led to a partnership with the Appalachian Regional Commission (ARC) to establish a job-training program.

In creating this program, NETL identified welding in the power industry as a high wage career opportunity. Thus, the program aims to:

- Create a workforce to install and service superalloy components in next-generation fossil-fueled power plants
- Meet the demand for welders with similar skills in the automotive and aerospace industries
- Prepare workers for long careers in growing or emerging industries
- Produce a well-trained workforce for good-paying jobs that support cleaner coal and gas power plants across Appalachia

ARC, in partnership with NETL, released a procurement action in the form of a Request for Proposals inviting other organizations to develop similar training programs.

NETL issued an RFI that led to their partnership with ARC

PARTNERS

CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

SYSTEMS ENGINEERING and ANALYSIS

NETL ESTABLISHED NEW ENERGY STORAGE PROGRAM TO ACCELERATE DEVELOPMENT OF ENERGY STORAGE TECHNOLOGIES

Identifying promising energy storage technologies that can be integrated with fossil energy assets to further the resiliency and flexibility of U.S. energy networks

THE FUTURE OF ELECTRICITY DEPENDS ON ENERGY STORAGE

Energy storage is integral to introducing both resiliency and flexibility to electricity networks and will continue to enable extraction of the maximum economic value from the Nation's fossil-fueled energy system assets, which have been historically challenged by intermittency.

MANAGING THE NEW ENERGY STORAGE PROGRAM

In Fiscal Year 2020, NETL was chosen by Department of Energy's (DOE) Office of Fossil Energy to establish and manage the Energy Storage program in order to accelerate the development of next-generation energy storage technologies. Under this program, NETL will work to develop an R&D roadmap to 2030 for a broad suite of storage technologies.

The goals of the Energy Storage Program include:

- Contribute to grid stability by accommodating for the variability in renewable energy availability
- Provide reliable fossil-based assets by leveraging and extending ongoing energy storage technology development
- Ensure reliable supplies of affordable, clean energy by recovering waste heat and enabling the optimal environmental footprint of base-load power plants

ACCELERATING NEXT GENERATION ENERGY STORAGE TECHNOLOGIES

DOE Energy Storage Grand Challenge

The critical undertaking of managing the Energy Storage program was a part of the Energy Storage Grand Challenge (ESGC), a comprehensive DOE program to accelerate the development, commercialization, and utilization of next-generation energy storage technologies.

NETL worked in close coordination with the ESGC, participating in an Request for Information (RFI) to provide comments and feedback on the ESGC Roadmap draft and leading the authorship on Use Case 6 on Facility Flexibility, Efficiency, and Value Enhancement, which directly impacted the program.

Energy Storage Grand Challenge Priorities

Technology Development	Manufacturing & Supply Chain	Technology Transitions	Policy & Valuation	Workforce Development
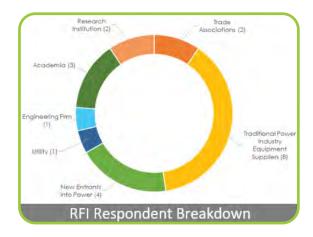
ASSESSING GAPS IN ENERGY STORAGE
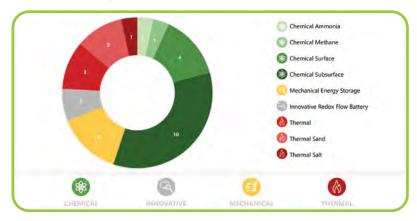
To kick off the new program, NETL released a RFI for energy storage opportunities and research needs that could lead to advances in energy storage technologies. The RFI aimed to identify and assess technology and knowledge gaps in energy storage.

Through the RFI, NETL engaged with numerous stakeholders in the energy storage space with a total of 23 individual responses from 21 different entities. It built upon the stakeholder outreach by holding a United States Energy Association webinar in which over 400 attendees registered, including many influential thought leaders in the space.

RFI Respondent Breakdown

MANAGING AN ENERGY STORAGE PROJECT PORTFOLIO

The DOE selected 29 projects to receive nearly $7.6 million in federal funding for research and development in advanced energy storage technologies. NETL will manage the projects and conduct a portfolio assessment for future pilot studies.

PARTNERS

CEATI INTERNATIONAL · EPRI · gti · ILLINOIS · SIEMENS · Southern Company · SwRI · USEA United States Energy Association

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

SYSTEMS ENGINEERING and ANALYSIS

NETL HELPS LEAD INTERNATIONAL CARBON CAPTURE AND UTILIZATION (CCU) ASSESSMENT HARMONIZATION GROUP
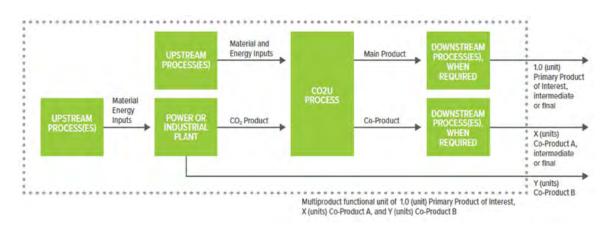
Aligning Carbon Utilization Life Cycle Analysis best practices between the European and U.S. research communities.

THERE ARE MANY PATHWAYS FOR TURNING CO_2 INTO USEFUL PRODUCTS

ENSURING A GLOBALLY CONSISTENT APPROACH TO ASSESSING LIFE CYCLE OF CARBON UTILIZATION PATHWAYS

NETL's Life Cycle Analysis competency, within the Research and Innovation Center, has teamed with the Global Carbon Utilization Initiative (GCI) led by the University of Michigan to lead a diverse group of 30 international researchers to **harmonize** the U.S. Department of Energy, Office of Fossil Energy **NETL LCA guidance** with the **GCI guidance** developed by the Technische Universität Berlin, RWTH Aachen University, The University of Sheffield, Institute for Advanced Sustainability Studies in Potsdam, and CO_2 Sciences Inc.

GATHERING GLOBAL LEADERS IN LIFE CYCLE ANALYSIS AND TECHNO-ECONOMIC ANALYSIS TO ACHIEVE DOE MISSION
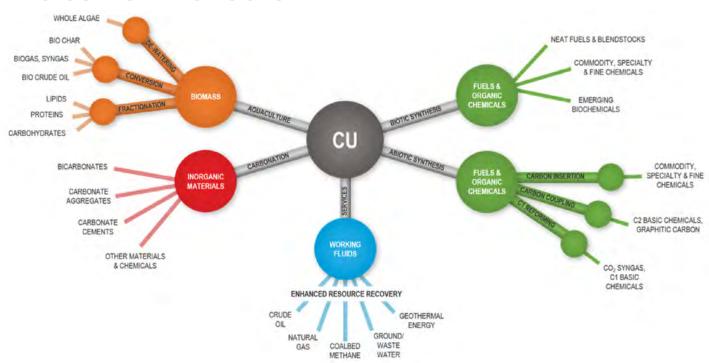
In addition to the aforementioned development organizations, the International CCU Assessment Harmonization Group includes participants from the Department of Energy's Office of Fossil Energy, Office of Energy Efficiency and Renewable Energy, Argonne National Laboratory, National Renewable Energy Laboratory, and the National Research Council of Canada.

Promoting research, development, and commercialization of carbon capture, utilization, and storage technologies requires assessing the environmental and economic opportunities and risks. Life cycle assessments and techno-economic assessments are means to quantify these opportunities and risks. **For consistent conduct and transparent reporting, a common framework is needed**. The mission of the International CCU Assessment Harmonization Group is to create this common framework by bringing together related efforts, analyzing differences, and seeking to eliminate them where possible. This effort will help enable the Department of Energy to achieve the mission of discovering and maturing technologies to ensure environmentally sustainable solutions for the use of captured carbon dioxide to reduce greenhouse gas emissions.

VISIT *www.netl.doe.gov/LCA/CO2U*

PARTNERS

CORE COMPETENCIES

PROGRAM EXECUTION and INTEGRATION

SYSTEMS ENGINEERING and ANALYSIS

MARKET ANALYSIS HIGHLIGHTS EXCITING NEW GROWTH MARKETS FOR COAL

Informing stakeholders of high-impact products and markets for carbon products from coal that are beyond traditional power and heat applications.
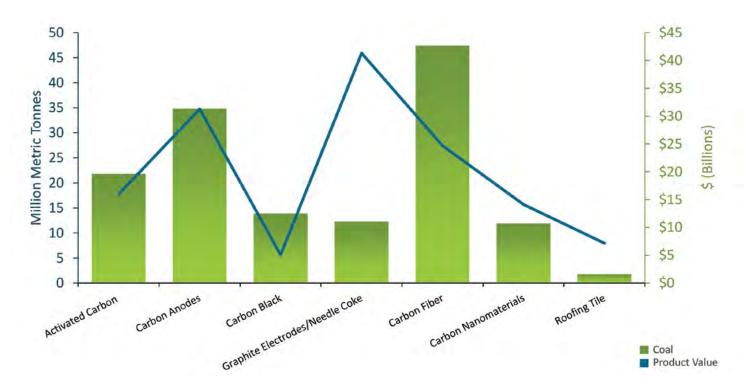
ASSESSING THE MARKET POTENTIAL OF CARBON PRODUCTS FROM COAL

NETL's Energy Markets Analysis Team developed a comprehensive market analysis with quantitative estimates of market size and growth for carbon products, and information on producers, importers, exporters, and the potential for coal-derived carbon products to satisfy this demand, as well as barriers to market entry.

The analysis already has informed programmatic decisions about future research directions and has highlighted markets that can consume significant amounts of coal exclusive of traditional thermal and metallurgical applications.
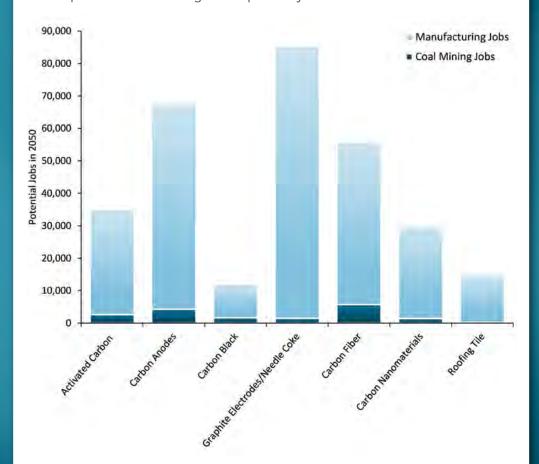
MARKET ANALYSIS IDENTIFIES HIGH-VALUE PRODUCTS WITH POTENTIAL TO UTILIZE MILLIONS OF TONNES OF DOMESTIC COAL

NETL's analysis of coal-based products indicates the potential for utilizing over 145 million metric tonnes of coal to produce products worth over $140 billion in year 2050. The values are reported in year 2050 and represent a high coal penetration scenario of 80 percent of the overall product market. Several products (e.g., anodes and carbon fiber) represent high demand growth scenarios.

LARGE JOB GROWTH POTENTIAL IS INDICATED

NETL investigated several coal-based products and found the potential for over 17,500 coal mining jobs and over 280,000 manufacturing jobs by 2050. This analysis enables NETL to focus on developing technologies and coal-based products with the highest impact on job and value creation.

PARTNERSHIPS ENABLE ACCESS TO CUTTING-EDGE DATA

A collaborative partnership was established with Ramaco Carbon and the Oak Ridge National Laboratory to access state-of-the-art data on novel coal-based carbon fiber technologies to support a Life Cycle Analysis of light vehicle materials. Life cycle analysis evaluates the environmental footprint of rapidly emerging coal-based manufacturing technologies.

PARTNERS

TESTING CAPABILITIES EXPANDED AT NATIONAL CARBON CAPTURE CENTER AND TECHNOLOGY CENTRE MONGSTAD IN NORWAY

Construction progressed on key testing capabilities for transformational carbon capture technologies.
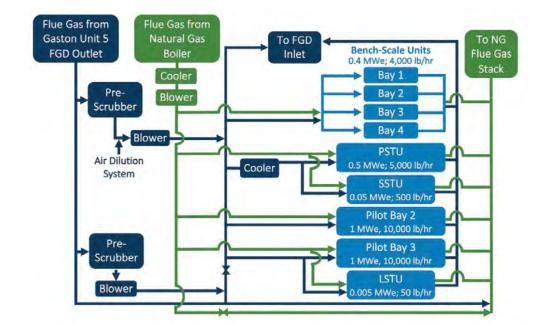
The Carbon Capture Program, which develops and optimizes carbon dioxide capture technology for industrial, coal, and natural gas sources and negative emissions technologies, supported expansion of technology testing capabilities.

NATIONAL CARBON CAPTURE CENTER

Natural Gas Flue Gas Carbon Capture

The National Carbon Capture Center (NCCC) completed construction of the natural gas infrastructure on a natural gas boiler capable of providing natural gas-derived flue gas to technology developers testing at the NCCC. The new facility will enable testing of transformational technologies for natural gas sources. This system also enables testing at the facility when the host power station, Plant Gaston, is offline. NCCC supports technology testing at laboratory, bench, and pilot scale.

Direct Air Capture

The NCCC actively pursued research agreements with national labs, universities, and other research institutions to provide a host site for direct air capture (DAC) technologies. This work will support program efforts to evaluate low-cost transformational DAC technologies.

TECHNOLOGY CENTRE MONGSTAD

Modular Transformational Carbon Capture Technologies

Program partner Technology Centre Mongstad (TCM), the world's largest pilot plant for verification of carbon capture and sequestration technologies, constructed components of a nearly-completed new facility to test modular, transformational carbon capture technologies. Testing enabled for 2021 includes NETL program-sponsored technologies developed by Membrane Technology & Research, Inc. (membrane), TDA Research, Inc. (hybrid membrane-sorbent), and Innosepra, LLC (sorbent). RTI International (solvent) will test at TCM's amine plant.

PARTNERS

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CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

ARTIFICIAL INTELLIGENCE FOR ENHANCED DATA ANALYTICS AND CONTROL OF COAL-FIRED POWER PLANTS

Advanced techniques such as artificial intelligence, data analytics, machine learning, and intelligent controls for enhanced control, monitoring, and diagnostics of power plants

DATA ANALYTICS-DRIVEN CONTROLS FOR IMPROVING EFFICIENCY, RELIABILITY, AND FLEXIBILITY OF EXISTING COAL-FIRED POWER PLANTS

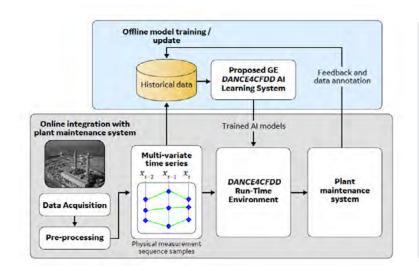NETL selected four projects to use software-based techniques such as artificial intelligence (AI) and machine learning for enhanced data analytics, improved process control, and condition-based monitoring for coal-fired power plants. AI and other methods, such as pattern recognition and predictive analytics, can help unlock and enable **improved power plant performance, reliability, and flexibility**.

AI-BASED MULTIVARIATE TIME SERIES LEARNING SYSTEM DESIGNED FOR ENHANCED FAULT DETECTION
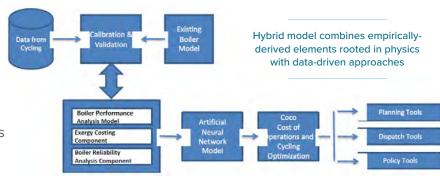

GE Research is developing the Deep Analysis Net with Causal Embedding for Coal-fired power plant Fault Detection and Diagnosis (DANCE4CFDD) system for **flexible and scalable coal power plant fault detection and root cause analysis**.

The system addresses challenges faced by today's asset health management systems for coal-fired plants with a combination of two novel components: a deep similarity net and a deep causal embedding net.

HYBRIDIZED MODELING TOOL FACILITATES FLEXIBLE, RELIABLE, AND COST COMPETITIVE COAL-BASED POWER GENERATION
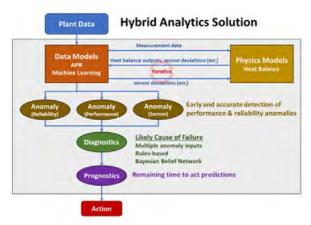
The National Rural Electric Cooperative Association is developing a Generation Plant Cost of Operations and Cycle Optimization Model (Coco) to accurately estimate the costs of cycling boilers in large coal plants.

The resource will allow large coal boilers to cycle safely to provide enhanced resiliency and reliability while utility systems accommodate increased penetration of renewable resources such as wind, solar photovoltaics, or other small generators.

Hybrid model combines empirically-derived elements rooted in physics with data-driven approaches

HYBRID ANALYTICS SOLUTION ENABLES OPTIMIZATION OF PLANT PERFORMANCE
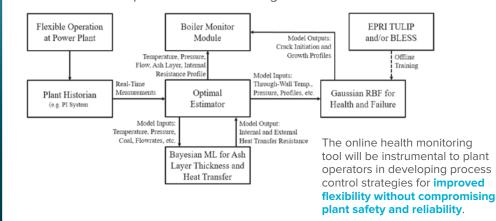
Expert Microsystems, Inc. is commercializing a hybrid analytics software tool to provide real-time information on the relationship between plant operational data and plant performance/reliability. The diagnostic platform integrates an established data-driven analytics product that includes advanced pattern recognition, machine learning, and artificial intelligence with a well-proven heat balance modeling product to create a **hybrid online monitoring solution for improving coal plant operations**.

Plant operators will be able to recognize patterns involving fuel composition, excess oxygen, air leakages, heat transfer rates, and boiler efficiency to identify "sweet-spots" for optimum performance and develop control strategies for flexible plant operation.

HYBRID FIRST PRINCIPLES-AI BASED APPROACH FOR BOILER HEALTH MONITORING

West Virginia University Research Corporation is generating an adaptive, real-time, accurate boiler health-monitoring framework that synergistically leverages physics-based/AI hybrid models and plant measurements to understand the impacts of load-following.

The online health monitoring tool will be instrumental to plant operators in developing process control strategies for **improved flexibility without compromising plant safety and reliability**.

PARTNERS

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CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING

PROGRAM EXECUTION and INTEGRATION
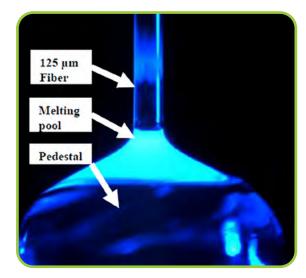
NETL'S SENSORS AND CONTROLS PROGRAM RECEIVES MULTIPLE AWARDS RECOGNIZING EXCELLENCE IN RESEARCH AND DEVELOPMENT
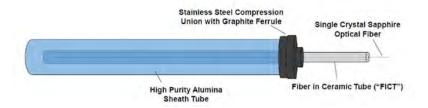
Advanced Sensors and Controls research supports condition-based monitoring of critical components to improve efficiency, reliability, and performance of fossil energy systems.

ROBUST FIBER OPTIC SENSING TECHNOLOGY IMPROVES POWER PLANT PERFORMANCE

NETL researchers received a prestigious award from Pittsburgh's Carnegie Science Center in the Innovation in Energy category for investigating single-crystal optical fibers capable of measuring numerous environmental parameters anywhere the fiber is installed — including the extreme environments of power generation systems.
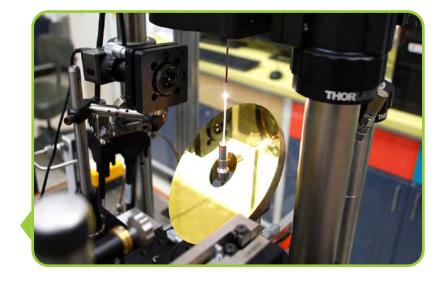
- Single-crystal optical fibers provide benefits such as greater mechanical strength, a higher laser damage threshold, power-delivering capabilities and better corrosion resistance at a reduced cost.
- Fiber optic sensors installed in a reactor or combustor can significantly **improve the efficiency and reliability of fossil energy plants**.
- The innovation has drawn significant interest from the U.S. military for use in high-energy lasers in missile defense systems.

A patent-pending computer-control algorithm invented by NETL enables the manufacture of single-crystal optical fibers of potentially infinite length, with improved diameter control and faster growth, using a laser-heated pedestal growth system.

The fibers can be used to fabricate sensors that can withstand the harsh environments of advanced energy systems.
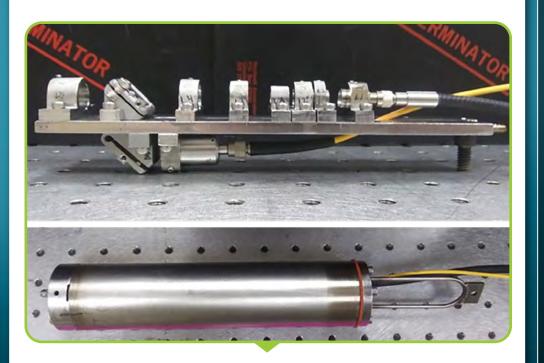
A sapphire seed crystal being lowered onto the molten sapphire rod to begin the growth of a single-crystal sapphire fiber.

ADVANCED LASER-BASED TECHNOLOGY ENABLES RAPID, PRECISE SUBSURFACE MONITORING

NETL received an R&D 100 award in the Analytical/Test category for a miniature, all-optical sensor based on laser induced breakdown spectroscopy (LIBS) that provides detailed information on elemental composition in subsurface environments.

This sensor enables the efficient performance of reliable analysis in the field without removing samples from the well, which saves time and reduces cost. Applications include carbon storage, process monitoring, rare earth element detection, and environmental monitoring.

The LIBS probe features simplified construction, reducing the cost of the laser head and maximizing the amount and quality of light returned for analysis.

Creating new monitoring systems that yield quick and effective information, even under harsh conditions in the field, builds on NETL's mission to discover and mature technology solutions that enhance the nation's energy foundation and protect the environment for future generations.

AWARD NUMBER
FWP-1022427

PROJECT BUDGETS EY20

FIBER OPTIC SENSOR
$485,000

SUBSURFACE LIBS
$335,000

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DUSTIN MCINTYRE (LIBS)

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

CARBONSAFE ACHIEVED A MAJOR MILESTONE BY ADVANCING FIVE PROJECTS INTO PHASE III

Learning-by-doing at these field projects is setting the stage for safe and reliable geologic storage of captured CO_2 on a broad scale.

ADDRESSING THE KEY CHALLENGES POSED BY CARBON CAPTURE, UTILIZATION, AND STORAGE (CCUS) DEPLOYMENT

The Carbon Storage Assurance Facility Enterprise (CarbonSAFE) Initiative:

- Demonstrates geographically widespread deployment of geologic storage with capacities of 50+ million metric tons (MMT) of CO_2.
- Provides all necessary activities to apply for and obtain a Class VI Underground Injection Control (UIC) permit-to-construct.
- Integrates CCUS projects by linking storage complexes with state-of-the-art capture technologies.

Comprised of Four Phases:

Phase I: Integrated Carbon Capture and Storage Pre-Feasibility – 13 projects awarded (Complete)

Phase II: Storage Complex Feasibility – 6 projects awarded (Active)

Phase III: Site Characterization and CO_2 Capture Assessment – 5 projects awarded (Active)

Phase IV: Construction and Permitting for Injection-Ready Operations – (Potential Future Funding)

CARBONSAFE PHASE III: ACCELERATING THE INTEGRATION OF CAPTURE AND STORAGE TECHNOLOGIES AT COMMERCIAL-SCALE SITES

Map of the contiguous U.S. showing locations of CarbonSAFE Phase III projects and Carbon Capture Program Front-End Engineering Design (FEED) studies.
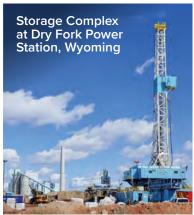
2 **MTR's Membrane CO_2 Capture Process –** MTR, Inc. Polymeric Membrane
Membrane Technology and Research

Accelerating CCUS at Dry Fork Station, Wyoming
University of Wyoming (UW)

4 **Illinois Storage Corridor**
The Board of Trustees of the University of Illinois

Retrofitting the Prairie State Generating Station with an 816 MWe Capture Plant Using Mitsubishi Heavy Industries – MHI Solvent
University of Illinois Geological Survey (ISGS)

5 **San Juan Basin CarbonSAFE:** Ensuring Safe Subsurface Storage of CO_2 in Saline Reservoirs
New Mexico Institute of Mining and Technology (NMT)

1 **North Dakota CarbonSAFE Phase III:** Site Characterization and Permitting
University of North Dakota Energy & Environmental Research Center (EERC)

Project Tundra Carbon Capture System – Fluor's amine-based Econamine FG Plus
Minnkota Power Cooperative

Large-Scale Commercial Carbon Capture Retrofit of the San Juan Generating Station – Commercial Solvent
Enchant Energy

3 **Establishing an Early CO_2 Storage Complex in Kemper County, Mississippi: Project ECO₂S**
Southern States Energy Board

Commercial Carbon Capture Design & Costing: Part Two – Ion Engineering Non-aqueous Solvent
Ion Engineering

Front-End Engineering Design Study for Retrofit Post-Combustion Carbon Capture on a Natural Gas Combined Cycle Power Plant – Fluor's amine-based Econamine FG Plus
Electric Power Research Institute

Piperazine Solvent/ Advanced Stripper Front-End Engineering Design (PZAS FEED)
University of Texas at Austin

Retrofit a 2x2x1 Natural Gas-Fired Gas Turbine Combined Cycle Power Plant for Carbon Capture Storage/ Utilization – MEA Solvent
Bechtel National

3 **Linde-BASF Advanced Post-Combustion CO_2 Capture Technology at a Southern Company Natural Gas-Fired Power Plant – Linde BASF Amine Solvent**
Southern Company Services

● CarbonSAFE Phase III Projects
● Capture Program FEED Studies
▲ Coal-based power plants
▲ Natural Gas-based power plants

THE 5 PROJECTS NOW IN PHASE III ESTABLISH OPTIMAL GEOLOGIC STORAGE LOCATIONS AND STRONG CORPORATE SUPPORT

- Comprehensive site characterization classifies the Kemper County Energy Facility as located in a world class geologic area capable of securely storing over 1,200 MMT of CO_2.
- Storage complexes in North Dakota and Wyoming have confirmed megaton storage potential from Phase II work.
- The Illinois Storage Corridor has proven geologic storage performance and numerous industrial carbon sources.
- In the San Juan region, there is stacked storage potential in alternating sequences of deep saline and oil-bearing formations.

Phase III projects successfully launched all necessary subsurface investigations to obtain six UIC Class VI permits to construct.

Storage Complex in Kemper County, Mississippi

Storage Complex at Milton R. Young Station, North Dakota

Storage Complex at Dry Fork Power Station, Wyoming

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

PROGRAM EXECUTION and INTEGRATION

PARTNERS

SOUTHERN STATES ENERGY BOARD

EERC

UNIVERSITY OF WYOMING

ILLINOIS
Illinois State Geological Survey
PRAIRIE RESEARCH INSTITUTE

NEW MEXICO TECH
SCIENCE • ENGINEERING • RESEARCH UNIVERSITY

SMART-CARBON STORAGE INITIATIVE SUCCESSFULLY LAUNCHED

Supporting near real-time decision making for geologic storage reservoirs to enable real-time visualization, real-time forecasting, and virtual learning.
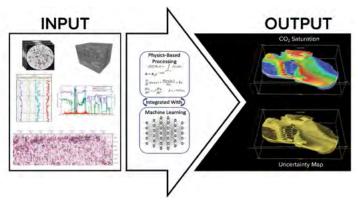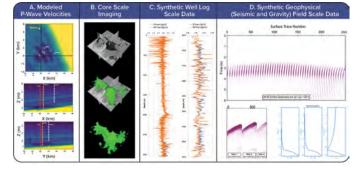
PROGRAM OVERVIEW

The Science-informed Machine Learning to Accelerate Real-Time Decisions in Subsurface Applications Carbon Storage (SMART-CS) Initiative aims to transform how people interact with subsurface data, improving decision-making, reducing costs and risk for field-scale carbon storage by application of science-based machine learning (ML) and data analytics. Impressive initial results have already been achieved in key areas by the SMART Teams.

ENABLING A 'GOOGLE EARTH FOR THE SUBSURFACE' PLATFORM

- A conceptual goal of the SMART team is to create a "Google Earth for the Subsurface" capability, allowing the user to explore geology and geography by being able to pan from the basin scale down to the pore scale.
- The team has completed an important first step towards realizing that goal by generating a comprehensive synthetic dataset for a realistic CO_2 injection site, building off the National Risk Assessment Partnership's Kimberlina 1.2 CO_2 Injection Simulation.
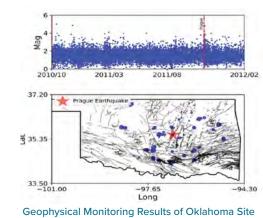
Conceptual Goal of Real-Time Visualization "Google-Earth for the Subsurface"

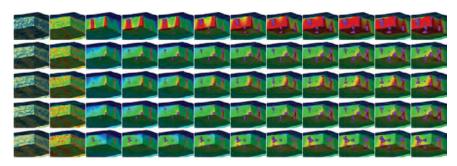Summary of Results of Generation of Synthetic Datasets

REAL-TIME IMAGING OF PRESSURE AND STRESS

- **Data Assimilation and Pressure Forecasting:** Produced a far-field pressure prediction using ensemble reservoir simulations and tested near-wellbore pressure prediction using gauge time series deconvolution.
- **ML-Enabled Geophysical Monitoring:** Developed a high accuracy convolutional neural network-based detection and location system for a site in Oklahoma to produce a more complete micro-seismicity catalog.
- **Developing a Platform to Manage Induced Seismicity Risk:** Combining stress and seismicity data with ML algorithms to develop a platform of the future to manage induced seismicity risk in a quantifiable way that is transparent to all stakeholders.

Geophysical Monitoring Results of Oklahoma Site
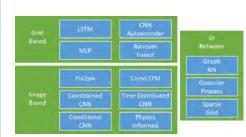
REAL-TIME FORECASTING TO OPTIMIZE CO_2 STORAGE

- Acquired and processed data to generate robust datasets for reservoir simulations of dedicated and associated storage projects; completed Phase I of training and testing ML models.
- Completed integration of three types of measurements to emulate a monitoring program.
- Developing a capability for real-time history matching and rapid prediction of reservoir performance and safety, leading to cost-saving operational decisions and improved safety and storage security.
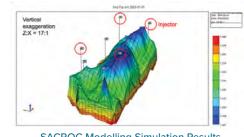
Outputs of Dedicated Storage Reservoir Simulations

CREATING A VIRTUAL LEARNING PLATFORM FOR CO_2 STORAGE

- Completed capacity scoping calculations utilizing SACROC (a carbonate reef deep saline system proxy model) to estimate optimal CO_2 storage capacity after 25 years of CO_2 injection.
- To date, the SMART Virtual Learning team has implemented rapid forecasting models using 13 different machine learning architectures on two sets of small synthetic reservoir simulation runs. These architectures range from traditional approaches (e.g., gaussian process and random forest models) to newer deep learning approaches.

13 types of ML algorithms tested for viability for virtual learning platform

SACROC Modelling Simulation Results

PARTNERS

BATTELLE · BERKELEY LAB · Carnegie Mellon University · EERC · Sandia National Laboratories · BUREAU OF ECONOMIC GEOLOGY · Los Alamos NATIONAL LABORATORY · OAK RIDGE National Laboratory · Pacific Northwest NATIONAL LABORATORY · ILLINOIS · F A C T · PennState · THE UNIVERSITY OF UTAH · COLORADO SCHOOL OF MINES · West Virginia University · UND UNIVERSITY OF NORTH DAKOTA · Lawrence Livermore National Laboratory

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CORE COMPETENCIES

- GEOLOGICAL and ENVIRONMENTAL SYSTEMS
- COMPUTATIONAL SCIENCE and ENGINEERING
- SYSTEMS ENGINEERING and ANALYSIS
- PROGRAM EXECUTION and INTEGRATION

FIRST ASSESSMENT OF STORAGE RESOURCES IN THE OFFSHORE ATLANTIC AND GULF OF MEXICO (GOM) COMPLETED

Storage resource estimates on the continental shelf off the U.S. Atlantic and Gulf coasts help advance commercial deployment of Carbon Capture and Storage.
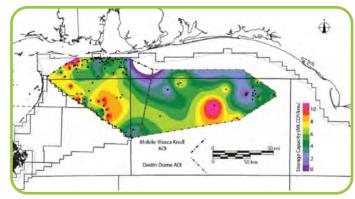
ADVANTAGES OF OFFSHORE CO_2 STORAGE

- Additional storage options for heavily populated and industrialized coastal areas while avoiding negative perceptions associated with storage beneath populated areas
- Reduced time and effort in negotiations since submerged land and mineral rights are owned by the state or federal government
- Reduced potential impacts to underground sources of drinking water since it is unlikely that fresh water will be found in strata beneath the ocean

GOM – A VAST, NATIONALLY SIGNIFICANT CO_2 STORAGE RESOURCE

Four studies focused on resource assessment of areas in the GOM. Results show a **potentially vast CO_2 storage resource** in both depleted oil and gas fields and saline formations, with aggregate storage **estimates of hundreds of billion metric tons or more**. More detailed resource studies were carried out for three locations offshore Texas and Louisiana, each capable of 30 million metric tons storage. Building on results, two Partnership projects have been undertaken to develop the knowledge required for secure, affordable, and safe large-scale offshore CO_2 storage in the GOM.
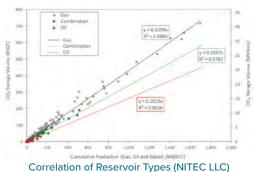

CO_2 storage resource in strata in the DeSoto Canyon Salt Basin, offshore Mississippi, Alabama, and the western Florida Panhandle (Southern States Energy Board)

RELATIONSHIP BETWEEN PRODUCTION AND CO_2 STORAGE ESTABLISHED FOR GOM OIL/GAS RESERVOIRS

Reservoir modelling showed a **strong correlation between cumulative oil/gas production and estimated CO_2 storage volumes** for the oil and gas reservoirs. The correlation showed that **significantly more CO_2 can be stored in depleted gas reservoirs than in depleted oil reservoirs** under similar conditions. The total CO_2 storage volume predicted by the studies of all 461 reservoirs is 1,129 million metric tons.

Correlation of Reservoir Types (NITEC LLC)

OFFSHORE ATLANTIC: POTENTIAL MULTI-GIGATON STORAGE RESOURCE

Still Largely Unexplored

The Atlantic Continental Shelf appears to hold **multi-Gt storage resource potential**, though many portions are largely unexplored. Three studies focused on four offshore basins that are known to have thick layers of potential storage rocks. These are the Georges Bank Basin, the Baltimore Canyon Trough, the Carolina Trough, and the Blake Plateau Basin (with Southeast Georgia Embayment).
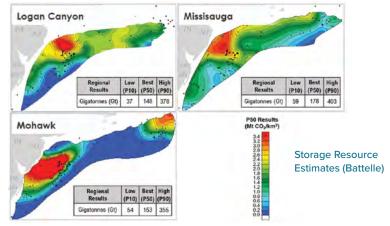

VERY PROMISING STORAGE PROSPECTS IN THE MID/NORTH ATLANTIC

The Missisauga, Logan Canyon, and Mohawk formations were identified as storage zones across the Georges Banks Basin, the Baltimore Canyon Trough, and the Long Island Platform separating the two basins. The **highest storage resource values** ($\geq$2.5 Mt CO_2/km^2) **occur near the Great Stone Dome in the Baltimore Canyon Trough** offshore New Jersey.

Storage Resource Estimates (Battelle)

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CORE COMPETENCIES

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

PROGRAM EXECUTION and INTEGRATION

PARTNERS

SOUTHERN STATES ENERGY BOARD
Transcending Boundaries

BATTELLE

TEXAS
The University of Texas at Austin

GeoMechanics Technologies

NITEC LLC

USGS, multiple industry, university, national laboratory and state geologic survey partners

GASIFICATION HANDBOOK— A MILESTONE IN PROMOTING COAL GASIFICATION-BASED SYSTEMS

Unprecedented Planning and Design Resource for Power, Hydrogen, Synthetic Natural Gas, and Liquid Fuels Advanced Coal Systems

HANDBOOK WILL SPARK DEVELOPER INTEREST IN NEW COAL GASIFICATION-BASED SYSTEMS

Defines and scopes design & development of modular coal-based gasification process plants & systems. Features detailed definitions & descriptions of systems with specific design guidelines for modules or unit operations in coal gasification process plants:

- Gasifier
- Coal handling
- Air/oxygen supply
- Syngas cleanup
- Syngas conversion
- Power/steam generation block
- Grid connection module
- Chemical conversion module
- Product upgrading
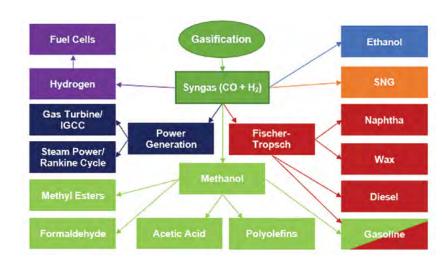- Environmental controls
- Carbon Capture and Storage

High Bay Reaction Lab, NETL
– *U.S. Department of Energy*

PROMOTES COAL USE FOR A RANGE OF POWER, FUELS, AND CHEMICALS PRODUCTION OPTIONS

Provides design aspects of varied options for coal gasification syngas-based production systems:

- Hydrogen production
- Power generation via turbines (gas combustion and steam) or reciprocating internal combustion engines
- Fischer-Tropsch fuels synthesis
- Synthetic natural gas
- Choice of types of gasifiers (entrained flow, fluidized bed, fixed bed, air or O_2 blown)

HIGHLIGHTS BEST PRACTICES TO ENHANCE PERFORMANCE, LOWER COST, AND OPEN MARKETS FOR GASIFICATION SYSTEMS

- Modular fabrication/construction, standardization, and use of "plug and play" process modules that simplify design, reduce costs, and speed project timelines
- Advantageous siting that leverages local resources, infrastructure, and markets
- Cutting-edge technologies (modeling and simulation, process intensification, and advanced manufacturing methods and materials) that provide efficiency and cost savings
- Streamlined and improved engineering and design, procurement, construction, partnering, and contracting
- Layout and engineering procedures enabling efficient O&M savings throughout plant lifecycle

Coal gasification-based integrated gasification combined cycle plant artist's conception
– *U.S. Department of Energy*

GASIFICATION SYSTEMS

FY20 FUNDING

$500K

GASIFICATION HANDBOOK
$500,000

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CORE COMPETENCIES

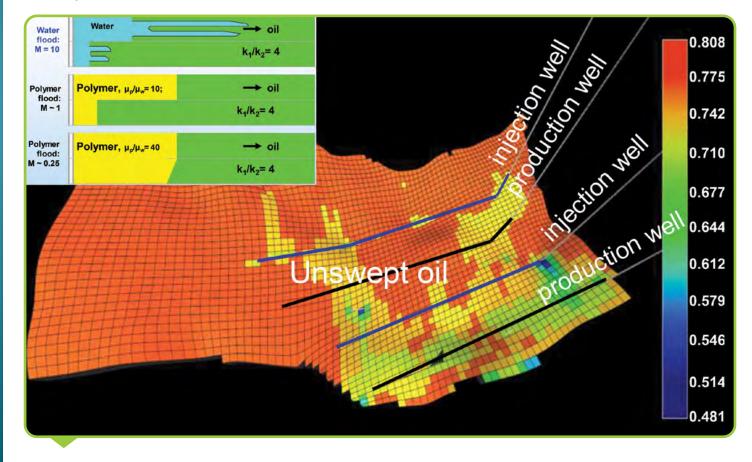ENERGY CONVERSION ENGINEERING

PROGRAM EXECUTION and INTEGRATION

POLYMER FLOODING INCREASES HEAVY OIL PRODUCTION ON ALASKA'S NORTH SLOPE

Large-Scale polymer flooding on Alaska's North Slope

IMPROVING SWEEP EFFICIENCY WITH LARGE-SCALE POLYMER FLOODING

Polymer fluid pilot testing to improve oil recovery on Alaska's North Slope has demonstrated the properties required to improve sweep efficiency and increase the volume of heavy-oil that can be produced there. This successful pilot test could enable the widespread application of the polymer flooding technology in heavy oil reservoirs on Alaska's North Slope to ensure the economic viability and operational reliability

Main Image: Reservoir simulations consist of history matching techniques of laboratory corefloods and waterfloods to optimize the polymer injection strategy for the field pilot.

Inset Image: Selection of polymer viscosity was made to overcome the permeability contrast and to make the flood mobility ratio (M) favorable, enabling efficient transport and increased production of heavy oil.

> **Results of this pilot injection project will have far-reaching implications and be useful in developing heavy oil fields throughout the North Slope.**

SUSTAINABLE PRODUCTION AND INCREASED ULTIMATE RECOVERY ACROSS THE NORTH SLOPE

Initial pilot testing demonstrated that the polymer increased production by 700 barrels of oil per day, which can significantly increase the estimated ultimate recovery of the reservoir with widespread deployment of this enhanced oil recovery method.

The polymer injection system delivered superior performance during the harsh Arctic winter when temperatures can drop to -50°F, demonstrating resiliency and ability to consistently support heavy-oil production on Alaska's North Slope.

The success of the polymer flooding technique has already provided an incremental increase in heavy oil production through more effectively sweeping the reservoir. As of August 2020, no polymer "breakthrough" has been observed at the production wells, indicating that this polymer flooding process will be a viable approach for moving more oil from Alaska's North Slope to downstream customers.
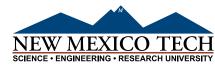
Due to the success of the pilot test, Hilcorp has implemented polymer floods on other well pads on Alaska's North Slope.

Polymer preparation equipment at NETL-supported field test on Alaska's North Slope.

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CORE COMPETENCY

PROGRAM EXECUTION and INTEGRATION

MARCELLUS SHALE FIELD LABORATORY FOCUSES ON ADVANCED CHARACTERIZATION AND COMPLETIONS
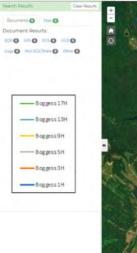
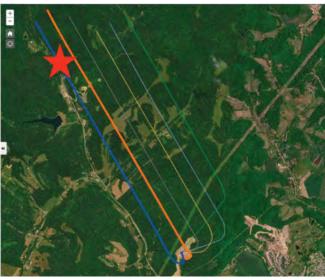Increased resource recovery through advanced modeling and improved completion techniques

WEST VIRGINIA FIELD LABORATORY USES INNOVATIVE STAGE DESIGNS TO COMPLETE HYDRAULIC FRACTURING OF SIX NEW MARCELLUS SHALE LATERALS

In late 2019, as part of the Marcellus Energy and Environment Laboratory (MSEEL) project, West Virginia University (WVU) and industry partner Northeast Natural Energy completed hydraulic fracturing of six 10,000+ foot Marcellus Shale laterals at the Boggess pad near Morgantown, WV, utilizing stimulation designs based on innovative logging techniques and advanced modeling. These advanced engineered stage and clustering designs are expected to lead to increased resource recovery. MSEEL will use the latest information technology to enable a broad, integrated program of open, collaborative science and technology development and testing.

Boggess Pad as shown in the MSEEL map viewer (*http://mseel.org/viewer/*) with the wells highlighted with colors used in subsequent production plots. The wells using the WVU completion design are the 1H and 3H with the bolder lines. The new generation permanent fiber is located in the central well (Boggess 5H, red star). A vertical pilot well (17H) was drilled, cored and logged prior to drilling the lateral.
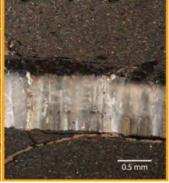
MSEEL COLLECTS AND ANALYZES SAMPLES TO IMPROVE UNDERSTANDING OF FRACTURE TRENDS WITHIN THE MARCELLUS

MSEEL retrieved 139 feet of 4-inch whole round core and 50 sidewall cores from the Boggess 17H pilot well. The core was delivered to NETL for CT imaging and core logging. Core samples from Boggess 17H were collected and crushed to 200 mesh size, and kerogen was isolated using chemical and physical separation techniques. MSEEL is integrating the core data received from the Schlumberger/Terra Tek lab and using that data to improve frack stage design, revise the production analysis, and to prepare for flow simulation in the Marcellus Shale.

Examples of the numerous calcite- and bitumen-filled fractures observed in the core from the MIP 3H pilot well. These fractures appear to influence hydraulic fracture stimulation efficiency.
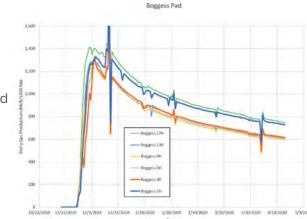
PRELIMINARY PRODUCTION RESULTS SHOW PROMISING RECOVERY IMPROVEMENTS

Total production ranges from 2.2 to 3.0 billion cubic feet through September 2020. Production data from the six laterals have been recorded since completion. Two of the six laterals (9H & 17H) were geometrically completed, two (5H & 13H) were engineered and completed by a private consultant, and two (1H & 3H) were engineered and completed using software developed by the MSEEL team.
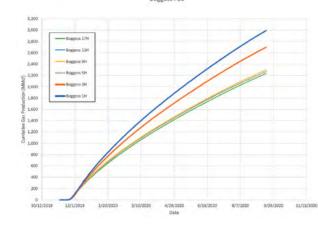
Early indications are that (based on rate transit analysis and production) the laterals engineered using software developed by the MSEEL team are the best producing laterals on the Boggess pad to date.

Initial daily net production from the Boggess Pad adjusted for Mcf per 1000' of completed lateral.

The MSEEL-completed laterals (1H and H3) have a higher gross production efficiency than the 9H/17H laterals (geometrically completed) and 5H/13H laterals (commercial design). Both MSEEL and the geometrically completed laterals contain identical 200 feet stages with with an identical number of clusters in each stage. While it is early in the production record, the laterals engineered using software developed by the MSEEL team are outperforming the other laterals on the pad.

Initial daily gross production from the Boggess Pad. The laterals engineered using the MSEEL software are highlighted with thicker lines (1H and 3H).

PARTNERS

CORE COMPETENCY

 PROGRAM EXECUTION and INTEGRATION

ASSESSING NATURAL GAS PRODUCTION POTENTIAL IN CENTRAL APPALACHIA

NETL project investigates the resource potential for multi-play production in emerging unconventional reservoirs.

INVESTIGATING EMERGING PLAYS

The Field Laboratory for Emerging Stacked Unconventional Plays (ESUP) project is focused on investigating the resource potential for multi-play production of emerging unconventional reservoirs in Central Appalachia.

The project is designed to extend our understanding of the multiple deep unconventional pay zones that exist in the established Floyd Embankment of the Rome Trough through the drilling, coring, and logging of a deep vertical stratigraphic test well to the Precambrian Basement (a depth of over 15,000 feet).

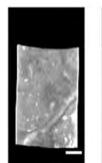*Basement Test Pad and Drilling Operations in Wise County, Virginia*

ADVANCED CHARACTERIZATION OF PROMISING FORMATIONS

The project team is utilizing multiple tools (both in-situ and in the laboratory) to assess the production potential of hydrocarbon resources within the stacked play, including multiple geophysical logging techniques and core analysis from samples collected throughout the borehole. Specific characterization elements included:

Borehole based tools: Quad Combo (G, N, D, Pe, LL), Dipole Sonic, LithoScanner, ELAN (Shale Evaluation), and Mechanical Properties logging tools.

Laboratory Assessment: A total of 90 cores were scanned with a Medical CT Scanner at two energies so that the dual energy density could be calculated. Eleven of those cores were selected to be scanned at high resolution with the Industrial CT Scanner.
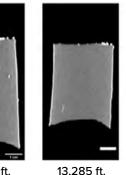
Grouping of Pumpkin Valley Shale scans.
Scale bar: 1 cm

| 13,270 ft. Core 34 | 13,280 ft. Core 32 | 13,285 ft. Core 31 | 13,270 ft. Core 29 |

Montage of ESUP scans and Mineralized Worm Burrows.
Scale bar: 1 cm

CT Scan Montage 13,185 ft.   Mineralized Worm Burrows within the shale.

Run 1, Core 17, 14,999 ft.

COMPREHENSIVE CHARACTERIZATION OF LOWER PALEOZOIC SECTION UNDERPINS ASSESSMENT OF RESOURCE DEVELOPMENT POTENTIAL

The data collected and analyzed from the ESUP test well provide valuable insights into the production potential and development strategies for multiple shale plays in Central Appalachia supporting industry's resource development efforts.

An illustration of drilling, completion, and lithofacies encountered as part of the basement test well. Formations with significant resource potential are noted in red.

PARTNERS

VIRGINIA TECH™

ENERVEST

NEW PIPELINE SURFACE TREATMENT PROVEN EFFECTIVE AND COMMERCIALLY DEPLOYED

Chemically resistant, water-and-oil repellent nanocomposite system

OCEANIT'S DRAGX™ IMPROVES PIPELINE INTEGRITY IN FIELD TRIAL

A public-private research effort managed by NETL with Oceanit Laboratories Inc., has produced an ultra-thin surface treatment that could significantly improve the reliability of the nation's extensive energy pipeline network by reducing corrosion and surface friction on pipe walls. Oceanit deployed the proprietary nanocomposite surface treatment technology, DragX™, in a commercial field trial with outstanding results. As the network of more than 2.5 million miles of pipeline delivering natural gas and oil across the U.S. ages, this collaborative effort is taking steps to help prevent disruptions in the flow of critical energy resources, ensure worker and public safety, and prevent negative environmental impacts.

Image of water droplet on untreated pipeline (left) vs DragX™ treated pipeline (right).

APPLICATION OF DRAGX™ ON FLOW TESTING FEEDER SHOWS PROMISING RESULTS

DragX™ protects carbon steel pipes from surface oxidation and rust buildup. The DragX™ solution has successfully been applied under various conditions (e.g., temperatures below 20°F) with no pitting or corrosion found after 6 months of deployment. The product has passed acceptance based on 3rd party Ultrasonic Test inspection, with long-term lifetime production still to be determined.

Representative image of test feeder line to simulate pig launcher (left), unprotected section (middle), and DragX™ treated section (right).

LARGE-SCALE DEPLOYMENT AND DRAG REDUCTION

DragX™ reduces the required pumping pressure, increases throughput, and increases service lifetime (corrosion due to high brine produced water and acidic gas). DragX™ was successfully tested in over 1 mile of <4" diameter coiled tubing. Pre-testing conducted in the laboratory showed optimal protection and chemical compatibility; this was verified during field testing.

Corrosion from Brine | **Corrosion from 10% HCl**

Untreated | DragX™ | Untreated | DragX™

Images comparing untreated and DragX™ treated pipes corroded by brine (left) and 10% HCl (right).

DRAGX™ APPLICATION VERSATILITY ALLOWS FOR FULL FIELD INTEGRATION

DragX™ is a scalable (+10 miles of pipeline at various diameters) process for in-situ treatment and does not require costly trenching and replacement of the pipelines. The process is compatible with complex geometry (90° bends), weld seams, and flanges, as well as existing pressures/temperatures and fluid compositions.

Recent field trials have helped Oceanit to broaden the use of this technology within and beyond the oil and gas domain. For instance, they have conducted field trials on wastewater lines and in hydrothermal and geothermal applications.

Typical Microbiological Influenced Corrosion damage to spool (left) vs. DragX™ application after 6 months (right)

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PROGRAM EXECUTION and INTEGRATION

PARTNER
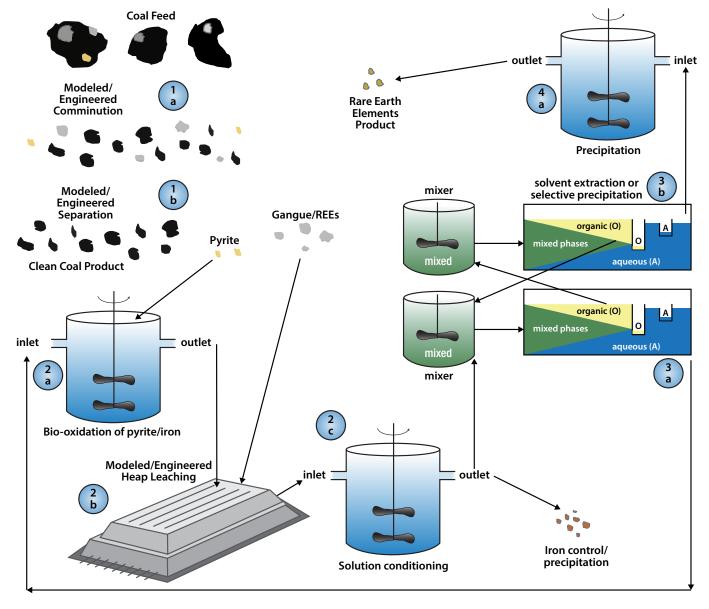

oceanit®
innovation through engineering & scientific excellence

BIO-OXIDATION TECHNIQUE GENERATES A BREAKTHROUGH IN RARE EARTH EXTRACTION TECHNOLOGIES

Enhanced bio-oxidation accelerates Rare Earth Element (REE) leaching and eliminates most acid rock drainage, improving economics and environmental sustainability.

LOW-COST TECHNOLOGY TO EXTRACT AND RECOVER MIXED RARE EARTH ELEMENTS (REE) GREATLY EXCEEDS GOALS

The University of Utah and Virginia Tech, in coordination with NETL, successfully demonstrated: (1) separation technologies to enrich pyrite for bio-oxidation; (2) column leaching with bio-oxidation and extraction of REEs; (3) concentration of REEs by solvent extraction; and (4) iron removal and REEs recovery by precipitation. The project goal of achieving a 2–8% by weight mixed REOs product was far exceeded with the successful production of 36.7% mixed REOs equivalent by weight.

Schematic diagram showing flow sheet and processing steps as well as task assignments for extraction, recovery, and upgrading of rare earth elements from coal-based resources

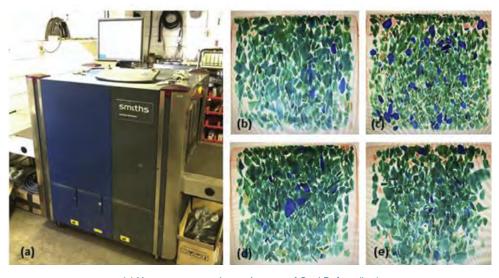## COAL-BASED MATERIALS FOUND TO BE ENRICHED WITH RARE EARTH ELEMENTS

Automated cross belt samplers collected eleven 55-gallon barrels of coal refuse representing six unique material types from four different mines in three states. Six different coal waste samples were found to have enriched REE content greater than 300 parts per million (ppm). Robust sampling and characterization of enriched REE samples enhance rapid technology development and evaluation.

REE enriched coal refuse samples

DUAL-SCAN X-RAY SORTING FURTHER IMPROVES ECONOMIC RECOVERY OF REES

Precise separation of REE-bearing coal refuse using dual-scan X-ray sorting, comminution, and spiral concentration concentrates pyrite-rich coal refuse improving process economics.

(a) X-ray scanner and x-ray images of Coal Refuse (b-e)

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VIRGINIA TECH

THE UNIVERSITY OF UTAH

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CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING
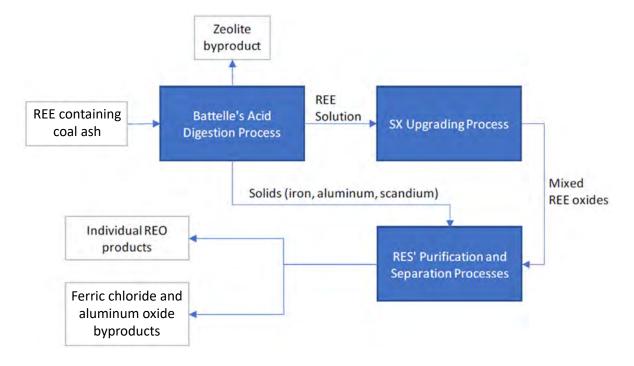
PROGRAM EXECUTION and INTEGRATION

HIGH PURITY RARE EARTH ELEMENTS (REE) RECOVERED FROM COAL ASH VIA A NOVEL ELECTROWINNING PROCESS

Generating and purifying environmentally benign and economically sustainable REE products from domestic coal ash resources

REE RECOVERY PROCESS DEVELOPED

Battelle Memorial Institute (BMI) and **Rare Earth Salts (RES)** worked together to develop and validate BMI's acid digestion process and RES's novel electrowinning separation and purification process, as well as overcome contaminant challenges.

ACID DIGESTION PROCESS IMPROVES REE DIGESTION

Acid digestion makes metals easier to separate by dissolving a coal ash sample into solution by adding acids and heating it until the metals break away from the other undesired materials. BMI successfully scaled up their acid digestion process to increase the concentration of mixed REE materials in solution and provided enough material for the RES facility.

Scaled-Up Acid Digestion Process

ZINC REMOVAL IMPROVES SOLVENT EXTRACTION (SX)

After acid digestion, aluminum and zinc remained in solution with the REEs. Aluminum was easily removed, but zinc presented a challenge. To overcome it, BMI used a new extractant composition selective for zinc over the REEs to be implemented prior to the traditional SX process as a pretreatment to remove zinc. BMI successfully scaled up their SX process 100x to 10 kg per batch.

REO Material for Purification

Electrowinning Produces High-Purity Rare Earth Oxides (REO)

During the electrowinning process, metal ions present in a solution are separated using a direct current. A concentrated, mixed REE solution was fed to RES's electrowinning process to obtain the final coal-based, high purity REO products.

TECHNOLOGY PRODUCES REO PRODUCT WITH A PURITY OF ~90%

With the zinc interference minimized, RES's electrowinning process recovered a concentrated REO product. A lanthanum oxide product with a purity of approximately 90% was generated. A purity of 90% renders the material suitable for further processing into a pure metal form for subsequent incorporation into commodity or national defense products.

~90% Pure REO Product

PARTNERS

CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION
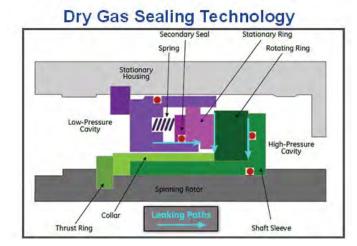
SUCCESSFUL DESIGN AND FABRICATION OF SCO$_2$ TURBINE SEALS

Effective seals for the high-pressure supercritical carbon dioxide power cycles give this efficient and cost-effective technology promise in future applications.

CRITICAL COMPONENTS FOR HIGH-EFFICIENCY POWER SYSTEMS

Effective seals limit pressure losses

- Lower cost electricity production can be achieved through indirect, coal-fired supercritical carbon dioxide (sCO$_2$) power cycles with thermodynamic cycle efficiencies over 50%.
- Achieving the system-level objectives for sCO$_2$ cycles requires development of low-leakage, large-diameter and split-segment face seals.
- Such face seals are not presently available for the operating environment of utility-scale sCO$_2$ turbines.

Dry Gas Sealing Technology

ADVANCED DESIGN LEADS TO OPTIMAL MANUFACTURED SEALS

- In collaboration with NETL, GE Research successfully designed and fabricated their 5-inch (approximately 10MWe size) radial sCO$_2$ turbine seals and supporting hardware.
- The seals initially underwent a series of static flow tests and demonstrated pressure lift-off and satisfactory secondary seal characteristics, with measured leakage as predicted in pre-test reviews.
- Following the successful seal static tests in May 2020, the seals were tested in two rounds of rotating tests: the first at 1/5 the full speed of the test rig and the second at 2/5 the full speed of the test rig.

APPLIED TEST ACHIEVES BREAKTHROUGH

- A testing rig was designed and assembled to analyze the performance of face and radial seals developed by researchers.
- The testing of the 5-inch radial seals in a rotating environment successfully demonstrated stable thermal operation.
- Completion of these tests advanced the sCO$_2$ seals' technology to TRL 3.

TEST SUCCESS CREATES OPPORTUNITIES TO ACHIEVE HIGHER TECHNOLOGY READINESS LEVELS

- GE has performed component development for larger seals and will start rotating tests at higher surface speeds and pressures to achieve TRL 4 in the near future.
- Development of this sCO$_2$ seal technology will close a critical technology gap necessary for enabling the high potential efficiency of indirect sCO$_2$ power cycles.

PARTNERS

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

PROGRAM EXECUTION and INTEGRATION

MAJOR MILESTONES ACHIEVED IN SUPERCRITICAL CARBON DIOXIDE (sCO$_2$) POWER CYCLES
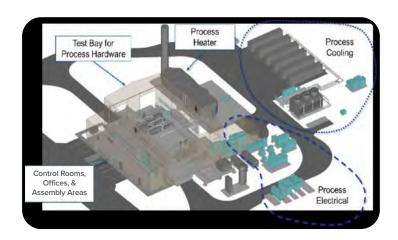
New sCO$_2$ power cycle pilot plant will prove critical capabilities of a novel technology for more efficient power generation at lower cost, making the United States a leader in domestic and global power generation.

IMPROVING DOMESTIC & GLOBAL POWER GENERATION

Supercritical CO$_2$ power cycles offer potential for power generation with increased efficiency, lower cost of electricity, reduced customer costs, and reduced water consumption.

- **S**UPERCRITICAL
- **T**RANSFORMATIONAL
- **E**LECTRIC
- **P**OWER

RECONFIGURABLE, FLEXIBLE STEP PILOT PLANT TEST FACILITY

Test Bay for Process Hardware — Process Heater — Process Cooling — Process Electrical — Control Rooms, Offices, & Assembly Areas

Path to Lower Cost of Electricity

The STEP pilot plant will demonstrate a fully integrated, functional, electricity-generating power plant using sCO$_2$ technology. This plant aims to show component performance and cycle operability over a range of operating conditions, as well as show progress toward a lower cost of electricity.

REDUCING BARRIERS & RISKS TO COMMERCIALIZATION

U.S. at Forefront of Cutting-Edge Power Cycle Technology

DOE's investment in sCO$_2$ power cycle technology through the 10 MWe sCO$_2$ power cycle pilot plant enables the U.S. to lead in developing and commercializing sCO$_2$ power cycle deployment for both domestic and global power generation.

MAJOR MILESTONES TOWARD COMMISSIONING THE LARGEST INDIRECT-FIRED sCO$_2$ POWER CYCLE TEST FACILITY IN THE WORLD

CERTIFICATE OF OCCUPANCY RECEIVED FOR STEP PILOT PLANT BUILDING

MECHANICAL INSTALLATION UNDERWAY

- **Installation** of process electrical equipment
- **Delivery** of main and bypass compressors, low temperature recuperator, and main process cooler
- **Major progress** toward addressing technical challenges associated with critical equipment
- **Turbine and High-Temperature Recuperator** designs completed for fabrication and delivery in FY21
- **All major equipment** expected for installation is planned for delivery by September 2021

DCS Cabinet

Turbine Stator Nozzle Machining

Main Process Valve

High Temperature Recuperator Cores

Turbine Rotor EDM First Stage Progress

Bypass Process Cooler

On Track For Simple Cycle Plant Commissioning

PARTNERS

CORE COMPETENCIES

ENERGY CONVERSION ENGINEERING

PROGRAM EXECUTION and INTEGRATION

START RIG MAPS TURBINE BLADE TEMPERATURES DURING OPERATION

The START Lab is the most sophisticated continuous flow research facility in the world for the study of advanced cooling and flow leakage in gas turbines – optimizing performance across the fleet.

STATE-OF-THE-ART FACILITY WITH UNMATCHED CAPABILITY

Steady Thermal Aero Research Turbine (START) Facility

The START Lab is a collaboration between NETL and Penn State University that pushes the boundaries of current experimental capabilities for gas turbine research because it is a continuous duration facility that operates at conditions representative of modern gas turbine engines.

DOE's investment in the START facility provides the United States with unmatched testing capability for improving cooling designs that will lead to improved turbine performance across the turbine fleet.

COLLABORATION IN NEXT-GENERATION TURBINE DESIGN RESEARCH

The National Experimental Turbine (NExT) rig, designed in collaboration with four turbine manufacturers, is a turbine testing platform focusing on US technology advancement. The NExT hardware will be designed to fit within the spatial envelope of the START turbine test section.

The project team has completed and approved preliminary conceptual designs for NExT. Agilis, a turbine design company, has completed a detailed design, including the aero and heat transfer analyses, which has been reviewed by the OEMs and other government agencies.

While all turbine geometries are highly proprietary, the goal for NeXT is to provide a modern turbine design that can be used by several organizations. The NExT geometry may also be used by companies quickly and cheaply to do proprietary research in the future.

FIRST-OF-ITS-KIND THERMAL IMAGING
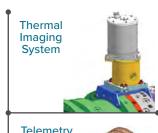

Baseline Cooling Design

The START's infrared camera system was fully calibrated and used to make detailed blade temperature measurements on the pressure surface of a rotating blade at full operating conditions. The data obtained is the first of its kind and showed the cooling performance of specific features.
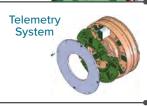
Software that provides a direct mapping of measured blade temperatures onto an image of the blade was developed. Instrumentation including infrared thermography, heat flux guages, and fast response pressure measurement devices have been installed and calibrated on the rig.
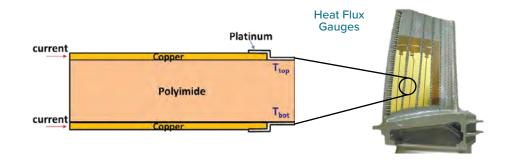
REAL-TIME OBSERVATION OF COOLING PERFORMANCE

The START team successfully captured spatially-resolved surface temperatures on a blade spinning at 10,000 rpm that illustrated the cooling feature performance.

The project team is working to improve the mapping accuracy with minimal computing time. This effort will enable experiments to be analyzed and cooling performance to be observed in real time.

Thermal Imaging System

Telemetry System

Heat Flux Gauges

current — Copper — Platinum — T_{top} — Polyimide — current — Copper — T_{bot}

CORE COMPETENCIES

 ENERGY CONVERSION ENGINEERING

 PROGRAM EXECUTION and INTEGRATION

PARTNERS

AGILIS — Revolutionary Insight

Honeywell AEROSPACE

Solar Turbines — A Caterpillar Company

PennState

SIEMENS — Ingenuity for life

ADVANCES AND DISCOVERIES MADE IN COAL-FIRED ROTATING DETONATION ENGINE OPERATION AND BEHAVIOR

Coal-fueled rotating detonation engines are an emerging technology for efficient and clean power generation through pressure gain combustion.

SUCCESSFUL OPERATION OF ROTATING DETONATION ENGINE (RDE) USING PRIMARILY SUB-BITUMINOUS COAL

The University of Central Florida successfully increased the use of 5 µm ground sub-bituminous coal to fuel their RDE, a pressure gain combustion system. Previously, the system had primarily used carbon black as a fuel. Compared to carbon black with size of 29 nm and low volatility of 1.18%, the larger coal particles with higher volatility of 34 to 44% represented a significantly more challenging operating scenario.

Coal RDE test fires: non-reacting (left), deflagration (center), detonation (right)
University of Central Florida

EVIDENCE FOUND PROVING SOLID CARBON IS DRIVING DETONATION WITHIN THE COAL RDE
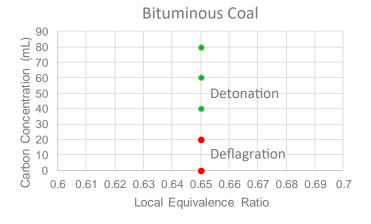
Presence of carbon required for detonation

Maintaining a constant equivalence ratio of hydrogen during engine firing, with and without carbon present, showed that detonation only occurred when carbon was present in the fuel mixture at certain equivalence ratios.
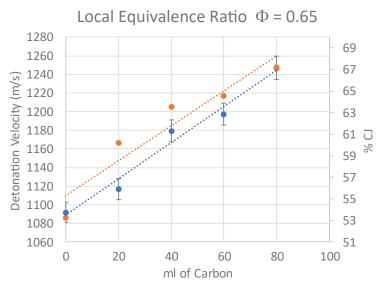

Imaging of detonation wave dynamics visualized by high speed imaging with carbon present,
University of Central Florida

CARBON CONCENTRATION CORRELATES TO DETONATION WAVE SPEED

Gradually increasing the carbon concentration while maintaining a constant equivalence ratio of hydrogen demonstrated that increasing the carbon concentration led to an increase in the detonation wave speed. (If the carbon was experiencing afterburn rather than detonation, the wave speed would decrease as the carbon concentration increased.)

Experimental data (blue points) showing that as carbon concentration increases (horizontal axis) the detonation velocity (left vertical axis) also increases,
University of Central Florida

PARTNERS

CORE COMPETENCIES

⚡ ENERGY CONVERSION ENGINEERING

PROGRAM EXECUTION and INTEGRATION

LONG-TERM MONITORING PROGRAM INDICATES GEOLOGIC CARBON STORAGE HAS NO EFFECT ON GROUND WATER QUALITY

MVA programs are demonstrating that commercial-scale pilot projects are protective of human health and the environment.

FIRST-OF-A-KIND FULLY INTEGRATED SALINE CARBON STORAGE

The Midwest Geological Sequestration Consortium (one of seven DOE Regional Carbon Sequestration Partnerships) concluded a 12-year monitoring, verification, and accounting (MVA) program at a site in Decatur, IL, where 1 million metric tons of carbon dioxide (CO_2) were injected over a 3-year period (2011–2014) into the Mt. Simon sandstone, a world class geologic storage reservoir. Monitoring activities also extended to the adjacent Illinois Industrial Carbon Capture and Storage Project (IL-ICCS). Major accomplishments include:

- Produced multiple lines of evidence, including more than **60,000 analyses in groundwater monitoring efforts**, to support the conclusion that CO_2 injection has not influenced **groundwater quality**.
- Demonstrated that project activities are protective of human health and the environment (in part by ensuring **that all regulatory conditions were met**).
- Established **pre-injection environmental conditions** (2008–2010) to evaluate potential impacts from CO_2 injection.
- Improved risk-based, adaptive monitoring programs necessary to **optimize monitoring costs** throughout a project life cycle.
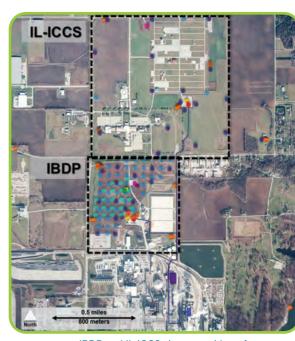- Field validated and improved the commercial readiness of **seven emerging technologies**.

MVA Activities at Illinois Basin - Decatur Project (IBDP) site

MVA ACTIVITY SUMMARY

| Monitoring Activity		Freq.	Pre-inj.	Injection	Post-inj.
SURFACE	Aerial imagery	SA	●	●	●
	Eddy covariance	C		●	
	Soil flux - network~	W-Q	●	●	●
	Soil flux - multiplexer~	C	●	●	●
	Tunable diode laser - single path~	C		●	
	Tunable diode laser - multi path~	C			●
	InSAR ~	BW		●	
	Continuous GPS~	C		●	
NEAR SURFACE	Soil gas sampling	Q-A		●	●
	Shallow groundwater sampling*^	M-Q	●	●	●
	Shallow electrical earth resistivity~	A	●		
SUBSURFACE	Pressure/temp. - VW1 and CCS1*^	C		●	●
	Pulsed neutron (CCS1, VW1, GM1)*^	Q-A	●	●	●
	Deep fluid sampling (VW1)^	SA		●	●
	Passive seismic monitoring (GM1)^	C	●	●	●
	Seismic/3D VSP imaging*^	SA-A	●	●	
	Mechanical integrity (CCS1, VW1)*^	A	●	●	●
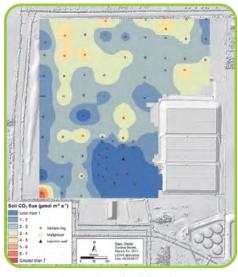
* required in the Class I permit. ^ required in the Class VI permit. ~experimental technique or deployment (Abbreviations: C = Continuous, W = Weekly, BW = Biweekly, M = Monthly, Q = Quarterly, SA = Semi-Annually, A = Annually, VW1 = Verification Well 1, CCS1 = Injection Well 1, and GM1 = Geophysical Monitoring Well 1.)

IBDP and IL-ICCS site map with surface and near-surface monitoring networks

NOVEL TECHNOLOGIES PROVIDE REAL-TIME SURVEILLANCE TO CARBON STORAGE INDUSTRY
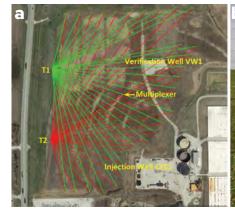
- Integration and automation methods have resulted in significant time savings when applied to near-surface field monitoring data.
- Successful deployment of cost-effective technologies for identifying anomalous temporal or spatial changes in atmospheric CO_2.
- Continuous monitoring of atmospheric CO_2 provides effective detection of locations where more detailed investigation would be justified.

Automation of soil flux data

Open-path sensor, applies tunable diode laser absorption spectroscopy

GreenLITE system. (a) layout showing chords from transceivers (T1 and T2) to reflectors, (b) transceiver installed, and (c) retroreflector installed at the IBDP site.

PARTNERS

CORE COMPETENCIES

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

SYSTEMS ENGINEERING and ANALYSIS

CARBON CAPTURE TECHNOLOGIES PROGRESS TO LARGE-SCALE TESTING AT TECHNOLOGY CENTRE MONGSTAD IN NORWAY

Long-term realistic testing at engineering scale is crucial for advancing technologies toward meeting DOE carbon capture performance goals.

THREE NEXT-GENERATION, POST-COMBUSTION CARBON DIOXIDE CAPTURE PROJECTS HEADING FOR LARGE-SCALE TESTING

Three next-generation, post-combustion carbon dioxide (CO_2) capture technologies, matured and de-risked by DOE, are slated for extended engineering-scale testing with actual flue gas at the Technology Centre Mongstad (TCM) in Norway via international collaboration.

Transformational Non-Aqueous Solvent-Based CO_2 Capture Process Testing at 10 MWe

TCM's existing 10 MWe amine-based CO_2 absorption facility will be modified by Research Triangle Institute (RTI) International to test their amine-based, non-aqueous solvent process. RTI, with support from Pressura AS, completed a Front-End Engineering Design study and developed cost estimates for installation of a CO_2 absorber intercooler and associated tie-ins to the seawater cooling system, addition of a forced recirculation pump to the thermosyphon reboiler, and tightening of the water wash section to reduce process emissions.

PARTNERS

TECHNOLOGY CENTRE MONGSTAD — SINTEF — CCSI² Carbon Capture Simulation for Industry Impact — PRESSURA — EPRI ELECTRIC POWER RESEARCH INSTITUTE
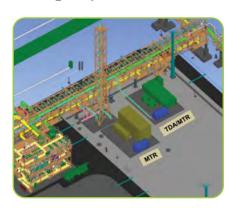
TDA RESEARCH, INC. AND MEMBRANE TECHNOLOGY AND RESEARCH, INC. (MTR) TEST 1 MWE MODULAR SYSTEMS

TDA and MTR will engineer and integrate 1 MWe modular systems at TCM's dedicated test bay to test their membrane-sorbent hybrid and advanced Polaris™ membrane processes. Data generated by modular systems is directly applicable to the design of full-scale systems.

Hybrid Membrane-Sorbent System for Post-Combustion CO_2 Capture

The hybrid process integrates MTR's polymeric membrane and TDA's low-temperature physical adsorbent. The polymer membrane removes the bulk of the CO_2 across a relatively low-pressure gradient, reducing the power consumption and cost of capture. The membrane residue gas is further treated by the sorbent, ensuring greater than 90 percent CO_2 capture overall.

PARTNERS

TECHNOLOGY CENTRE MONGSTAD — MTR MEMBRANE TECHNOLOGY & RESEARCH — gti — UCI University of California, Irvine

Advanced Polaris Membrane CO_2 Capture Technology

MTR's membrane-based capture system uses advanced membranes and compact, low-pressure-drop plate-and-frame modules contained in a modular unit that can be repeated in future commercial systems at low cost.

PARTNERS

TECHNOLOGY CENTRE MONGSTAD — TRIMERIC CORPORATION — DRESSER-RAND A Siemens Business — Advisian Worley Group

PROJECT BUDGETS

AWARD NUMBER
DE-FE0031590 (RTI)

$17.4M
- DOE $10,013,513
- PERFORMER $7,371,000

AWARD NUMBER
DE-FE0031603 (TDA)

$11.5M
- DOE $9,198,799
- PERFORMER $2,299,725

AWARD NUMBER
DE-FE0031591 (MTR)

$10.7M
- DOE $8,166,304
- PERFORMER $2,579,429

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FEDERAL PROJECT MANAGERS
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ANDREW O'PALKO (TDA)
ANDREW AURELIO (MTR)

PRINCIPAL INVESTIGATORS
MARTY LAIL (RTI)
GOKHAN ALPTEKIN (TDA)
TIM MERKEL (MTR)

CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

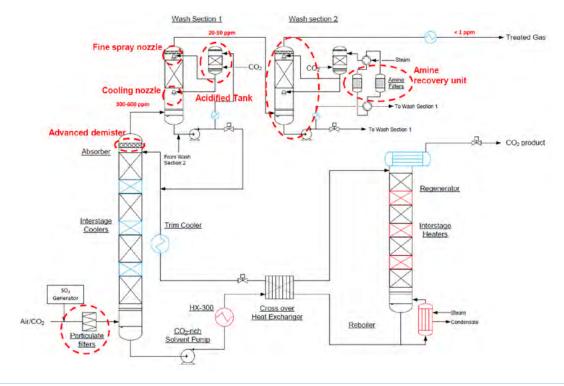# RTI INTERNATIONAL (RTI) DEMONSTRATES LOWER AMINE AEROSOL EMISSIONS IN SOLVENT SYSTEMS
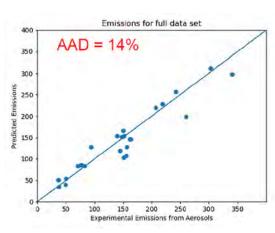
Comprehensive solvent emission mitigation tool set specifically designed for water-lean solvent CO_2 capture systems minimizes amine loss & aerosol formation

INTEGRATED APPROACH FOR EFFECTIVE AMINE EMISSIONS CONTROL

RTI achieved lower amine emissions by incorporating emission control technologies (ECTs) in a solvent-based CO_2 capture system. Following the installation of particulate filters, CO_2-acidified water washes, amine recovery beds, and advanced demisters in their Bench-scale Gas Absorption System, approximately 980 hours of parametric testing was conducted with water-lean solvents and simulated flue gas, resulting in **amine emissions <5 ppm**, a significant reduction compared to baseline testing without ECTs.

EMPIRICAL MODEL FOR PREDICTING AEROSOL-BASED EMISSIONS

RTI developed an empirical process model that predicts aerosol-based emissions based on solvent physical and chemical properties and on critical operating parameters from the absorber and wash section.

A regression model based on data from the parametric testing campaign on RTI's Non-Aqueous Solvent (NAS-5) shows an average absolute deviation of 14%.

ACIDIFIED WATER WASH ENABLES ADEQUATE AMINE SCRUBBING

- A CO_2 slipstream acidifies the wash water, increasing amine solubility, leading to more amine captured from the treated-flue gas.

- The CO_2-acidified water wash significantly lowers amine aerosols emissions from ~25 ppm to ~2 ppm – **a ~90% decrease from baseline aerosol emissions with regular water washes**.

Mitigating amine losses by treating flue gas emissions addresses both **environmental and operating expense** issues.

Emission control serves as an **enabling technology** for the ongoing development of transformational water-lean solvents for CO_2 capture.

PARTNERS

CORE COMPETENCIES

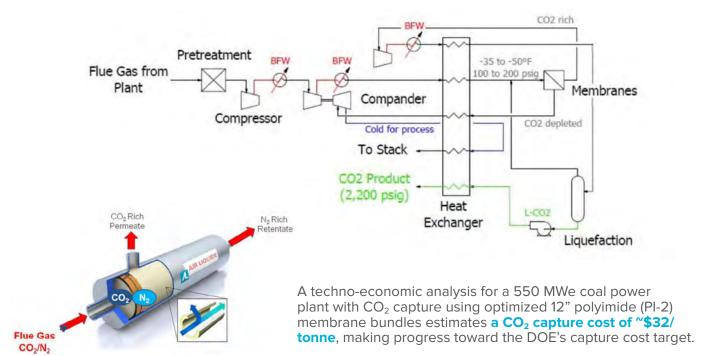MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

NEXT GENERATION HOLLOW FIBER MEMBRANE MODULES REDUCE COST OF CO_2 CAPTURE

Polyimide-based membrane material for application in hybrid cold membrane/ cryogenic distillation process yields cost-effective CO_2 separation from flue gas

IMPROVED ECONOMICS FOR CARBON CAPTURE

Air Liquide's hybrid process combines cold membrane operation with cryogenic separation technology for CO_2 liquefaction to achieve 90% CO_2 recovery at >58% purity.

A techno-economic analysis for a 550 MWe coal power plant with CO_2 capture using optimized 12" polyimide (PI-2) membrane bundles estimates **a CO_2 capture cost of ~$32/ tonne**, making progress toward the DOE's capture cost target.
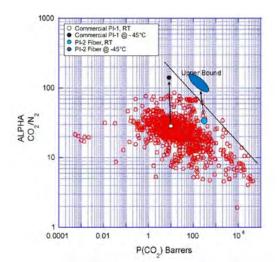
STABLE MEMBRANE PERFORMANCE AT SUB-AMBIENT TEMPERATURES

Air Liquide completed testing of next generation hollow fiber membrane modules at the National Carbon Capture Center. Field testing on 6" PI-2 membrane bundles at 0.3 MWe scale was performed using actual flue gas. The membranes exhibited stable performance at -40°C for >700 hours and were capable of processing >650 Nm^3/ hr of flue gas at 90% CO_2 recovery and with a permeate composition of 59+% CO_2 purity.
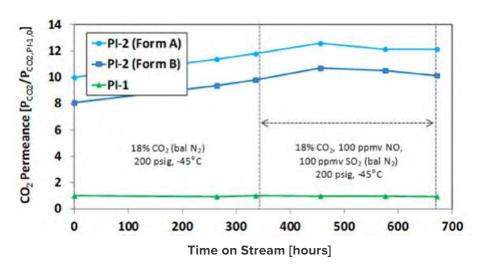

6" commercial bundle

Membrane Skid

POLYIMIDE MEMBRANES EXHIBIT COMBINATION OF HIGH PERMEANCE AND CO_2/N_2 SELECTIVITY

- Polyimide (PI)-based membrane bundles show a two-to-four times higher CO_2/N_2 selectivity with minimal loss of CO_2 permeance when operated at temperatures below -20°C, as compared to ambient temperature operation.
- PI-2 material exhibits CO_2 permeance >5x higher than PI-1 material.

MEMBRANES RESISTANT TO ACIDIC COMPONENTS IN FLUE GAS

PI-2 membrane fibers are stable at 100 ppm NO and SO_2 and tolerant to 20 ppm NO_2

PARTNERS

Air Liquide

PARSONS

NATIONAL CARBON CAPTURE CENTER

MEDAL

Delaware Research & Technology Center

CONTACTS

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ALEX AUGUSTINE

CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

NOVEL UPCYCLED CO$_2$-NEGATIVE CONCRETE PRODUCTION SYSTEM CONSTRUCTED

Utilizing CO$_2$ and industrial byproducts to create CO$_2$-negative upcycled concrete that performs as well, or better, than traditional construction materials

NEW, VALUE-ADDED PRODUCT FOR THE COAL INDUSTRY TO REDUCE EMISSIONS AND OPEN MARKETS

Flue gas-borne CO$_2$ and repurposed abundant industrial wastes, such as crystalline slags and fly ash, can be used to create "upcycled concrete." This value-added product **provides the coal power industry with a viable path to significantly reduce its carbon emissions**.

The "upcycled concrete" production process also **minimizes external energy needs** by fully utilizing low-grade heat sourced from the flue gas, which **decreases operating costs**.

Examples of Industrial Waste Feedstocks
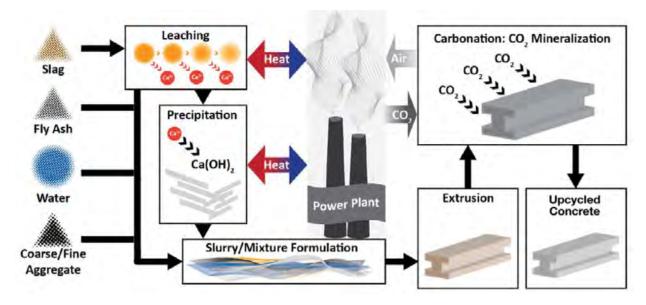
Basic Oxygen Furnace Slag

Co-Mingled Steel Slag

Upcycling Process Outcome

Cylindrical Mortar Specimens

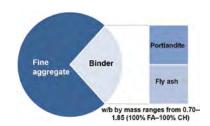## INTEGRATED TECHNOLOGY PRODUCTION PROCESS

- Completed construction of a novel laboratory-scale upcycled concrete production system.
- The integrated "bolt-on" technology incorporates calcium leaching, portlandite precipitation, mixture formulation, and structural shape stabilization—while maximizing CO$_2$ uptake.

CARBONATED MORTARS HAVE HIGHER COMPRESSIVE STRENGTH THAN TRADITIONAL MORTARS

Mechanical compaction tests of **carbonated** and non-carbonated mortar samples composed of fly ash-portlandite binders show that **compressive strength increased upon mineral carbonation** (>15 MPa target achieved).

- Direct correlation between strength and CO$_2$ uptake and carbonate formation; higher CO$_2$ uptake is attributed to higher levels of portlandite (Ca(OH)$_2$) in the mixture.

Upcycled concrete mixture

Compacted 2-inch cube specimens

$$Ca(OH)_2 + CO_2 \longrightarrow CaCO_3 + H_2O$$

Max CO$_2$ uptake = 59% by mass

Carbonation Process

REDUCED EMISSIONS AND LOWER COSTS

While maintaining **equivalent or superior performance** to ordinary Portland cement (OPC)-based concrete, **"Upcycled Concrete"** enables the following:

- **CO$_2$ uptake >6% by mass** due to an integrated CO$_2$ mineralization process that facilitates low-temperature portlandite precipitation.
- Reduces the 100-year Global Warming Potential by 175–250 kg CO$_2$e/m^3, equivalent to a **57–82% CO$_2$ emissions reduction**.
- The fully loaded production cost for 140 m^3/day of upcycled concrete is estimated at **$97/m^3**, which is below the OPC concrete block market price ($100–170/m^3).
- Utilization of flue gas CO$_2$ and the ability to repurpose abundant industrial wastes **opens new markets for coal products**.

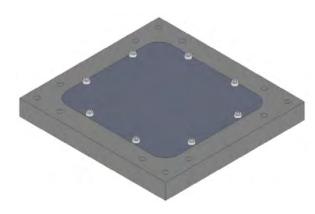### PARTNERS

BORAL RESOURCES

ASU Arizona State University

UCLA

AI ENABLED ROBOTS FOR AUTOMATED NONDESTRUCTIVE EVALUATION (NDE) AND REPAIR OF POWER PLANT BOILERS
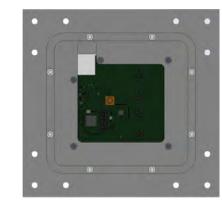
The autonomous robotic platform will be capable of attaching to and navigating on vertical boiler furnace walls.

NDE SENSING AND ASSESSMENT

NDE Sensor Integration with the Robot

NDE sensing and assessment: efforts focus on (1) design of robust eddy-current based sensors on a robotic platform to detect cracks and assess their repair and (2) signal processing for detection and assessment of repair. **The NDE sensor has been identified, quoted, and is in the procurement process**. **The sensor housing and printed circuit board (below) have been designed**.
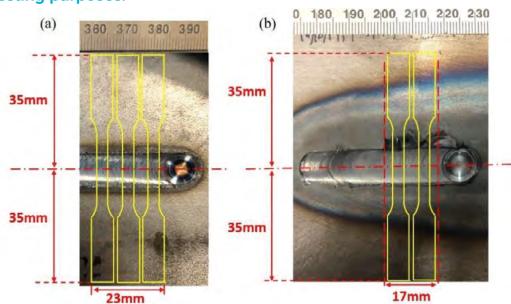

REPAIR DEVICE DESIGN AND CONTROL

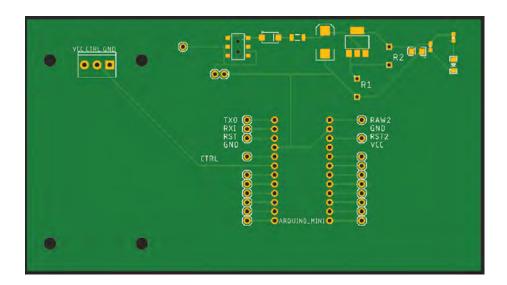### Welding and Joining Systems for Repair

Efforts focus on designing and evaluating a repair technology as the compact live repair tool to repair cracks. The induction heating assisted friction stir welding method is being utilized. **Friction stir weld repairs have been made with the prototype welding parameters for tensile testing purposes**.

ROBOT PLATFORM INTEGRATION

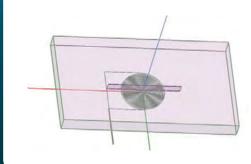### Brush Cleaning Mechanism-Electrical Component

The brush cleaning mechanism cleans the scale off the vertical inspection surface. **The brush cleaning mechanism printed circuit board (below) was designed** based on a revised wiring diagram.
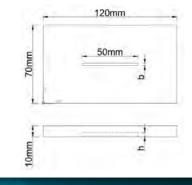
AI ALGORITHM DEVELOPMENT

Autonomous Robot Control under Uncertainties

AI algorithm development efforts focus on developing AI algorithms and software packages for (1) 3-D mapping and information fusion, (2) spatiotemporal crack tracking and map updating, and (3) smart damage analysis by robot learning. **Different neural network methods have been designed and tested** to find the optimized machine learning structure for crack identification. **A steel plate (below) with a crack at the center has been created as the sample**.

PARTNERS

COLORADO SCHOOL OF MINES

MICHIGAN STATE UNIVERSITY

CONTACTS

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HAO ZHANG

CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING

MATERIALS ENGINEERING and MANUFACTURING

SYSTEMS ENGINEERING and ANALYSIS

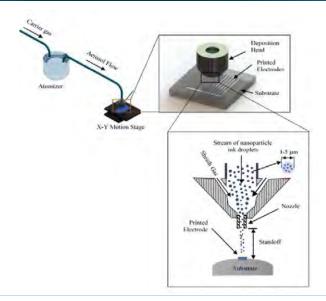# LOW-COST, EFFICIENT, AND DURABLE HIGH-TEMPERATURE WIRELESS SENSORS BY DIRECT WRITE ADDITIVE MANUFACTURING FOR APPLICATION IN FOSSIL ENERGY SYSTEMS

Develop next-generation sensors and controls that can sustain temperatures up to 500 degrees Celsius (°C)

MANUFACTURING METHOD AND MATERIAL SYSTEMS
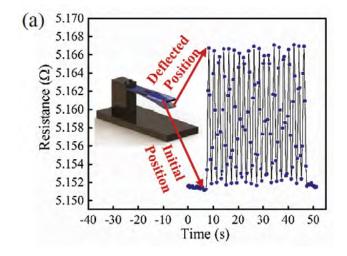
Additive Manufacturing of 2-D Films

An Aerosol Jet® printer was used to print nanoparticles onto substrates such as glass, ceramics, Kapton®, and metals. **This technique was used to print 2-D films at a lateral resolution as low as 10-15 μm.** Nanoparticle materials used for printing were silver, nickel, nichrome, carbon nanotubes, copper, and copper-nickel.

3-D PRINTED HIGH-TEMPERATURE STRAIN SENSOR AND ANTENNA

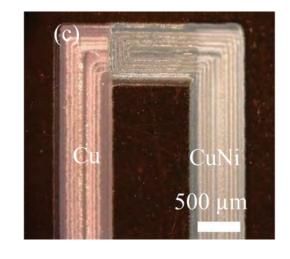### Fabrication, Characterization and Performance of 3-D Printed High Temperature Strain Sensor

Strain sensors were fabricated by Aerosol Jet printing and sintering of silver nanoparticles on a rectangular cantilever beam substrate for deflection testing at elevated temperature. The synthesized high temperature strain sensors **show stable and superior performance up to 500 °C.** Further, 3-D printed passive antenna designs **demonstrated transmission at a distance on the order of a foot.**

3-D PRINTED TEMPERATURE SENSORS

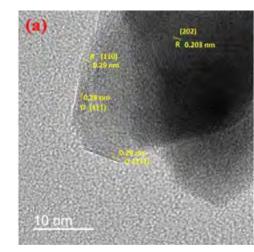### Using Nanoparticles to Create a Fabrication Platform for High-Performance Temperature Sensors

Solvent-based Cu and CuNi nanoparticle inks were printed by an Aerosol Jet printer to realize the two elements/films of the sensor. The printed nanoparticle films were laser sintered after printing. Sensor performance measurement testing measured sensor output at different temperatures. The printed sensors **showed a highly linear performance with the highest sensitivity of any film-based temperature sensors in literature.**
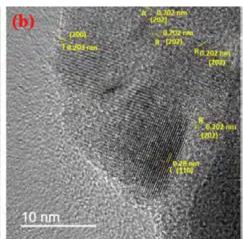

BA-PEROVSKITE (BFTO) COMPOUNDS FOR HIGH-TEMPERATURE SENSING

Materials provide stability to improve reliability

Due to their high melting point and decomposition temperature, perovskite oxides are particularly attractive for high-temperature sensor applications. $Ba(Fe0.7Ta0.3)O_3$-δ [$BFTO_30$] compounds were synthesized and extensive characterization was performed. The **detailed understanding of the phase transformations and crystal physics as derived in this work could be useful to develop chemical sensors with optimum performance for high-temperature and corrosive environments.**

SENSOR RELIABILITY

Interfacial Adhesion Energy of Printed Metal Films

Silver nanoparticle samples were prepared on alumina and glass substrates with various thermal exposures (sintering times and thermal cycling). Samples were tested by applying a vertical load. Results showed that the **separation energy increased upon high-temperature exposure,** concluding that the strain **sensor films investigated in this work show reliable operation at temperatures up to 500 °C.**

CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

SYSTEMS ENGINEERING and ANALYSIS

PARTNERS

Carnegie Mellon University

THE UNIVERSITY OF TEXAS AT EL PASO

WASHINGTON STATE UNIVERSITY

MAJOR MILESTONES ACHIEVED TOWARD COMPLETING FULL-SCALE ADVANCED ULTRASUPERCRITICAL (AUSC) COMPONENT DEMONSTRATIONS

Demonstrating commercial readiness by testing full-scale versions of key AUSC power plant components.

PUSHING BOUNDARIES ON TEMPERATURE AND PRESSURE

By 2021, AUSC materials will be developed to operate at high pressures and temperatures to meet global electricity demand, reduce overall emissions, and increase efficiency in coal-fired power plants. AUSC power plants are 25% more efficient than average power plants, and 10% more efficient than state-of-the-art power plants.

CONTRIBUTING TO THE FUTURE OF POWER PLANTS

The ComTest project is a six-year effort that focuses on building full-scale versions of key components and sub-assemblies of an AUSC boiler, steam turbine and steam piping system, which has been identified as the final step necessary to demonstrate the readiness of AUSC technology for a commercial-scale demonstration power plant. The materials technology that NETL is developing is not only applicable to AUSC plants but also to other advanced fossil energy plants, like supercritical CO_2.

The ComTest project is advancing AUSC technology by:

- Expanding a qualified domestic supply chain **to manufacture nickel superalloy components for AUSC power plants**.
- Validating that AUSC components can be designed and built for reliable operation under both steady-state and varying load operating conditions for the 30-year design life of an AUSC boiler.
- Developing fabrication, installation, and repair methods for cast and forged nickel superalloy AUSC components and sub-assemblies.

ILLUSTRATING THE UNIQUE CAPABILITY OF BUILDING AUSC COMPONENTS

① AUSC steam turbine nozzle carrier casting

② AUSC superheater/ reheater assembly

PHASE 1: COMPLETE
Completed front-end engineering design and detailed engineering. Began developing a domestic supply chain for AUSC nickel superalloy components and determined that operational testing of an AUSC steam turbine and AUSC superheater was not required.

PHASE 2: CURRENT
In Phase II the key components and sub-assemblies of an AUSC boiler, steam turbine, and steam piping system will be fabricated at sizes equivalent to an 800-MWe power plant. Fabrication of AUSC boiler components began in FY2019. Production of these components will demonstrate the capability of U.S. manufacturers to produce AUSC power plant parts.

BUILDING POWER PLANTS OF THE FUTURE: AUSC COMPONENTS TESTING FOR FULL-SCALE COMMERCIAL USE

Key Successes

- Subcontractors in place and domestic fabrication shops identified for all components within project scope.
- Design and materials selection for AUSC superheater section finalized. Welding qualification tests nearly completed.
- Two Inconel 740 ingots made for steam pipe headers. First ingot extruded into 22-inch OD x 3.7-inch wall thickness, which makes it the largest Inconel 740 pipe produced to date.
- Pressure Relief Values (PRV) for AUSC boiler fabricated and first round of ASME flow certification testing completed.
- Haynes 282 steam turbine carrier casting pour conducted. Mold run out occurred after half of casting completed. Reasons for mold run out determined and plan to conduct second casting prepared.

22-inch OD x 3.7-inch wall thickness x 14-foot-long nickel superalloy pipe extruded in October 2020

Continuing Progress:

- Extrude Inconel 740 Reheater pipe (28-inch OD) and bend into an elbow fitting.
- Cast triple melt Inconel 740 ingot for a forged Wye pipe fitting and fabricate the Wye fitting.
- Cast triple melt H282 ingot and forge the ingot into an AUSC steam turbine rotor forging.
- Conduct second pour of H282 steam turbine nozzle carrier casting.
- Fabricate AUSC superheater section.
- Complete final flow qualification testing of AUSC PRVs.

PARTNERS

AECOM | ALSTOM | MetalTek INTERNATIONAL
EPRI ELECTRIC POWER RESEARCH INSTITUTE | Riley Power a Babcock Power Inc. company | GE | Energy Industries Of Ohio
McConway & Torley, LLC CRAFTSMANSHIP & INNOVATION | SPECIAL METALS

HOLISTIC, LOWER COST/ENERGY EFFLUENT WATER MANAGEMENT APPROACHES FOR COAL-FIRED ENERGY PLANTS

Yielding lower-cost clean water and reduced energy consumption compared to conventional systems, with reusable/safely disposable salts and solid byproducts
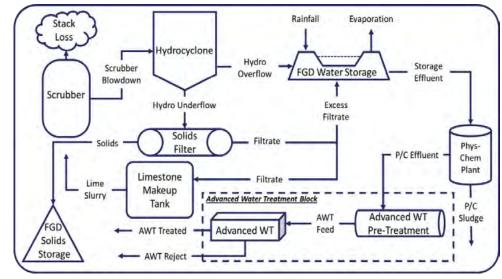
HOLISTIC APPROACH TO FLUE GAS DESULFURIZATION DISCHARGE TREATMENT

This project successfully completed a 60-day demonstration of a flue gas desulfurization discharge treatment system for significant cost/energy savings, as well as developed and tested approaches to make unusable byproducts safer and cheaper to dispose of as non-hazardous materials.
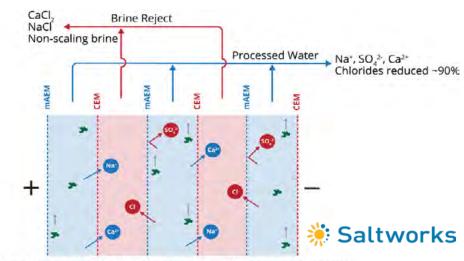
STATISTICAL-BASED WATER MASS BALANCE MODEL

Identifying Opportunities for Reducing Water Consumption and Meeting Discharge Requirements

Integrated water volume and chemical composition model with flexible input/output module to support site-specific scenarios.

HIGHLY EFFECTIVE, LOWER COST ENERGY TECHNOLOGY FOR TREATING FLUE GAS DESULFURIZATION DISCHARGE

At Pilot Scale at the Georgia Power Plant (Bowen) Water Research Center

Monovalent Electrodialysis (mEDR) with FlexEDR Selective
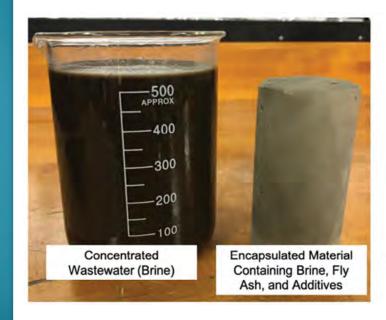Remove chlorides at high recovery with minimal pre-treatment
mAEM Monovalent anion exchange membrane (blocks sulphate, passes chloride)
CEM Cation exchange membrane
Organics do not transit or foul membranes

ENCAPSULATION OF SOLID BYPRODUCTS OF WASTEWATER TREATMENT FOR SAFE DISPOSAL

Developed and Tested for Process Byproducts

EPRI partnering with Golder, performed geochemical modeling, benchtop and mineralogical testing, and field lysimeter deployment to enable comparisons of modeling and field-derived results, generating insights to support enhanced modeling capabilities and data on long-term material properties.

Concentrated Wastewater (Brine) — Encapsulated Material Containing Brine, Fly Ash, and Additives — Scanning Electron Microscope Image of a Sample from the Encapsulated Material

SOFTWARE TOOLS AND GUIDELINES HELP TO DEVELOP WATER SYSTEMS VIEW

The software models and associated guidelines developed in the project will help energy plants utilize wastewater treatment and byproduct encapsulation as components of a holistic approach to water management.

PARTNERS

EPRI | ELECTRIC POWER RESEARCH INSTITUTE

GOLDER

Saltworks

CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION
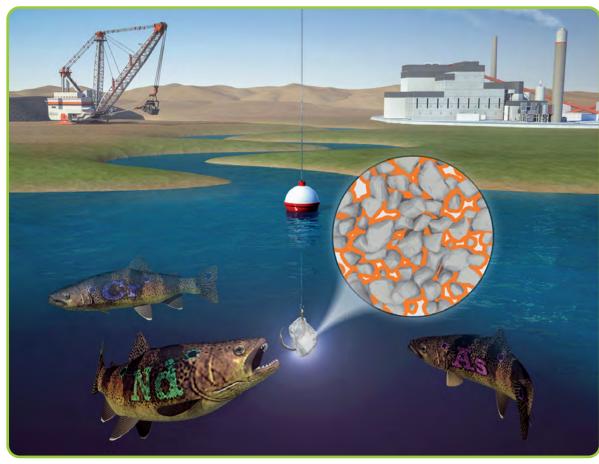
SYSTEMS ENGINEERING and ANALYSIS

RARE EARTH EXTRACTION FIELD TESTS PROVE VERSATILITY OF NOVEL SORBENT

Unique sorbents recover valuable rare earth elements from acid mine drainage (AMD) waters and heavy metals from flue gas desulfurization (FGD) discharge.

MULTIPLE PROCESSES BENEFIT FROM BASIC IMMOBILIZED AMINE SORBENT (BIAS) DEVELOPMENT

Rare earth elements (REE) and heavy metals are selectively recovered utilizing a highly adaptable sorbent that is also designed to efficiently capture CO_2. Successful demonstration of cyclic adsorption and desorption of ~90% REE from a synthetic AMD solution, and >90% successful removal of lead from spiked tap water further prove the efficacy of this sorbent for commercial applications. These critical advancements in BIAS technology represent exciting progress towards the realization of a commercial-scale, efficient REE extraction or CO_2 capture process.
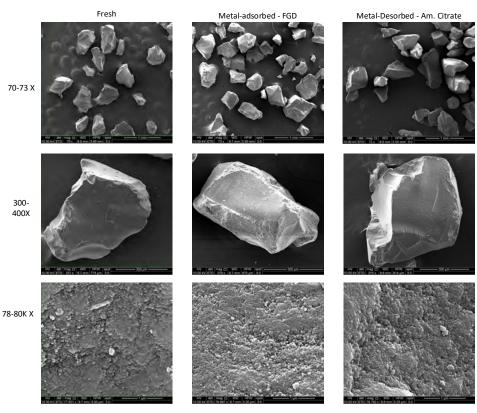

Novel sorbents can selectively remove heavy metals and rare earth elements from industrial wastewater, improving environmental sustainability and economics

PITTSBURGH BOTANIC GARDEN FIELD TEST ACHIEVES SUCCESSFUL EXTRACTION AND ENRICHMENT OF REE FROM ACID MINE DRAINAGE

Solid sorbent from a field test conducted at the Pittsburgh Botanic Garden achieved REE concentration enrichments in the evaporated, eluted effluent at 400 to 8,000 times the concentration of the authentic AMD. With ~100% of the bound REE released from the sorbent, the results indicate reusability and commercial viability of the sorbent for REE extractions.

UNIQUE DESIGN ENHANCES SORBENT STABILITY

The BIAS sorbents utilize robust amine–epoxide cross-linkages and are designed to be H_2O-stable materials. Advanced technical characterization work with a Scanning Electron Microscope reveals no appreciable change in the sorbent's structure upon adsorbing metals from real FGD discharge. Stable flow-through sorbent properties during cycling ensures smooth process performance and reduces potential for column plugging.

Images of sorbents before and after metal adsorption from FGD discharge and after metal desorption provide evidence of sorbent stability

PRINCIPAL INVESTIGATOR HONORED, PATENTS ISSUED, AND TECHNOLOGY LICENSED

In Fiscal Year 2020, McMahan Gray received a Distinguished Alumni Award from the University of Pittsburgh's Chemistry Department for his contributions to chemistry and sorbents. Unprecedented sorbent results have led to a second patent being issued on the BIAS pelletization process for CO_2 capture applications in 2020. The patent "Stable immobilized Amine Sorbents for REE and Heavy Metal Recovery from Liquid Sources" is pending and currently licensed by PQ Inc.

AWARD NUMBER
FWP-1022420
TASK 3

PROJECT BUDGET
FY20 FUNDING

$2.3M

● TASK 3 ·················· $983,000

CONTACTS

HQ PROJECT MANAGER
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TECHNICAL PORTFOLIO LEAD
THOMAS TARKA

PRINCIPAL INVESTIGATOR
MCMAHAN GRAY

CORE COMPETENCIES

MATERIALS ENGINEERING and MANUFACTURING

PROGRAM EXECUTION and INTEGRATION

GROUND-BREAKING TECHNOLOGIES ACCELERATE COMMERCIALIZATION OPPORTUNITIES FOR RARE EARTH EXTRACTION FROM COAL
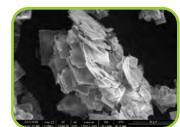
NETL researchers advance extraction technologies, producing high-purity (>95%) rare earth oxides from a diverse array of coal wastes.

STAGED LEACHING TECHNIQUE MINIMIZES THE COST OF EXTRACTING RARE EARTH OXIDES (REO) FROM ASH

NETL researchers produced high purity REO via a novel extraction technique for Powder River Basin (PRB) ash. By dissolving only a small portion of the ash and operating at ambient conditions, chemical and equipment costs are minimized, improving commercialization possibilities. PRB coal comprises 50% of the coal produced in the U.S. and is consumed throughout America.

PRB Fly Ash

96 wt.% REO

ACID MINE DRAINAGE TECHNOLOGY TRANSFORMS AN ENVIRONMENTAL ISSUE INTO AN ECONOMIC OPPORTUNITY

Researchers surpassed a major milestone in producing a 95wt% REO concentrate from acid mine drainage (AMD) both by treating AMD directly and processing the solid waste from passive AMD treatment systems. Each pathway can eliminate an expensive processing step—solvent extraction—to reduce cost, paving the way to address a widespread environmental issue in Appalachia.

AMD and AMD Sludge (Photos courtesy of B. Hedin)

TAKING INNOVATIONS FROM THE LABORATORY TO COMMERCIALIZATION

NETL's Staged PRB Ash Leaching project was one of 222 projects selected for a Technology Commercialization Fund award, resulting in $1.6 million of DOE and partner-matched funding. The project will result in a small pilot facility that validates and de-risks the commercialization of NETL's PRB extraction inventions. Separately, the ability of NETL's BIAS sorbent is being validated for rare earth elements (REE) recovery from AMD in a field test.
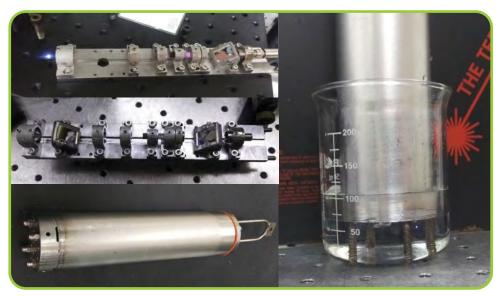
TECHNOLOGY TO "WASH" REE OUT OF CLAY MINERALS AND COAL REFUSE

A patent was filed for a minimally invasive technology to extract REE from clays and coal refuse using mild acids at room temperature and pressure. The technique doesn't dissolve the host material, which translates to reduced costs, and may be broadly applicable to non-coal resources domestically and abroad (particularly in South America).

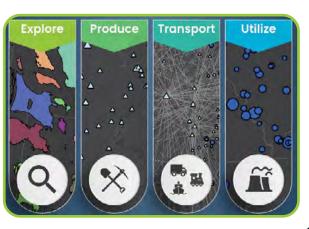## REAL-TIME SENSING CAPABILITIES SPARK INTEREST FROM INDUSTRY

NETL's real-time sensors enable the analysis of REE-containing resources in minutes (instead of hours), enabling innovation in REE separation processes and rapid identification of which feed sources warrant processing. The opportunity to leverage these sensors for rapid analysis and process control have led to industry interest and potential licensing opportunities.

Submersible laser-induced breakdown spectroscopy prototype

IDENTIFYING HIGH PRIORITY REE-CRITICAL MATERIALS RESOURCES THROUGH MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE

NETL has implemented a revision of their REE sedimentary resource assessment method, which leverages 21st century capabilities to identify promising REE resources in sedimentary systems. Modeling results for the PRB are being validated using geologic cores, and the method is being applied to other basins.

PARTNERS

CORE COMPETENCIES

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

MATERIALS ENGINEERING and MANUFACTURING

SYSTEMS ENGINEERING and ANALYSIS

MFiX SOFTWARE SUITE – PUSHING THE CODE FORWARD FOR INDUSTRIAL-SCALE SYSTEMS
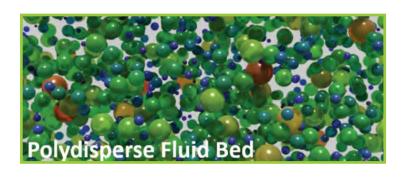
Enabling Accelerated Energy Systems Development with Modeling-based Rapid Scale-up and Design Optimization

SIGNIFICANT ENHANCEMENTS TO ENABLE CHALLENGING DESIGN AND OPTIMIZATION APPLICATIONS AT LARGE SCALES

Enhancements for Speed and Accuracy

- MFiX Releases 20.1-20.3 are designed for complex industrial problems
- New preprocessing for enhanced mesh quality
- **Set up time reduced significantly, less potential for user error**
- Particle-in-Cell and Coarse-Grained DEM techniques provide **10x speed increase**
- Polydispersity provides accurate **particle size distribution for large systems**
- Moving geometries address **complex industrial flow applications**
- All-time MFiX User Registrations now top 6,300 in FY 2020
- Annual software downloads continue to be strong—topping 3,900 in FY2020, even during a pandemic
- MFiX is now being used to support the 5x scale-up of an industrial gasifier for Office of Fossil Energy (FE) program support
- MFiX used to evaluate novel gasifier configurations hydrogen production with negative carbon emission
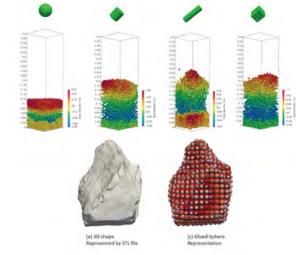

Polydisperse Fluid Bed

Rotating Bed - Mixing
Conveyor – Feed Systems
Impellers - Mixing
Valves – Flow Control

ADVANCED MODELS FOR COMPLEX PARTICLES – INCREASED ACCURACY FOR ADVANCED REACTOR DESIGN

NETL's MFiX Suite can now model large systems with complex particle shapes for greatly improved accuracy – SuperDEM
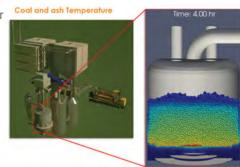
- Represent a broad range of particle shapes and can be used for modeling collisions and trajectories
- Demonstrated for fluid beds of over 100 million particles on 6800 supercomputer cores
- More accurately model behavior of complex reactor feedstocks like **coal, biomass, plastics, municipal solid waste**
- Runs on supercomputing systems using large core-count jobs to address industrial reactor systems of complex feedstock particles
- Greatly increased accuracy of feedstock flow physics in complex fossil energy reactors

(a) 3D shape Represented by STL file
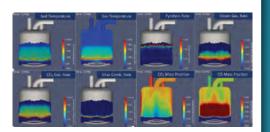(c) Glued-Sphere Representation

RECENT APPLICATIONS

Simulation for Gasifier Design: Industrial Scale Up and Next-Generation Systems

- A comprehensive simulation program has provided key insight into coal gasifier performance for a **5x scale up**.
- Transient gasifier performance over a range of loads was studied to evaluate impact on product gas — critical for designing balance of plant.
- Oxygen enrichment and biomass co-feed performance are being evaluated for the potential to achieve negative carbon emissions.
- Oxygen-blown gasification with steam enrichment is being studied for hydrogen production.
- Simulation support for the University of Alaska project will greatly de-risk FE's investment in this technology.
- Simulations can help identify key gasification reactor concepts that can be used for CoalFIRST and hydrogen production initiatives.

Coal and ash Temperature
Time: 4.00 hr

NETL and Natural Resources Canada (NRCan)-CanmetENERGY have teamed to study circulating fluidized bed (CFB) combustion systems with coal-biomass co-feed with potential for carbon capture.

- NETL is simulating the 50kWth pilot CFB system being operated at NRCan over a range of coal-biomass blends and oxygen-enrichment conditions.
- The collaboration provides NETL with high quality, detailed data and provides NRCan with valuable insight into conditions inside the system to help guide system optimization.
- Once validated at the small pilot scale, these MFiX models running on FE's JOULE2 supercomputer will be used to study scale-up and performance optimization of coal-biomass CFB combustion systems designed for negative CO_2 emissions.

PARTNERS

SOTACARBO SUSTAINABLE ENERGY RESEARCH CENTRE

NVIDIA.

OAK RIDGE National Laboratory

Natural Resources Canada

NREL NATIONAL RENEWABLE ENERGY LABORATORY

CORE COMPETENCY

COMPUTATIONAL SCIENCE and ENGINEERING

REALIZING FOSSIL ENERGY'S (FE) DATA-DRIVEN FUTURE

EDX Energy Data eXchange®

Visit **edx.netl.doe.gov** to learn more.

SUPPORTING THE ENTIRE DATA LIFECYCLE BY OFFERING R&D PROJECTS SECURE, VIRTUAL COLLABORATIVE WORKSPACES & CURATED LIBRARIES

EDX is FE's Smart Portal, Accelerating Data-Driven R&D

Meeting the need for improved and secure access to data for knowledge discovery, FE is investing in its future to drive the next-generation of applied energy technologies and research.

EDX **preserves over $20 billion** in research products, **preserving almost 125,000 public models, tools, datasets and publications** that have been **downloaded over 2 million times**.

EDX products comply with Federal data orders and regulations and international *FAIR* data standards.

WATT The Power of Ai

EDX Energy Data eXchange®

JOULE NETL SUPERCOMPUTER

SAMi SCIENCE-BASED AI/ML INSTITUTE

In FY20, Demand for EDX Capabilities & Resources Increased:
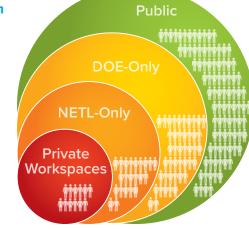
- **53.1% in Annual Data Downloads** (~2.1M total data downloads)
- **32.2% in New Data Resources** (131,152 total data resources)
- **31.8% in New Workspaces** (871 total workspaces)
- **23.5% in New Registered Users** (2,465 total EDX users)

Inform
Analyze & Optimize
Integrate & Label
Explore & Transform
Move & Store
Discover & Collect

EDX V.3 Launched, March 2020 — marking a major platform update

- **Enhanced search, filter, and data access capabilities aligned to the CKAN platform** EDX is built on
- Sets a foundation for **future, virtualized analytical capabilities** beyond current capabilities
- Optimized infrastructure to support future **data store with cloud backup**

Public
DOE-Only
NETL-Only
Private Workspaces

EDX Introduced Tiered Workspaces

Offers role-based security for the platform's diverse user community

To Date, EDX has

- **800+ active research projects** via EDX Collaborative Workspaces and **80,000+ secure, private data files**
- **20,000+ published resources** (digital files or external source links)

UNITED STATES PATENT AND TRADEMARK OFFICE

uspto

In 2020, EDX was granted a registered trademark

2020 R&D DATA HIGHLIGHTS

Harnessing AI/ML to Develop Big Data Foundation

NETL used AI/ML to **collect, label, organize, and catalogue** thousands of data resources, establishing a **strong foundation for carbon storage R&D**.

- These efforts have **increased the value, discoverability, accessibility, and integrity of large volumes of data** critical for carbon storage R&D and driving next-generation carbon storage breakthroughs.

In August 2020, EDX published the **Open-Carbon Storage Data Collection**.

- Including public release of *FutureGen 2.0 datasets*
- **Consists of nearly 7,000 files and millions of features**
- Integrated with strategic open-source resources
- **Key source of subsurface data and model simulations**
- Already being utilized for **R&D in NRAP, SMART-CS, oil, gas, geothermal, and other projects**

Powering Virtualized, Data-Driven Models & Tools

EDX continued to support the *Offshore* Spill Prevention Portfolio's **goals, hosting custom advanced spatio-temporal analytical tools, tapping into the power of EDX's big data cluster computing**.

- Simplified access and usability for end-users
- Combining **big datasets** and **analytics**, in a secure **platform**
- **Virtual access to custom models and tools** from NETL's R&D 100 award-winning *Offshore Risk Modeling Suite*

Capturing Data Quality Rankings

Metadata to characterize data quality is key to reuse. Published method developed by eXtremeMAT was used to inform capability deployed for all EDX users in FY20.

Overall	Completeness	Source	Accuracy	Accessibility
4.75 (4)	5.0 (1)	5.0 (1)	5.0 (1)	4.0 (1)

ENGAGEMENTS

BROOKHAVEN NATIONAL LABORATORY · eXtremeMAT · NRAP · SMART · Marcellus Shale Energy and Environment Laboratory · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · NREL · OAK RIDGE National Laboratory · Pacific Northwest NATIONAL LABORATORY · INL Idaho National Laboratory · Sandia National Laboratories · USGS science for a changing world · OSTI · U.S. DEPARTMENT OF ENERGY · ENERGY Energy Efficiency & Renewable Energy · ENERGY Office of TECHNOLOGY TRANSITIONS · ENERGY Office of ENVIRONMENTAL MANAGEMENT · ENERGY Office of Science · NGDS National Geothermal Data System · THE GENERAL COUNSEL · OpenEI Open Energy Information · DOE CODE · EPA · BOEM · ENERGY Office of THE CHIEF INFORMATION OFFICER · BSEE · BOSCH · CITRINE INFORMATICS · Chevron · UN environment · EDF ENVIRONMENTAL DEFENSE FUND · MGSC · EPRI ELECTRIC POWER RESEARCH INSTITUTE · gti · SECARB · MRCSP · PCOR · West Coast Regional Carbon Sequestration Partnership · ExxonMobil · Big Sky Carbon Sequestration Partnership · westcarb.org

CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

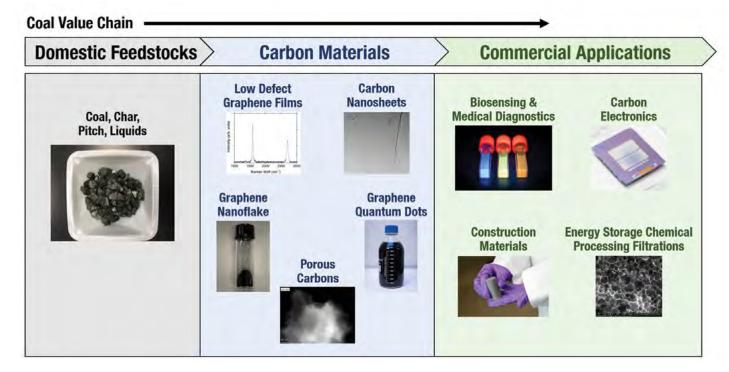MATERIALS ENGINEERING and MANUFACTURING

MANUFACTURING CARBON MATERIALS AND CONSUMER PRODUCTS FROM COAL

Cost-competitive, high-value products from coal create new jobs, products, and markets for domestic coal.

COAL-BASED MANUFACTURING CREATES NEW BUSINESS OPPORTUNITIES

NETL's Advanced Coal Processing Program develops technologies that convert coal into salable carbon materials and consumer products instead of burning it to produce electricity and greenhouse gas emissions. Products manufactured from coal range from high-volume construction materials, such as concrete additives, to high-value dielectric materials used in miniaturized computer electronics.

Coal is not traditionally used to manufacture high tech materials. As such, coal-based manufacturing creates new business opportunities for the coal industry at a time when demand for coal-based electricity is rapidly declining. Coal's use as a manufacturing feedstock also creates opportunities to reduce manufacturing costs and improve the performance of carbon materials and products over what can be achieved with conventional feedstocks.

NETL MANUFACTURES ADVANCED CARBON MATERIALS DIRECTLY FROM DOMESTIC COAL

NETL researchers develop physical and chemical processing methods to make high-performance carbons from coal. Current materials manufactured by NETL include: atomically-thin dielectric materials for memristor computer memory devices, low-defect graphene films for sensor and medical diagnostic applications, engineered graphene flake to improve the strength and durability of concrete construction materials, and porous sorbents for hydrogen energy storage and water remediation applications.
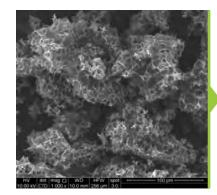
NETL'S COAL TO GRAPHENE (C2G) PROCESS WINS AN R&D 100 AWARD

NETL's low-cost Coal to Graphene (C2G) technology was recognized with a prestigious R&D 100 Award. The technology produces bulk quantities of nanostructured, graphene-like, carbon from anthracite, bituminous, and sub-bituminous ranks of coal. NETL is partnering with Ramaco Carbon through a Cooperative Research and Development Agreement to further develop this technology for commercial applications.

COAL-BASED POROUS CARBONS SHOW POTENTIAL FOR ENERGY STORAGE AND WATER PURIFICATION APPLICATIONS

Using Powder River Basin Coal as a feedstock, NETL researchers synthesized a series of porous carbons with narrow and tunable pore size distributions ranging from 1 to 50 nanometers. This allows researchers to design sorbent materials with pore sizes that are matched to small gas molecules (e.g., hydrogen), atomic ions (e.g., S^{2-}), and larger organic molecules (e.g., polycyclic aromatic hydrocarbons). This tunability opens opportunities to use these materials for increasing the amount of hydrogen gas that can be safely stored inside vehicular fuel tanks, enhance the efficiency and durability of LiS batteries, and to remove salts and organic waste from industrial waste water streams. NETL is currently collaborating with industrial partners to evaluate the commercialization potential of this technology.

Electron Microscopy Image of Coal-derived Porous Carbons: These carbon materials have high surface areas (1500-3500 m^2/g) and can be utilized in energy storage applications for batteries and supercapacitors.

PARTNERS

ADVANCEMENTS IN NETL CO_2 STORAGE ESTIMATOR TOOLS IMPROVE SPEED AND ACCURACY OF U.S. CO_2 STORAGE CAPACITY ASSESSMENTS

NETL researchers are developing advanced methods and tools to better assess storage resource potential (volume of CO_2) for onshore and offshore areas.

ENSURING SUCCESSFUL, LONG-TERM STORAGE USING DATA-DRIVEN ANALYTICS

Accurately **determining CO_2 storage potential and capacity is critical** to the overall success of any carbon capture, utilization, and storage (CCUS) effort. This information allows stakeholders to determine whether conditions are not only **advantageous, but also financially feasible** for CCUS operations. NETL has developed and released three **publicly available** tools designed to rapidly assess storage resource potential and capacity.

Enhanced oil recovery (EOR) settings

FE/NETL CO_2 Prophet Model

Select "FE/NETL CO_2 Prophet Model" under collection name and then hit the search button.
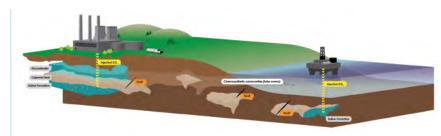
Multiple onshore geologic settings

CO_2 SCREEN

Offshore saline environments

NETL CARBON STORAGE

Offshore CO_2 Storage Calculator

THE OFFSHORE CO_2 STORAGE CALCULATOR*: APPLYING BIG, SPATIAL DATA TO ESTIMATE LONG-TERM STORAGE EFFICIENCY AND RESOURCE POTENTIAL IN SALINE RESERVOIRS

- Accounts for differences in the offshore environment, including how **CO_2 density** changes with the overlying water column and how **sediment behaves differently** in offshore environments (ex. Gulf of Mexico sediment is unlithified, more porous and permeable)
- Integrates **spatial data**, including features unique to offshore saline environments (bathymetric data and leakage pathways)
- **Calculates distributions for estimated storage efficiency** and **long-term resource potential** (in gigatons) at the local to regional spatial scale
- **User-friendly stand-alone tool**, tutorial, and help documentation all available for **download** through NETL's Energy Data eXchange*
- **Industry interest demonstrated**: tool has been downloaded over 15 times since it was released (March 2020)
- Custom built to **compliment NETL CCUS tools**
- Can be streamlined with **NETL's R&D 100 award-winning Offshore Risk Modeling** suite to **quantify uncertainty** and **down-select optimal injection sites** by accounting for **favorable infrastructure** while avoiding potential hazards
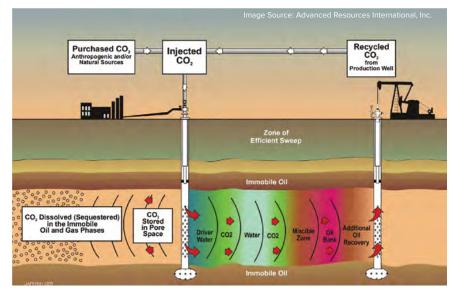
Sample Modeling Outputs

Tool outputs include comprehensive data table, overall percentiles (P10, P50, P90) for efficiency and storage potential, spatial data, and distribution graphs (shown below)

Example Results

A. Data table
B. Summary table
C. Variable distributions*
D. Phase distributions*
E. Spatial setbacks*

A.
B.
C. Storage resource potential — Overall efficiency
D. CO_2 density — Phase *(vapor, liquid, supercritical)* based on PT-regime and CO_2 Density
E.

* Optional outputs

FE/NETL CO_2 PROPHET MODEL* ENABLES USERS TO QUICKLY MODEL OIL PRODUCED AND CO_2 STORED AT AN OIL FIELD

- A streamline/stream tube reservoir simulator that can **simulate water flooding and CO_2 EOR** for a pattern at an oil field
- The outputs of the Prophet model are used as inputs to the FE/NETL Onshore CO_2 EOR Cost Model to estimate the CO_2 stored, oil produced and project economics for the oil field
- Model does not **require proprietary oil field datasets or models**, allowing for the transparent generation of results.
- **Model is fast**, requiring 5 to 20 seconds to simulate 30 years of CO_2 EOR at an oil field

Image Source: Advanced Resources International, Inc.

*Updated version of the CO_2 Prophet model developed by Texaco E&P for DOE.
Morgan, David; Remson, Donald; McGuire, Thomas. *Conceptual and Mathematical Foundation for the FE/NETL CO_2 Prophet Model for Simulating CO_2 Enhanced Oil Recovery, Version 2.* United States: N. p., 2020. Web. doi:10.2172/1572936.

CO_2SCREEN* OPENS DOOR FOR PREVIOUSLY UNRECOGNIZED LARGE-SCALE CCUS PROJECTS

- **Updated tool** provides a robust, user-friendly platform to estimate CO_2 resources and storage efficiency
- Can be used to **assess a variety of geological environments**, including saline formations, shale formations, and residual oil zones
- **More accurately estimates CO_2 storage potential in previously overlooked locations**, opening the door for additional storage opportunities

*Sean Sanguinito, Angela Goodman, Foad Haeri, CO_2-SCREEN, 1/28/2020, https://edx.netl.doe.gov/dataset/co2-screen, DOI: 10.18141/1719097

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OFFSHORE CO_2
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CORE COMPETENCIES

GEOLOGICAL and ENVIRONMENTAL SYSTEMS

SYSTEMS ENGINEERING and ANALYSIS

IDAES SPEARHEADED CUTTING-EDGE RESEARCH AND MODELING TO IMPROVE POWER PLANT COSTS AND PERFORMANCE

IDAES employs advanced process systems engineering capabilities to optimize fossil energy systems.

The Institute for the Design of Advanced Energy Systems (IDAES) Integrated Platform **accelerates cost-effective technology deployment needed to support critical DOE missions**.

IDAES enables the design and optimization of complex, interacting technologies and systems by providing **rigorous modeling** capabilities **to increase efficiency, lower costs, increase revenue, and improve sustainability** of power generation and electricity distribution.
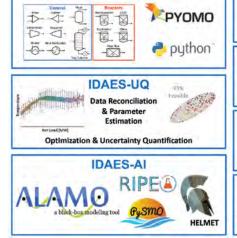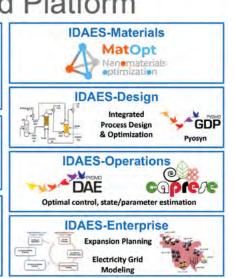
IDAES
Institute for the Design of Advanced Energy Systems

NEXT-GENERATION COMPUTATIONAL FRAMEWORK

IDAES builds on fundamental advances in algorithms and computing technology to address a critical capability gap in process modeling tools.

The IDAES Integrated Platform includes tools for the **large-scale optimization** of complex **dynamic systems, machine learning,** and **uncertainty quantification**.

Integrated Platform

IDAES-Core — PYOMO, python
IDAES-Materials — MatOpt Nanomaterials optimization
IDAES-UQ — Data Reconciliation & Parameter Estimation, Optimization & Uncertainty Quantification
IDAES-Design — Integrated Process Design & Optimization, GDP, Pyosyn
IDAES-Operations — DAE, caprese, Optimal control, state/parameter estimation
IDAES-AI — ALAMO a black-box modeling tool, RIPE, PySMO, HELMET
IDAES-Enterprise — Expansion Planning, Electricity Grid Modeling

FY20 EFFORTS ADDRESSED PRESSING NEEDS OF THE POWER INDUSTRY...

Improved Operation of Existing Plants

Through a Cooperative Research and Development Agreement with Tri-State Generation and Transmission Association, Inc., advanced computational tools were applied to their Escalante Generating Station. This effort identified a process bottleneck **enabling a 44% improvement in the plant's minimum operating load**.
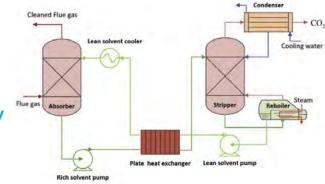
Continued Recognition and Growth

IDAES was the recipient of a **2020 R&D 100 Award**, and has thousands of downloads with an active, growing **global user community** from multiple industries.

R&D 100 2020 WINNER

...AND SOLVED CRITICAL U.S. ENERGY CHALLENGES

Reduced Cost of Carbon Capture

IDAES enabled the optimization of an amine-based post-combustion CO_2 process, **reducing the operating cost by 15–18%** using models validated against data from the National Carbon Capture Center.
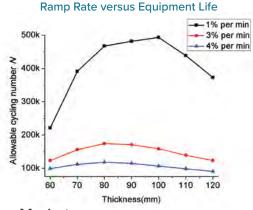

Improved Process Efficiency

Through efficient, automatic exploration of 42 million process alternatives, **the energy demand** of a complex separation system was **reduced by more than 40%**.

Demonstrated Advantages of Hybrid Energy

Demonstrated how retrofitting existing generators with energy storage has the potential to **reduce equipment wear and tear by 30%** by reducing stresses caused by equipment cycling.

Ramp Rate versus Equipment Life

Designed Plants for Future Energy Markets

Modeling of **generator interactions with the bulk power market** has shown that these interactions are **more complex than previously thought** — a finding with the potential to radically change how new power plants are designed and valued.

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CORE COMPETENCY

SYSTEMS ENGINEERING and ANALYSIS
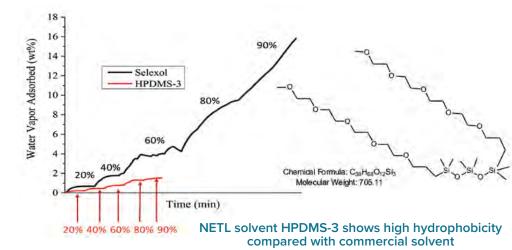
INNOVATIVE MATERIALS DEVELOPED TO IMPROVE CO$_2$ CAPTURE PERFORMANCE

Progress towards 2030 DOE program goal of demonstrating 95% CO$_2$ purity with a cost of capture less than $30/tonne

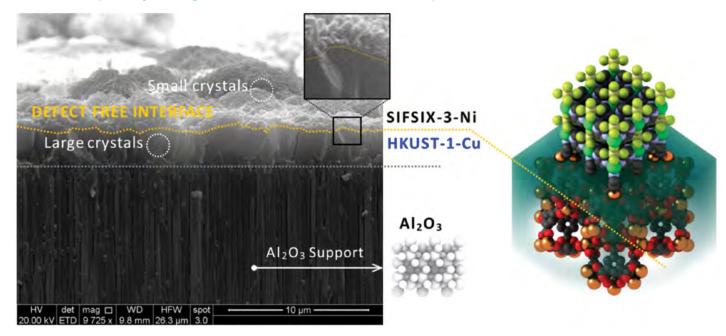## PATENT OBTAINED FOR NOVEL HYDROPHOBIC SOLVENT

NETL researchers obtained U.S. Patent #10,589,228 for a new solvent (HPDMS-3) for capturing CO$_2$ from fuel gas streams, such as downstream of coal gasifiers or at petroleum refineries. The solvent is hydrophobic, can operate at and above room temperatures, and can be regenerated using waste heat, **significantly reducing the cost of CO$_2$ capture at IGCC powerplants and plants that generate hydrogen from fossil fuels**.

Chemical Formula: C$_{30}$H$_{68}$O$_{12}$Si$_5$
Molecular Weight: 705.11

NETL solvent HPDMS-3 shows high hydrophobicity compared with commercial solvent

NEW TECHNIQUE FOR GROWING METAL-ORGANIC FRAMEWORK (MOF) THIN FILMS

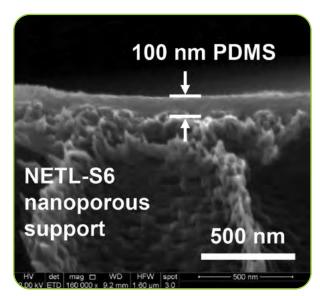**Application to post-combustion CO$_2$ capture membranes**
NETL developed a technique for growing a planar MOF thin film on the surface of a second type of MOF film, with chemical binding between them, to improve membrane permeance and selectivity performance for post-combustion CO$_2$ capture. **This novel technique was published in *Cell Reports Physical Science* and subsequently recognized as one of their "Best Papers of 2020."**

Dual layer MOF films form a layer of small crystal SIFSIX-3-Ni over HKUST-1-Cu

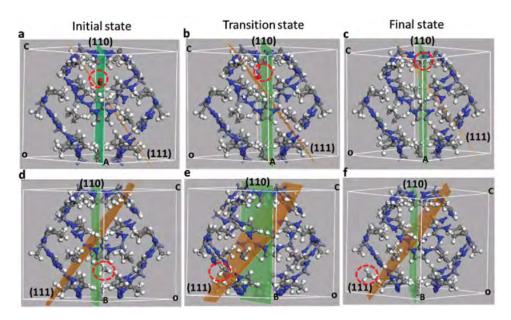## INVENTION OF NEW POLYMER SUBSTRATE FOR CO$_2$ SELECTIVE MEMBRANES

NETL researchers invented a new high permeance (260,000 GPU), chemically and thermally stable porous polymer support that is optimized to serve as the substrate for a CO$_2$ selective membrane. A composite membrane with a Polydimethylsiloxane (PDMS) selective layer **achieved the highest CO$_2$ permeance (12,600 GPU) of any known defect-free PDMS membrane**.

PDMS/NETL support thin film composite

STUDIES ILLUMINATE GAS SEPARATIONS BEHAVIOR IN KEY MATERIALS

Research on CO$_2$ and methane (CH$_4$) gas adsorption and diffusion in bulk zeolitic imidazolate framework-8 (ZIF-8) materials using a density functional theory approach found that **CO$_2$ has higher adsorption energy and diffusion barriers than CH$_4$**.

Modeling of CO$_2$ (a, b, c) and CH$_4$ (d, e, f) molecules (indicated with red dotted circles) diffusing in ZIF-8, with reference to the miller planes (111) (orange) and (110) (green)

CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING

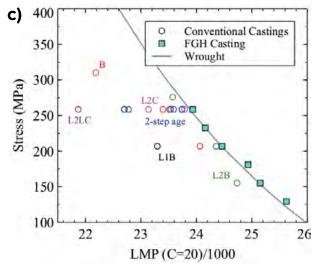MATERIALS ENGINEERING and MANUFACTURING

SYSTEMS ENGINEERING and ANALYSIS

ADVANCED ALLOY DEVELOPMENT

NETL utilized its extensive alloy development and manufacturing capabilities to improve alloys and processes that enable advanced energy systems and advanced technologies.
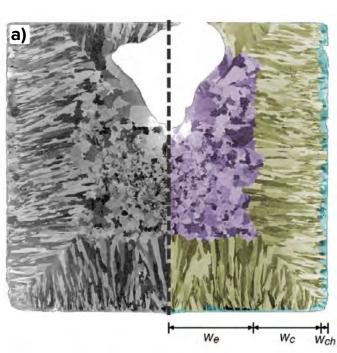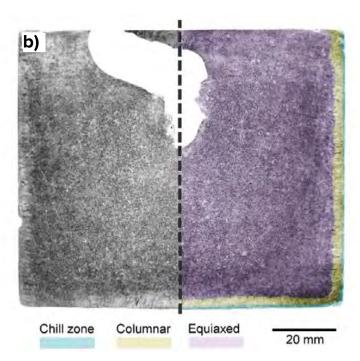
ACHIEVING CASTABLE HEAT-RESISTANT SUPERALLOYS

Cast Version of Alloy IN 740H - Expanding supply chain options for large castings for advanced energy systems

NETL developed an alternative method to manufacture cast components from superalloy. The method enables additional alloys to be used for manufacturing components for advanced high-efficiency energy systems, and helps to diversify the supply chain by providing original equipment manufacturers with alloy options. Currently, advanced ultra-supercritical and sCO$_2$ (Supercritical Transformational Electric Power) projects are using Haynes 282 to demonstrate large castings of superalloy components. NETL played a role in developing large castings of Haynes 282, a traditional wrought (forged, rolled, extruded) alloy, by demonstrating that the cast forms of the alloy could achieve similar performance to wrought form. In part this was achieved by NETL developing an award-winning computational method to specify homogenization heat-treatment of casting. However, unlike Haynes 282, cast versions of other superalloys, such as IN740H, did not perform as well in the cast and heat-treated condition compared to the wrought condition. Consequently, NETL developed a modified casting method that promotes a homogeneous grain structure, grain boundary carbide repartition, and enhanced chemical homogeneity within the cast ingot. The material produced through NETL's Fine Grain Homogenization (FGH) process outperformed conventional castings and showed comparable creep resistance to wrought IN740H.

Grain structure of (a) conventional casting and (b) the NETL FGH casting. (c) Larson-Miller plot (figure of merit for creep behavior) for conventional and NETL developed FGH.
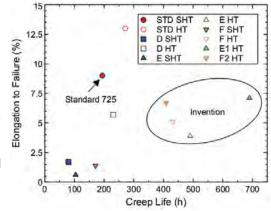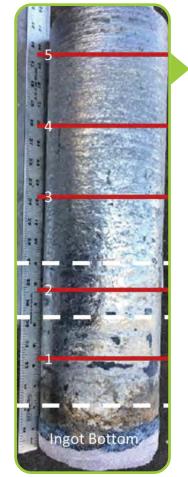

OPTIMIZING THE PERFFORMANCE OF SUPERALLOYS

For Strength, Ductility, Stability, and Temperature Capability. Lowering the Cost of Advanced Energy Systems

NETL is improving the performance of high-temperature alloys to enable operation of plants at higher temperatures while also reducing the thickness required to meet existing designs, making advanced systems more affordable.
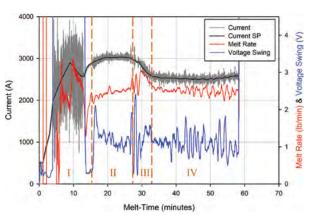
As an example, NETL modified corrosion-resistant alloy 725 to increase its strength and creep resistance at elevated temperatures and obtain an alloy with a unique set of properties, including an increase in creep life of up to 256% at 700°C / 483 MPa. A provisional patent application has been filed for the NETL technology.

LEVERAGING CAPABILITIES TO ASSIST AMERICA'S ALLOY MANUFACTURERS

Through strategic partnership projects, NETL continues to partner with America's specialty alloy manufacturers, end users, and other research organizations to improve advanced alloys. As an example, in 2020, through a 100% cost reimbursable project with a Ni alloys manufacturer, NETL successfully performed electro-slag remelting (ESR) of a Ni alloy as a lower cost method to produce high-purity Ni alloy for critical medical, aerospace, and defense applications.

Above, controlled ESR melt recording enabled through slags and process parameters designed for the alloy. Left shows the ESR ingot produced at NETL. NETL 's ingot metallurgy capabilities readily scale to industrial practice.

ACCELERATING THE DEVELOPMENT OF EXTREME ENVIRONMENT MATERIALS

Visit **edx.netl.doe.gov/extrememat** to learn more.

eXtremeMAT is a US DOE National Laboratory effort harnessing the DOE's unparalleled breadth of world-leading materials science and engineering expertise and capabilities to realize affordable and durable materials for fossil energy applications.

MATERIALS DISCOVERY & QUALIFICATION

eXtremeMAT is developing and demonstrating advanced computational tools **to accelerate the development cycle of cost-effective alloys for harsh environments needed to enable highly efficient advanced energy systems**.
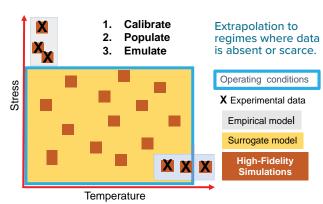
THRUSTS

1 Materials Lifetime & Performance Predictors
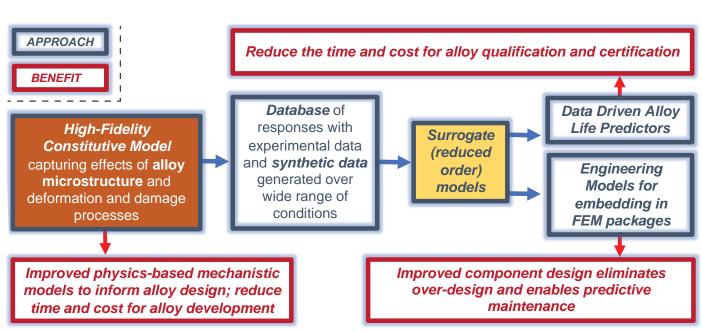
2 Component Lifetime & Performance Predictors

3 Data Science & Analysis Tools

4 Guidelines for Designing New Alumina Forming Alloys

eXtremeMAT's MODELING FRAMEWORK & APPROACH

1. Calibrate
2. Populate
3. Emulate

Extrapolation to regimes where data is absent or scarce.

Operating conditions

X Experimental data

Empirical model

Surrogate model

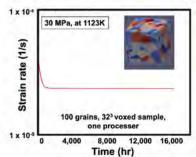High-Fidelity Simulations

Stress / Temperature

The *eXtremeMAT* models are intended to be predictive in arbitrary loading conditions, sensitive to microstructure and composition, and account for operative alloy deformation and damage processes. **The model framework is applicable to multiple alloys**.

APPROACH

BENEFIT

Reduce the time and cost for alloy qualification and certification

High-Fidelity Constitutive Model capturing effects of **alloy microstructure** and deformation and damage processes

→ **Database** of responses with experimental data and **synthetic data** generated over wide range of conditions

→ **Surrogate (reduced order) models**

→ **Data Driven Alloy Life Predictors**

→ **Engineering Models for embedding in FEM packages**

Improved physics-based mechanistic models to inform alloy design; reduce time and cost for alloy development

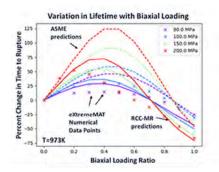*Improved component design eliminates over-design and enables predictive maintenance*
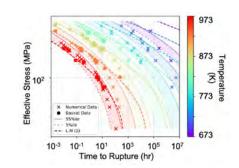
eXtremeMAT's CONSTITUTIVE MODEL

The mechanistic model, initially developed for alloy P91 and implemented in a finite element solver, has been extended **to account for second phase strengthening, to predict primary secondary and tertiary creep,** and implemented in a **numerically efficient** Fast Fourier Transform (FFT)-based formulation.

The code can **simulate the response of an alloy subjected to creep loading conditions for a time period of 10 years in approximately 5 hours.** The model has been successfully calibrated for alloy 347H and is being used to produce a database of expected rupture life as a function of stress and temperature.
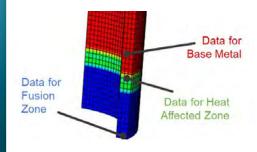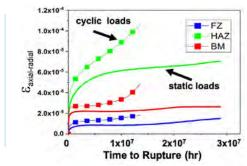

30 MPa, at 1123K
100 grains, 32³ voxed sample, one processer

eXtremeMAT's PERFORMANCE PREDICTORS

Variation in Lifetime with Biaxial Loading

As demonstrated above for alloy P91, a **rupture life criterion** that **considers uncertainty** and is applicable to **multi-axial loading** was derived **using limited experimental data**.

Data for Base Metal
Data for Fusion Zone
Data for Heat Affected Zone

Using LaRomance (Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations), a **surrogate model** was developed for **embedding into commercial finite element packages** and can account for **cyclical loading** (demonstrated above for an **idealized weld**).

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CORE COMPETENCIES

COMPUTATIONAL SCIENCE and ENGINEERING

MATERIALS ENGINEERING and MANUFACTURING

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