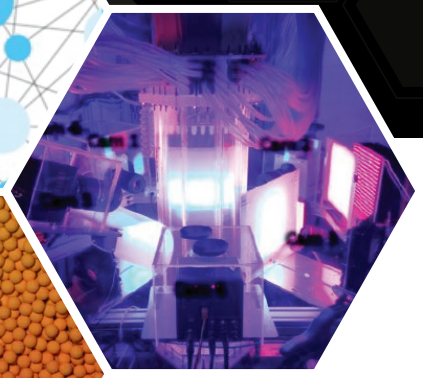
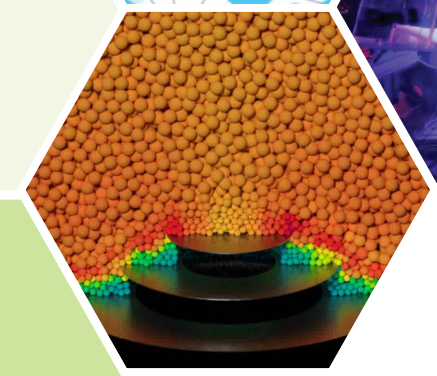
CROSSCUTTING RESEARCH

2022

SIMULATION-BASED ENGINEERING





PROJECT PORTFOLIO

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

DISCLAIMER

This project was funded by the United States Department of Energy, National Energy Technology Laboratory, in part, through a site support contract.

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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.

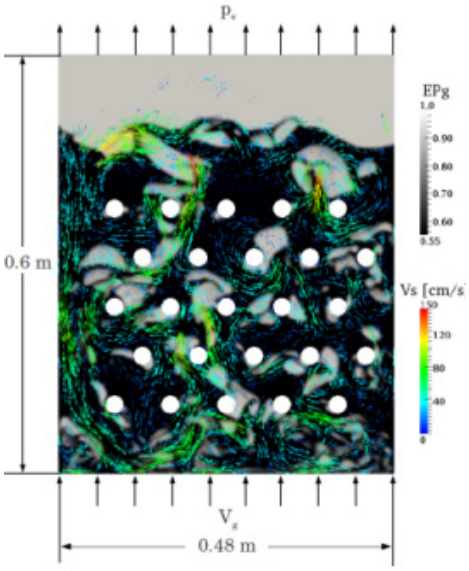
This effort combines theory, computational modeling, advanced optimization, experiments, and industrial input to simulate complex advanced energy processes, resulting in virtual prototyping. The research conducted in the SBE R&D develops accurate and timely computational models of complex reacting flows 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.

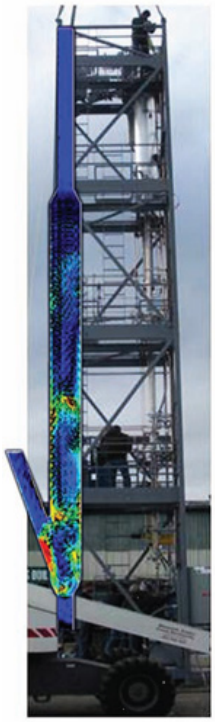
University Training and Research: University Training and Research supports two of the longest-running university training programs, the Historically Black Colleges and Universities and Other Minority Institutions (HBCU-OMI) and the University Coal Research (UCR) programs, to support the education of students in the area of coal science. 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.

SIMULATION-BASED ENGINEERING

Modeling efforts have been demonstrated to reduce the development costs and time required by the iterative use of expensive lab set-ups in research and physical prototypes in the design and engineering phase of projects. NETL is seeking improvements in all aspects of modeling from algorithms to software engineering. NETL's Simulation-Based Engineering area combines the technical knowledge, software development, computational power, data repository, experimental facilities, and unique partnerships to support research into timely and accurate solutions for complex power systems. Understanding the performance of complex flows and components used in advanced power systems and having the means to impact their design early in the development process provides significant advantages in product design. Computational models can be used to simulate the device and understand its performance before the design is finalized. During new technology development—for instance, the development of a new sorbent adsorber/desorber reactor for carbon dioxide capture—empirical scale-up information is not available because the device has not yet been built at the scale required. Traditional scale-up methods do not work well for many of the components of complex power systems. Therefore, science-based models with quantified uncertainty are important tools for reducing the cost and time required to develop these components.



The simulation of a bubbling fluidized bed with heat transfer tubes used for model validation.



CFD model of a pilot-scale carbon dioxide adsorber (shown in the background).

Research through Simulation-Based Engineering 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 nation, such as NETL's University Training and Research programs. Partnerships have also been formed with other national laboratories through the Institute for the Design of Advanced Energy Systems (IDAES).

The vast computational resources available to NETL ensure timely solutions to the most complex problems. The NETL Joule supercomputer is one of the world's fastest and most energy-efficient, intended to help energy researchers discover new materials, optimize designs, and better predict operational characteristics. Speed-up is also achieved through research in modern graphical processing unit computing as well as the implementation of reduced-order models when appropriate. Simulation-Based Engineering also exploits on-site, highly instrumented experimental facilities to validate model enhancements. Models are made available to the public through the laboratory's computational fluid dynamics (CFD) code Multiphase Flow with Interphase eXchanges (MFiX), developed specifically for modeling reacting multiphase systems.

Simulation-Based Engineering personnel work closely with stakeholders and partners to outline issues, emerging trends, and areas of need. NETL has sponsored multiphase flow workshops annually to bring together industry and academia to identify R&D priorities and ensure that key technologies will be available to meet the demands of future advanced power systems. The research areas under Simulation-Based Engineering are Advanced Process Simulation, Computational Materials Design (with High Performance Computing), and Multiphase Flow Science.

ADVANCED PROCESS SIMULATION

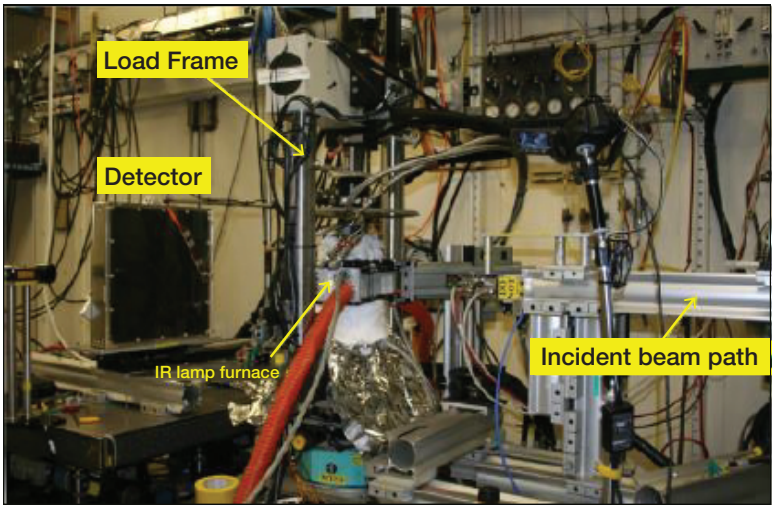
Damage Accumulations Predictions for Boiler Components Via Macrostructurally Informed Material Models

Performer	General Electric (GE) Company	Argonne National Laboratory
Award Number	FE0031823	FWP-31961.2
Project Duration	10/01/2019 – 09/30/2022	10/01/2019 – 09/30/2022
Total Project Value	$ 907,084	$ 30,000
Total Project Value	$ 937,084	
Collaborator	Energy Industries of Ohio	
Technology Area	Plant Optimization Technologies	

The goal of this project is to develop accurate models of the physical and mechanical behavior and degradation of nickel-based superalloys during cyclic operations in fossil energy power plants where thermo-mechanical fatigue and creep damage are occurring at the same time. The project will build on knowledge and models developed in previous DOE-funded projects to expand current microstructure-based models and predict hold time cyclic loading for nickel-based superalloy Haynes 282 at temperatures between 1100 and 1400 degrees Fahrenheit. Enhanced material model capabilities will be demonstrated by analyzing a superheater header component, comparing total strain evolution in time in the highest-strained regions for various wall thicknesses.

The project focus is on an alloy (Haynes 282) that is increasingly used in boiler and piping components of fossil power plants. Researchers will provide physically informed models, capturing the microstructural changes taking place in components under cyclic loading and exposure to high stress and temperature for operating life up to 300,000 hours.

Validated software tools will be developed that can be used to increase accuracy in predicting the life of high temperature nickel components in the long term and subject to significant cycling operation as well as to improve the design of new high-temperature components for new power plants or for use in existing power plants.

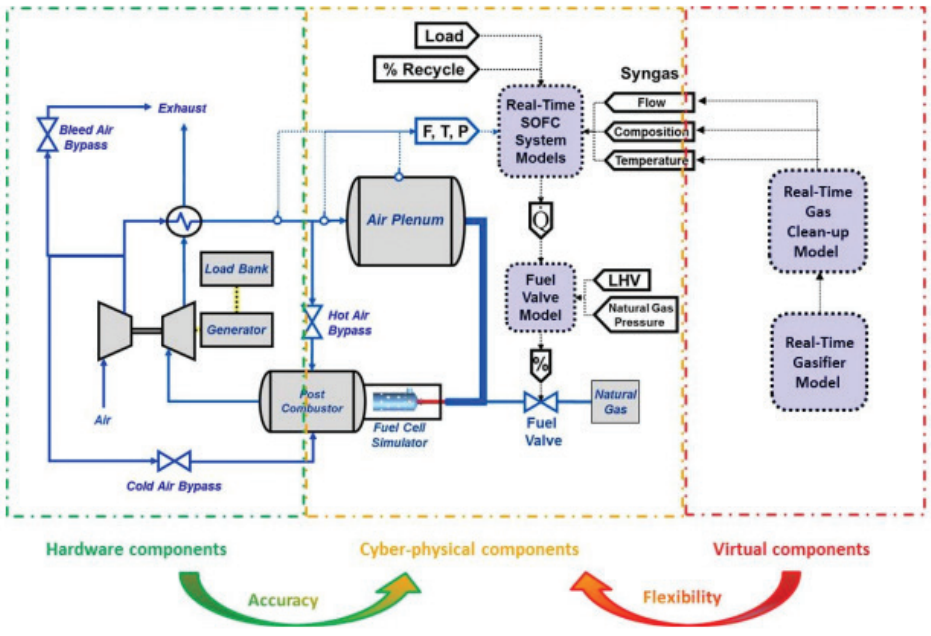


Cyclic loading test setup.

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
Technology Area	University Training and Research

The primary objective of the proposed project is to provide the National Energy Technology Laboratory's Hybrid Performance (HYPER) Facility the needed numerical methods algorithm(s), 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. Each of these three classes will be attempted independently as options for improvement, yet 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.



Layout of the HYPER project facility at NETL illustrating the connectivity of the cyber-physical fuel cell system and real-time model.

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

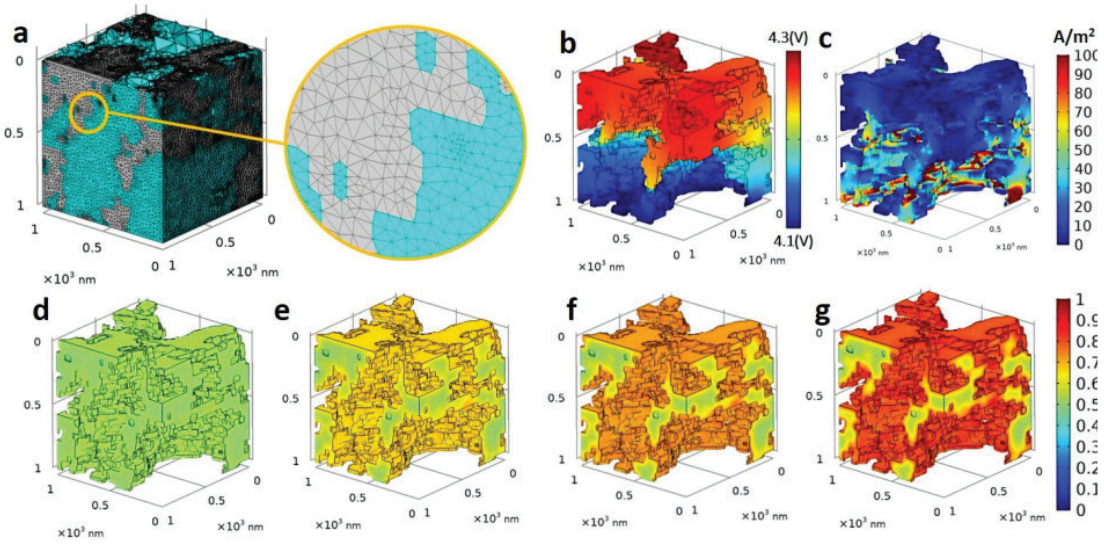
Performer	**Howard University**
Award Number	FE0032092
Project Duration	09/01/2021 – 08/31/2024
Total Project Value	$ 399,935
Technology Area	University Training and Research

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.

The Institute for the Design of Advanced Energy Systems (IDAES)

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022423
Project Duration	01/01/2018 – 3/31/2023
Total Project Value	$ 6,783,221
Collaborator	Carnegie Mellon University; Lawrence Berkeley National Laboratory; Notre Dame; Sandia National Laboratories; West Virginia University
Technology Area	Coal Utilization Science

The National Energy Technology Laboratory's Institute for the Design of Advanced Energy Systems (IDAES) was formed in 2016 to develop new advanced process systems engineering (PSE) capabilities to support the design and optimization of innovative new processes that go beyond current equipment/process constraints, including process intensification concepts and the optimization of materials and material properties. The IDAES framework leverages advances in computing hardware and algorithms to move from modeling and simulation to one of modeling and optimization. These capabilities are applied to improve the efficiency and reliability of the existing fleet of coal-fired power plants while accelerating the development of a broad range of advanced fossil energy systems by enabling their large-scale optimization.

The open-source IDAES PSE framework addresses the capability gap between state-of-the-art simulation packages and general algebraic modeling languages (AMLs) by integrating an extensible, equation-oriented process model library within the open-source, Department of Energy (DOE)-funded Pyomo AML, which addresses challenges in formulating, manipulating, and solving large, complex, structured optimization problems.

The IDAES framework includes tools for (1) process synthesis and conceptual design, including process intensification, (2) process design and optimization, including process integration, (3) process control and dynamic optimization, (4) use of advanced solvers and computer architectures, (5) automated development of thermodynamic, physical property, and kinetic submodels from experimental data, (6) integration of multi-scale models, (7) comprehensive, end-to-end uncertainty quantification, including stochastic optimization, (8) maintenance of complete provenance information, and (9) the ability to support multiple scales, from materials to process to market.

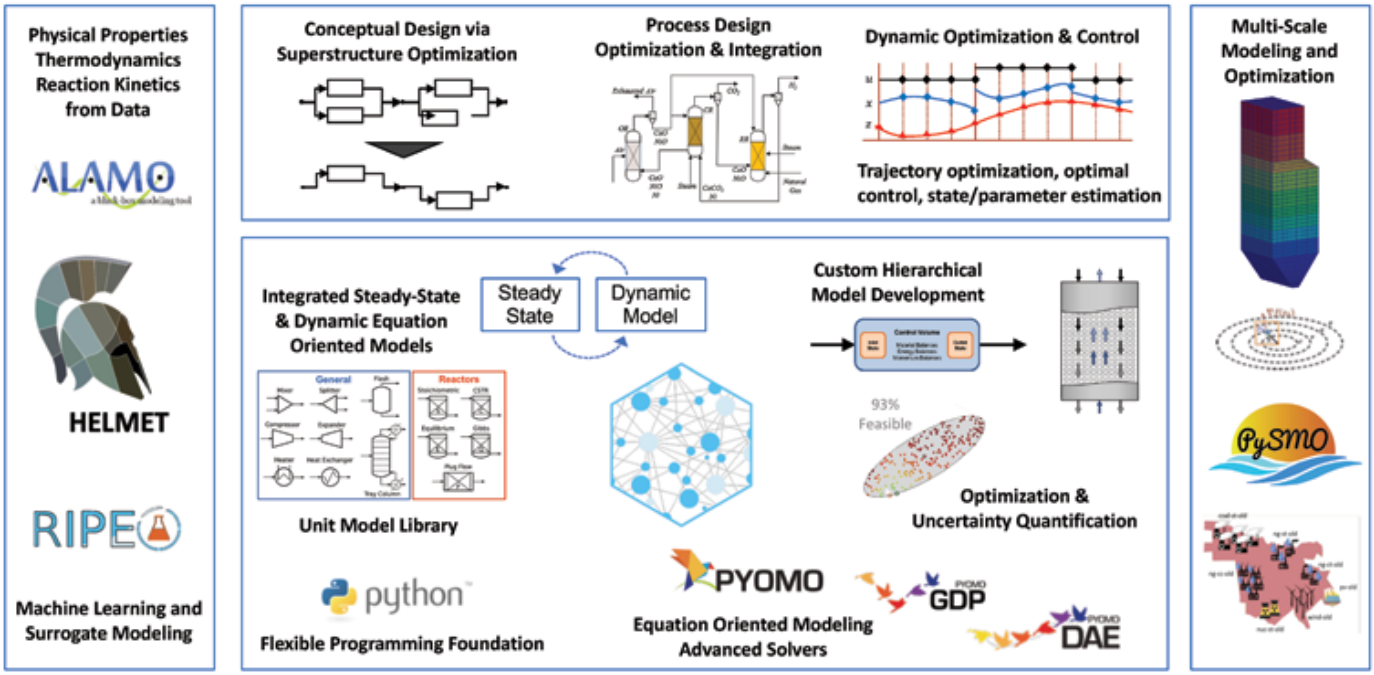
During EY 2021, the IDAES team plans to achieve the following milestones:

- Public release of general-purpose dynamic power plant modeling library along with example flowsheets.
- Demonstrate expanded market-based nonlinear model predictive control to evaluate fuel cost, revenue opportunities, and equipment health impacts.
- Demonstrate software that, at minimum, generates highly usable daily reports of process anomalies in measured process variables.
- Demonstrate conceptual design workflow including surrogate model construction for property calculations.
- Validate dynamic models for Ohio State University's reactors using experimental data.
- Validate the multi-scale dynamic liquid-gas contactor model using plant data.
- Public release of IDAES process costing methodology, codes, and documentation.
- Complete the evaluation of a candidate power system design using the integrated market/operations rolling horizon simulation platform.
- Deploy enhanced usability features for IDAES, including IDE integration, flowsheet/data visualization, and data management enhancements for data reconciliation, parameter estimation, and validation.
- Demonstrate improved Pyomo solver interface to support the efficient, scalable repeated solution of linear and nonlinear IDAES models.
- Conduct user workshops and tutorials.

IDAES

Institute for the Design of Advanced Energy Systems

NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Sandia National Laboratories · Carnegie Mellon University · West Virginia University · UNIVERSITY OF NOTRE DAME · U.S. DEPARTMENT OF ENERGY



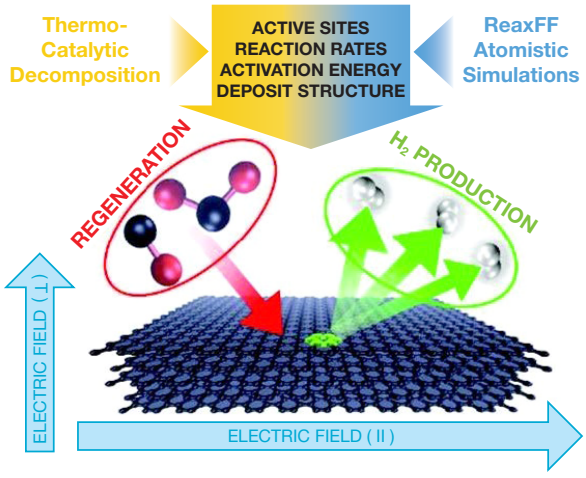
Electric Field Assisted Thermo-Catalytic Decomposition: Comparisons with Reaxff Atomistic Simulations

Performer	**Pennsylvania State University**
Award Number	FE0032070
Project Duration	08/01/2021 – 07/31/2024
Total Project Value	$ 399,435
Technology Area	University Training and Research

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_20 (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.

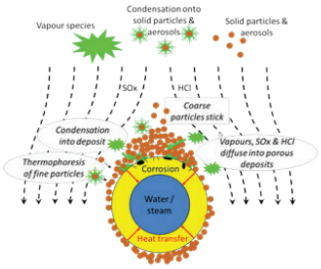
Component Level Modeling of Materials Degradation for Insights into Operational Flexibility of Existing Coal Power Plants

Performer	Siemens Corporation
Award Number	FE0031831
Project Duration	10/15/2019 – 10/14/2022
Total Project Value	$ 952,815
Collaborator	Cranfield University
Technology Area	Coal Utilization Science

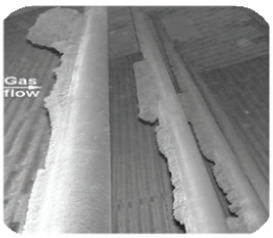
Siemens will develop a computational fluid dynamics/finite element (CFD/FE) modeling toolkit for component-level models of the boilers and low-pressure steam turbines in coal power plants that can tackle multidisciplinary failure mechanisms occurring concurrently for extreme environment materials. The research objective is to develop a component-level modeling toolkit for materials-based degradation for two key mechanisms that can accelerate with cyclic operations. This includes the fireside corrosion, steam oxidation, erosion, creep, and fatigue of superheaters/reheaters and steam pipework, and water droplet erosion and fatigue of last-stage steam turbine blade degradation mechanisms.

The lifetime assessment model will be validated using data gleaned from destructive analysis. The validated model can be extrapolated to coal/fossil plants with similar environmental conditions and failure mechanisms to enable these plants to operate for longer periods of time under flexible load conditions, and the model can also be extended to combined-cycle power plants.

Boilers/Heat Exchangers

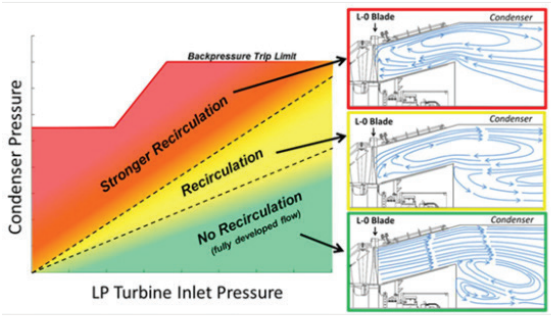


Fouling in heat exchangers

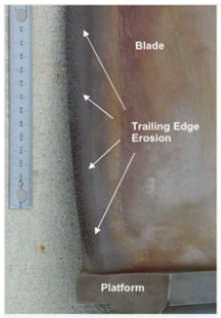


Deposit on real superheater tubes

Steam Turbines



Steam exhaust recirculation causing erosion and cracking



Eroded trailing edge of last row blade

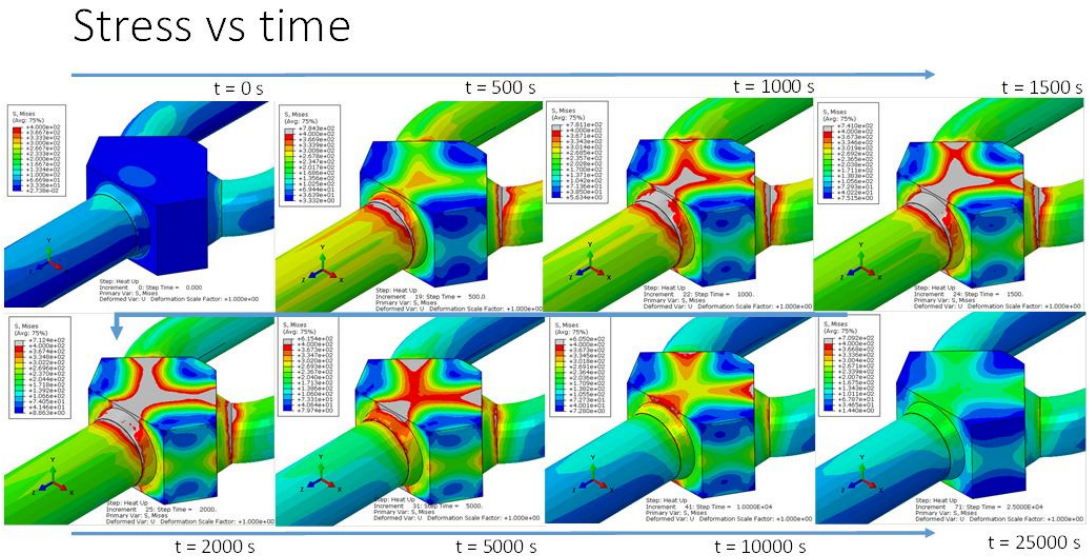
Life Modelling of Critical Steam Cycle Components in Coal-Fueled Power Plants

Performer	**Southern Research Institute**
Award Number	FE0031811
Project Duration	10/01/2019 – 09/30/2022
Total Project Value	$ 862,345
Technology Area	Coal Utilization Science

The objective of this work is to calibrate an existing damage accumulation and component life model to a high-pressure turbine disk/rotor alloy (used in a steam-cycle turbine of a coal-fueled plant) and a steam cycle Y-block alloy. The component life model accounts for coupled thermomechanical damage accumulation, material microstructural evolution, and material/component erosion/corrosion damage to determine component life predictions. The damage accumulation model, complete with lifetime prediction capabilities, will be implemented in Microsoft Excel or MATLAB format, and will only require input data (inelastic strain, hydrostatic stress, temperature-time waveforms, initial microstructure, etc.) from a component-specific finite element analysis to predict component lifetime. The modelling tool will then enable lifetime prediction as a function of historical plant steam cycle operational data as well as any potential proposed future operational cycling.

Activities proposed as part of this work include material testing and characterization, damage accumulation and component model calibration and verification, and component life model implementation within a user-friendly format (Microsoft Excel or MATLAB).

This project proposes to calibrate an existing environmental-fatigue life model to the metals and operational conditions found in the steam cycle of coal-fired power plants. The existing physics-based life model has the ability to predict cycles to failure as a function of varying mechanical load/load rates/load waveforms, varying temperature, and metal microstructural evolution. The successful completion of this work will provide coal-fired power plant engineers and operators with a tool to perform component-specific safe-life and retirement-for-a-cause analysis as a function of actual operating conditions, thereby mitigating failure induced component downtime.

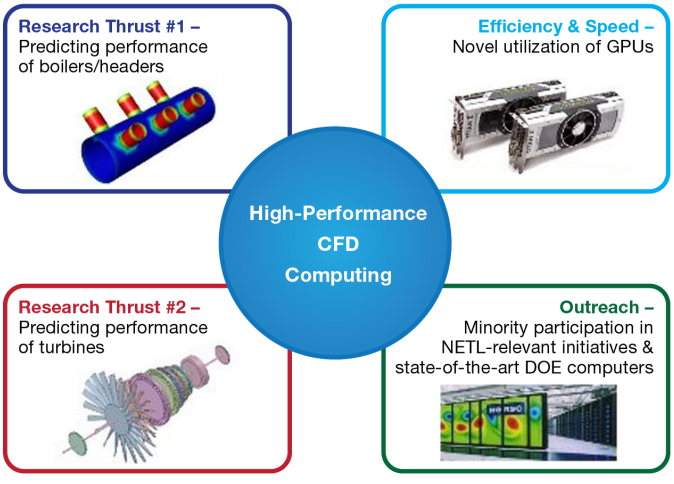


Probing Particle Impingement in Boilers and Steam Turbines Using High-Performance Computing with Parallel and Graphical Processing Units

Performer	**University of California–Riverside**
Award Number	FE0031746
Project Duration	09/01/2019 – 08/31/2022
Total Project Value	$ 400,000
Technology Area	University Training and Research

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 computational fluid dynamics (CFD) ANSYS Fluent 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 advantage 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.



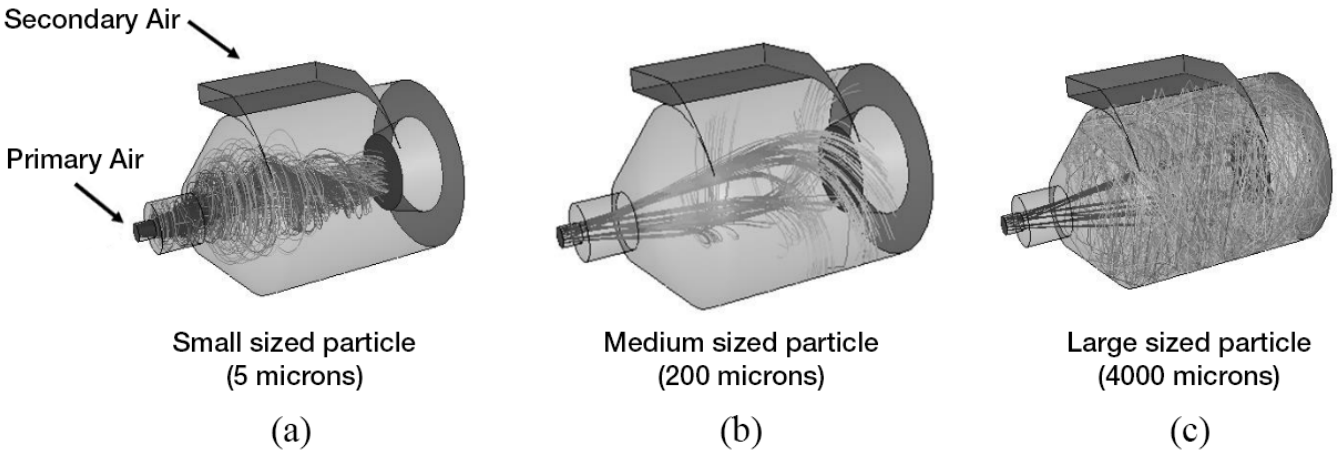
High-performance CFD computing forms a central theme and unifies research thrusts, efficiency, outreach, and technological impact in this HBCU-OMI project.

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
Collaborator	Microbeam Technologies, Inc.
Technology Area	University Training and Research

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.

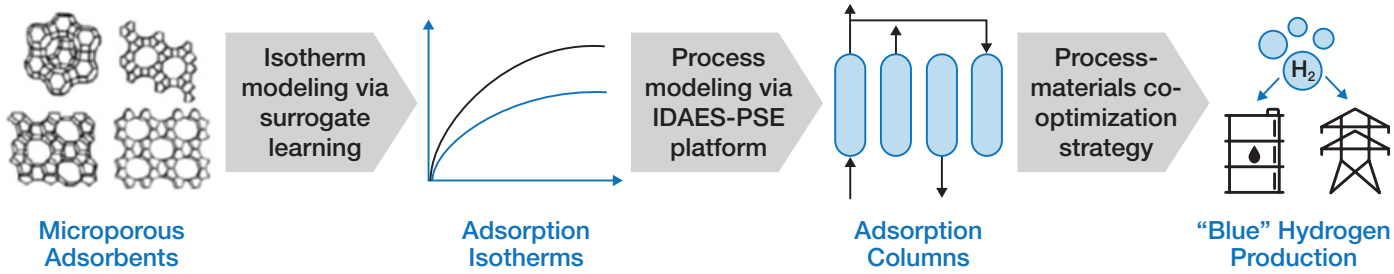
COMPUTATIONAL MATERIALS DESIGN

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
Technology Area	Coal Utilization Science

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.

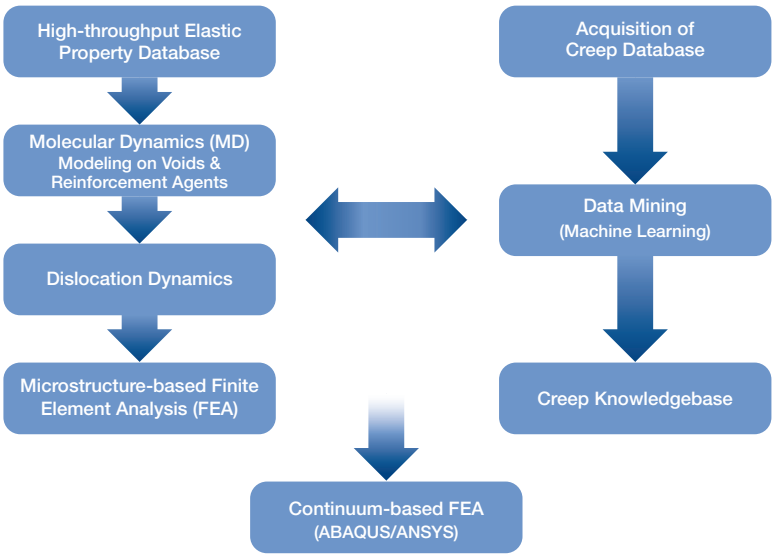


Multi-modal Approach to Modeling Creep Deformation in Ni-Base Superalloys

Performer	**Missouri State University**
Award Number	FE0031554
Project Duration	12/15/2017 – 03/31/2022
Total Project Value	$ 918,370
Collaborators	Missouri University of Science and Technology; University of Missouri–Kansas City
Technology Area	Plant Optimization Technologies

NETL partnered with Missouri State University to develop a new multi-modal approach to modeling of creep deformation in nickel-base superalloys. The approach is based on a two-pronged strategy combining a bottom-up, multi-scale, physically based modeling approach and a data-mining-driven top-down approach, backed by experimental database and correlation connectivity with strength augmented by data mining/machine learning protocols. The overarching goal is to integrate these two strategies to create quantitatively better predictive creep models that are not only sensitive to the microstructural evolution during various stages of creep, but also based on physically sound creep modeling that judiciously encompasses the strength of each modeling scale and provides a more comprehensive creep deformation analysis via finite element analysis.

The main advantage of the project's approach is to establish a new framework within which the adaptation of data mining tools for predicting the creep property of nickel-base alloys can be accelerated using a rigorous step-by-step atomistic-mesoscale continuum-based simulation. This approach will reduce the level of uncertainty of experimental creep data and facilitate a better linkage between the experimentally acquired creep data and the creep models that are established through the hierarchical multi-scale modeling. Ultimately, it will provide better diagnostics on the slow progression of creep deformation and will help to improve the quantitative predictive capability for the onset of creep failure during the tertiary creep stage. The approach can also be applied to a wider range of material candidates for fossil energy power plants.



Schematics of overall multi-modal workflow of proposed new roadmap to integrate the use of experimental creep database ("top-down" approach) with multi-scale modeling ("bottom-up" approach).

eXtremeMAT: Extreme Environment Materials

Performer	National Energy Technology Laboratory	Ames National Laboratory	Idaho National Laboratory	Lawrence Livermore National Laboratory	Los Alamos National Laboratory	Oak Ridge National Laboratory	Pacific Northwest National Laboratory
Award Number	FWP-1022433	FWP-AL-17-510-091	FWP-B000-17016	FWP-FEW0234	FWP-FE-850-17-FY17	FWP-FEAA134	FWP-71133
Project Duration	10/01/2018 – 09/30/2022	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020	10/01/2018 – 09/30/2020
Total Project Value	$ 2,496,921	$ 981,000	$ 628,000	$ 590,000	$ 2,063,000	$ 1,604,000	$ 1,090,000
Total Project Value (All)	$ 9,452,921						
Technology Area	Coal Utilization Science						

Affordable, durable, heat-resistant alloys are necessary for improving the existing fleet of fossil energy power plants and enabling advanced fossil energy systems such as advanced ultra-supercritical steam cycles and supercritical carbon dioxide (sCO_2) power cycles. Advanced alloys will continue to be needed for fossil energy plants of the future, flexible plants operating cyclically, as needed, at temperatures in excess of 700 °C (approaching 800 °C), and under complex mechanical loading conditions in harsh oxidizing environments for lifetimes exceeding 100,000 hours (12 years). Accelerating the development of improved steels, superalloys, and other advanced alloys is of paramount importance in deploying materials solutions to meet the challenges facing fossil energy power generation.

The eXtremeMAT collaboration brings together leading national laboratories to harness the unparalleled breadth of unique capabilities across the DOE complex associated with materials design, high-performance materials computing, data science and analytics, manufacturing process development, basic and advanced materials characterization, and life cycle performance assessment into an integrated, mission-focused team in order to revolutionize alloy development for fossil energy applications. Specifically, the collaboration intends to:

- develop a suite of improved heat-resistant alloys for fossil energy components in existing and future power plants.
- improve models to predict long-term materials performance in existing and future fossil energy power cycles.

eXtremeMAT will achieve these goals by developing advanced physics-based, multi-scale computational models and simulations with machine learning approaches to more accurately predict performance under realistic service conditions. The technology breakthrough lies in the ability of these tailor-made models to predict the influence of initial microstructure on microstructural evolution and performance during component service. This approach constitutes a significant departure from existing empirically driven lifetime standards in which accuracy and sensitivity to microstructure and complex non-monotonic and non-uniaxial loading is either limited or altogether absent.

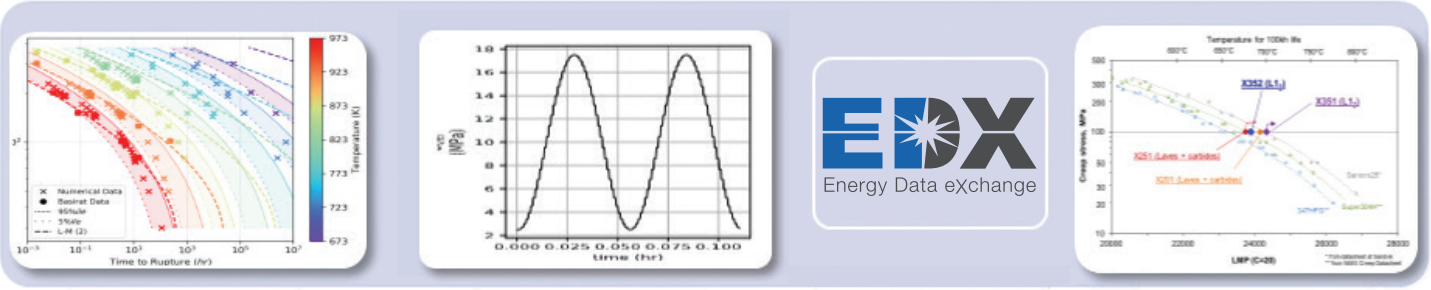
Over the last two years, eXtremeMAT has made significant progress on achieving its goals as follows:

- A suite of eXtremeMAT models was developed to predict creep rupture life using a minimum of short-term creep tests. This model has been extended to multi-axial stresses and cyclic loading (i.e., ratcheting) conditions.
- A platform (database) is in place (on the NETL EDX site) to curate experimental and simulated data and metadata required for material data analytics in expediting design and development, as well as, material property life prediction.
- eXtremeMAT has accelerated the design of an alumina-forming alloy (AFA) with exceptional creep life compared to existing commercial alloys, e.g. 347H, Super 304H, and Sanicro25.

eXtremeMAT will demonstrate and deliver by end of project (September 30, 2023):

- **Alloy Lifetime Predictor: A mechanistically based (i.e.,** physics and microstructure derived) multi-axial lifetime model for 347H and P91 steels. This model and its life prediction aspects will incorporate the complexities of stress loading, temperature, and microstructure.
- **Engineering Scale Lifetime Predictor:** A reduced order model for 347H stainless steel that can be implemented into commercial finite element codes. The tool will predict the performance lifetime of steel components subjected to multi-axial and cyclical loading and temperature in high-temperature steam environments, including mechanical and oxide spallation failure mechanisms.
- **Materials Database and Analysis Tools:** A curated database of experimental and simulation data for FE materials of interest. eXtremeMAT will also develop and demonstrate algorithms for automated detection of features in alloy microstructures that change with time, which can be used to predict how long a component may survive under differential operating conditions.
- **Accelerated Discovery of Alloys:** Demonstrate AFA stainless steels developed through the eXtremeMAT framework.

For more information visit the eXtremeMAT website at: https://edx.netl.doe.gov/extrememat/



Material lifetime and performance predictors

Component lifetime and preformance predictors

Materials database and analysis tools

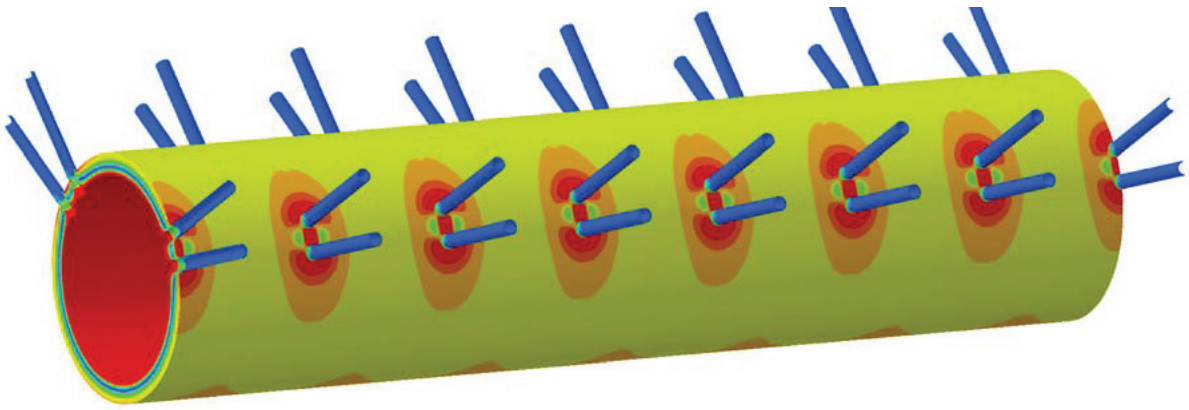
Rapid discovery of new alumina forming alloys

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
Collaborator	University of North Carolina Charlotte
Technology Area	University Training and Research

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.



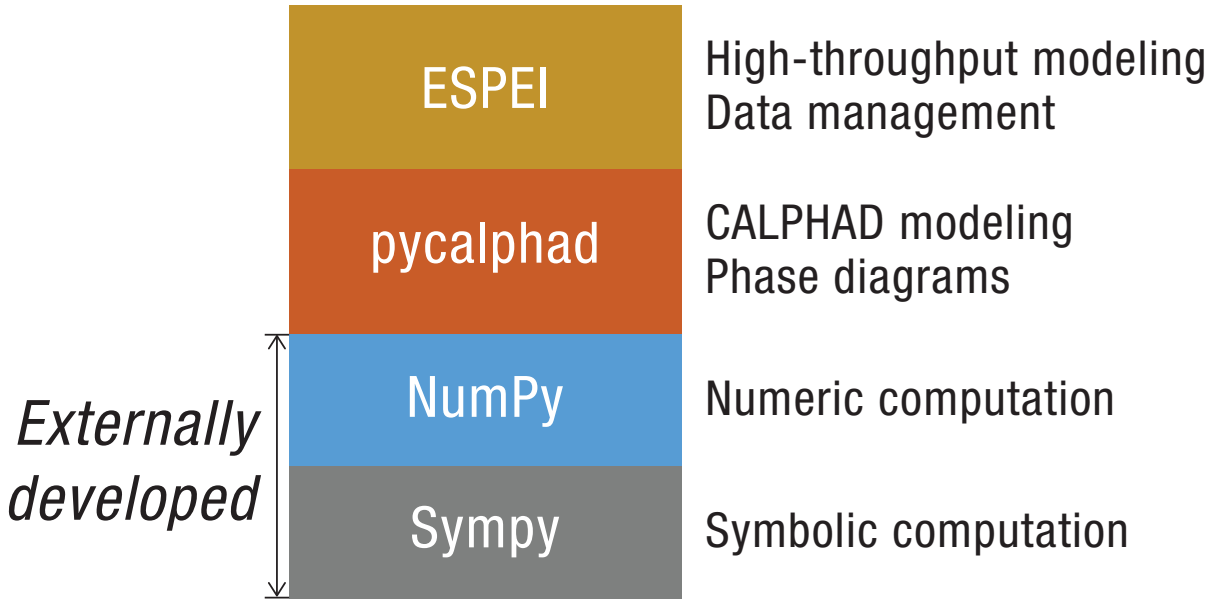
Stress contour plot of a steam header.

High Throughput Computational Framework of Materials Properties for Extreme Environments

Performer	**Pennsylvania State University**
Award Number	FE0031553
Project Duration	12/15/2017 – 08/31/2022
Total Project Value	$ 937,836
Technology Area	Plant Optimization Technologies

NETL is partnering with Pennsylvania State University to establish a framework capable of efficiently predicting the properties of structural materials for service in harsh environments over a wide range of temperatures and long periods of time. The approach will be to develop and integrate high-throughput first-principles calculations based on density functional theory in combination with machine learning methods, perform high-throughput calculation of phase diagrams (CALPHAD) modeling, and carry out finite-element method simulations. In regard to high-temperature service in fossil power systems, nickel-based superalloys Inconel 740 and Haynes 282 will be investigated.

The framework has the potential to enable high-throughput computation of tensile properties of multi-component alloys at elevated temperatures, resulting in significant reduction in computational time needed by the state-of- the-art methods. Once successfully completed, the project will deliver an open-source framework for high-throughput computational design of multi-component materials under extreme environments. This framework will enable more rapid design of materials and offer the capability for further development of additional tools due to its open-source nature.



ESPEI-2.0 software stack.

Integrated Computational Materials and Mechanical Modeling for Additive Manufacturing of Alloys with Graded Structure Used in Fossil Fuel Power Plants

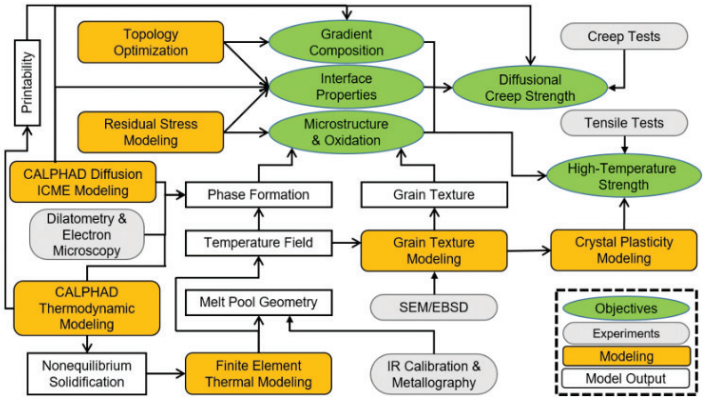
Performer	**University of Pittsburgh**
Award Number	FE0031637
Project Duration	11/01/2018 – 10/31/2021
Total Project Value	$ 937,500
Collaborator	United Technologies Research Center
Technology Area	Coal Utilization Science

University of Pittsburgh (Pitt) researchers developed an integrated computational materials engineering modeling framework through a combination of materials and mechanical models for relevant advanced ultra-supercritical components and materials processed by wire-arc additive manufacturing (WAAM). Physics-based process-structure-property models were developed to predict thermal history, melt pool geometry, phase stability, grain morphology/texture, high-temperature oxidation, tensile and creep strength, and residual stress. In addition to bulk properties for single materials, interfacial properties between two dissimilar alloys joined together were modeled and employed to design the compositional profile in the interfacial zone using phase transformation modeling and topology optimization techniques. All the models developed were validated by characterization experiments on both coupon and prototype samples, and their uncertainty were quantified via sensitivity analysis.

Development of a simulation tool that can predict the structure-property relationships of extreme environment materials for fossil energy infrastructure manufacturing could lead to a framework and manufacturing methods that can be used in other energy unit manufacturing, such as concentrated solar power plants and ultra-supercritical and supercritical boiler systems.

The developed model will support the joining of dissimilar alloys that are vitally important in the welding and joining industry; the manufacture of functionally graded alloys that are not limited to the fossil fuel energy infrastructure; and further development of an additive manufacturing technique for repairing critical fossil fuel energy generating components. Also, this project is expected to lead to the design and manufacture of superior alloy components with excellent creep-rupture strength and oxidation resistance at elevated temperatures as required for the efficient operation of fossil fuel power plants.

Overall, this effort demonstrated feasibility for additively manufactured materials suited for power generation applications. Several multi-material and gradient combinations were explored, including joints between P91 steel and Inconel 740H superalloy. This provided a method for integrating both materials in future designs, to improve both performance and cost.



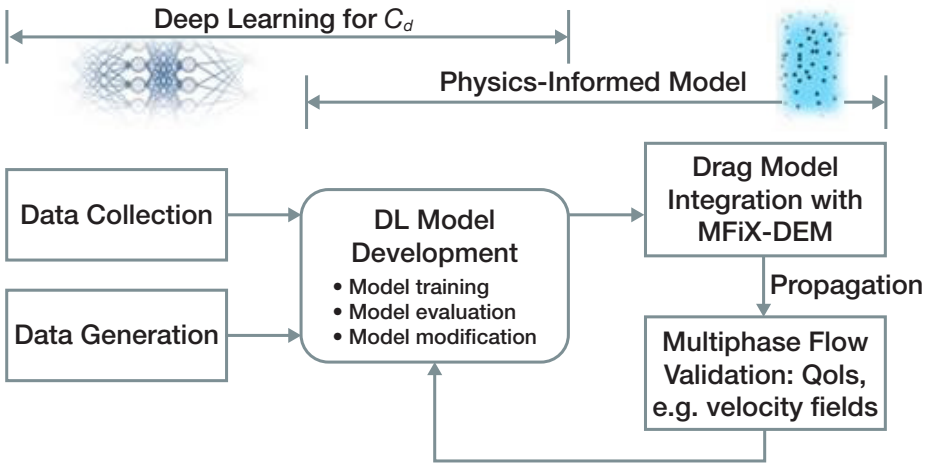
Integrated Computational Materials Engineering model framework for additive manufacturing of alloys with graded structure.

MULTIPHASE FLOW SCIENCE

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
Technology Area	University Training and Research

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. The research 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.

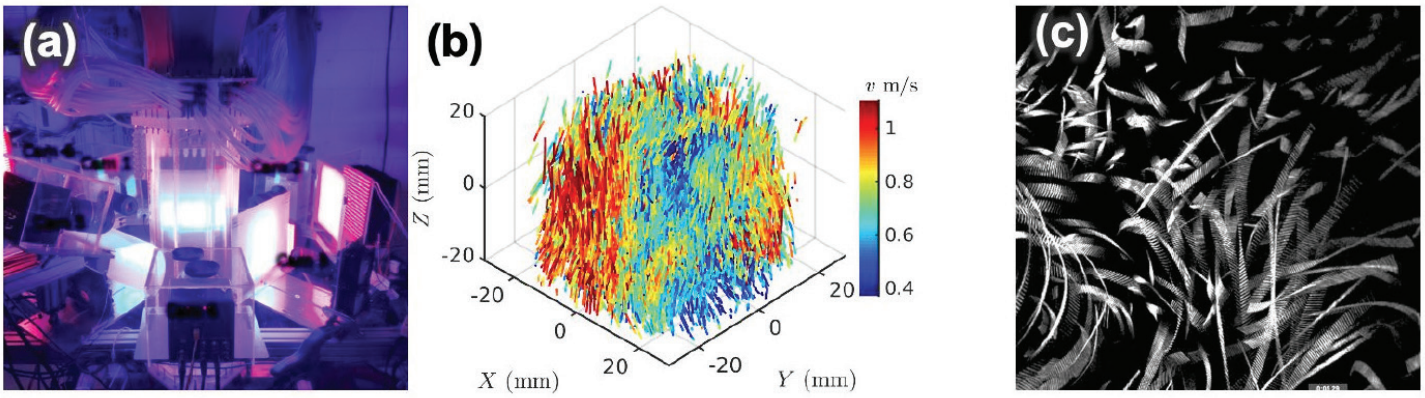


A physics-informed deep learning framework for a drag coefficient model.

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
Technology Area	University Training and Research

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.

Advanced Reaction Systems

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022405
Project Duration	04/01/2019 – 03/31/2023
Total Project Value	$ 6,485,000
Technology Area	Gasification Systems

Design and optimization of complex reactors for fossil energy applications is a challenging and expensive process. Understanding the performance of complex multiphase flow reactors used in fossil energy technology and having the means to impact their design early in the developmental process is important for two reasons. First, about 75 percent of the manufacturing cost of any product is committed at the conceptual design stage, even when the incurred cost might be very small. Once the conceptual design stage is completed, opportunities for cost savings are substantially diminished. Second, during innovative technology development, empirical scale-up information is not available because reactors at large scales have not been built. It is well known that traditional scale-up methods do not work well for multiphase flow reactors, such as the ones used for fossil energy applications. Given these challenges, computational models can be used to simulate the device and understand its performance before the design is finalized, which is important for reducing risk and cost. Science-based models are critical tools for reducing the cost and time required for development. The objectives of this work are to:

- Develop, validate, apply, publicly distribute, and support the Multiphase Flow with Interphase eXchanges (MFiX) suite, a multiphase flow software suite capable of modeling large-scale reactor systems that include chemical reactions and complex geometries. These modeling tools will support the design and optimization of novel reactor systems that will meet Advanced Reaction Systems (ARS) Field Work Proposal (FWP) and Office of Fossil Energy programmatic goals.
- Continue development and application of the Software Quality Assurance Program for the MFiX suite to ensure that the software provides physically accurate predictions. The Quality Assurance Program includes verification, validation, and uncertainty quantification processes and uses the capabilities of the multiphase flow analysis laboratory facilities for generation of high-quality validation data.

NETL researchers and the MFiX suite of codes provide the FECM program with required critical modeling capability. The MFiX suite includes the following set of complementary modeling tools that can be brought to bear on fossil energy technologies:

- *MFiX-TFM (Two-Fluid Model)*: An Eulerian-Eulerian code capable of dealing with the range of small-scale through industry-scale reacting simulations. It is presently the most mature code and includes a broad range of capabilities for dense reacting multiphase flow. The approximation of the solid phase as a continuum allows for faster simulation time but it also introduces the need for more complex model closures to accurately represent solid phase behavior. Development of faster and more accurate algorithms to accomplish this is one of the key research program objectives for this approach.
- *MFiX-DEM (Discrete Element Model)*: An Eulerian-Lagrangian code that treats the fluid phase as a continuum and models the individual particles of the solids. While the treatment of individual particles can provide higher fidelity over a broad range of flow regimes (from dilute to pack), it is also very challenging when dealing with very large numbers of particles for large-scale simulations. These large-scale applications require high-performance computing resources and substantial amounts of computer time. Therefore, code optimization and speed-up are critical research fronts to support industrial-scale applications.
- *MFiX-PIC (Particle-In-Cell)*: An Eulerian-Lagrangian code that treats the fluid phase as a continuum and models solids as discrete parcels of particles, with each parcel

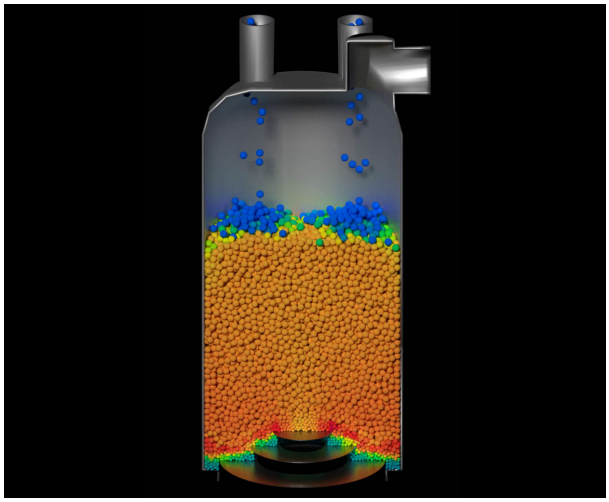
representing a group of real particles with the same physical characteristics. This is an emerging capability that will be brought to maturity for use in advanced reactor simulations in the proposed work. The MFiX-PIC approach greatly reduces the computational cost. However, modeling approximations are required for the PIC technique, which will affect accuracy. Development, validation, and optimization of these modeling approximations are critical research fronts.

In this research effort, NETL is providing an advanced suite of multiphase flow CFD models that enable the required capability. These models provide detailed predictions of reactor performance including temperature, velocities, chemical composition, reaction rates, and heat transfer for both fluid and solid phases in the reactors.

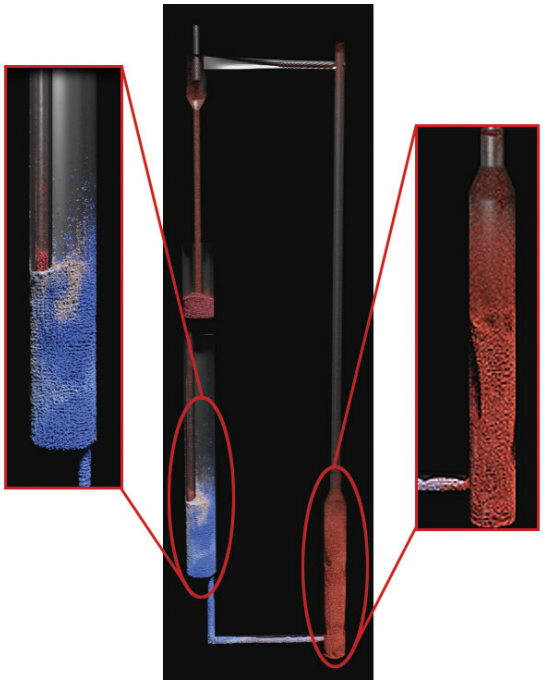
In contrast to expensive, proprietary CFD software, the MFiX suite and associated toolsets are open-source codes that are developed, validated, and supported in-house by NETL's software development and application specialists and can be customized for novel applications. The suite is available on NETL's Joule supercomputer, enabling advanced large-scale, challenging, computer-intensive applications. There are over 4,600 registered users of the MFiX suite and associated toolsets including industry, academic, and national laboratories. User applications span a broad range of topics including chemical process, energy conversion, and even volcanology. Members of the user group exchange information through support mailing lists which helps to ensure that code problems are found and addressed quickly.

Densely-loaded multiphase flows are very demanding applications for CFD codes. This is made even more challenging in this work due to the need to model chemical kinetics and heat transfer in very complex, reacting systems. The systems of interest can span laboratory-scale through pilot- and commercial-scale systems.

Multiphase flow CFD requires substantial amounts of computer time so the ability to perform simulations on supercomputing systems is mandatory for larger applications. These codes are quite complex in both quantity of code and complexity of the physics and numerical approaches to obtain a solution. A quality assurance program including systematic verification, validation, and uncertainty quantification is required to ensure integrity and acceptability of the model predictions. NETL has maintained a multiphase flow modeling program for over 30 years, starting from CFD in its infancy until the present day in which CFD has become a well- accepted tool for studying reacting flows. NETL's expertise in dense, reacting multiphase flow is unique and continues to be one of NETL's and FE-CM's key capabilities. In the past 5 years, there has been renewed emphasis on the expansion of the MFiX family of codes to include more accurate and capable modeling approaches, such as MFiX-DEM and MFiX-PIC.



MFiX-DEM simulation of coal gasification in a 1 megawatt moving bed gasifier.



MFIX-PIC simulation of a pilot-scale circulating fluid bed reactor.

CFD for Advanced Reactor Design (CARD)

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022463
Project Duration	04/01/2020 – 03/31/2023
Total Project Value	$ 2,643,000
Technology Area	Coal Utilization Science

The efforts of CFD for Advanced Reactor Design (CARD) continue the development, enhancement, and application of the suite of multiphase computational fluid dynamics (CFD) software tools based on the National Energy Technology Laboratory (NETL) Multiphase Flow with Interphase eXchange (MFiX) software suite that is used for design and analysis of novel reactors and devices for fossil energy applications.

Science-based models are critical tools for reducing the risk, cost, and time required for development of novel fossil energy reactors. In this research effort, NETL is providing an advanced suite of multiphase flow CFD models that enable this capability. These models provide detailed predictions of reactor performance including temperature, velocities, chemical composition, reaction rates, and heat transfer for both fluid and solid phases in the reactors.

In contrast to expensive, proprietary commercial CFD software, the MFiX Suite and associated toolsets are open source codes that are developed, validated, and supported in-house by NETL's software development and application specialists. These specialists are experts in application of CFD tools to FE technologies. As an open source code, the MFiX Suite can be customized for novel applications. The MFiX Suite is available on NETL's Joule 2.0 supercomputer, enabling advanced, large-scale, challenging, computer-intensive applications. There are over 5,600 registered users of the MFiX Suite and associated toolsets including industry, academic, and national laboratories.

The CARD portfolio pursues the following primary tasks:

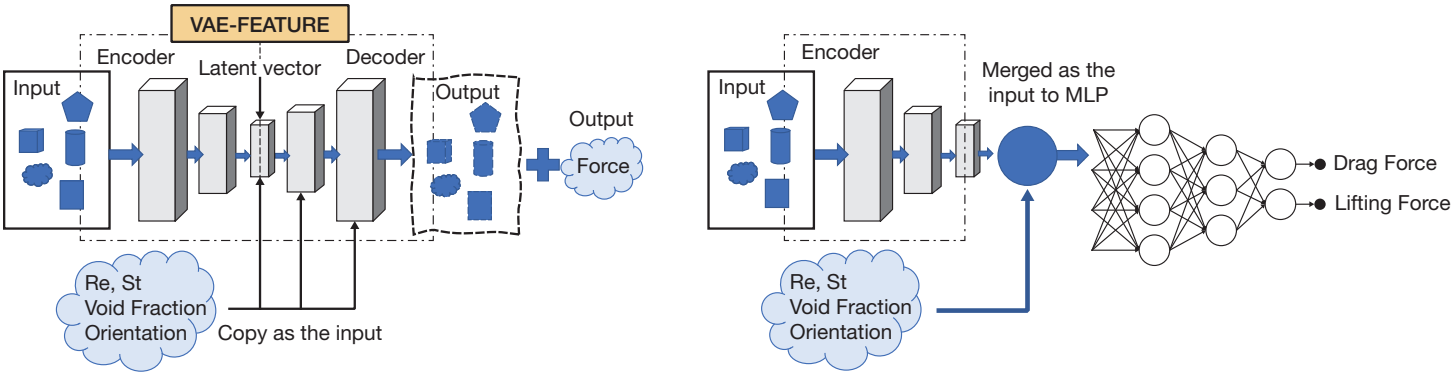
- Develop, validate, apply, publicly distribute, and support the MFiX Suite of multiphase flow modeling software capable of modeling large-scale, reactor systems that include complex chemical reactions and realistic geometry to support the design and optimization of novel reactor systems supporting DOE FECM's programmatic goals.
- In collaboration with industry partners, apply computational tools and FECM/NETL supercomputing resources to aid in understanding and optimizing circulating fluidized bed boiler performance under challenging operating conditions of interest to operators.
- Google's TensorFlow™ software library will be linked to NETL's MFiX and the solvers will be written in TensorFlow to achieve significant code acceleration on the latest hardware.

This work is focused on building the ability to optimize a reactor based on reaction chemistry, reactor flows, and/or reactor geometries to ensure a valuable product is delivered to the U.S. taxpayer. The modeling tools are also made available to industry and academic stakeholders as part of the publicly available MFiX Suite of codes that are provided through NETL's Multiphase Flow Science web portal (https://mfix.netl.doe.gov).

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
Technology Area	University Training and Research

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.



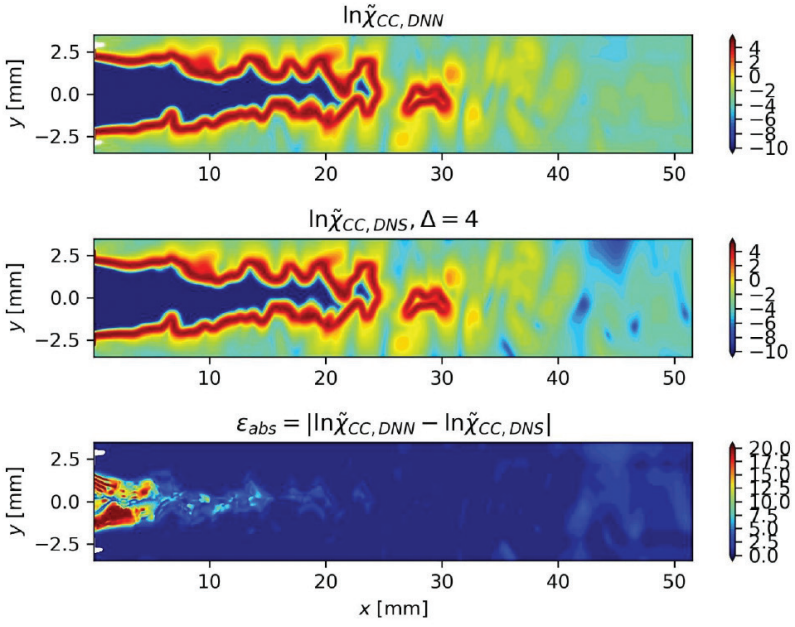
Variational auto-encoder (VAE) will be utilized to extract the primitive geometrical factors of a non-spherical particles. A multi-layer perceptron (MLP) will then be supplied as a regressor for both the drag and lifting force of the non-spherical particles.

Adaptive Depth Neural Networks for Scale-Bridging Modeling of Multiphase Reacting Flows

Performer	**Pennsylvania State University**
Award Number	FE0026825-06-01
Project Duration	02/01/2021 – 01/31/2023
Total Project Value	$290,000
Technology Area	University Training and Research

The overarching goal of this research program is to develop a general automated databased framework for scale-bridging modeling between full-fidelity simulations and coarse-grained simulations. The framework will be developed within the specific context of multiphase reacting flows bridging the Discrete Element Model (DEM) to develop data-based closure models for the filtered Two-Fluid Model (TFM). The novel data-based modeling framework consists of three distinct components: (1) automatic identification of model inputs based on optimal estimator analysis; (2) automatic design of just-deep-enough neural network topologies termed Adaptive Depth Neural Networks (ADNN) to avoid underfitting yet prevent overfitting; and (3) three distinct strategies for imposing physical constraints on data-based models including careful selection of inputs and outputs, "shielding" quantities of interest by instead modeling terms in their transport equations, and direct integration of "physics" hidden layers into neural networks.

As part of the MFiX and Nodeworks suite of tools, the data-based scale-bridging modeling approach will be immediately available to stakeholders in numerous commercial sections including fossil energy where multiphase reacting flows represent key scientific and technological challenges. Looking more broadly, the data-based scale-bridging modeling framework could also be integrated into other computational simulation and modeling workflows in virtually any domain.

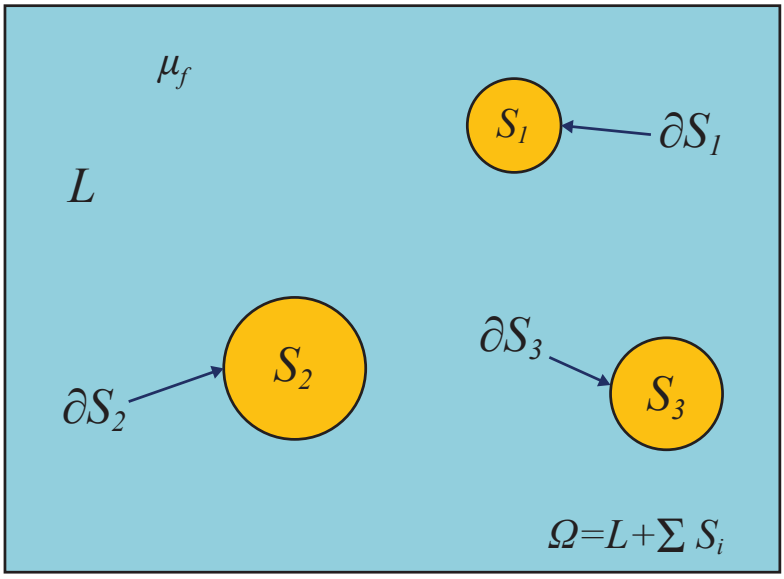


Models of Multiphase Reacting Flows.

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
Technology Area	University Training and Research

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.

ABBREVIATIONS

ADNN ..... adaptive depth neural networks

AL ..... aluminum

AM ..... additive manufacturing

AML ..... algebraic modeling language

ANN ..... artificial neural network

ARS ..... Advanced Reaction Systems

AUSC ..... advanced ultra-supercritical

CALPHAD ..... calculation of phase diagrams

CARD ..... CFD for Advanced Reactor Design

CFB ..... circulating fluidized bed

CFD ..... computational fluid dynamics

CO_2 ..... carbon dioxide

Co ..... cobalt

Cr ..... chromium

CSE ..... creep strength enhanced

DEM ..... discrete element model

DOE ..... Department of Energy

E ..... electric

ESPEI ..... extensible self-optimizing phase equilibrium infrastructure

FE ..... finite element

Fe ..... iron

FECM ..... Office of Fossil Energy & Carbon Management

FWP ..... Field Work Proposal

FY ..... fiscal year

GPU ..... graphics processing unit

HBCU-OMI ..... Historically Black Colleges and Universities -Other Minority Institutions

HYPER ..... Hybrid Performance

ICME ..... integrated computational materials engineering

IDAES ..... Institute for the Design of Advanced Energy Systems

IN ..... Inconel

INL ..... Idaho National Laboratory

MFiX ..... Multiphase Flow with Interphase Exchanges

MFS ..... Multiphase Flow Science

Mn ..... manganese

MTI ..... Microbeam Technologies Incorporated

MWth ..... megawatt thermal

NETL ..... National Energy Technology Laboratory

Ni ..... nickel

OTP ..... Otter Tail Power

PIC ..... particle-in-cell

Pitt ..... University of Pittsburgh

PR-DNS ..... particle-resolved direct numerical simulation

PSE ..... process systems engineering

R&D ..... research and development

sCO_2 ..... supercritical carbon dioxide

TCD ..... Thermo-catalytic decomposition

TFM ..... Two-Fluid Model

UCR ..... University Coal Research

UND ..... University of North Dakota

UNDEERC ..... University of North Dakota Energy and Environmental Research Center

VAE ..... variational auto-encoder

WAAM ..... wire-arc additive manufacturing

NOTES

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https://netl.doe.gov/onsite-research/computational

https://netl.doe.gov/carbon-management/crosscutting

https://MFiX.netl.doe.gov/

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