CROSSCUTTING RESEARCH

2022

UNIVERSITY TRAINING AND RESEARCH

PROJECT PORTFOLIO

DISCLAIMER

CONTENTS

CROSSCUTTING RESEARCH

NETL's Crosscutting Research Program matures novel technologies that can enhance the efficient performance and eliminate or reduce the environmental impacts of fossil energy power plants. On behalf of the U.S. Department of Energy's Office of Fossil Energy and Carbon Management (FECM), NETL pursues crosscutting research and development (R&D) by collaborating with other government agencies, world-renowned national labs, entrepreneurs, industry, and academic institutions. Efforts are focused on five primary research areas: High Performance Materials; Sensors, Controls, and Novel Concepts; Simulation-Based Engineering; Energy Storage; and University Training and Research (UTR).

The goals are to create transformational technologies under a single research umbrella that improve plant efficiency, flexibility, and security; reduce water consumption; reduce costs; and better enable dependable fossil power systems to maintain the stability and resilience of the electricity grid while maximizing use of variable renewable power sources. The research is leading to enhancements to the fleet such as new ways to address the challenges of load following, better ways to counter cyber intrusions, and advancements in affordable, scalable technical solutions. Because of the broad scope of the Crosscutting Research Portfolio, its technologies often have applicability to other energy-related sectors such as renewable and nuclear power generation, oil and natural gas infrastructure, and aviation (both commercial and military).

Crosscutting Research efforts include sponsorship of two long-running university training programs that prepare the next generation of scientists and engineers to meet future energy challenges. These are the University Coal Research (UCR) program and the Historically Black Colleges and Universities and Other Minority Institutions (HBCU-OMI) program. By working with students on the university level, the efforts ensure that key technologies in areas including advanced manufacturing, cybersecurity, smart data analytics, and high-performance computing will be integrated into fossil plants of the future.

In combination, these investments in innovation, informed by private sector stakeholders, enable more comprehensive risk assessment and techno-economic analysis, increase the resiliency of the nation's energy infrastructure, and enable the adoption of cutting-edge data harnessing technologies for plant owners and operators.

High Performance Materials: The High Performance Materials program drives to characterize, produce, and certify cost-effective alloys and other high-performance materials suitable for the extreme environments found in fossil-based power-generation systems. NETL supports and catalyzes a robust domestic materials supply chain that prepares materials for advanced ultra-supercritical (AUSC) steam cycles and spinoff applications. The work also enables research in suitable materials for supercritical carbon dioxide (sCO_2) cycles that yield higher thermal efficiencies.

The Crosscutting Materials program works to accelerate the development of improved steels, superalloys, and other advanced alloys to address challenges of both the existing fleet and future power systems. Materials of interest are those that enable components and equipment to perform in the high-temperature, high-pressure, corrosive environments of an advanced energy system with specific emphasis on durability, availability, and cost both within and across each of four primary platforms: Advanced Manufacturing, Advanced Structural Materials for Harsh Environments, Computational Materials Design, and Functional Materials for Process Performance Improvements.

Sensors, Controls, and Novel Concepts: The Sensors, Controls, and Novel Concepts program is conducting research and development for technologies that will provide pivotal insights into optimizing performance, reliability, and availability of integrated energy and carbon management systems. NETL develops, tests, and matures novel sensor and control technologies that are operable in next-generation energy systems, including hybrid plants incorporating components such as hydrogen-powered turbines and fuel cells, renewables, and energy storage applications. These sensors enable responsiveness to varying conditions in real time, maintaining high efficiencies and reducing emissions.

The Crosscutting Sensors, Controls, and Novel Concepts program explores advances within and the integration of technologies across the following primary research areas: Harsh Environment Sensors, Advanced Controls and Cyber Physical Systems, and Novel Concepts.

Simulation-Based Engineering: Simulation-Based Engineering (SBE) focuses on developing and applying advanced computational tools at multiple scales: atomistic, device, process, grid, and market scales, to accelerate development and deployment of fossil fuel technologies. Research in this area provides the basis for the simulation of engineered devices and systems to better predict and optimize the performance of fossil fuel power generating systems.

Computational design methods and concepts are required to significantly improve performance, reduce the costs of existing fossil energy power systems, and enable the development of new systems and capabilities such as advanced ultrasupercritical combustion and hydrogen turbines.

This effort combines theory, computational modeling, advanced optimization, experiments, and industrial input to simulate complex advanced energy processes, resulting in virtual prototyping. The research conducted in the SBE R&D develops accurate and timely computational models of complex reacting flows and components relevant to advanced power systems. Model development and refinement is achieved through in-house research and partnerships to utilize expertise throughout the country.

Energy Storage: Energy Storage aims to develop a comprehensive strategy to expand FECM's current portfolio of technologies and programs in order to better enable fossil power plants to maintain the electricity grid's stability and resilience while increasingly utilizing variable renewable power. Energy storage at the generation site will be essential to a resilient and flexible electricity network and NETL's Energy Storage program aims to address the needs and challenges of site storage. The goal of this program is to leverage over a century of investment in fossil energy infrastructure, extend the useful lifetime of existing fossil energy assets, enhance the role of fossil assets as contributors to grid stability and reliability, and provide the nation with a reliable fossil-based option by leveraging and extending ongoing energy storage technology development.

University Training and Research: University Training and Research supports two of the longest-running university training programs, the Historically Black Colleges and Universities and Other Minority Institutions and the University Coal Research programs, to support the education of students in the area of carbon management. Both programs are promoted through research grants to U.S. colleges and universities that emphasize FECM strategic goals. These training programs were designed to increase the competitiveness of universities in fossil energy research and discoveries. The student-led research programs advance energy technologies and allow for expansion of energy production while simultaneously facilitating energy sector job growth.

UNIVERSITY TRAINING AND RESEARCH PROGRAM

The University Training and Research (UTR) program within the Crosscutting Research portfolio supports novel early-stage research at U.S. colleges and universities that advances the Office of Fossil Energy and Carbon Management (FECM) mission to deliver integrated solutions that enable transformation to a sustainable, low-carbon energy future.

With a special emphasis on inclusion and diversity, the UTR program provides opportunities for traditionally underrepresented communities in STEM fields. By investing in the education and training of America's future scientists and engineers, this program highlights the key role technology plays in addressing America's energy challenges, promotes the development of innovative and disruptive technologies, reinforces workforce development as a part of our nation's continued economic prosperity, and furthers the aims of the Justice40 Initiative, which seeks to advance environmental justice and revitalize the economies of disadvantaged communities.

The University Training and Research program comprises the Historically Black Colleges and Universities and Other Minority Institutions (HBCU-OMI) and the University Coal Research (UCR) programs. The core mission of both programs is:

- To develop the next generation of engineers and scientists as contributors to a highly skilled, inclusive, and competitive U.S. workforce and economy
- To support novel early-stage research at U.S. colleges and universities that advances FECM's mission and minimizes the environmental impacts of fossil fuels while working to achieve net-zero emissions
- To tap into the innovative and diverse thinking of student researchers
- To ensure that students are being equipped with cutting-edge, translatable skill sets that will allow them to contribute to the U.S. workforce and greater economy over the course of a long and enduring career.

The HBCU–OMI program's mission is further dedicated to increasing research and development (R&D) opportunities for traditionally underrepresented communities within the United States. The UCR program's emphasis on R&D structured to achieve FECM strategic goals seeks more broadly to promote student interest in energy topics.

Current key technology focus areas and their subfocus emphases within the University Training and Research program include:

- Materials, with subfocuses on hydrogen production and materials supply chains
- Water Management: wastewater contaminants partitioning, hydrogen production, and effluent water reuse
- Sensors and Controls: 5G wireless, emissions control, cyber-physical systems, cybersecurity for power generation, flexible power generation, robotics for non-destructive evaluation, quantum energy systems and technologies, and direct power extraction
- Energy Storage: gasification and hydrogen production
- Simulation-Based Engineering: computational fluid dynamics, hydrogen production, and plant modeling

This project portfolio highlights 43 projects that are active as of October 1, 2021 (start of FY22) categorized into the following technology research areas:

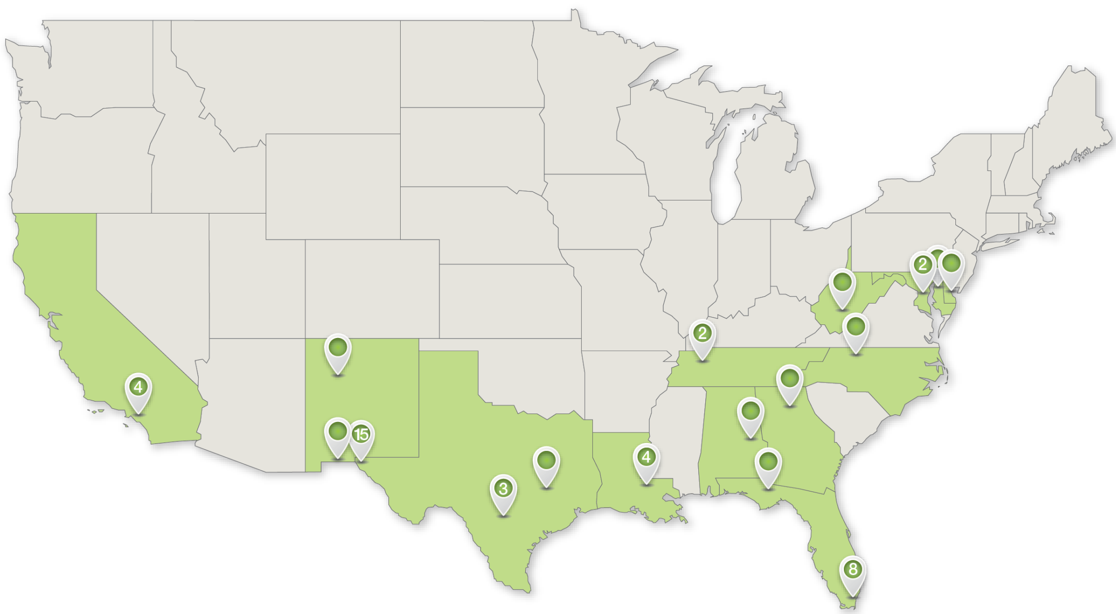
- Energy Storage
- Gasification
- High Performance Materials
- Sensors, Controls, and Novel Concepts
- Simulation-Based Engineering
- Water Management

Table 1: UTR Key Technologies—AOIs (Active Projects as of October 1, 2021)

Key Technologies	Areas of Interest	# of Projects
Energy Storage	Energy Storage	1
Gasification	Hydrogen Production	4
High Performance Materials	5G Wireless	1
	Hydrogen Production	1
	Supply Chain	2
Sensors, Controls, and Novel Concepts	5G Wireless	3
	Cyber-Physical Systems	1
	Cybersecurity for Fossil Power Generation	3
	Emissions Control	2
	Flexible Fossil Power Generation	5
	Quantum Energy Systems and Technologies	2
	Robotics for Non-Destructive Evaluation	5
Simulation-Based Engineering	Computational Fluid Dynamics	4
	Hydrogen Production	1
	Plant Modeling	4
Water Management	Effluent Water Reuse	1
	Hydrogen Production	1
	Waste-water Contaminants Partitioning	2

HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND OTHER MINORITY INSTUITUTIONS PROGRAM

NETL has supported the HBCU-OMI program for more than 30 years, making it one of the longest-running university training initiatives within FECM. Activities align with the Biden Administration's Justice40 Initiative. Since 2010, the HBCU-OMI program has supported 160 students.



HBCU-OMI Participating Universities Locations 2010-2021

Table 2: HBCU-OMI Key Technologies—AOIs (Active Projects as of October 1, 2021)

Key Technologies	Areas of Interest	# of Projects
Gasification	Hydrogen Production	3
Sensors, Controls, and Novel Concepts	5G Wireless	2
	Cybersecurity for Fossil Power Generation	1
	Flexible Fossil Power Generation	1
	Quantum Energy Systems and Technologies	2
	Robotics for Non-Destructive Evaluation	3
Simulation-Based Engineering	Computational Fluid Dynamics	2
	Plant Modeling	2
Water Management	Hydrogen Production	1

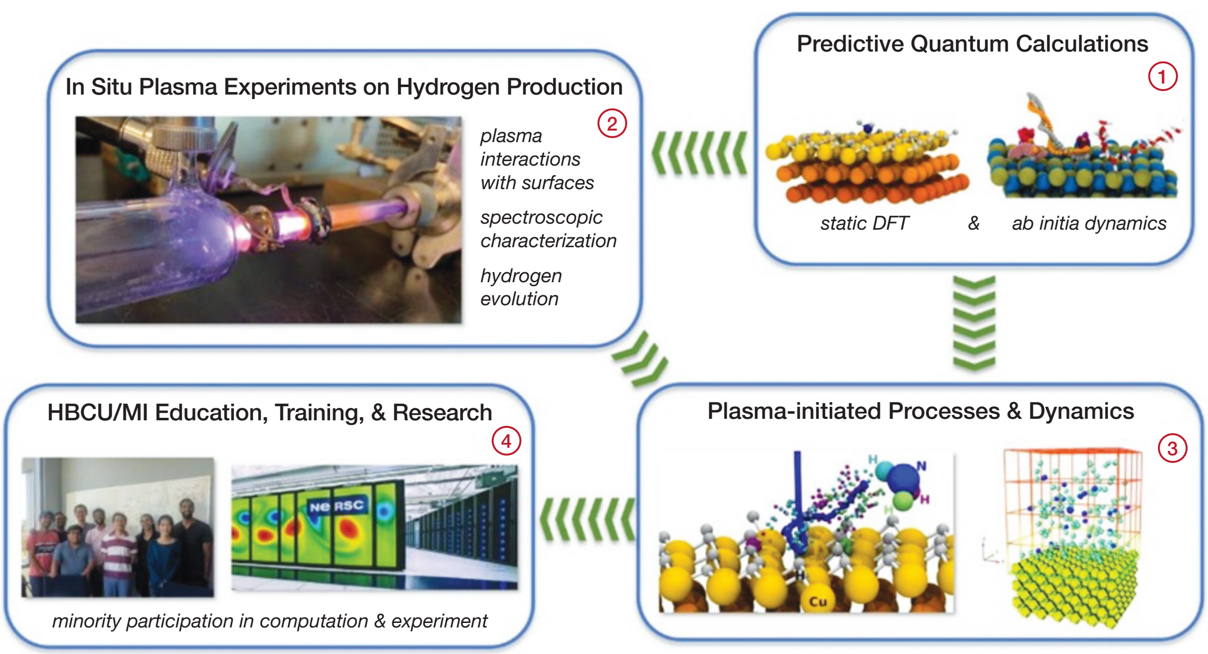
HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND OTHER MINORITY INSTITUTIONS (HBCU–OMI)

Harnessing Plasma Experiments with Quantum Calculation for Low-Cost Hydrogen Production

Performer	**University of California - Riverside**
Award Number	FE0032091
Project Duration	08/18/2021 – 08/17/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	Hydrogen Production

In response to the pressing need for improved technologies for clean hydrogen generation, this project will combine experiment and ab-initio quantum calculations in order to understand the interaction between methane-containing plasma and a carbon-based catalyst. Predictive quantum calculations for the case of a methane plasma impinging onto a carbon surface will be performed, in addition to in-situ diagnostic techniques to experimentally characterize the interaction between the plasma and the carbon surface. These results of both computation and experiment will be used to leverage the design of an improved process for the plasma-driven pyrolysis of methane for low-cost hydrogen production.

The prospect of activating graphite as a catalyst for the decomposition of methane into hydrogen would open the possibility of leveraging a readily available resource such as coal to enable a cost-effective process for the production of hydrogen from natural gas which is cost competitive with water electrolysis.



Overall scope and approach for utilizing plasma experiments and quantum calculations for low-cost hydrogen production from fossil fuels.

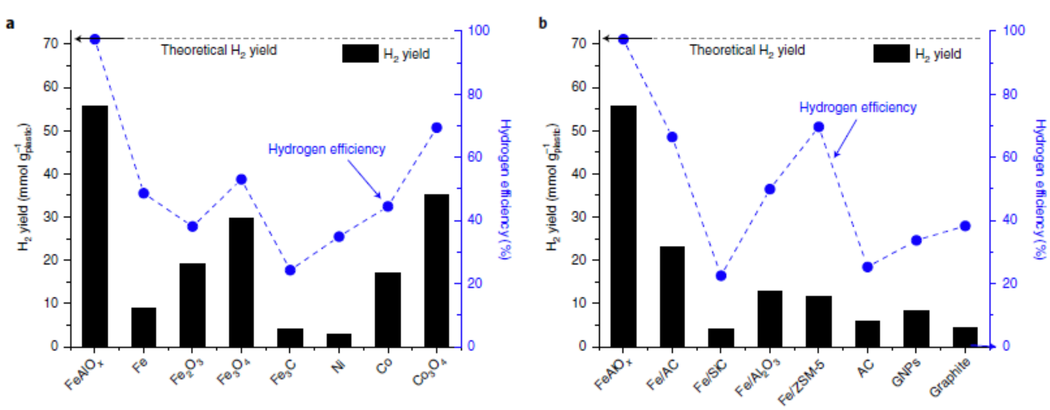
Microwave-Assisted Dehydrogenation of Fossil Fuels Using Iron-Based Alumina Nanocomposites

Performer	**University of Texas at El Paso**
Award Number	FE0032086
Project Duration	08/15/2021 – 08/14/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	Energy Storage

The primary goal of this research is to develop a microwave-assisted technology for low-cost production of hydrogen from fossil fuels. The research objectives are: (1) to determine optimal parameters of solution combustion synthesis for the fabrication of iron-based alumina nanocomposites with superior catalytic activity, microwave absorptivity, and ferrimagnetic properties; (2) to determine the effectiveness of the iron-based alumina nanocomposites in the microwave-assisted catalytic decomposition of coal tar, crude oil, diesel fuel, and gasoline in terms of hydrogen selectivity and yield; and (3) to investigate regeneration of the iron-based alumina nanocomposites by microwave-assisted gasification of the formed carbon and by magnetic separation of the catalyst particles from the carbon byproducts.

The work will include fabrication of iron-based alumina nanocomposites by solution combustion synthesis using nitrates of iron and aluminum as the precursors and oxidizers. Citric acid will be used as the fuel. For optimization of the composition, morphology, and properties of the nanocomposites, the Fe-Al and oxidizer-fuel ratios will be varied. For comparison, iron-based catalysts supported on silicon carbide (Fe/SiC) will be prepared by incipient wetness impregnation. There will be a study of microwave-assisted dehydrogenation of coal tar, crude oil, diesel fuel, and gasoline using the fabricated materials as microwave susceptors and catalysts, and the effectiveness of the iron-based alumina nanocomposites in terms of hydrogen selectivity and hydrogen yield will be determined and compared with that of the Fe/SiC catalysts.

The laboratory-scale studies will physically validate the effectiveness of the SCS-fabricated iron-based alumina nanocomposites in the main components of the proposed technology, namely, the microwave absorption, the catalytic effect, and the magnetic separation from carbon. Since the involved materials are abundant, inexpensive, and not toxic, the proposed method has the potential to become a competitive technology for hydrogen production from fossil fuels.



The effects of (a) different metal catalysts and (b) various supported iron catalysts and carbons on the H_2 yield and hydrogen efficiency.

Multiphysics and Multiscale Simulation Methods for Electromagnetic Energy Assisted Fossil Fuel to Hydrogen Conversion

Performer	**Howard University**
Award Number	FE0032092
Project Duration	09/01/2021 – 08/31/2024
Total Project Value	$ 399,935
FOA Number	DE-FOA-0002398
Area of Interest	Hydrogen Production

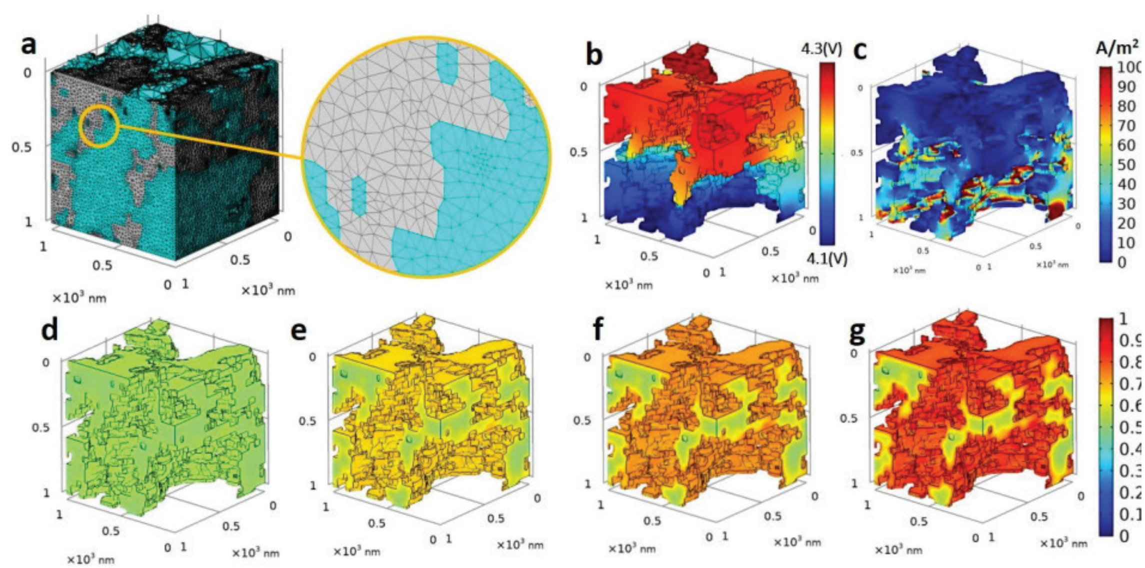
This project will develop and apply multiphysics and multiscale simulation methods for efficient electromagnetic (EM) energy assisted conversion from fossil fuel to low-cost hydrogen. This will entail the development and investigation of computational methods in two major thrust areas:

1. Modeling and simulation methods for coupled multiphysics phenomena involving EM, plasma physics, thermal and fluid dynamics, and quantum chemistry across multiple spatial scales from macro, meso, to microscopic scales and temporal scales from nanoseconds to minutes.

2. Simulation-guided designs for EM energy assisted high-throughput, high-yield, and low-cost hydrogen generation from fossil fuels such as methane and methanol.

Together, these will be used to target four specific objectives: (1) understanding 3D structures of catalysts and their supports; (2) characterization of EM hotspots within heterogeneous catalysis; (3) multiphysics investigation of EM energy assisted catalytic active sites enhancement; and (4) system design and optimization for high-yield and low-cost hydrogen generation

By developing advanced multiphysics and multiscale simulation methods, the fossil fuel-to-hydrogen conversion process can be optimized for both higher yields and lower costs.



Example of a successful multiphysics simulation of solid-state battery performed by the PI. The same type of simulation will be performed for EM assisted conversion of fossil fuels to hydrogen through the use of a solid-state catalyst. The size of the simulated battery is 1 μm cubic. a. mesh. b-c. potential and current distribution. d-g. the state of charge at different potentials.

5G Integrated Edge Computing Platform for Efficient Component Monitoring in Coal-Fired Power Plants

Performer	**University of Texas at El Paso**
Award Number	FE0032089
Project Duration	08/23/2021 – 08/22/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	5G Wireless

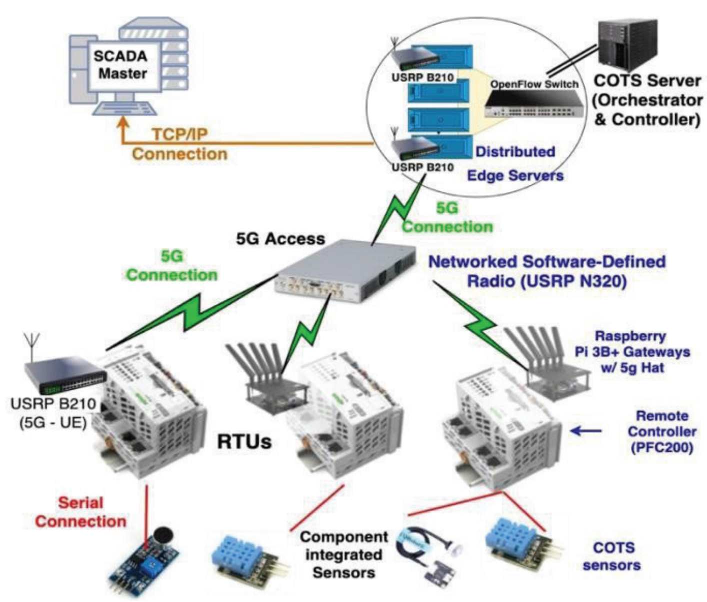
The goal of this project is to develop a 5G integrated distributed edge computing framework that facilitates real-time monitoring of critical components in coal-fired power plants (CFPPs). The objectives are as follows:

(1) Distributed Edge Computing Service (DECS) Orchestration for CFPP Component Monitoring – Develop an on-demand distributed edge computing platform to gather, process, and efficiently analyze the component health data in the CFPPs.

(2) Deploy and Integrate 5G networking to enable QoS (Quality of Service)-Aware Network Slicing – Leverage software-defined networking and network function virtualization mechanisms of 5G to instantiate a logically separated component monitoring network slice that will be integrated with DECS for time-sensitive and efficient transfer of CFPP component health data.

(3) Prototype Development and Empirical Evaluation – Develop a customizable 5G-capable distributed edge computing prototype with a separate network slice for efficient plant component monitoring. In addition, extensive performance evaluation of the developed platform will be conducted by measuring several critical metrics.

The project will involve development of a reconfigurable prototype for efficient component monitoring in CFPPs using cutting-edge 5G and edge computing technology. This technology could be used to monitor the health of the components of any power plant in real time allowing for quicker detection and replacement of worn components with reduced downtime and a reduced need for manual monitoring, The proposed system is an improvement over current solutions due to its underlying resource virtualization and reconfigurability characteristics. This will allow plant operators to dynamically instantiate and manage the QoS needs of the component monitoring traffic in real time. This platform would inherently enhance resiliency of the SCADA network because of the network slicing functionality.



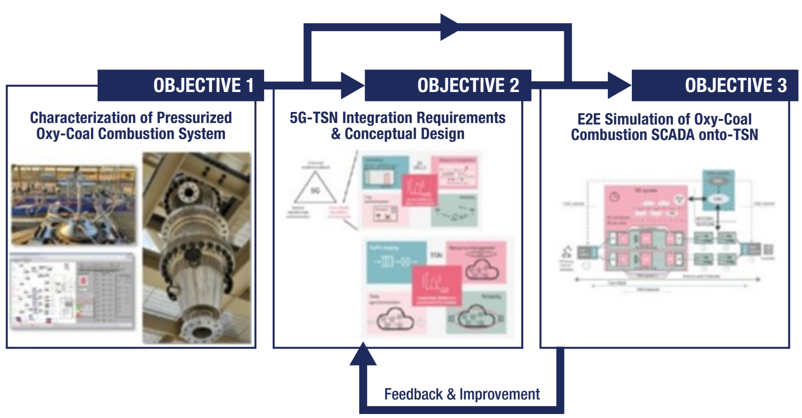
5G Capable Edge Computing Testbed for Component Monitoring.

5G-Time Sensitive Networking Architecture Capable of Providing Real-Time Situational Awareness to Fossil-Energy (FE) Generation Systems

Performer	University of Texas at El Paso
Award Number	FE0032090
Project Duration	09/23/2021 – 09/22/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	5G Wireless

The overall goal of the project is the delivery of an integrated fifth-generation time-sensitive networking architecture (5G-TSN) capable of supporting coal-fired power generation systems' operational data while providing the required deterministic quality of service. Requirements formulation and design will be based on a thorough network performance and emitted electromagnetic interference (EMI) characterization of the University of Texas at El Paso (UTEP) Center for Space Exploration and Technology Research (cSETR) pressurized oxy-coal combustion system and the high-pressure oxy-natural-gas combustor. Recorded data and EMI profiles will then be played back into an end-to-end (E2E) simulation of the 5G-TSN network. The proposed research will demonstrate the ability to design a 5G-TSN network capable of providing the necessary quality of service and security for measurement and control of an oxy-coal and oxy-natural gas combustor systems. The UTEP team will advance this technology by simulating end to end, live combustor data through a 5G-TSN network. The goal will be fulfilled by the following specific objectives: (i) operational characterization of the pressurized oxy-coal combustion system, (ii) 5G-TSN integration Requirements and conceptual design, and (iii) E2E simulation of oxy-coal combustion SCADA onto 5G-TSN ontology.

As power plants evolve, the ability to monitor them in real time is critical to increasing their efficiency and minimizing down time due to maintenance and repairs. Fifth-generation networks established in the harsh operating conditions can give operators a way to monitor equipment that have needed to be shut down for inspection and pro-active response to maintenance issues. The effort undertaken in this body of work will aim to characterize and deliver a novel 5G-TSN architecture capable of critical control and real-time measurement. The proposed design will be validated not only through industry-standard simulation but through the characterization of a pilot-scale oxy-coal combustor system during the course of this project. The introduction of a physical system to an otherwise simulated environment paves the way to practical implementation of 5G-TSN networks.



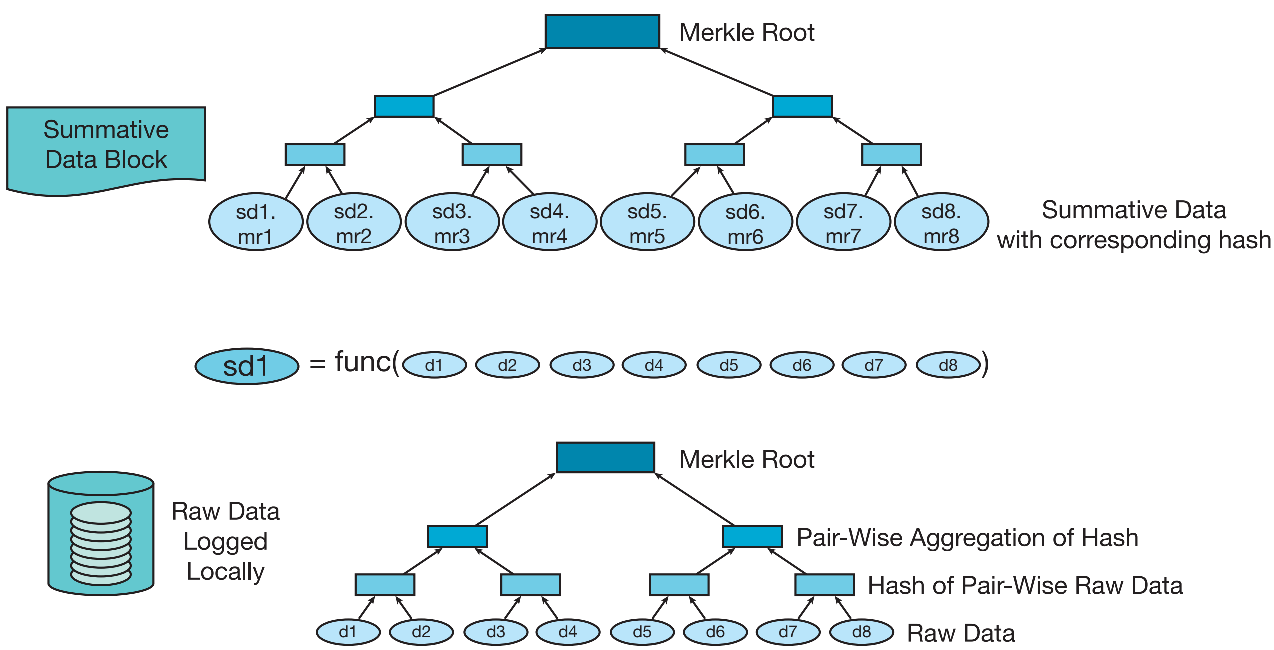
Schematic flowchart showing the overarching objectives of the project.

Secure Data Logging and Processing with Blockchain and Machine Learning

Performer	Florida International University
Award Number	FE0031745
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Cybersecurity for Fossil Power Generation

The scope of work of this project includes (1) secure data logging for 'smart' sensors and wireless communications; (2) authentication and identity verification of sensor nodes, actuators, and other equipment within a network; and (3) decentralized data storage. Florida International University will develop a novel platform that integrates two emerging technologies, namely blockchain and machine learning. This platform will incorporate a mechanism that ensures that only data sent by legitimate sensors are accepted and stored in the data repository, a suite of data aggregation methodologies using machine learning/deep learning algorithms to minimize noise and faulty data, and a two-level secure logging mechanism supported by an energy-aware blockchain solution.

If the project is successful, the fossil energy community will be able to develop a better understanding of how to securely store sensor data from various equipment in the power generating infrastructure. It will reduce data theft while increasing data logging efficiency.



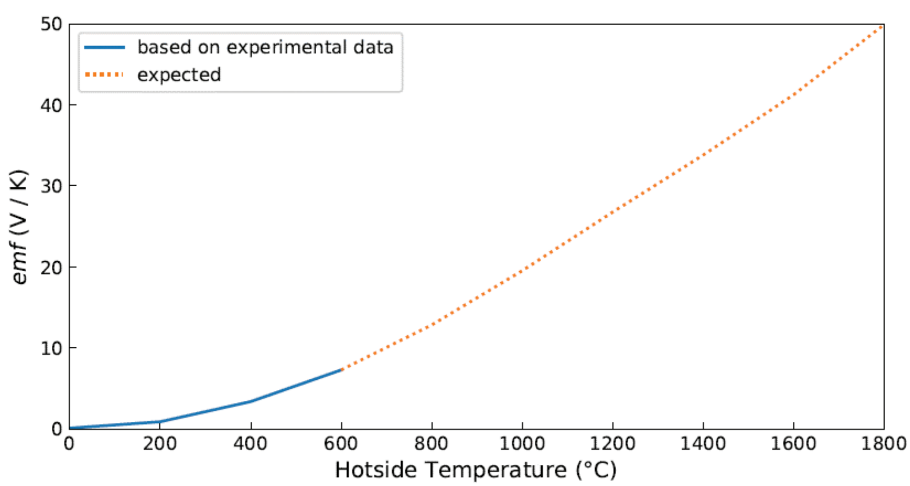
The two-level secure logging mechanism.

Ceramic-Based Ultra-High Temperature Thermocouples in Harsh Environments

Performer	**Morgan State University**
Award Number	FE0031906
Project Duration	08/01/2020 – 07/31/2023
Total Project Value	$ 500,000
FOA Number	DE-FOA-0002193
Area of Interest	Flexible Fossil Power Generation

Researchers will develop novel, durable, low cost, ceramic-based super high-temperature thermocouples (up to 2000 °C) for use in high-temperature (750–1800 °C) and 1000 PSI and above coal-based energy systems under high corrosion and erosion conditions. The materials, Zirconium diboride (ZrB2) and samarium hexaboride (SmB6) thermoelectric refractory materials will be employed as n- and p-type thermocouple legs. The materials will be compacted into isotropic thermoelectric nanocomposites as thermocouple legs with excellent Seebeck coefficient. The legs will be fabricated into ceramic-based thermocouples with p-n junctions. The thermocouples will also have good oxidization and sulfidization resistance, no protective outer layer, and cost less than acoustic and optical devices. Thermocouple performance will be evaluated in oxygen, carbon oxide, and sulfide atmospheres at high pressure and temperature. In addition, the effects of heat flow, flow rate, and mass flux found in coal power generation on the performance of the thermocouples will be investigated. Physical behaviors and long-term stability will be evaluated.

Accurate and reliable temperature measurements and controls are essential to operating coal-based energy systems at high efficiency and optimal performance. However, present thermosensors, utilizing expensive acoustic and optical techniques, usually do not work well under such harsh conditions. Development and application of new kinds of thermocouples are essential elements for low-cost maintenance and long-term stable thermo-sensing devices. The proposed ceramic based super-high thermocouples will lead to the development of low-cost thermosensors and significant reduction in maintenance costs.

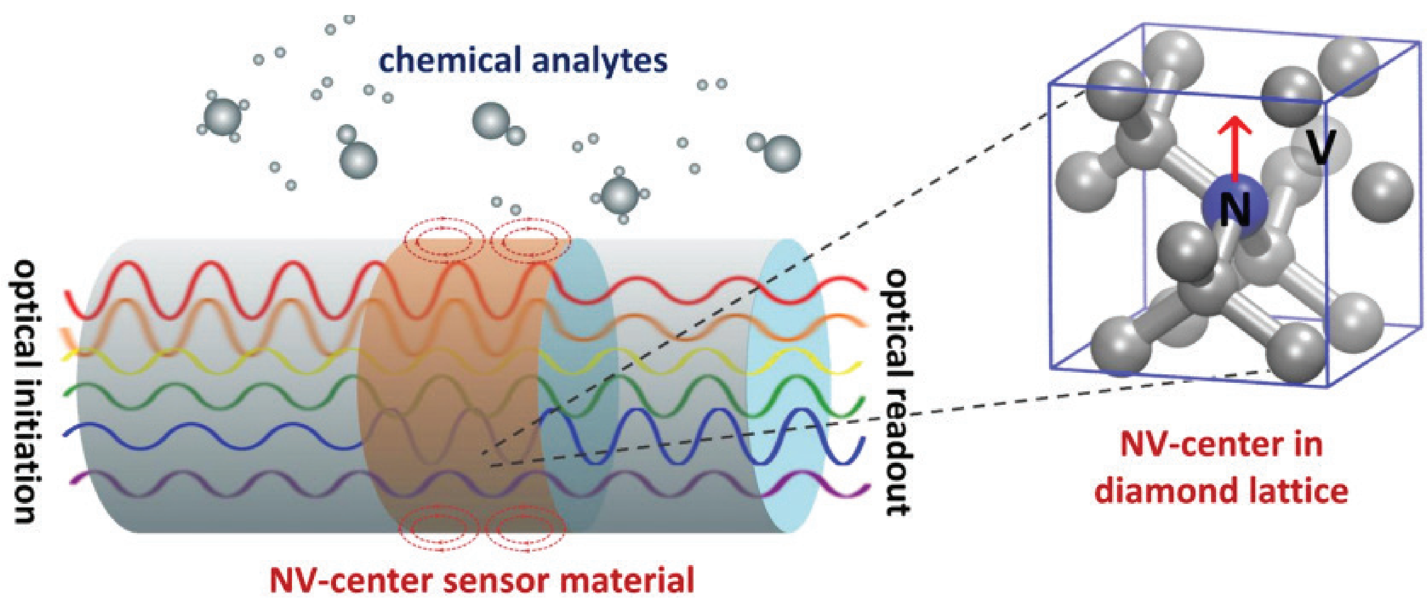


Expected emf of ZrB2-SmB6 thermocouples.

Harnessing Quantum Information Science For Enhancing Sensors In Harsh Fossil Energy Environment

Performer	University of California - Riverside
Award Number	FE0031896
Project Duration	09/20/2020 – 09/19/2023
Total Project Value	$ 500,000
FOA Number	DE-FOA-0002193
Area of Interest	Quantum Energy Systems and Technologies

The project plans to utilize real-time quantum dynamics simulations and quantum optimal control algorithms to (1) harness near-surface nitrogen vacancy (NV) centers to detect chemical analytes in harsh fossil energy environments and (2) design optimally constructed electromagnetic fields for initializing these near-surface NV center spins for efficient sensor performance and detection. Together, these objectives will leverage quantum information science to enable new sensing modalities for the extremely sensitive monitoring (i.e., below classical measurement limits) of critical operating parameters of fossil energy infrastructures in harsh environments. Quantum information science is leveraged to enable new sensing modalities for the extremely sensitive monitoring (i.e., below classical measurement limits) of critical operating parameters of fossil energy infrastructures in harsh environments.



Improving sensing modalities in fossil energy infrastructures.

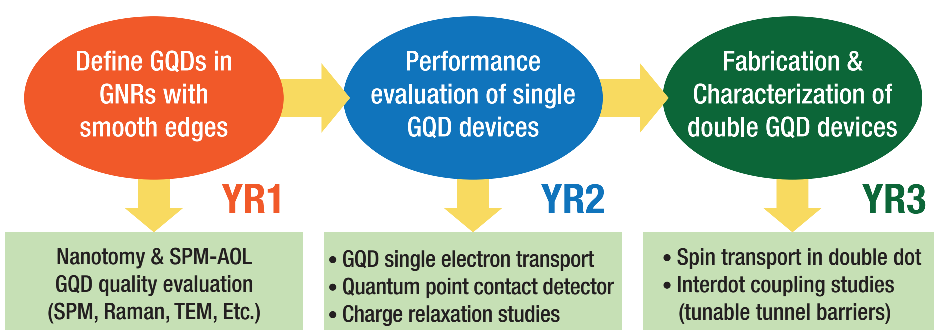
Ultra-Low Disorder Graphene Quantum Dot-Based Spin Qubits for Cyber Secure Fossil Energy Infrastructure

Performer	**University of Texas at El Paso**
Award Number	FE0031908
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$ 499,546
FOA Number	DE-FOA-0002193
Area of Interest	Quantum Energy Systems and Technologies

The specific research objectives of the project will be to define graphene quantum dots (GQDs) on graphene nanoribbon (GNR) with ultralow local defects and characterize the edge roughness and local disorder by diverse microscopic and spectroscopic techniques; conduct low-temperature characterization of quantum transport and spin relaxation times in GQDs to evaluate the effect of lower local disorder; and develop a multi-GQD-based qubit platform and analyze coupling effects and performance improvements achieved through the new synthetic protocols for quantum communication applications. To achieve the objectives, the team will first leverage the nanotomy technique to prepare GNRs of various widths and characterize its superiority by comparing their structural and disorder status with lithographically prepared GNRs (which will function as the baseline in the project). Subsequently, scanning probe microscopy-based oxidation lithography (SPM-OL) will be used to fabricate geometrically confined GQDs with tunnel barriers on the GNRs. Then the team will fabricate electrode patterns that connect the quantum dots to source and drain electrodes.

An in-depth study will be conducted characterizing the local density of states and conductance of the GQDs with variable widths. Cumulatively, these studies will help developing an optimized GQD qubit system fabricated using nanotomy and SPM-OL. Quantum transport and spin relaxation measurements conducted at mK temperatures will reveal the superiority of the present GQDs with ultralow defects. Further, the optimized GQD fabrication process will be extended to develop an array of GQDs integrated with local gate electrodes and quantum point contact to study the inter-dot coupling effects in the GQD arrays.

The primary benefit of the project is that it will result in a significantly improved strategy to formulate GQD qubits (individual and multi-GQDs) with ultralow local defects and higher spin relaxation times (>μ-seconds). The development of such GQD platforms is expected to advance state-of-the-art graphene quantum structure fabrication technologies and semiconductor spin qubits. This project will also be beneficial for ongoing research efforts to develop highly secured communication systems and thus enable the implementation of GQD spin qubits in quantum processors for cyber-resilient grid infrastructure.



Outline of the overall effort of the proposed project.

Development of a Pipe Crawler Inspection Tool for Fossil Energy Power Plants

Performer	**Florida International University**
Award Number	FE0031651
Project Duration	09/01/2018 – 05/31/2022
Total Project Value	$ 398,333
FOA Number	DE-FOA-0001842
Area of Interest	Robotics for Non-Destructive Evaluation

Florida International University researchers are developing a robotic inspection tool to evaluate the structural integrity of key components in fossil fuel power plants. The tool will consist of multiple modular crawlers that can navigate through the 2-inch-diameter superheater tubes typically found within power plant boilers—which are often subject to corrosion and micro cracks—and provide information regarding the health of the pipes. Design modifications to reduce the tether load and maximize the pull force will be made. Multiple systems will then be synchronized to increase the length of pipe that can be inspected. The base system will house a camera for video feedback and contain a module that utilizes thumbnail-size ultrasonic sensors for measuring pipe thickness, and a LiDAR (light detection and ranging) sensor to detect any pipe buildup, damage, and/or misalignment. In addition, the module will provide a means to prepare the surface prior to measuring. The team will develop and conduct bench-scale tests to optimize the design of the crawler and its modules and conduct engineering-scale tests to validate the system.

The robotic system will improve the state of the art for inspection tools in pipes that are subject to extreme conditions and for which structural integrity assessments are difficult to obtain. The technology will lead to better understanding of the health of critical components, and plant downtime will be reduced, efficiency increased, and cost savings realized.

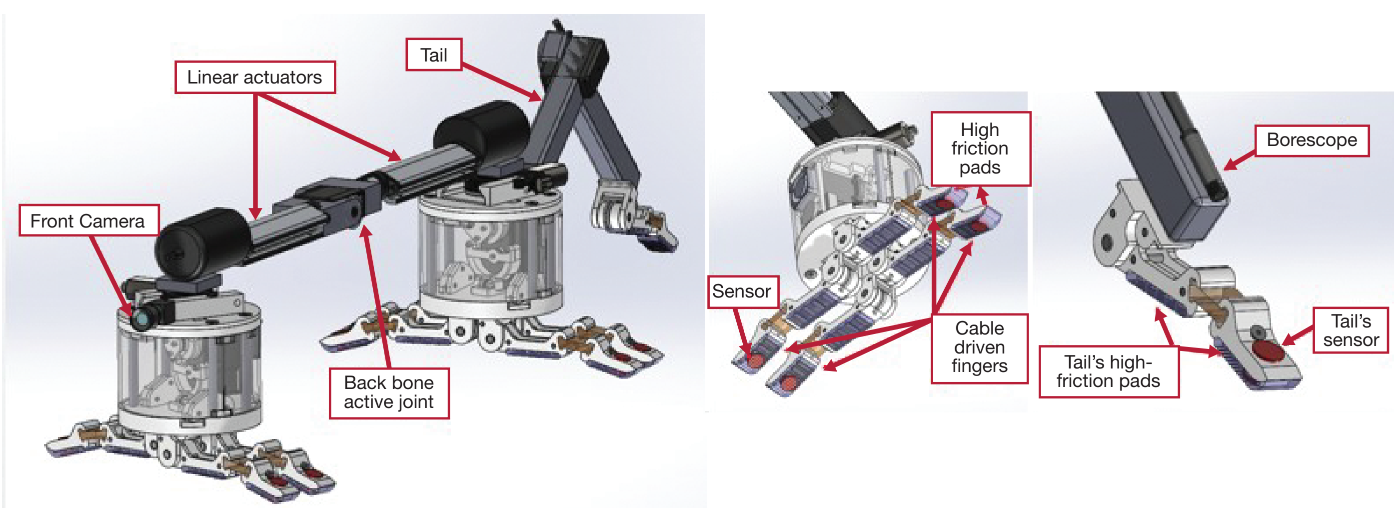
3- and 4-inch pneumatic pipe crawler developed at Florida International University.

A Lizard-Inspired Tube Inspector (LTI) Robot

Performer	**New Mexico State University**
Award Number	FE0031649
Project Duration	09/01/2018 – 08/31/2022
Total Project Value	$ 470,000.00
FOA Number	DE-FOA-0001842
Area of Interest	Robotics for Non-Destructive Evaluation

New Mexico State University researchers are developing a versatile lizard-inspired tube inspector (LTI) robot with embedded inspection sensing components that will eliminate the need for point-by-point scanning of tube surfaces for detecting and evaluating cracks and erosion. Inspired by lizards which have evolved to live within tight spaces with complex geometries and rough surfaces, the robot will integrate couplant-free ultrasound sensing and transmission, advanced Lamb wave-based ultrasound imaging, and a friction-based mechanical mobility component to eliminate the need for smooth surfaces and simple geometries for mobility and scanning. This project will replace the wheel-based approach to tube inspection with friction and/or adhesion-based mobility to significantly increase the flexibility and maneuverability of the LTI robot, providing easy access to a power plant unit such as a boiler to inspect components of interest (e.g., curved and flat surfaces, non-ferromagnetic or ferromagnetic materials, and tubes with rough surfaces and complex geometries). In addition, advanced imaging will enable the robot to image the entire area between and around the robot's multi-functional mobility system (grippers) using Multi Helical Ultrasound Imaging and a Lamb wave-based Total Focusing Method recently developed by the principal investigator.

The results of the current project may revolutionize robotic inspection technology used to inspect power plant components. The advanced imaging and mobility of the LTI robot makes it a unique tool that can be adopted for inspection of other power plants' hard-to-reach components such as steam turbines, heat recovery steam generators, gas turbines, and electrical generators without a need for overhaul.



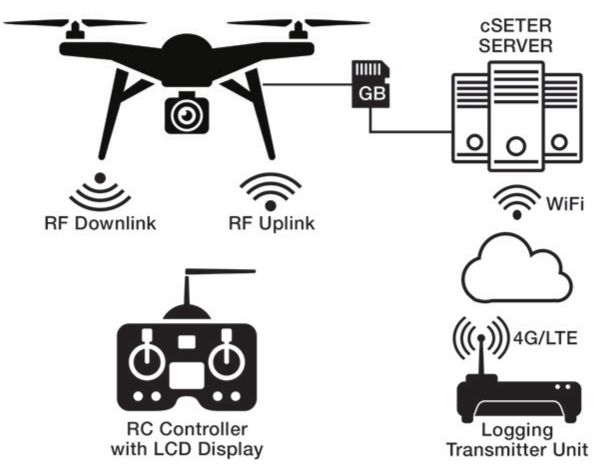
Conceptual design of the LTI robot.

Autonomous Aerial Power Plant Inspection in GPS-Denied Environments

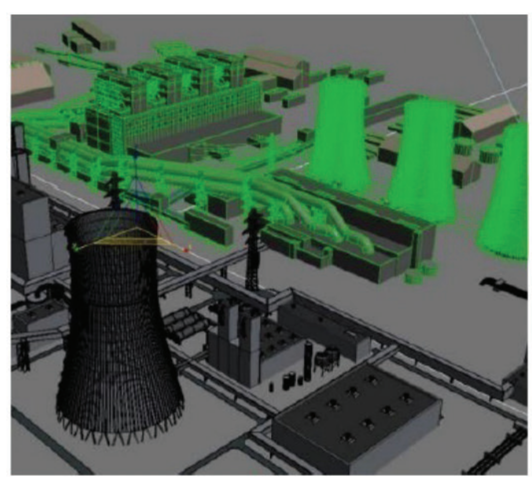
Performer	**University of Texas at El Paso**
Award Number	FE0031655
Project Duration	09/01/2018 – 05/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001842
Area of Interest	Robotics for Non-Destructive Evaluation

University of Texas at El Paso (UTEP) researchers will test and validate the performance of UTEP's global positioning system (GPS)-denied inspection system, outfitted with electro-optical and infrared inspection sensors, in a representative coal-fired power component that will be determined in conjunction with the El Paso Electric Company. Researchers will use rotary wing flying robots for outdoor inspection and airships for indoor inspection of GPS-denied environments to test the system's guidance and navigation and obstacle avoidance capabilities. The objectives are to develop computer assisted design (CAD)-based inspection profiles for space-constrained and GPS-denied areas of a power plant; test and validate the capability to keep a pre-set distance from complex surfaces (within sub-15-centimeter tolerances in all six directions); and test and validate the capability to perform an automated inspection of uneven vertical and horizontal surfaces in enclosed and GPS-denied areas.

The aerial system will leverage current robotic-based inspection technology in power plants by potentially increasing the area and the types of structural components that can be inspected with unmanned aerial systems; access dangerous and difficult-to-reach structures; inspect areas where GPS is not available; and enable inspection of cluttered and space-reduced areas, internal and external components such as cooling towers and flue gas stacks, and areas with high ash content without disturbing particulate matter.



Data logging and telemetry system.

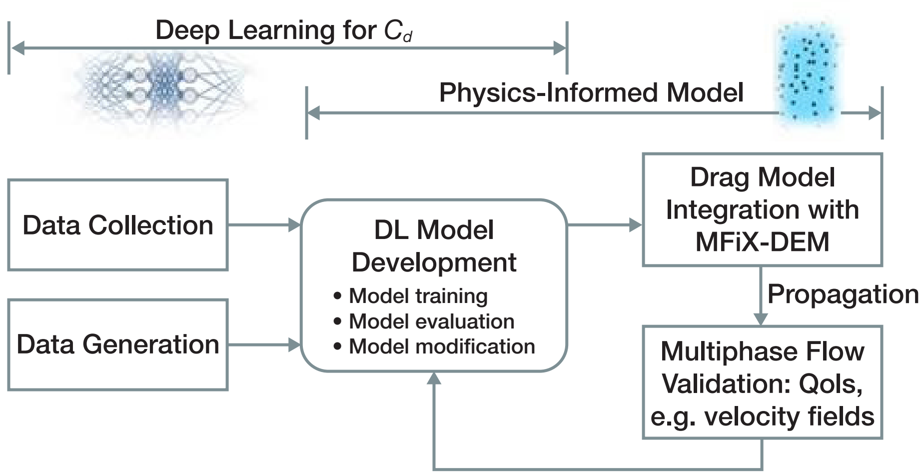


Model of a power plant (courtesy of Turbosquid).

Development and Evaluation of a General Drag Model for Gas-Solid Flows Via Physics-Informed Deep Machine Learning

Performer	**Florida International University**
Award Number	FE0031904
Project Duration	08/01/2020 – 07/31/2023
Total Project Value	$500,000
FOA Number	DE-FOA-0002193
Area of Interest	Computational Fluid Dynamics

The objective of this project is to develop, test, and validate a general drag model for multiphase flows in assemblies of non-spherical particles by a physics-informed deep machine learning approach using an artificial neural network (ANN). Once implemented in computational fluid dynamics (CFD) code, the model aims to accurately predict a particle's drag coefficient and flow fields in the simulation of gas-particle flows, with a wide range of parameters including Reynolds number, Stokes number, solid volume fractions, particle densities, particle orientations, and particle aspect ratios. The project will involve the following research and development activities: (1) data collection and generation of drag coefficients for non-spherical particles; (2) ANN-based drag model development through deep learning neural networks (DNN), algorithm identification and evaluation, and model tests using different data sets; (3) integration of the best DNN model into the open source CFD software MFiX-DEM; and (4) validation of selected multiphase flows using the new drag model. Completion of the project will result in a deep machine learning-based general drag model for non-spherical particles in gas-solid flow simulation by CFD. The general drag model will overcome the limitations of existing models, which are problem specific and work only within narrow parameter ranges. This research project provides the students and faculty at Florida International University, a minority-serving institution, great opportunity to work on cutting-edge research related to applications of emerging machine learning technologies in gas-particle multiphase flows.

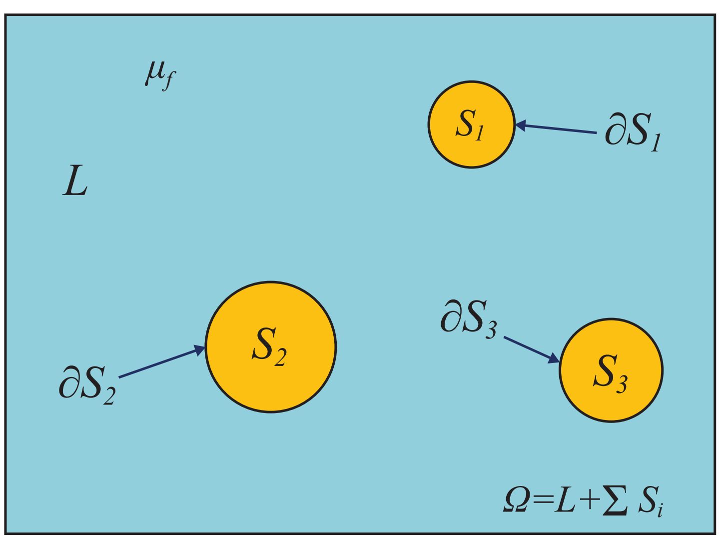


A physics-informed deep learning framework for a drag coefficient model.

A General Drag Model for Assemblies of Non-Spherical Particles Created with Artificial Neural Networks

Performer	University of Texas at San Antonio
Award Number	FE0031894
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$499,982
FOA Number	DE-FOA-0002193
Area of Interest	Computational Fluid Dynamics

The project plans to develop a more accurate artificial neural network (ANN)-based method for modeling the momentum exchange in fluid-solid multiphase mixtures to significantly improve the accuracy and reduce the uncertainty of multiphase numerical codes and, in particular, of MFiX by developing and providing a general and accurate method for determining the drag coefficients of assemblies of non-spherical particles for wide ranges of Reynolds numbers, Stokes numbers, and fluid-solid properties and characteristics. The research team will achieve this aim by conducting numerical computations with a validated in-house CFD code and using artificial intelligence methods to develop an ANN that will be implemented in TensorFlow™ and linked with the MFiX code. The main objectives of this project are to use a validated computational fluid dynamics (CFD) code to perform computations and to derive accurate expressions for the drag coefficients of single non-spherical particles and assemblies of non-spherical particles for wide ranges of the parameters of interest. A second objective of the work is to educate and train several graduate and undergraduate students in the science of multiphase flow and the use of in-house CFD codes, the MFiX code, and TensorFlow.



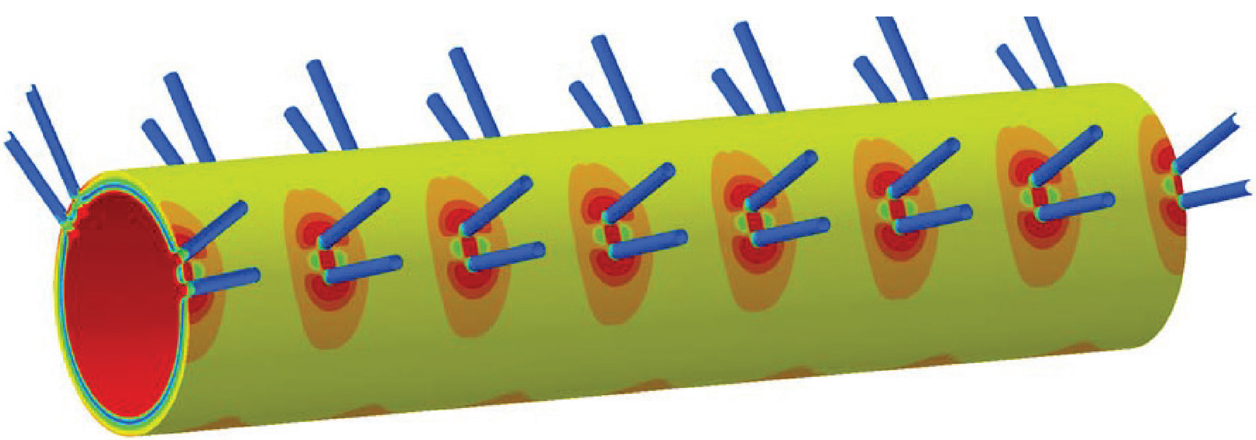
Conceptual model of three particles suspended in a fluid.

Alloy for Enhancement of Operational Flexibility of Power Plants

Performer	**North Carolina Agricultural and Technical State University**
Award Number	FE0031747
Project Duration	08/15/2019 – 08/14/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Plant Modeling

North Carolina Agricultural and Technical State University will employ advanced computational techniques to address the challenge of higher material deterioration facing the existing coal-fired power plants due to a shift in their operational mode from baseline steady state to cycling. The cycling operation of coal-fired power plants promotes thermo-mechanical fatigue damage in boiler headers. As a result, materials deteriorate at a higher rate and ligament cracking occurs in headers in a shorter time. The main objective of this project is to employ computational fluid dynamics and finite element analysis to conduct a comprehensive and advanced study of the applicability of Inconel (IN) 740H superalloy in steam headers to improve the operating flexibility of power plants. The project team will use the results of the analysis to optimize the geometry of headers to minimize the quantity of material used.

A cost-benefit analysis of headers designed with IN740H (employing both traditional and optimized shapes) in comparison with creep-strength-enhanced ferritic (CSEF) steels such as Grade 91 will be conducted. This analysis will consider the higher cost of IN740H with respect to CSEF steels and the lower maintenance cost of IN740H during operation of the power plant.



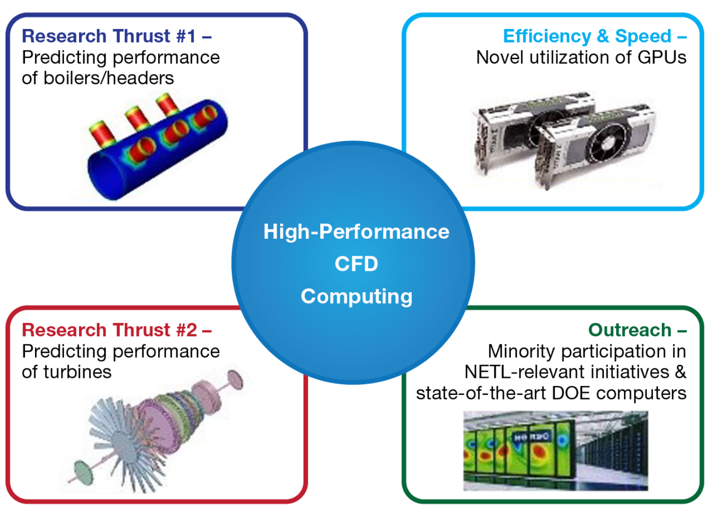
Stress contour plot of a steam header.

Probing Particle Impingement in Boilers and Steam Turbines Using High-Performance Computing with Parallel and Graphical Processing Units

Performer	**University of California - Riverside**
Award Number	FE0031746
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Plant Modeling

This project encompasses four complementary objectives that will employ a high degree of coordination and communication to realize a final, rigorously sound, and validated computational capability for identifying plant inefficiencies upon completion that will subsequently be communicated and validated with industrial partners for technology transfer. Objective 1 will utilize massively parallelized graphics processing units (GPUs) in the laboratories of both the recipient and partners to efficiently execute the ANSYS Fluent computational fluid dynamics (CFD) code used in this project. A sizeable portion of operational damage in fossil fuel power plants occurs in the boiler's superheater/reheater headers; therefore, Objective 2 will be to make use of these GPU-parallelized simulations to understand the durability of and damage mechanisms to these header structures under various cycling and operational modes. Objective 3 will be to assess subsequent damage mechanisms by quantifying and calculating the effects of particulates within "steam in" boilers as a function of both boiler geometry and operating conditions. Objective 4 will combine the results of the previous three objectives to create a holistic, comprehensive, and systems-level assessment of damage rates under different cycling modes.

The methodology and computational approaches used in this project will provide a new computational analysis to identify and develop insight into the inefficiencies of specific physical processes in existing coal plants and propose mitigation solutions using advanced modeling tools. These advanced approaches have significant advantages compared to conventional physical/experimental diagnostics, which are time-consuming due to the nearly limitless number of erosion processes and power-plant control variables. The predictive computational approaches for understanding inefficient power-plant mechanisms in this project are significantly more cost-efficient and lead to a rational and more logical approach for understanding and mitigating plant inefficiencies. Moreover, the use of massively parallelized GPUs plays a critical role in accelerating the computational efficiency of the calculations performed on the immense mechanical structures examined in this project. Together, these benefits directly support the Department of Energy's (DOE's) Historically Black Colleges and Universities – Other Minority Institutions programs and create an exciting opportunity for DOE and National Energy Technology Laboratory leadership to improve the operating efficiency of critical fossil energy power plants.



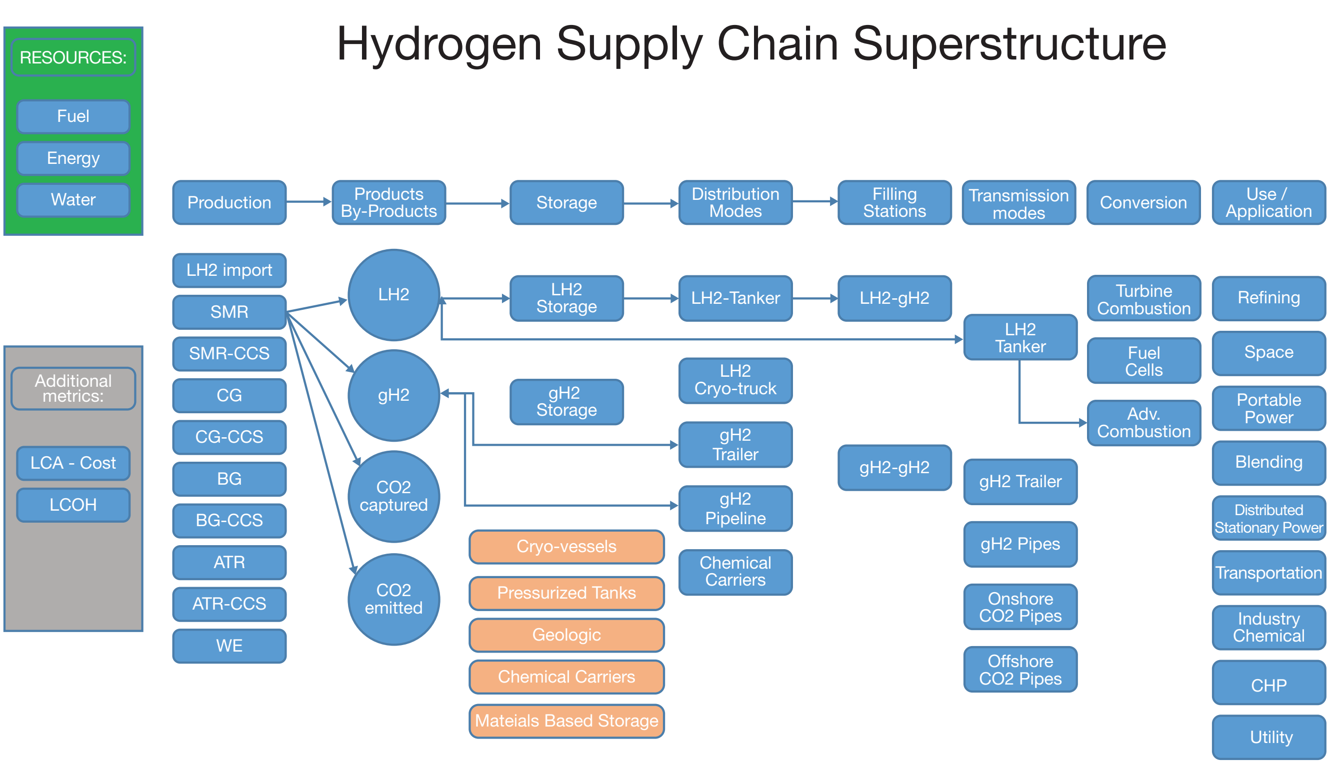
High-performance CFD computing forms a central theme and unifies research thrusts, efficiency, outreach, and technological impact in this HBCU-OMI project.

Fossil Energy in the Hydrogen Economy - A Carbon-Water-Energy Nexus Adaptive Evaluation Platform

Performer	**Florida A&M University**
Award Number	FE0032084
Project Duration	07/16/2021 – 07/15/2023
Total Project Value	$ 399,943
FOA Number	DE-FOA-0002398
Area of Interest	Hydrogen Production

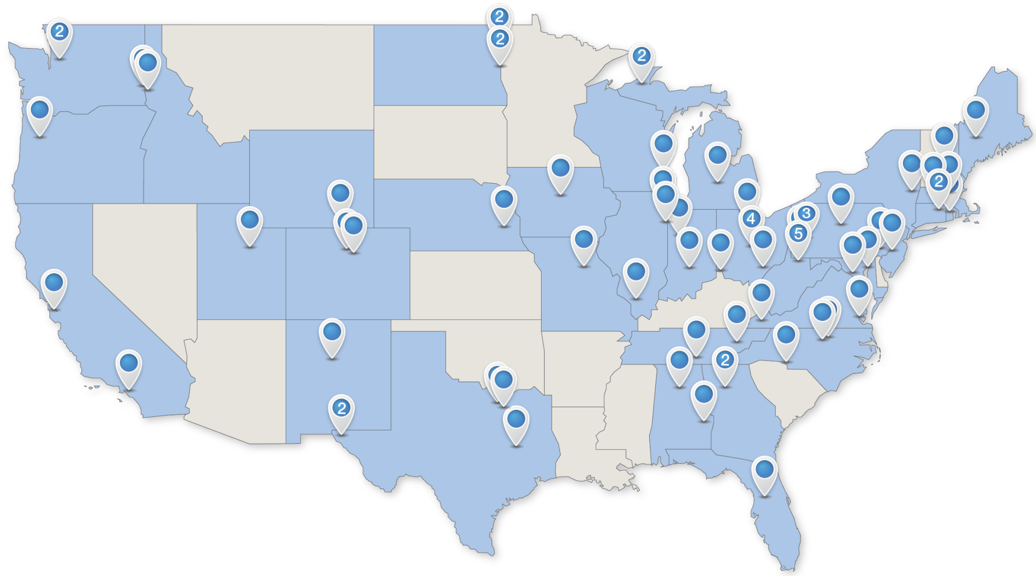
The objective of the project is to survey and document the current technologies that enable the integration of fossil fuels into the hydrogen economy with emphasis on tracking their potential for carbon neutrality and reduced water intensity. The project will develop tools to aid in planning and decision making including an adaptive evaluation platform to evaluate sensitivity of technology options to mitigate water consumption and to reduce cost and greenhouse gas emissions. A second tool developed under this project will be a dynamic Sankey-like diagram to visualize hydrogen production, transport, storage, and use. The project also aims to involve and educate undergraduate and graduate students on the hydrogen economy.

The project will quantify the water demands associated with integration of hydrogen into the energy system, a critical step in enabling a transition to a hydrogen economy. Furthermore, the project will train a diverse group of engineering students on the challenges and benefits of hydrogen as a fuel.



UNIVERSITY COAL RESEARCH PROGRAM

The UCR program emphasizes research and development efforts that are structured to achieve FECM strategic goals in concert with student education in relevant carbon management topics. Key research areas supported include (but are not limited to) near-zero-emission power plants, carbon capture, computational energy sciences, development of advanced high-performance materials, sensors and controls, and the development of hybrid power generation systems.



UCR Participating Universities Locations (2010-2021)

Table 3: UCR Technologies—AOIS (Active Projects as of October 1, 2021)

Key Technologies	Areas of Interest	# of Projects
Energy Storage	Energy Storage	1
Gasification	Hydrogen Production	1
High Performance Materials	5G Wireless	1
	Hydrogen Production	1
	Supply Chain	2
Sensors, Controls, and Novel Concepts	5G Wireless	1
	Cyber-Physical Systems	1
	Cybersecurity for Fossil Power Generation	2
	Emissions Control	2
	Flexible Fossil Power Generation	4
	Robotics for Non-Destructive Evaluation	2
Simulation-Based Engineering	Computational Fluid Dynamics	2
	Hydrogen Production	1
	Plant Modeling	2
Water Management	Effluent Water Reuse	1
	Waste-Water Contaminants Partitioning	2

UNIVERSITY COAL RESEARCH (UCR)

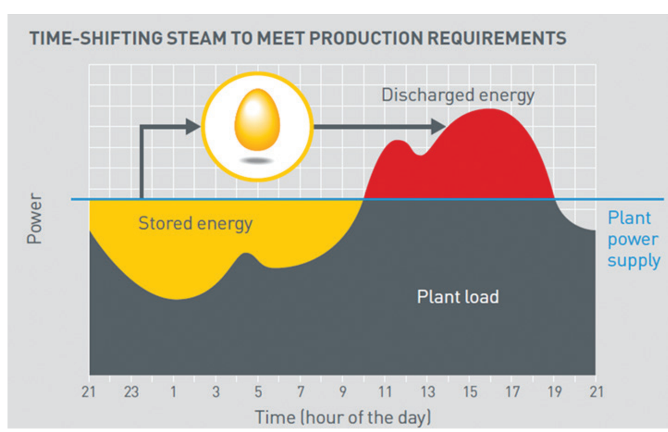
Techno-Economic and Deployment Analysis of Fossil Fuel-Based Power Generation with Integrated Energy Storage

Performer	**University of North Carolina Charlotte**
Award Number	FE0031903
Project Duration	09/01/2020 – 08/31/2022
Total Project Value	$ 499,998
FOA Number	DE-FOA-0002193
Area of Interest	Energy Storage

Improving the flexibility of conventional power plants is a key challenge in transforming current energy system towards a high share of renewable energies in electricity generation. In the current energy system, mainly dispatchable coal- and gas-fired power plants compensate for fluctuating renewable power generation to ensure the stability and reliability of the electrical grid. Considering the expected capacity growth of renewable energy resources and corresponding reduction in the capacity of conventional power plants, the remaining dispatchable power plant fleet has to meet increasingly higher flexibility and reliability requirements. Energy storage integrated with a power plant partially decouples plant power output and boiler (steam generator) firing rate thus improving flexibility of the plant (lowering minimum load, providing peak power when needed, time-shifting peak power generation, and allowing load changes at constant or nearly constant firing rate), reducing cycling damage, reducing emissions, and improving plant economic performance.

This project will analyze four energy storage technology options and six sub-options, and determine their impact on operation and economics of a representative (reference) coal-fired power plant. A coal-fired steam plant was selected for the analysis because it may provide the greatest benefits from the integration of energy storage and can be used as a foundation for other fossil fuel facilities. The savings due to the integrated energy storage resulting from improved operating efficiency, improved system reliability, reduced CO_2 and other pollutant emissions, lower operating costs, more efficient plant participation in frequency control, and increased participation in the ancillary services market will be considered. As the penetration of renewables increase over the next decades, the efficient, flexible, and reliable operation of existing fossil power generating plants is critical for a smooth cost-effective decarbonization of the power generation sector.

Results obtained from this project will be highly relevant for future advancements of energy storage application and integration with the power generation assets. Technical analysis performed by using high-fidelity plant models will be verified against actual operating data, and augmented with deep understanding of the power plant operation, resulting in a realistic incremental cost curve for the plant. An economic analysis will be performed using actual grid data and market prices to simulate operation of the reference plant with and without integrated energy storage to determine the actual value of storage under realistic grid operating conditions. Revenues due to increase in energy output (achieved by reducing inefficiencies caused by variable load operation and improved performance) and increased participation in the ancillary services market will be documented.



Visual representation of the energy storage concept.

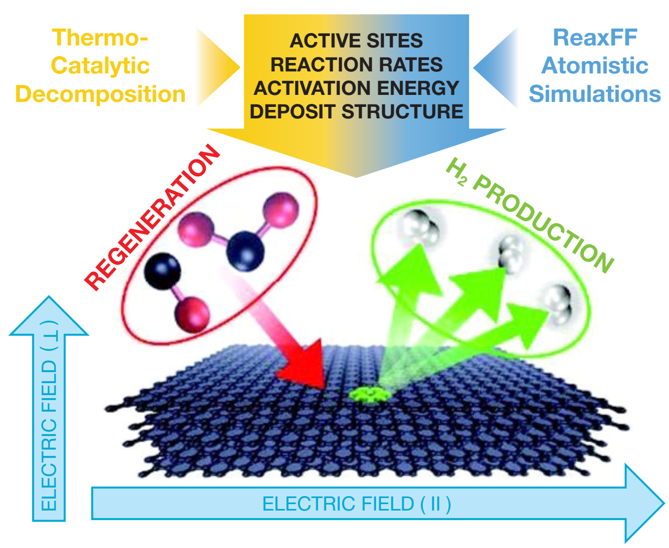
Electric Field Assisted Thermo-Catalytic Decomposition: Comparisons with Reaxff Atomistic Simulations

Performer	**Pennsylvania State University**
Award Number	FE0032070
Project Duration	08/01/2021 – 07/31/2024
Total Project Value	$ 399,435
FOA Number	DE-FOA-0002398
Area of Interest	Hydrogen Production

Thermo-catalytic decomposition (TCD) is an alternative energy technology to produce (blue) hydrogen by decarbonizing fossil fuels, providing a bridge to the hydrogen economy. A limitation is the ongoing deactivation of the carbon catalyst as deposited carbon from the decomposition reaction reduces the number of catalyst active sites. Cyclic regeneration complements the TCD reaction by creating new active sites through partial oxidation by CO_2, renewing carbon catalyst activity. Moreover, partial gasification of deposited carbon by H_2O (generating H_2, the desired end product) also regenerates the catalyst. This establishes applicability of electric (E)-field enhancement to a coal feed and serves as a baseline for gasification of coal. Neither TCD nor carbon oxidation has been tested under an E-field for change in activation energy or mechanism. For both reactions, an imposed electric field may maintain and potentially increase the reaction rate, either by an increase in active site number or a shift in component energy level and the associated activation energy for reactions.

It is hypothesized that an applied E-field changes the reaction mechanism. This project will test two field configurations, perpendicular imposing only voltage stress and parallel imposing current stress. Active site and kinetic dependence upon reactive gases and their concentrations will be mapped parametrically as a function of applied E-field strength, polarity, direction, and frequency. Changes in rates may be resolved by active site number or activation energy. ReaxFF (reaction force field)-based molecular dynamics simulations will be compared to experimental measurements of activation energy and kinetics of deposition to test the hypothesis that the E-field changes the reaction mechanism, manifested by activation energy and kinetics of deposition, for both TCD and regeneration reactions.

A steady or increased catalytic rate produced by an applied E-field removes a critical barrier to TCD implementation at scale and its potential to negate regeneration. Similarly, gains in gasification rates and their origin(s) under an applied E-field will be probed. Improved regeneration rates can benefit CO production for syngas or H_2 production by gasification of feedstocks such as coal with greater energy efficiency and reduced CO_2 footprint. Measurement of active sites and predictions by atomistic simulations will provide mechanistic insights for carbon surface reactions relevant to both TCD and regeneration reactions, addressing the mechanism of E-field enhancement for carbon surface reactions for H_2 generation from fossil fuels.



Combined experiment plus modeling for E-field enhanced thermo-catalytic decomposition of methane for hydrogen production.

Hybrid Structured Nickel Superalloys to Address Price Volatility and Weld/Weld Repair Based Supply Chain Issues

Performer	Michigan Technological University
Award Number	FE0032071
Project Duration	09/03/2021 – 09/02/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	5G Wireless

Two key factors affecting the fossil power high-temperature material supply chain are the volatility of nickel-based alloy prices and the challenges in welding precipitation-strengthened alloys. This project seeks to use integrated computational materials engineering (ICME) design strategies to solve these challenges by designing, casting, forging, welding, and validating the properties of hybrid eta-gamma prime-strengthened nickel superalloys optimized for cost and weldability. Specifically, significant reduction in cobalt to less than 5 wt% versus 10–20 wt% in candidate alloys for advanced energy systems is sought. Performance in high-temperature strength and creep will be maintained within 10 wt% compared against existing candidate alloys designed for extreme environments. Weldability criteria will be evaluated through use of various susceptibility indices (solidification cracking, liquation, stress relief cracking) with the goal of broadening the welding and post-weld heat treat processing windows to be more forgiving.

Benefits are focused on providing alternatives to existing alloys with significant weldability issues which will enhance fabrication of new components, on-site assembly, and in-service repairs. Additional impacts include training graduate students in hybrid real-world/theoretical design methodologies to better prepare for advanced materials development.

Electromagnetic Energy-Assisted Thermal Conversion of Fossil-Based Hydrocarbons to Low-Cost Hydrogen

Performer	University of North Dakota
Award Number	FE0032061
Project Duration	08/01/2021 – 07/31/2023
Total Project Value	$ 398,969
FOA Number	DE-FOA-0002398
Area of Interest	Hydrogen Production

Hydrogen can be produced from the decomposition of hydrocarbons such as methane, without the production of carbon oxides. This represents a highly favorable route for hydrogen production compared to industrial production methods based predominantly on steam-methane reforming (SMR). Breaking hydrogen-oxygen bonds in water requires about seven times the energy compared to breaking carbon-hydrogen bonds in methane. SMR and methane decomposition processes both require indirect heating to provide the overall endothermic heat of reaction for hydrogen formation, but the heat of reaction for the SMR is more than double that for methane decomposition. In contrast to the SMR process, the methane decomposition process offers a promising path for economical and environmentally sound production of hydrogen without production of carbon dioxide.

The goal of this project is to make targeted improvements to the conventional thermo-catalytic hydrocarbon conversion process using an electromagnetic energy assisted mechanism; resulting in the reduction of downtime associated with catalyst reactivation or replacement due to poisoning. State-of-the-art solid catalysts exhibit short process lifetimes that are not suitable for commercial application. This project uses both experimental and computational tools to understand the fundamental interactions between fossil fuels and their interactions with an electromagnetic energy source. This technology can utilize natural gas or volatiles obtained from coal decomposition to provide carbon dioxide-free hydrogen. The first objective of this project is to identify catalyst supports that enhance the electromagnetic energy-assisted mechanism to ensure in-situ catalyst reactivation to near-initial fresh conditions. The performance of these prepared catalysts will be tested in laboratory units and the results will be used to validate computational fluid dynamics (CFD) and chemical kinetics models. Finally, CFD will be used to investigate the electromagnetic energy-assisted conversion mechanism as a function of catalyst structure and operating conditions for hydrogen production.

This study will provide future researchers with a cost-effective tool to explore a multitude of yet-to-be-conceived electromagnetic systems to ensure long-term catalytic activity. The proposed technology has the potential to extend the longevity of catalyst materials, thereby reducing overall catalyst replenishment costs. With these improvements to the conventional thermo-catalytic hydrocarbon conversion process, it is hoped to enable a wider adoption of hydrogen-related technologies from fossil resources. This project will also support two graduate students focused on fossil energy research.

High-Speed and High-Quality Field Welding Repair Based on Advanced Non-Destructive Evaluation and Numerical Modeling

Performer	**Ohio State University**
Award Number	FE0032067
Project Duration	09/24/2021 – 09/23/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	Supply Chain

The goal of the project is to establish the experimental and computational foundations that are crucial to implementation of high-speed and high-quality field welding repair based on advanced non-destructive evaluation (NDE) and numerical modeling. The scope of work of the project is focused on developing two enabling techniques for repair of CSEF grades 91 and 92 steel components: (1) microstructure detection using ultrasonic NDE, and (2) hardness prediction using a computational model for multi-pass, multi-layer welding.

Weld coupons will be fabricated using a high-deposition-rate process based on hot wire gas tungsten arc welding (GTAW). These weld coupons will be characterized for microstructure and hardness, which provides the baseline data for Gleeble® physical simulation to produce a bulk weld microstructure. Through the control of peak temperature and time, individual microstructures (especially martensite) with different levels of tempering will be produced. This simulated microstructure is needed since the actual weld comprises a highly inhomogeneous microstructure that is difficult for analysis by raw ultrasonics. Samples containing different microstructures will be scanned using ultrasonic testing and advanced data processing algorithms such as machine learning will be used to find ultrasound parameters that are unique to the susceptible microstructures. The physics-based models will consider the heat transfer and molten pool fluid flow in a multi-pass, multi-layer dissimilar metal welding repair. The Gleeble testing results will also be used to develop a tempering kinetic model to predict the as-welded hardness distribution as well as that after post-weld heat treatment (PWHT).

High-quality field welding repairs on CSEF steel components are critical to the reliable and efficient operation of the current fleet of power plants in the United States. Development of a reliable field-usable NDE technique will ensure that the required microstructure is achieved after onsite welding. Additionally, establishing knowledge of weld reparability for newer CSEF steels such as Grade 92 based on advanced numerical models of welding processes will facilitate their adoption. The tools and knowledge to be generated in the project will establish experimental and computational foundations to achieve the overall goal of detecting and controlling microstructure and properties for welding repair onto CSEF steel components.

Conformal Coatings on Additive Manufactured Robust Alloys for Significant Mitigation of Oxidation, Erosion, and Corrosion

Performer	**West Virginia University Research Corporation**
Award Number	FE0032068
Project Duration	09/15/2021 – 09/14/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	Supply Chain

The project aims to develop novel high-temperature alloys from Ni-based alloys that further integrate additive manufacturing (AM) fabrication, creating novel nanoscale oxide precipitation for strengthened mechanical integrity and enhanced oxidation resistance, and subsequent application of conformal protective coatings on the additive- manufactured alloys. To increase the strength and oxidation resistance of nickel alloys, erbium and titanium oxide (Er2O3 and TiO) precipitants will be added to the AM powders for the Inconel 625 alloy and will result in dense nano-oxide precipitation of Er2O3 and Er2Ti2O7, which will result in a solution-strengthened novel Ni-based alloy. Furthermore, a conformal protective oxide coating layer will be simultaneously applied on both the internal and external surface of the additive manufactured heat exchangers with complex geometry using atomic layer deposition (ALD). The ALD layer will be conformal, uniform, pin-hole free, dense, and ultra-thin with negligible weight gain to increase both the oxidation and corrosion resistance at elevated temperatures.

The project is organized into 5 Tasks. Task 1 is project management. Task 2 is devoted to introducing the dense precipitates into the Ni-based alloys through AM. Task 3 is devoted to ALD coating of the newly additive manufactured 3D printed Ni-based alloys and ALD repairing and recoating the alloys after oxidation exposure. Task 4 is the oxidation resistance testing of the additive manufactured and ALD coated Ni-based alloys. Task 5 is the comprehensive physical properties testing, and nanostructure analysis of the additive manufactured alloys (including those with precipitates), ALD coated alloys, and the alloys after exposure to the oxidation and corrosion environments.

The developed high-temperature materials are expected to possess superior strength, high resistance to external surface oxidation, internal surface carburation, and corrosion, and can be applied to heat exchangers for operation in supercritical carbon dioxide at high temperatures (over 750 °C) and pressure (30 MPa). For after-service heat exchangers that have damaged surfaces, the proposed ALD coating can also be utilized to repair/ refurbish the heat exchanger parts that may have been impacted by surface oxidation and dramatically increase their lifetime and reduce costs.

Enabling the Next Generation of Smart Sensors in Coal Fired Power Plants Using Cellular 5G Technology

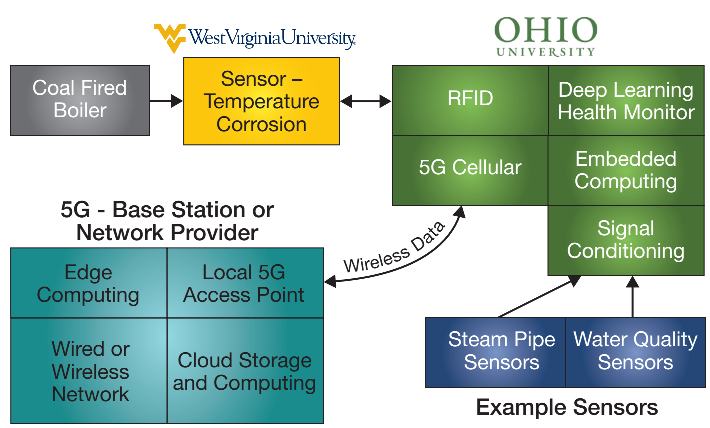
Performer	Ohio University
Award Number	FE0032078
Project Duration	08/16/2021 – 08/15/2024
Total Project Value	$ 414,481
FOA Number	DE-FOA-0002398
Area of Interest	5G Wireless

This project will build upon existing experience with cellular based systems, power plant water quality sensing, and high-temperature sensors developed during past projects. The main objective of this project is to demonstrate the effectiveness of 5G cellular embedded, cloud, and edge computing-based sensors specific to coal-fired power plant needs where harsh, noisy radio frequency (RF) conditions are encountered. Sensors that utilize 5G for data communications are the first logical step in revolutionizing wireless connectivity that will enable robust operations in coal-fired power plants. Working together, Ohio University and WVU will focus on a high-priority in-situ boiler temperature measurement system that relies on chipless radio-frequency identification (RFID) technology and much-needed temperature, pressure, environmental, and water quality industrial sensors.

The specific project objectives are (1) investigate specific needs of interfacing and data collection of identified sensing areas of significance within coal-fired power plants that would immediately benefit from 5G wireless data communications, (2) enable 5G data communication for 'peel-and-stick' chipless RFID-based boiler temperature and corrosion sensors, (3) demonstrate effectiveness and performance of 5G enabled Internet-of-Things (IoT) sensors used in coal-fired power plants, (4) investigate sensor-driven deep learning/artificial intelligence using laboratory conditions that simulate power plants for system health monitoring, and (5) determine the limits of 5G systems in harsh environments–hot, humid, and cold.

The duty cycle style of power plant operation combined with a need to lower operating costs has left several components of coal-fired power plants vulnerable to unscheduled maintenance. More advanced, intelligent, inexpensive, and simple-to-install monitoring equipment based on wireless data transfers will support the current and future coal power plant needs. Right now, coal power plant operators could greatly benefit from retro-fitting of existing sensors and additional sensor and control systems throughout. In addition, the intelligent health monitoring capabilities that occur at the sensor (embedded computing) or base station (edge computing) will give operators more prediction tools about scheduling maintenance.

Graduate students at both universities will be employed and trained on our respective technologies and will cross-collaborate to exchange information and gather laboratory results.



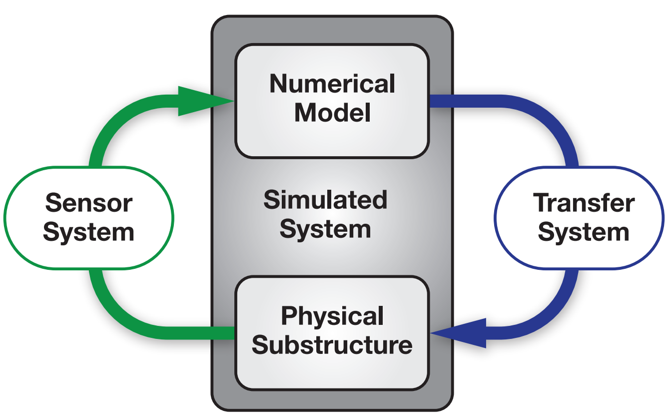
Proposed system integration - identifying contribution.

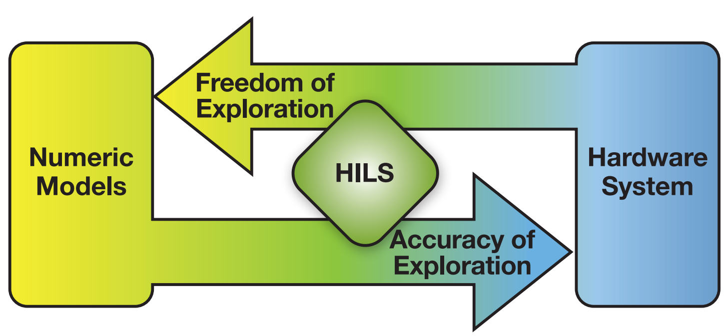
Expedited Real Time Processing for the NETL Hyper Cyber-Physical System

Performer	**Georgia Tech Research Corporation**
Award Number	FE0030600
Project Duration	08/01/2017 – 07/31/2022
Total Project Value	$ 504,130
FOA Number	DE-FOA-0001715
Area of Interest	Cyber-Physical Systems

The primary objective of this project is to provide the National Energy Technology Laboratory's Hybrid Performance Facility (HYPER) with needed numerical methods algorithms, software development, and implementation support to enact real-time cyber-physical systems that simulate process dynamics on the order of five milliseconds or smaller. The proposed paths forward comprise three distinct approaches to faster transient simulations. They fall under the numerical methods categories of (1) optimizing key parameters within the facility's present real-time processing scheme; (2) introducing an "informed" processing approach wherein a priori computations expedite real-time attempts; and (3) implementing alternatives to the presently employed explicit-implicit blended finite difference (spatio-temporal) approach. Although each of these three classes will be attempted independently as options for improvement, in some cases one may complement another.

The three approaches provide individual paths that will expedite critical computational steps. They are also anticipated to have points of compatibility to synergistically speed processing. Achieving the five-millisecond time-step threshold for the pioneering HYPER cyber-physical system would afford dynamic operability studies that capture higher-time-resolution phenomena (e.g., electrochemical-fluidic dynamics) at the full response capability of the HYPER system.





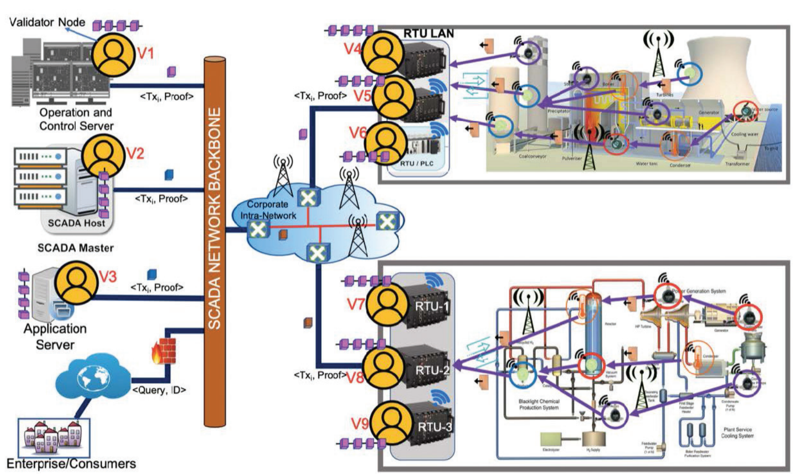
Cyber-physical simulation.

Blockchain Empowered Provenance Framework for Sensor Identity Management and Data Flow Security in Fossil-Based Power Plants

Performer	**Old Dominion University**
Award Number	FE0031744
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Cybersecurity for Fossil Power Generation

Old Dominion University will develop a blockchain-based provenance platform that would track data flow traffic from sensors deployed in fossil-based power plants and detect identity violations, unauthorized communication, and process integrity violation. The proposed platform will be scalable across a geographically distributed footprint. The blockchain-based platform would detect the presence of rogue or unauthorized sensors and unauthorized communication among the authorized sensors based on identity profiles derived from the analysis of network traffic. The proof-of-stake consensus protocol in the blockchain platform will be customized to ensure that validation of transactions would take place on the order of milliseconds and achieve a balance between scalability and resilience based on the optimal number of validating nodes. Finally, the team will provide empirical evaluation of the proposed identity management, process integrity, and scalability by testing the system on both uncongested and congested networks.

The proposed framework will ensure high availability of a distributed ledger, which will be used to verify validity of process/signal data. A trusted framework with integrity assurance that is resilient against cyber-attacks will be developed. Analytics software can query the blockchain ledger and be assured that the process data integrity, which cannot be altered by a single malicious entity, is maintained. The provenance capability within the blockchain platform would provide the ability to audit equipment operations to ensure that they are operating according to terms and conditions of a service agreement. This capability would provide real-time validation of sensor data and detect incidental/accidental/malicious incidents that could cause the equipment to operate in violation of the service level agreement.



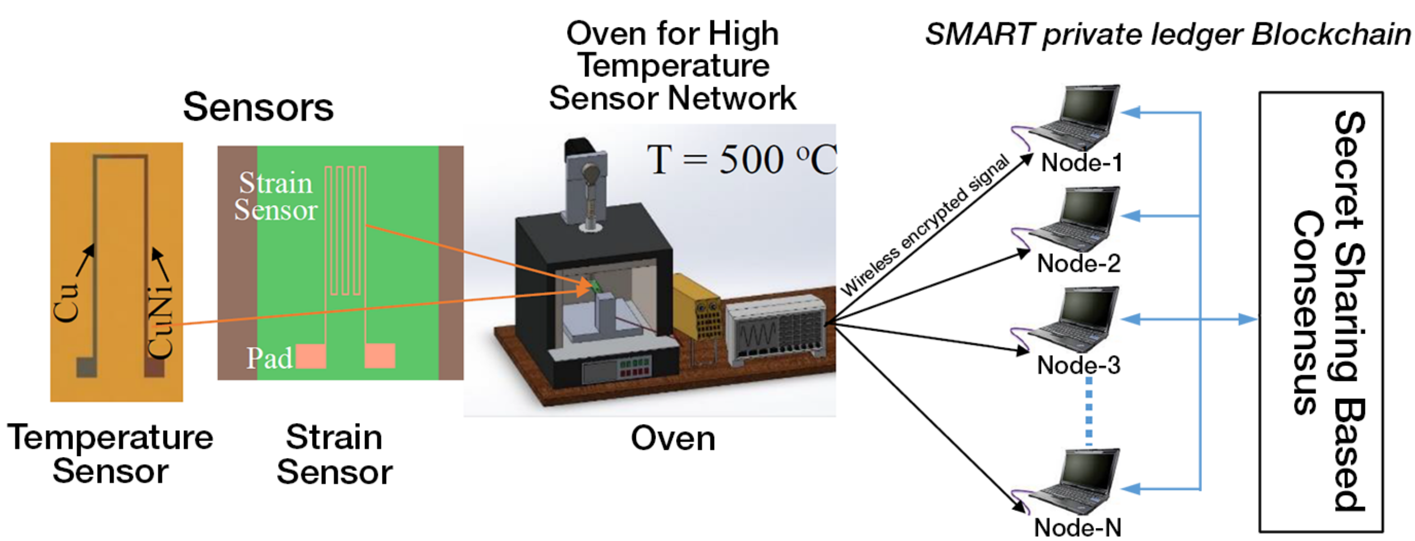
Blockchain architecture for fossil power plants.

A Novel Access Control Blockchain Paradigm to Realize a Cybersecure Sensor Infrastructure in Fossil Power Generation Systems

Performer	**Carnegie Mellon University (CMU)**
Award Number	FE0031770
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Cybersecurity for Fossil Power Generation

The goal of this project is to demonstrate a secure private blockchain protocol designed for fossil power generation systems. The specific objectives include (i) design and implementation of a secure private blockchain architecture that can secure process signal data and other information flows within distributed sensor networks for fossil-based power generation systems, (ii) a simulated power plant environment that uses sensor data with cryptographic digital signatures and integration of the secure blockchain developed by the project team with this system, and (iii) demonstration of the effectiveness of the developed blockchain technology by simulating a cyber-attack on the sensor infrastructure.

Benefits include a more secure system for data management for fossil power generation systems, and preparation of the next generation of researchers and engineers with highly interdisciplinary and complementary skills in these important areas for their own careers and maintenance of U.S. leadership in fossil energy sciences and technology.



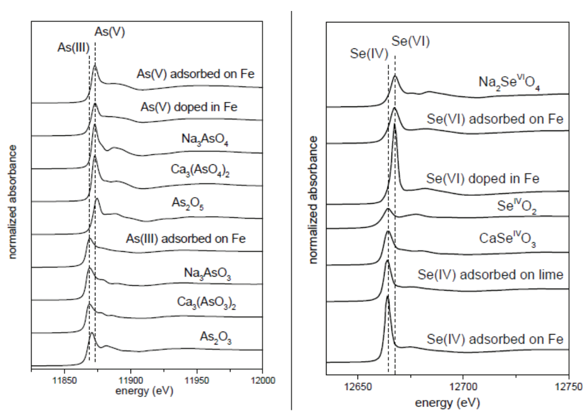
Integration in data acquisition system.

Elucidating Arsenic and Selenium Speciation in Coal Fly Ashes

Performer	Georgia Tech Research Corporation
Award Number	FE0031739
Project Duration	07/01/2019 – 06/30/2022
Total Project Value	$ 399,706
FOA Number	DE-FOA-0001991
Area of Interest	Emissions Control

This research will systematically characterize arsenic (As) and selenium (Se) speciation within a representative matrix of coal fly ashes using state-of-the-art synchrotron X-ray spectroscopic and microscopic techniques in order to develop a comprehensive correlation and searchable database for coal source/type, generation condition, As/ Se speciation, and As/Se mobility. The project will be implemented in three phases. Phase I will establish a detailed survey documenting the current state of knowledge on fossil power generating units as a function of coal type/source, operating conditions, environmental control systems, additive use, and fly ash handling methods, as well as common existing techniques for analyzing As and Se concentration. Based on this survey, a matrix of fly ash samples representing a range of conditions will be chosen, collected, and used for Phase I studies. Phase II is composed of three main tasks: (1) traditional characterization techniques will be conducted to provide bulk characteristics of the fly ash samples, such as elemental composition, microstructure, chemical and mineralogical composition, surface area, and particle size distribution, (2) state-of-the-art synchrotron X-ray microscopy and spectroscopy techniques will be applied to reveal the molecular-scale speciation information of As and Se, such as oxidation state, association with other elements/minerals, embedded mineral phase, and complexation states, and (3) the mobility of As and Se in the fly ash samples will be evaluated using different leaching methods. Phase III will incorporate the information obtained from phases I and II and establish a searchable database, detailing the correlations among coal type/source, utility operating conditions, As/Se speciation, and As/Se mobility.

When successfully completed, this technology will allow plant operators to quickly assess the amount and valence state of heavy metals in their coal fly ash.



As K-edge XANES spectra of selected reference compounds (left), Se K-edge XANES spectra of selected reference compounds (right).

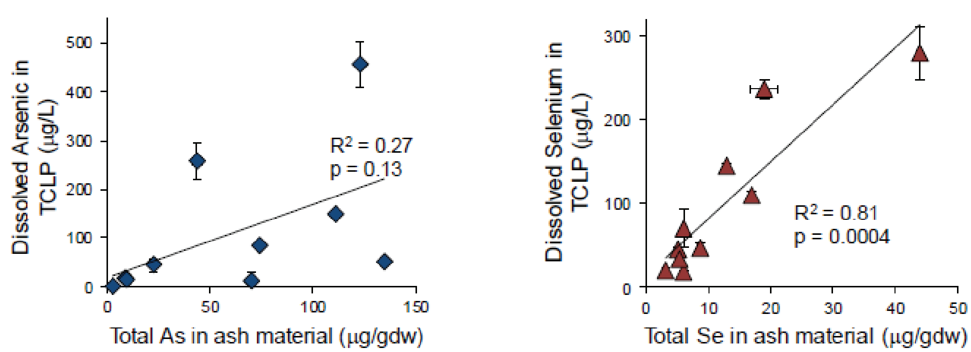
Characterization of Arsenic and Selenium in Coal Fly Ash to Improve Evaluations for Disposal and Reuse Potential

Performer	Duke University
Award Number	FE0031748
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Emissions Control

This project aims to establish high throughput characterization methods for arsenic (As) and selenium (Se) species in coal fly ash and understand how coal combustion parameters might influence leachable As and Se contents from fly ash. Specifically, the project will (1) compare methods for determining As and Se concentration, chemical speciation, and mass distribution in fly ash and establish the efficacy of these methods taking into account data quality and operator accessibility, (2) evaluate As, Se, and fly ash characteristics and measurement methods that can improve indications of leachability and mobilization potential from fly ash, and (3) perform a survey of As and Se characterization for fly ashes representing a variety of coal feedstocks, combustion conditions, and emissions controls. Duke University will study methods to quantify the chemical forms of As and Se by comparing a series of state-of-the-art quantitative methods (e.g., synchrotron-based X-ray spectroscopy and microscopy) with alternative 'benchtop' spectroscopy methods that are commonly employed in the materials and geological sciences.

The evaluation will consider benefits and trade-offs of each method, including quantitative versus qualitative determination, throughput capacity, and ease of sample processing. These characterization techniques will be compared to As and Se mobilization potential from fly ash as indicated by waste leaching protocols established by waste disposal regulations. These evaluations of As and Se concentration, speciation, mass distribution, and mobilization potential will be applied to a large variety of coal fly ashes that represent a range of coal sources, boiler types, ash collection systems, emissions controls, and combustion conditions.

Results obtained from this work will enable practitioners to understand data generated from qualitative methods that may be more accessible than state-of-the-art synchrotron techniques. A comprehensive database of As and Se speciation in a variety of coal fly ashes and other residuals will be generated. The study will outline advantages and tradeoffs for each method and establish correlations to leaching potential.

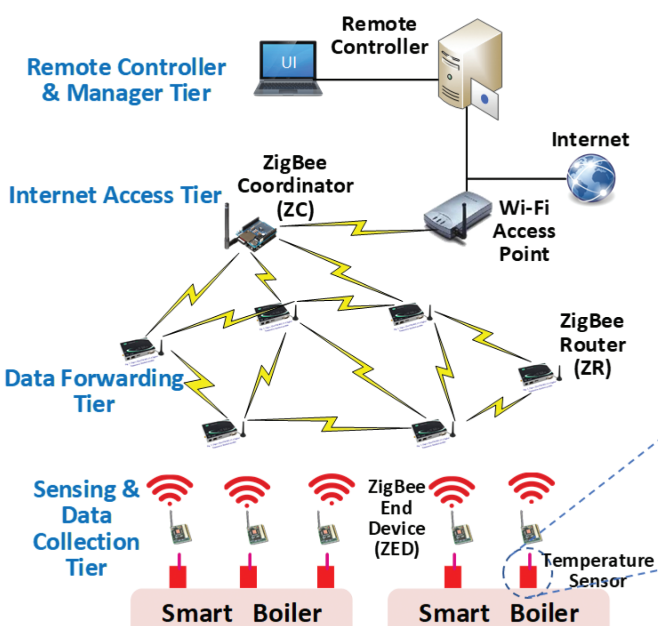


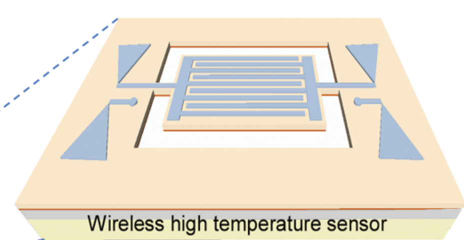
Leachable As and Se from 10 coal ash samples subjected to the toxicity characteristic leaching procedure. Data from Schwartz et al. 2018

Wireless High Temperature Sensor Network for Boiler Systems

Performer	**University of Massachusetts**
Award Number	FE0031895
Project Duration	09/04/2020 – 09/03/2023
Total Project Value	$ 499,958
FOA Number	DE-FOA-0002193
Area of Interest	Flexible Fossil Power Generation

This project aims to develop a new wireless high-temperature sensor network for real-time continuous boiler condition monitoring in harsh environments. The wireless high-temperature sensor network consists of wireless radio frequency (RF) high-temperature sensors with integrated attached antennas for wireless internet-based continuous remote monitoring. Each of the new RF high-temperature sensors is based on a high-quality factor RF filter fabricated on 4H silicon carbide semiconductor material capable of measuring high temperatures over 1,800 °C. The integrated antennas are broadband bow-tie RF antennas that can provide efficient signal transmission and reception. The wireless sensor network enables real-time and continuous monitoring of boiler conditions to achieve smart boiler system management. The high-temperature sensor network enables network-based automatic temperature sensing and data collection, which combined with artificial intelligence algorithms allow the construction of smart boiler systems with boiler condition management and optimization for significant energy-saving and reliability improvements. The research will also train graduate students in the critical technology areas of high-temperature materials, advanced manufacturing of integrated RF sensors, wireless sensor network communication, cloud computing with high security, and AI-enabled smart systems.





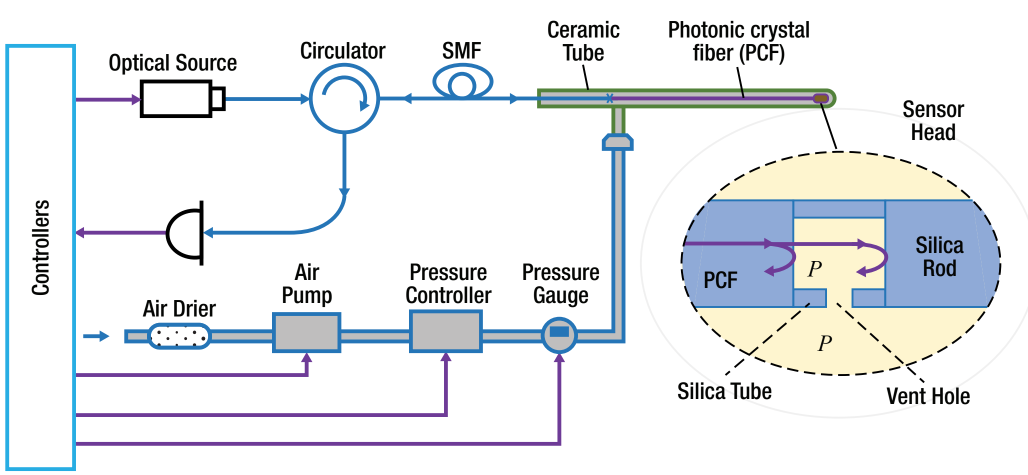
Schematic architecture of the smart boiler wireless sensor network. Each wireless high-temperature sensor is coupled with a ZigBee end device (ZED) to collect and continuously transmit the boiler temperature data in real time. The temperature data will be routed to the remote controller through the wireless mesh network and the internet as well as Wi-Fi access points. Inset: schematic structure of the wireless high-temperature sensor in boilers. It is based on a Lamb RF filter with integrated broadband bow-tie antennas for wireless temperature transfer.

High-Accuracy and High-Stability Fiber-Optic Temperature Sensors for Coal Fired Advanced Energy Systems

Performer	**Michigan State University**
Award Number	FE0031899
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$ 496,475
FOA Number	DE-FOA-0002193
Area of Interest	Flexible Fossil Power Generation

The objective of this project is to develop a revolutionary gas-based fiber-optic temperature sensor technology with the required accuracy and long-term stability for temperature control and condition monitoring of the next generation of coal-fired power systems. The temperature sensor technology is based on a Fabry-Perot (FP) cavity filled with a gas (e.g., air) the pressure of which can be changed. An FP cavity is formed by a silica tube that is filled with air and sandwiched between a side-hole fiber and a capping fiber. The holey fiber has air channels in its cladding running along the length of the fiber through which the air pressure in the FP cavity can be tuned. The light coming from the holey fiber is partially reflected at the two fiber/tube interfaces and coupled back into the holey fiber. The system then measures the reflection spectrum which contains the interference fringes of the FP cavity by a white-light source, a fiber-optic coupler, and a spectrometer.

Accurately controlling the temperature is critical for the reliable and efficient operation of future highly efficient coal-fired energy systems. An accurate temperature sensor with long-term operating reliability is key for temperature control. Temperature is also a critical parameter for condition monitoring and lifetime prediction of energy systems. However, the extreme conditions present in advanced energy systems often lead to accelerated degradation in the performance and lifetime of current sensors. Most sensors used today show unacceptable drift and require frequent calibration or replacement, often leading to costly power plant shut down. The movement toward advanced energy systems requires that new temperature sensors be developed which can maintain accuracy and long-term stability comparable to or even better than low-temperature sensors over extended periods of operation under extreme conditions.

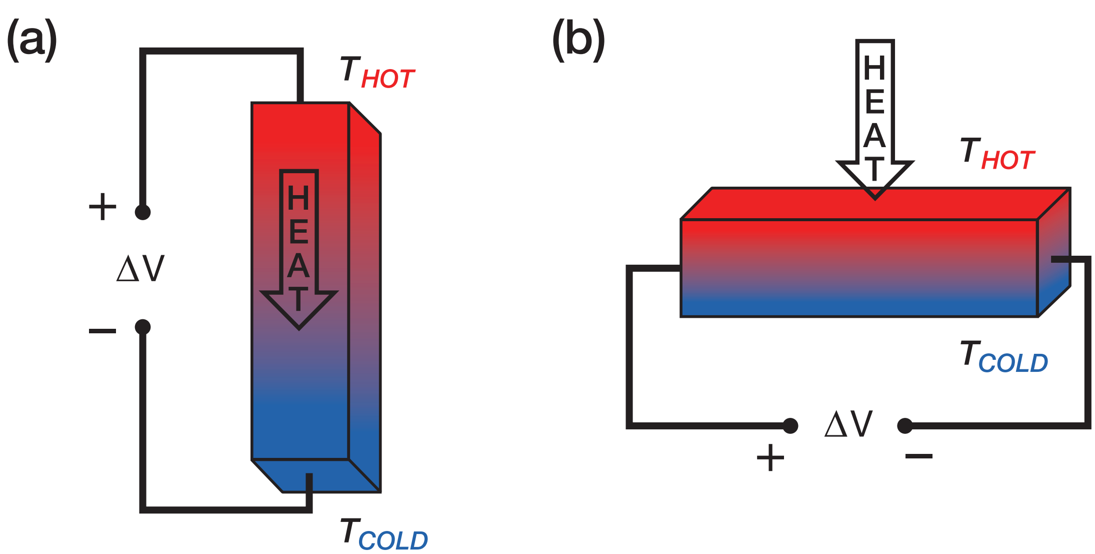


Developed a temperature sensor system that can operate at a temperature level above 1000 °C with accuracy and long-term stability comparable to the sensors of low-temperature version.

Robust Heat-Flux Sensors for Coal-Fired Boiler Extreme Environments

Performer	**University of Maryland**
Award Number	FE0031902
Project Duration	01/01/2021 – 12/31/2023
Total Project Value	$ 500,000
FOA Number	DE-FOA-0002193
Area of Interest	Flexible Fossil Power Generation

Researchers will develop robust heat flux sensor elements, based on the wire-wound Schmidt Boelter gauge architecture and the transverse Seebeck effect, capable of operating in the challenging high-temperature, corrosive environments within the boilers of coal-fired power plants. The heat-flux sensors will utilize thermoelectric effects to directly transduce the heat-flux input to analog electrical voltage signals and will be constructed from dedicated materials that can withstand oxidative atmospheres at temperatures from 700 to 1200°C and maintain adequate performance under these conditions for prolonged periods. Rigorous testing and calibration protocols in furnaces and medium-scale fire research facilities will be employed to understand the significance and reliability of the output signal under a range of dynamic environmental conditions. These conditions will include a range of heat-flux values, temperatures, surface emissivity, cooling rates, flow rates, and concentrations of carbon particulates. If successful, the project will help extend the power industry's real-time heat-flux sensing capabilities to a challenging regime of extreme environments, offering new opportunities to understand the mechanisms by which operational parameters affect the power generation efficiency. Furthermore, adverse effects of overheating, uneven burner operation and deposition of soot and slag can be detected and remediated before experiencing irreversible damages that could lead to shut down.

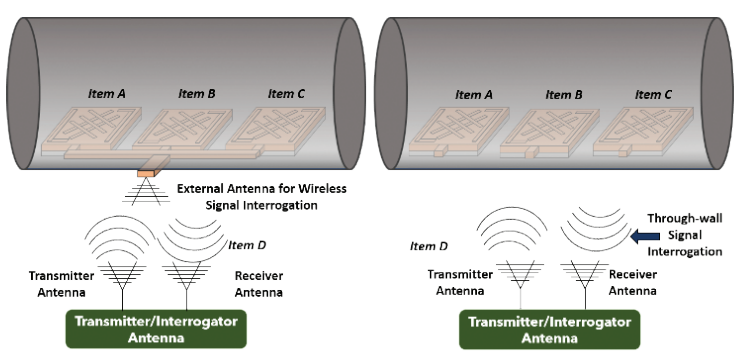


(a) Schematic of the Seebeck effect, (b) Schematic of the transverse Seebeck effect.

Passive Wireless Sensors for Realtime Temperature and Corrosion Monitoring of Coal Boiler Components Under Flexible Operation

Performer	**West Virginia University Research Corporation**
Award Number	FE0031912
Project Duration	08/17/2020 – 08/16/2023
Total Project Value	$ 500,000
FOA Number	DE-FOA-0002193
Area of Interest	Flexible Fossil Power Generation

This project will develop an inexpensive wireless, high-temperature sensor for real-time monitoring of the temperature and corrosion of metal components that are commonly used in coal-fired boilers. This work will focus on the fabrication and testing of harsh-environment, chipless radio-frequency identification (RFID) sensors that will function between 25 °C and 1300 °C in high steam and/or combustion gas environments. Sensor arrays will also be evaluated where each RFID sensor will be designed with a specified frequency band to spatially differentiate the testing site on the metal specimen. Specifically, this project will: (1) design passive wireless RFID patch and interrogator antennas for high-temperature sensing of temperature and corrosion/crack propagation at temperatures up to 1300 °C; (2) develop materials and methods to fabricate a microstrip patch antenna sensor composed of a robust conductive electroceramic pattern and interlayer ceramic coating, and then incorporate this sensor into “peel-and-stick” preforms that will efficiently transfer and bond to the metal specimens of interest; (3) investigate the wireless RFID sensor response in accelerated high-temperature and high steam environments, and correlate corrosion and cracking mechanisms (and kinetics) with the response of the sensors; (4) investigate the wireless signal acquisition and processing of data transferred in various configurations by multiple sensors within the same environment and through-wall transmission of the signal by a singular RFID sensor; and (5) investigate the passive wireless sensor system developed (and method of transferring the sensor system) for monitoring the temperature and health of metal components in service within a coal-fired power plant. Applications for the passive wireless sensors are numerous within a coal boiler power plant, and these sensors will provide operators additional information over the current state-of-the-art temperature and corrosion sensors. An important strategy for managing cycling damage for flexible operation is through real-time monitoring of localized temperature and health of the various pipework, headers, rotors, and steam chests. This technology permits simplified monitoring of these components, which would greatly reduce the cost and provide valuable localized knowledge of thermal conditions.



Left: Schematic of the multi-sensor array deposited onto the inner wall of a metal pipe to monitor corrosion rates, where each sensor focuses on a specific band range read by an external interrogator antenna; Right: schematic of the alternative interrogation method, where through-wall transmission will be tested in order to eliminate the need for an access hole.

A Robotics Enabled Eddy Current Testing System for Autonomous Inspection of Heat Exchanger Tubes

Performer	**University of Missouri**
Award Number	FE0031645
Project Duration	09/01/2018 – 12/31/2021
Total Project Value	$ 410,864
FOA Number	DE-FOA-0001842
Area of Interest	Robotics for Non-Destructive Evaluation

University of Missouri researchers developed a robotics-enabled eddy current testing (ECT) system for autonomous inspection of heat exchanger tubes. The system was capable of precisely controlling the location and speed of the ECT probe into or out of tubes of various sizes and geometries. An imaging system and adaptive control algorithm was employed to quickly identify the outer geometry of the tubes and their positions relative to the probe, enabling precise movement of the ECT probe to the inlet of each tube. Insertion and extraction speeds will be controlled for fast and more consistent scanning during testing. A convolutional neural network or other machine learning algorithms were developed to enable autonomous inspection via a feedback loop, which will be employed to learn from historical data categorized by the signatures of the various failure modes (e.g., cracking and corrosion; abrasive and erosive wear). If measured data from suspicious regions of the tubes match these signatures, the controller will make a real-time decision on insertion and extraction speeds and probe location for more detailed scanning, thus increasing measurement accuracy while enhancing testing efficiency.

The developed robotic platform could enable automated eddy- current testing, thus reducing labor time and cost. Well-controlled testing speeds will reduce human inconsistencies in data gathering and analysis. The artificial intelligence algorithm could enable deep mining of historical data for in- situ analysis and real-time decision making.

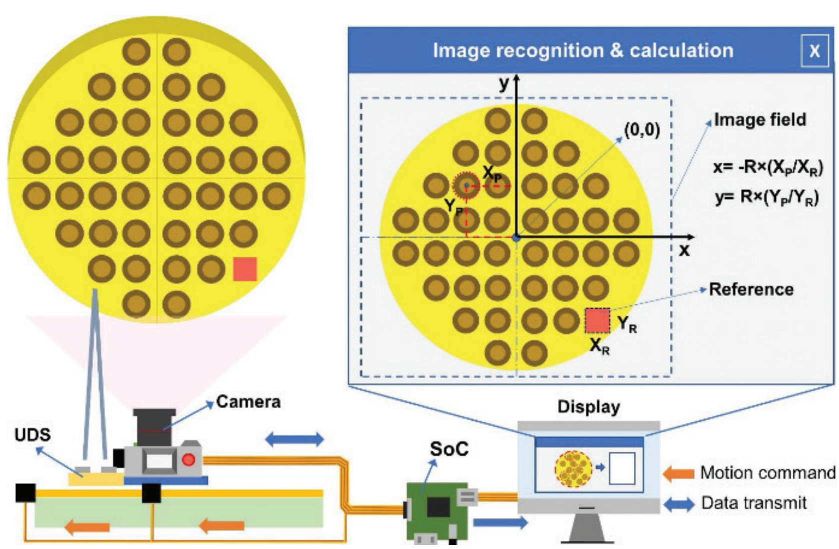


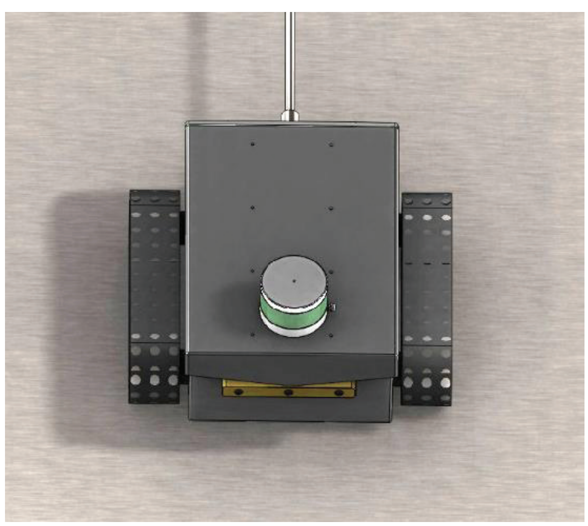
Image processing steps for recognizing geometry and location of tubes' inlets.

AI Enabled Robots for Automated Nondestructive Evaluation and Repair of Power Plant Boilers

Performer	Colorado School of Mines
Award Number	FE0031650
Project Duration	09/01/2018 – 08/31/2022
Total Project Value	$ 473,972
FOA Number	DE-FOA-0001842
Area of Interest	Robotics for Non-Destructive Evaluation

Colorado School of Mines researchers are collaborating with partners from Michigan State University to develop an integrated autonomous robotic platform that (1) is equipped with advanced sensors to perform live inspection, (2) operates innovative onboard devices to perform live repair, and (3) uses artificial intelligence (AI) for intelligent information fusion and live predictive analysis for smart automated spatiotemporal inspection, analysis, and repair of furnace walls in coal-fired boilers. The autonomous robotic platform will be capable of attaching to and navigating on vertical boiler furnace walls using magnetic drive tracks. Live non-destructive evaluation (NDE) sensors and repair devices will be developed and integrated in the robot. In addition, the robot will be empowered with AI to automate data gathering (e.g., mapping and damage localization), and live predictive analysis will incorporate end-user feedback to continuously improve performance and achieve smart autonomy. Performance will be verified on vertical steel test structures in the principal investigators' laboratories and at facilities provided as in-kind support by Xcel Energy and EnergynTech.

Successful robotic inspection will limit or eliminate the need to send inspectors to assess difficult-to-access or hazardous areas, enable automated live inspection, reduce risk to human operators during maintenance or unplanned outage, and enable smart collection of comprehensive and well-organized data. The impact is increased boiler reliability, usability, and efficiency.

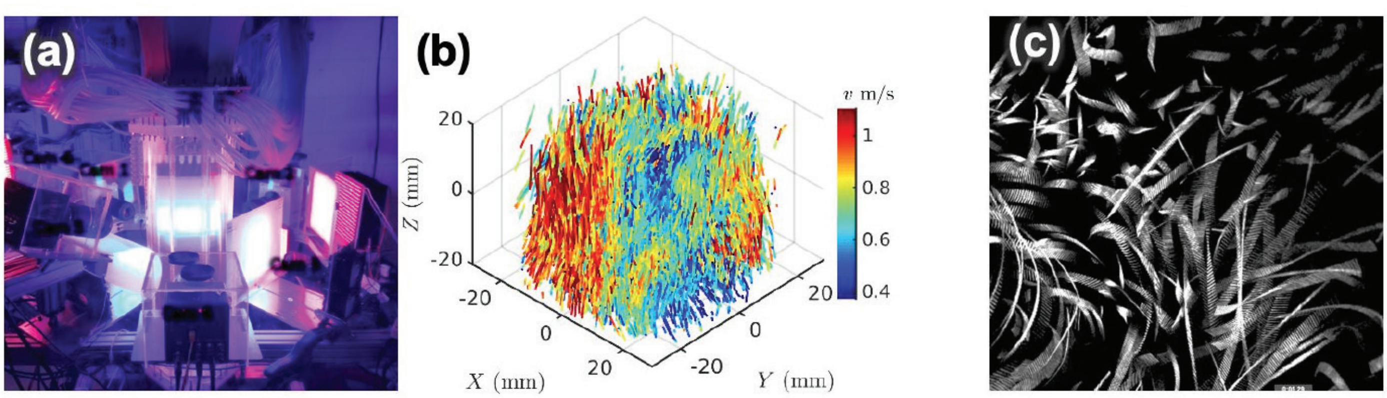


Concept image of the tracked robot platform without the NDE or repair equipment attached traversing a steel plate.

Developing Drag Models for Non-Spherical Particles through Machine Learning

Performer	**Johns Hopkins University**
Award Number	FE0031897
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$500,000
FOA Number	DE-FOA-0002193
Area of Interest	Computational Fluid Dynamics

The overarching goal of this project is to produce comprehensive experimental and numerical datasets for gas-solid flows in well-controlled settings to understand the aerodynamic drag of non-spherical particles in the dense regime. The datasets and the gained knowledge will be utilized to train deep neural networks in TensorFlow™ to formulate a general drag model for use directly in NETL MFiX-DEM module. This will help to advance the accuracy and prediction fidelity of the computational tools that will be used in designing and optimizing fluidized beds and chemical looping reactors. The unique combination of DNS and high-resolution experiments, the capability to reduce the number of parameters, and the machine-learning-based data processing, will allow for developing a drag model that has unprecedented accuracy and breadth of regimes to which it can be applied. It will critically advance the physical understanding of particle-particle and particle-gas interaction in gas-solid flows. This research program will also provide a comprehensive database to inform and validate MFiX and other numerical models for multiphase flows. Finally, students that will be involved in this project will gain experience in modern computational, experimental, and machine learning methods. The rigorous scientific training will prepare the students to become future leaders in promoting and revolutionizing fossil energy.

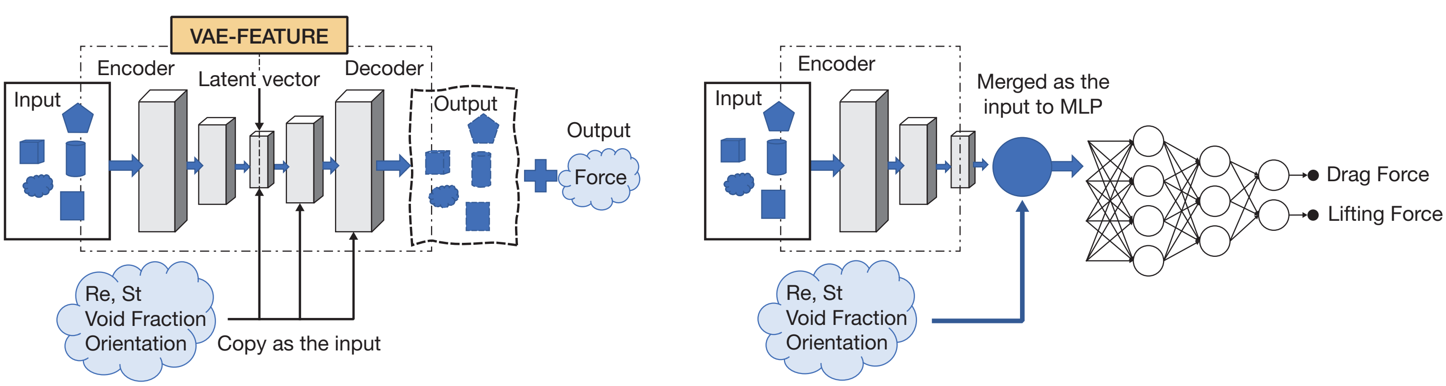


a) Picture of the 3D dense particle tracking system that has already been integrated in another similar vertical setup. (b) Dense particle trajectories collected from the same system in (a), color-coded by individual's particle velocity. (c) Long-exposure picture of dense fibers moving in turbulence conducted by PI Ni.

Unsupervised Learning Based Interaction Force Model for Non-spherical Particles in Incompressible Flows

Performer	**Ohio State University**
Award Number	FE0031905
Project Duration	08/01/2020 – 07/31/2023
Total Project Value	$500,000
FOA Number	DE-FOA-0002193
Area of Interest	Computational Fluid Dynamics

The objective of this project is to develop a neural network-based interaction (drag and lifting) force model. The project seeks to firstly construct a database of the interaction force between the non-spherical particles and the fluid phase based on the particle-resolved direct numerical simulation (PR-DNS) with immersed boundary-based lattice Boltzmann method. An unsupervised learning method, i.e., variational auto-encoder (VAE), will be used to improve the diversity of the non-spherical particle library and to extract the primitive shape factors determining the drag and lifting forces. The interaction force model will be trained and validated with a simple but effective multi-layer feed-forward neural network: multi-layer perceptron, which will be concatenated after the encoder of the previously trained VAE for geometry feature extraction. The interaction force model obtained by the accurate DNS-based database will be supplied as a more general and robust gas-solid coupling correlation than the currently used empirical and semi-empirical correlations in computational fluid dynamics coupled with discrete element method simulations. The PR-DNS code developed in this project will broaden the modeled range of the Stokes number from 0 to infinity and thus improve the generality of the current non-spherical interaction force model. Additionally, with PR-DNS, the effect of orientation and volume fraction can be readily considered for each individual particle, whereas experimentally, only the averaged value can be obtained.



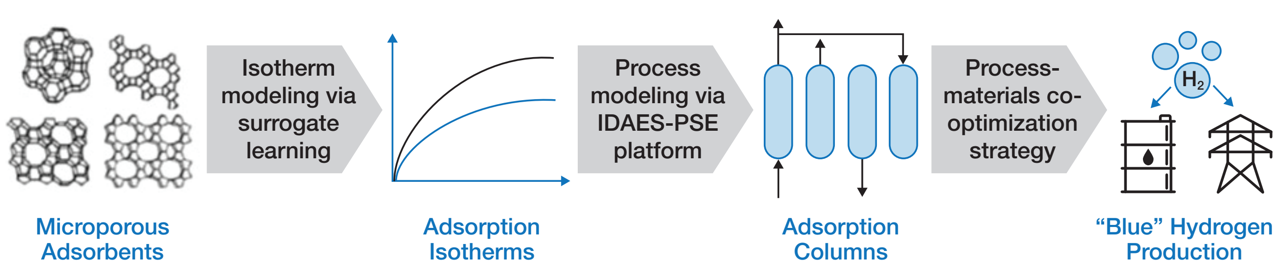
Variational auto-encoder (VAE) will be utilized to extract the primitive geometrical factors of a non-spherical particles. A multi-layer perceptron (MLP) will then be supplied as a regressor for both the drag and lifting force of the non-spherical particles.

Advanced Modeling and Process-Materials Co-Optimization Strategies for Swing Adsorption Based Gas Separations

Performer	Carnegie Mellon University (CMU)
Award Number	FE0032069
Project Duration	09/13/2021 – 09/12/2024
Total Project Value	$ 400,000
FOA Number	DE-FOA-0002398
Area of Interest	Hydrogen Production

Integrating carbon capture with fossil fuel-based technologies currently stands as the most realistic pathway for enabling a hydrogen economy. To realize this, it is crucial to develop novel, energy-efficient, adsorption-based gas separation processes that are coupled with purpose-designed microporous materials serving as the adsorbents, in order to enable needed efficiencies in either a pre-combustion, oxyfuel combustion, or post-combustion carbon capture setting. In this project, mathematical models and computational methodologies are developed to enable the design of novel gas separation processes, along with the microporous materials they rely upon, in a co-optimization paradigm. This project specifically focuses on swing adsorption, considered to be the most promising technology for selectively adsorbing and separating gases at massive scales. Swing adsorption achieves the gas separation by utilizing the difference in pressure-dependent and/or temperature-dependent equilibria and kinetics that different gases exhibit when adsorbing inside solid sorbents. The high-fidelity process modeling effort will be coupled with data-driven materials design methodologies, realizing a novel integrated process-materials co-optimization framework that will be implemented within DOE's IDAES Integrated Platform, an open-source computational platform for the modeling and optimization of advanced energy systems. Harnessing data from open-source databases, the materials optimization effort will involve the automated learning of high-quality adsorption isotherms in forms that can be seamlessly incorporated within high-fidelity process models, in order to enable the direct search over the material's molecular structure. Such materials optimization will be conducted simultaneously, in an integrated fashion, with process optimization that considers both cycle configuration and flowsheet design. Specific emphasis will be given to the development of a smart hierarchy of models that navigates the trade-off between model tractability and model fidelity, in a user-configurable model interface that empowers IDAES users to control this trade-off in their own application.

The proposed framework will enable the ever-growing base of IDAES users, from industry to government to academia, to design gas separation processes at multi-scale levels, supporting their efforts to develop new technologies and systems for hydrogen production and to determine the most cost-efficient pathways toward a hydrogen economy. Example systems in which the developed methodologies could be applied include carbon capture for combustion-based power generation and hydrogen purification for gasification and syngas-based technologies. There are numerous other application contexts that require gas separations and for which innovations resulting from this project could also be leveraged.

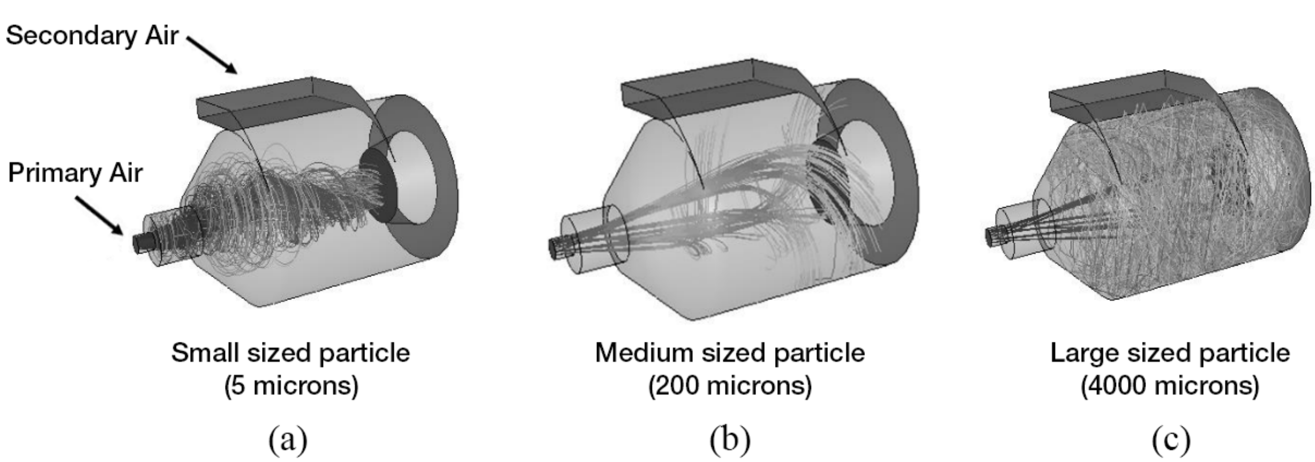


An Integrated Approach to Predicting Ash Deposition and Heat Transfer in Coal-Fired Boilers

Performer	**University of North Dakota Energy and Environmental Research Center (UNDEERC)**
Award Number	FE0031741
Project Duration	08/01/2019 – 07/31/2022
Total Project Value	$ 399,238
FOA Number	DE-FOA-0001991
Area of Interest	Plant Modeling

The overall goal of this project is to develop an advanced online technology to predict, monitor, and manage fireside ash deposition that allows for more efficient operations under a range of load conditions. Today a significant number of coal-fired plants are required to follow load and cycle the units as a result of the intermittent availability of power from wind or solar sources. These plants are faced with new challenges associated with decreased efficiency during low-load conditions as well as degradation of system components due to cycling. The project team consisting of the University of North Dakota (UND), Microbeam Technologies Incorporated (MTI), and Otter Tail Power (OTP) will model ash deposition formation processes occurring at Otter Tail Power's Coyote Station using computational fluid dynamics (CFD) over a range of load conditions and coal properties to develop algorithms to augment current online predictive methods.

This project has the potential to economically improve the environmental performance of cyclone-fired boilers by managing lignite properties that will allow for optimum cyclone performance. Developing these tools will enable personnel associated with lignite mining and plant operations to operate the systems more efficiently.



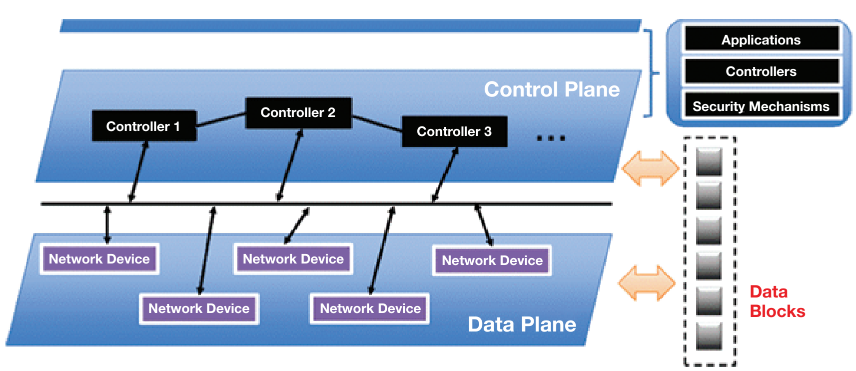
Typical particle trajectories of (a) small; (b) medium; (c) large-sized particles within the cyclone barrel.

Incorporating Blockchain/P2P Technology into an SDN-Enabled Cybersecurity System to Safeguard Fossil Fuel Power Generation Systems

Performer	University of North Dakota Energy and Environmental Research Center (UNDEERC)
Award Number	FE0031742
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Cybersecurity for Fossil Power Generation

This project will investigate the functionality and performance of a blockchain/peer-to-peer (P2P)-enhanced, software-defined networking (SDN)-enabled cybersecurity protection system. This cybersecurity system will operate on a group of controllers which form the control plane of an SDN system. The group of SDN controllers determine how traffic flows are handled passing through switches in the SDN forwarding plane. The forwarding switches relay the communications traffic flows among the cyber-capable devices (e.g., monitors and actuators) deployed in the industrial control system (ICS) for managing and controlling the power plant, transformer yard and power bus functions, transmission system, and distribution substations. The actions of handling traffic flows reflect the purpose of an ICS in allowing legitimate flows and blocking suspicious traffic flows pertaining to possible network intrusions or denial-of-service attacks. The actions are expressed in the form of rules which can be programmed into the forwarding switches by the SDN controllers. Cybersecurity protection based on the present SDN technology is susceptible to attacks targeting the control plane or targeting the communications between the forwarding and the control planes. However, the PIs believe that blockchain/P2P technology can be incorporated into an SDN-based cybersecurity protection system to mitigate the security risks. The prototype of a blockchain/P2P-enhanced cybersecurity protection system can be used to demonstrate a cost-effective reinforcement of the security protection safeguarding the operations of fossil fuel power generation systems. A testbed needs to be developed to examine the technical feasibility of incorporating blockchain/P2P technology into an SDN-enabled cybersecurity protection system, from both inter-operability and performance perspectives.

This project will also create a synergy between the University of North Dakota and its project partner, Minnkota Power Cooperative, for addressing the practical need of cybersecurity protection over fossil fuel power generation systems. In the long term, the project is expected to facilitate sustained efforts in advancing ongoing research in emerging technologies to enhance cybersecurity protection in a broader range of applications.



The generic framework of blockchain-based SDN.

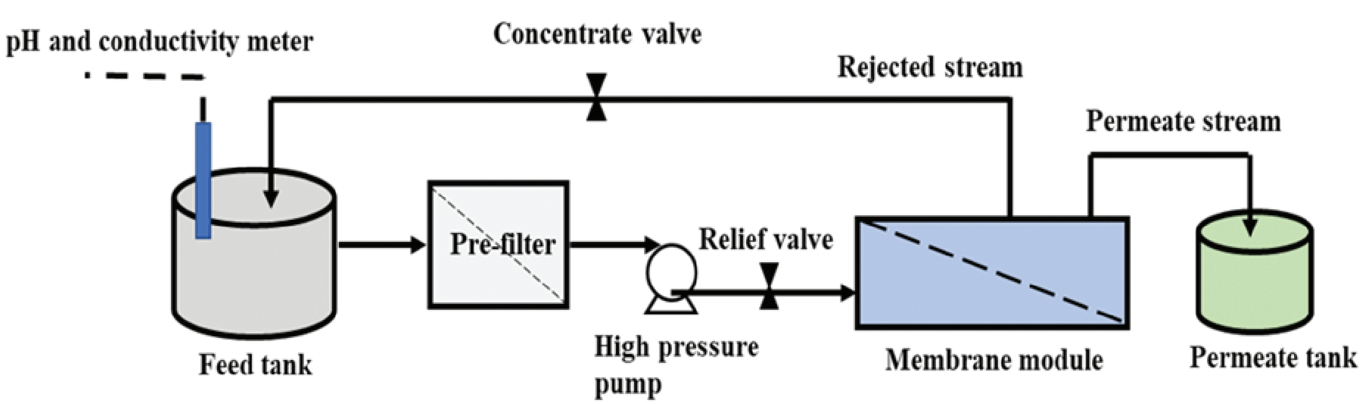
Produced Water and Waste Heat-Aided Blowdown Water Treatment: Using Chemical and Energy Synergisms for Value Creation

Performer	**West Virginia University Research Corporation**
Award Number	FE0031740
Project Duration	09/01/2019 – 04/30/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Effluent Water Reuse

West Virginia University Research Corporation will develop and test an innovative treatment process that utilizes produced water (PW) to create chemical and energy synergisms in blowdown (BD) water treatment. The project goal is to maximize generation of a product stream low in fouling potential for reuse and a concentrated stream of commercial value (i.e., 10-lb brine) while reducing chemical and energy costs for the treatment. This treatment process consists of mature treatment technology and innovative use of mature technology (i.e., brine electrolysis) to enable step improvement in cost and energy requirements for BD water treatment over the baseline process. Specifically, the proposed treatment process consists of softening, organics and suspended solids removal, reverse osmosis, brine electrolysis, and thermal desalination. These treatment units are integrated to sequentially treat the PW and BD water from their raw water conditions to those of a product stream suitable for reuse and 10-lb brine as a saleable product.

Each treatment unit will be tested to quantify its treatment efficiency and chemical and energy requirements. The treatment units will be integrated together into a single, packaged, prototype module that will also be tested using simulated or actual cooling tower blowdown water. In addition, the Recipient will develop a process model and conduct process simulations based on the experimental results and literature values to optimize the treatment process. The model will include a cooling tower and a condenser in addition to the PW-aided BD water treatment subsystem. A techno-economic analysis will be performed to quantify chemical and energy savings compared to the baseline as well as potential revenue generation.

If successfully implemented, this project will demonstrate a model process for closing unsustainable, open-ended waste streams generated in an industrial sector (i.e., gas production) by utilizing the waste streams in another sector (i.e., power generation) for value creation through technology innovation.



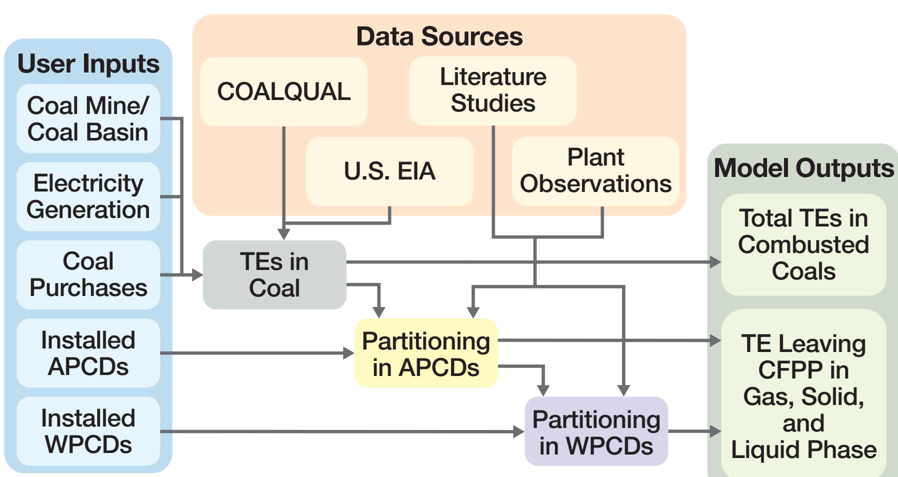
Schematic diagram of the RO treatment system.

Trace Element Sampling and Partitioning Modeling to Estimate Wastewater Composition and Treatment Efficacy at Coal Generators

Performer	Stanford University
Award Number	FE0031646
Project Duration	09/10/2018 – 09/09/2022
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001842
Area of Interest	Waste Water Contaminants Partitioning

Stanford/Carnegie Mellon University researchers will sample pulverized-coal-fired power plants (CFPPs) owned and operated by Louisville Gas & Electricity–Kentucky Utilities (LGE-KU) to build a predictive model that will enable utility decision makers, academic researchers, and policymakers to simulate trace element (TE) emissions from such plants. Samples taken during baseload and cycling conditions will be used to develop and validate an open-source, easy-to-implement trace element partitioning model using publicly available datasets, literature studies of trace element partitioning, and sampling data from LGE-KU coal-fired plants to estimate trace element partitioning in air pollution control devices (APCDs) between the gas, liquid, and solid phases exiting boilers and flue gas treatment trains. The project team will use estimates of the liquid phase trace element concentration in flue gas desulfurization (FGD) wastewater to estimate trace element behavior in water pollution control devices (WPCDs) and evaluate treated wastewater effluent concentrations for compliance with the Effluent Limitations Guidelines and Standards for the Steam Electric Power Generating Point Source Category (ELGs). The team will then develop cost estimates of established and emerging wastewater treatment trains to identify the most cost-effective approaches to comply with the ELGs.

It is anticipated that this project will create an open-source predictive model of trace element partitioning to solid, liquid, and gas phases at coal-fired power plants, establish a range of FGD wastewater chemistries for existing and new plants, model costs for biological and emerging selenium removal technologies, and quantify the impact of non-steady state operation on trace element partitioning.



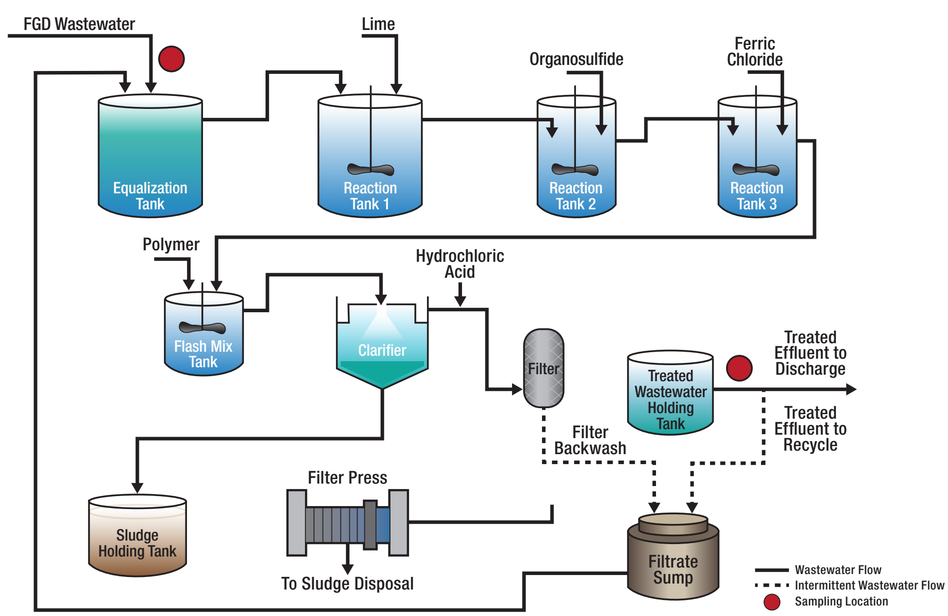
Framework for the Trace Element Partitioning Model.

Coal-Fired Power Plant Configuration and Operation Impact on Plant Effluent Contaminants and Conditions

Performer	**Lehigh University**
Award Number	FE0031654
Project Duration	09/01/2018 – 12/31/2021
Total Project Value	$ 400,000
FOA Number	DE-FOA-0001991
Area of Interest	Waste Water Contaminants Partitioning

Lehigh University, working with Western Kentucky University, characterized coal contaminants in power plant wastewater as a function of coal type, plant type, plant operational profile, environmental controls, water treatment technology, and effluent species. Multiple utility companies provided access to their coal-fired power plants and in- kind support for testing and data and sample collection from flue gas desulfurization wastewater discharge and treated water tank discharge effluent streams. Effluent samples were analyzed for mercury, arsenic, selenium, nitrate/nitrite, and bromide. Coal sample analyses included proximate analysis (moisture, volatile matter, ash, and fixed carbon); ultimate analysis (carbon, hydrogen, nitrogen, sulfur, ash, and oxygen); trace elemental analysis (mercury, arsenic, and selenium); and anions analysis (bromide, nitrate plus nitrite).

The project provided results of effluent conditions as a function of coal type, unit configuration, and unit operation profile, and identified the levels of uncertainty in the effluent results. These results will provide feedback information about the impact of fuel type on effluents and help future decisions on wastewater compliance. Participation of students will encourage new research ideas and provide valuable training opportunities for future U.S. scientists and engineers.



Sampling locations for wastewater chemical precipitation system.

ABBREVIATIONS

5G-TSN .... fifth-generation time-sensitive networking
ALD .... atomic layer deposition
AM .... additive manufacturing
ANN .... artificial neural network
APCD .... air pollution control devices
As .... arsenic
AUSC .... advanced ultra-supercritical
BD .... blowdown
CAD .... computer assisted design
CFD .... computational fluid dynamics
CFPP .... coal-fired power plant
CO .... carbon monoxide
CO_2 .... carbon dioxide
CSEF .... creep-strength-enhanced ferritic
cSETR .... Center for Space Exploration and Technology Research
DECS .... distributed edge computing service
DNN .... deep neural network
DNS .... direct numerical simulation
DOE .... U.S. Department of Energy
E2E .... end-to-end
ECT .... eddy current testing
ELG .... Effluent Limitations Guidelines and Standards for the Steam Electric Power Generation Point Source Category
EM .... electromagnetic
EMI .... electromagnetic interference
FECM .... U.S. Department of Energy's Office of Fossil Energy and Carbon Management
FGD .... flue gas desulfurization
FP .... Fabry-Perot
GNR .... graphene nanoribbon
GPS .... global positioning system
GPU .... graphics processing unit
GQD .... graphene quantum dot
GTAW .... gas tungsten arc welding
H_2 .... hydrogen
H_2O .... water
HBCU-OMI .... Historically Black Colleges and Universities and Other Minority Institutions
HYPER .... Hybrid Performance (NETL program)
ICME .... integrated computational materials engineering
ICS .... industrial control system
IDAES .... Institute for the Design of Advanced Energy Systems
IN .... Inconel
LGE-KU .... Louisville Gas & Electricity–Kentucky Utilities
LTI .... lizard-inspired tube inspector
MFiX .... Multiphase Flow with Interphase eXchanges
MFiX-DEM .... Multiphase Flow with Interphase eXchanges Discrete Element Model
MLP .... multi-layer perceptron
MTI .... Microbeam Technologies Incorporated
NDE .... non-destructive evaluation
NETL .... National Energy Technology Laboratory
NV .... nitrogen vacancy
OTP .... Otter Tail Power
P2P .... peer-to-peer
PR-DNS .... particle-resolved direct numerical simulation
PW .... produced water
PWHT .... post-weld heat treatment
QoS .... quality of service
R&D .... research and development
RF .... radio frequency
RFID .... radio-frequency identification
SBE .... Simulation-Based Engineering (NETL program)

SDN .... software-defined networking

Se ....selenium

SCADA .... supervisory control and data acquisition

SCS................................. solution combustion synthesis

SPM-OL ....scanning probe microscopy-based oxidation lithography

STEM ....science, technology, engineering, and mathematics

sCO_2.................................... supercritical carbon dioxide

TCD...............................thermo-catalytic decomposition

TE .... trace element

UCR ....University Coal Research

UND ....University of North Dakota

UTEP................................ University of Texas at El Paso

UTR.....University Training and Research (NETL program)

VAE .... variational auto-encoder

WPCD ....water pollution control devices

WVU..West Virginia University

ZED ....ZigBee end device

NOTES

NOTES

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