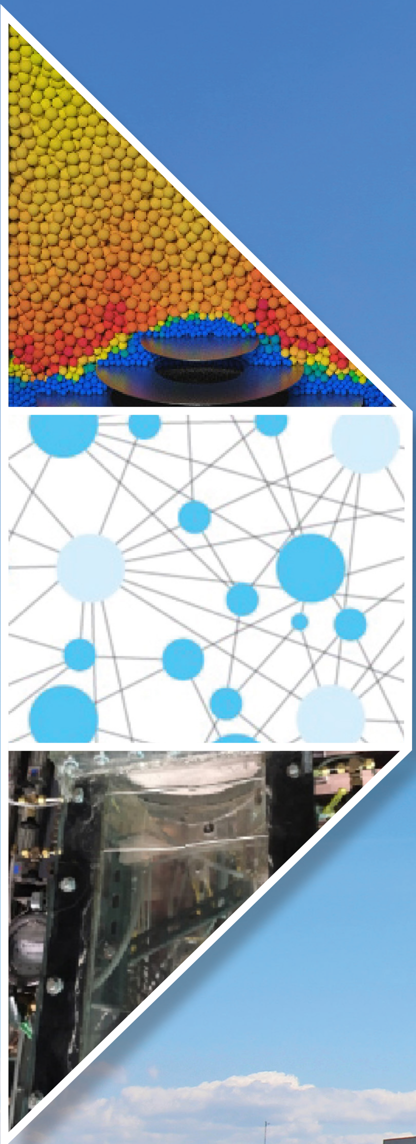
CROSSCUTTING RESEARCH

SIMULATION-BASED ENGINEERING PROJECT PORTFOLIO 2021



U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

DISCLAIMER

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INTRODUCTION

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 six primary research areas: High Performance Materials; Sensors, Controls, and Novel Concepts; Simulation-Based Engineering; Water Management; 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 improves fossil energy power generation with sensors, distributed intelligent control systems, and increased security. Advanced sensors and controls provide pivotal insights into optimization of plant performance and increasing plant reliability and availability. NETL tests and matures novel sensor and control systems that are operable in power plants and capable of real-time measurements and that can improve overall plant efficiencies and allow for more effective ramp rates. Given the crosscutting nature of sensors and controls, these technologies will benefit power plants across the spectrum of fossil generation and other harsh-environment applications.

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, Robotics-based Inspection, Advanced Controls and Cyber Physical Systems (Distributed Intelligent Controls), and Cybersecurity/Blockchain.

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.

Water Management: Water Management addresses competing water needs and challenges through a series of dynamic and complex models and analysis that are essential in informing and deciding between priority technology R&D initiatives. The program encompasses the need to minimize any potential impacts of power plant operations on water quality and availability. Analyzing and exploring plant efficiency opportunities can reduce the amount of water required for fossil energy operations.

New water treatment technologies that economically derive clean water from alternative sources will allow greater recycling of water within energy extraction and conversion as well as carbon storage processes. This helps reduce the amount of total water demand within fossil energy generation.

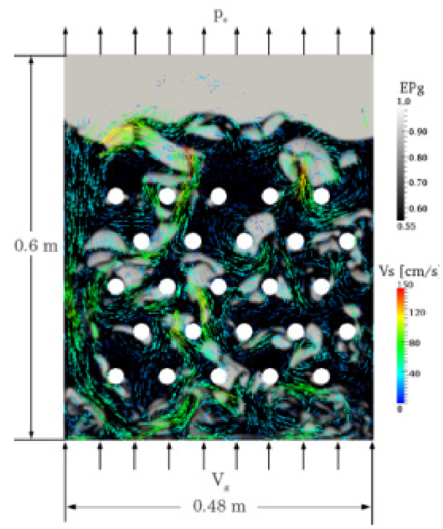
The program leads a critical national effort directed at removing barriers to sustainable, efficient water and energy use; developing technology solutions; and enhancing the understanding of the intimate relationship between energy and water resources. Water Management R&D focuses its research in three chief areas: increasing water efficiency and reuse, treatment of alternative sources of water, and energy-water analysis. These research areas encompass the need to minimize potential impacts on water quality and availability.

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.

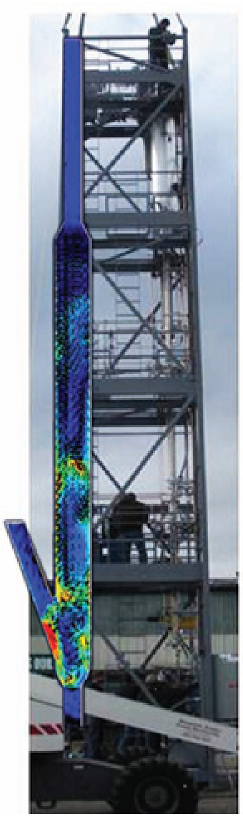
University Training and Research: University Training and Research supports two of the longest-running university training programs, the Historically Black Colleges and Universities and Other Minority Institutions (HBCU-OMI) and the University Coal Research (UCR) programs, to support the education of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

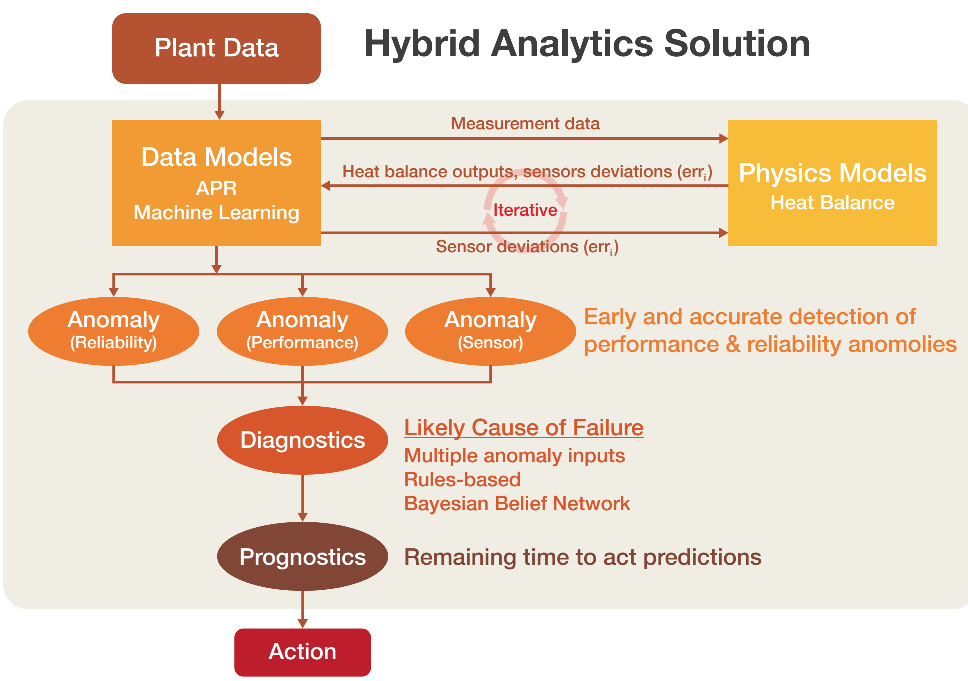
Simulation-Based Engineering personnel work closely with stakeholders and partners to outline issues, emerging trends, and areas of need. NETL has sponsored multiphase flow workshops annually to bring together industry and academia to identify R&D priorities and ensure that key technologies will be available 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

Hybrid Analytics Solution to Improve Coal Power Plant Operations

Performer	**Expert Microsystems, Inc.**
Award Number	FE0031753
Project Duration	10/01/2019 – 09/30/2021
Total Project Value	$ 989,616
Collaborator	MapEx Software, Inc.; XMPLR Energy LLC
Technology Area	Plant Optimization Technologies

The goal of this project is to develop, demonstrate and commercialize a new real-time monitoring approach, the Hybrid Analytics Solution, to improve coal plant operations. This hybrid analytics software tool will provide real-time information on the relationship between plant operational data (such as measured temperatures, pressures, and flow rates) and plant performance and reliability. The hybrid analytics solution will integrate machine-learning-based data analytics with thermal analysis in a manner that enables increased accuracy and scope of the thermal analysis, resulting in improved ability of the data analytics to monitor changes affecting plant operations. The anticipated outcome of this project will be a plant monitoring and modeling system that will be able to recognize patterns of operation involving the fuel composition, excess oxygen, measured gas temperatures, air leakages, tube bank metal temperatures and heat transfer rates, steam/water temperatures, and boiler efficiency. With the hybrid analytics solution, operators will be able to understand these patterns to find "sweet spots" where plant performance is optimized and to optimize control strategies for flexible plant operation.



The data analytics and heat balance analysis exchange information as part of the data-driven advanced pattern recognition analysis.

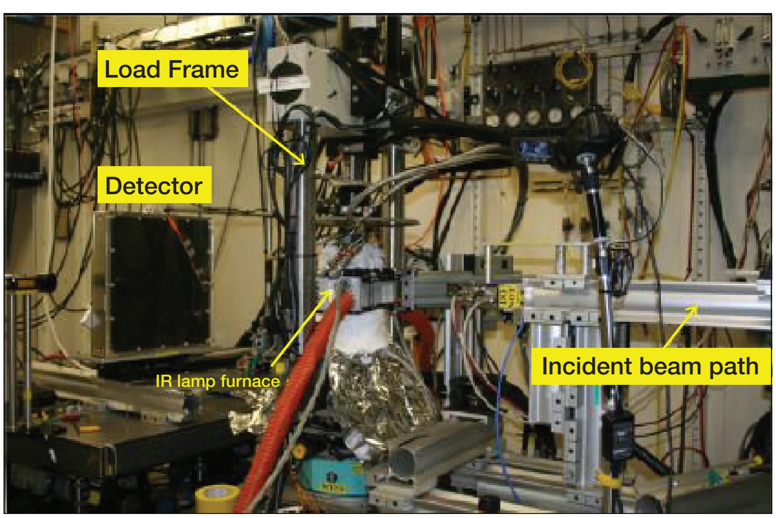
Damage Accumulations Predictions for Boiler Components Via Macrostructurally Informed Material Models

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.

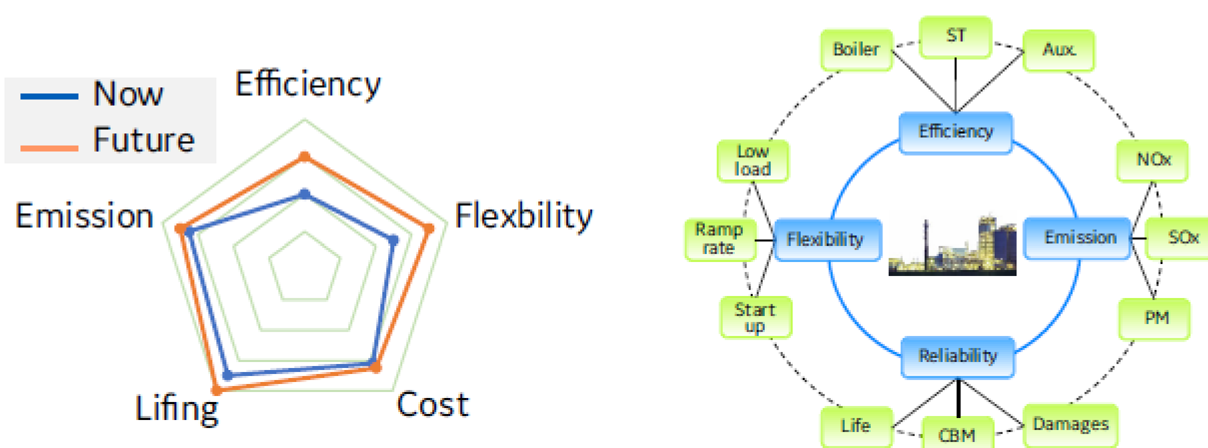
Investigation of Cycling Coal Fired Power Plants Using High-Fidelity Models

Performer	**General Electric (GE) Company**
Award Number	FE0031822
Project Duration	10/01/2019 – 03/31/2021
Total Project Value	$ 937,429
Technology Area	Coal Utilization Science

Using General Electric (GE) Company's existing process models (both transient and steady state) and mechanical integrity models, an integrated high-fidelity simulation platform was built to enable critical component analysis. An automated data processing and model calibration tool was developed to allow easy adaption of the models built under this program to other units, thereby saving future engineering project costs. An economics model was developed and integrated to evaluate the financial impact of cycling operations in coal power plants. Using the integrated simulation platform, analytical results and insights into existing coal-fired power plant challenges impacted by cycling operations were generated. The primary focus of this program was the critical component analysis of the drums and headers in the boiler island for a representative subcritical coal-fired power plant.

A representative plant between 200 and 600 MW was investigated. Results obtained from the investigation will be applicable to multiple units with close megawatt scales and similar plant configurations. Model-based analyses will be performed for critical components to determine plausible damage and remedial solutions.

The analyses will reveal valuable information about how existing coal power plants are impacted by cycling operations and could lead to development of practical and cost-effective solutions to reducing plant failures due to cycling, thereby extending plant life. A potential benefit is the development of a requirement and specification document that will serve as a new industrial standard process that can be used by the entire U.S. coal fleet.

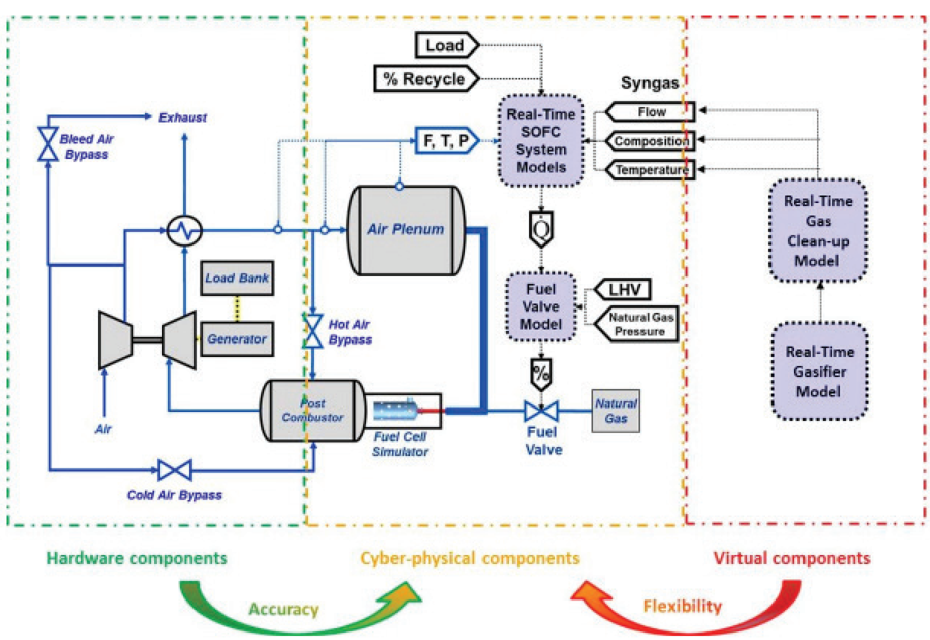


Multi-dimensional analysis for critical components.

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

Performer	Georgia Tech Research Corporation
Award Number	FE0030600
Project Duration	08/01/2017 – 07/31/2021
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.

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 – 3/31/2022
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.

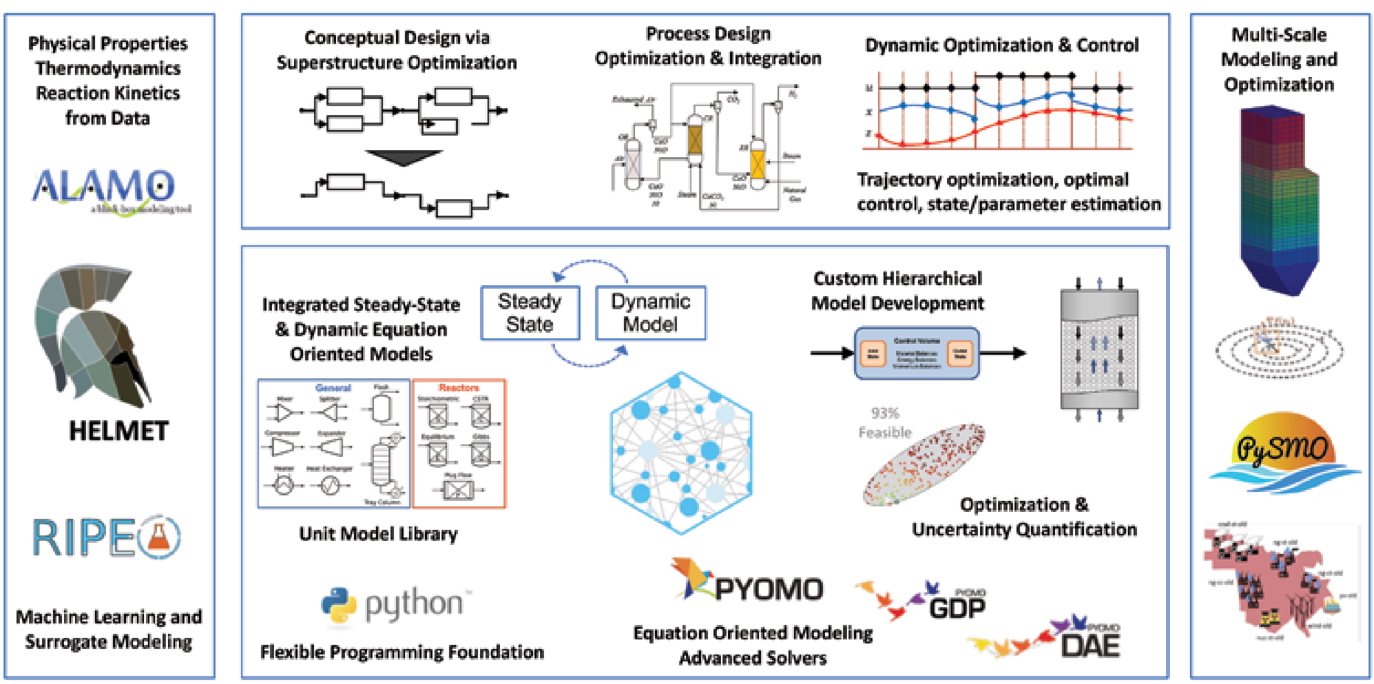
The IDAES framework includes tools for (1) process synthesis and conceptual design, including process intensification, (2) process design and optimization, including process integration, (3) process control and dynamic optimization, (4) use of advanced solvers and computer architectures, (5) automated 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 2020, the IDAES team anticipates achieving 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.

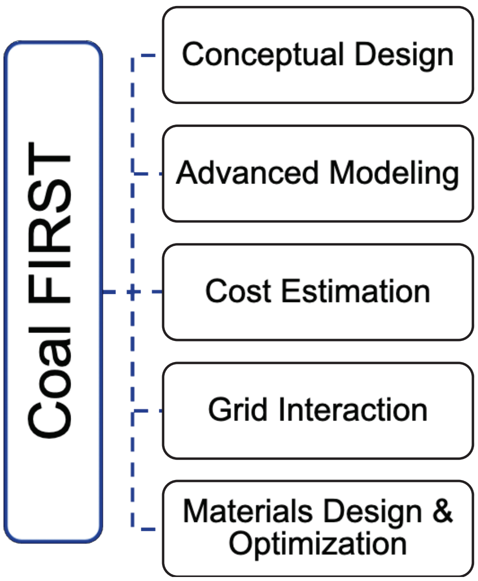
IDAES

Institute for the Design of Advanced Energy Systems



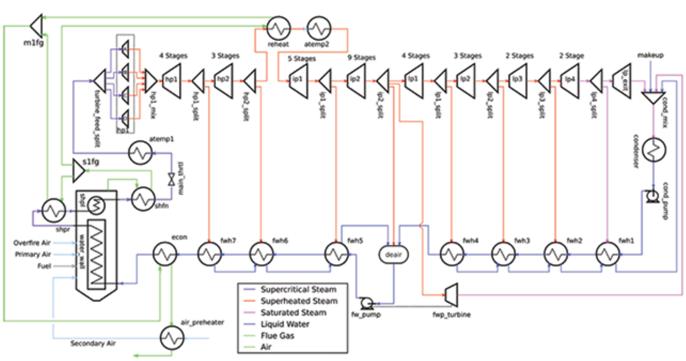
Designing Coal FIRST Power Plants

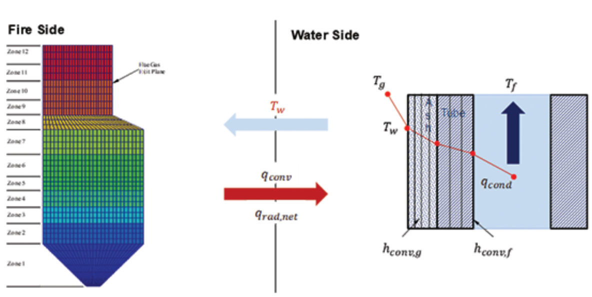
Flexible, Innovative, Resilient, Small and Transformational



- Synergistic advantages when producing power + synthetic chemicals + fuels + storage
- Develop robust conceptual design tools to identify the flexible design (< 400 MW)
- Create advanced models for transformational technologies (Chemical Looping, Carbon Capture) that enable optimal design and analysis
- Develop reliable cost-estimating methodologies for new and existing candidate technologies
- Develop design targets that best integrate with the evolving needs of the electric grid
- Identify innovative materials using optimization that might help meet high performance metrics

Support for the Existing Fleet





- Power plant optimization model
  - Boiler fire side (combustion, NO_x, SO_x formation)
  - Boiler water side (vertical tubes, convective superheaters, economizer)
  - Steam cycle (turbines, condenser, feedwater heaters, deaerator)
  - Pollution controls (SCR, FGD)
- Key features
  - Suitable for optimizing baseload & part load conditions
  - Hybrid 1-D/3-D zonal model of boiler fire-side
  - 1st-principles equation-oriented models for rest of flowsheet
  - Rigorous physical properties calculations (e.g., IAPWS-95 for water and steam, must handle phase change)
- Established workflows for
  - Data reconciliation
  - Parameter estimation
  - System-wide optimization
  - Fault detection and diagnosis

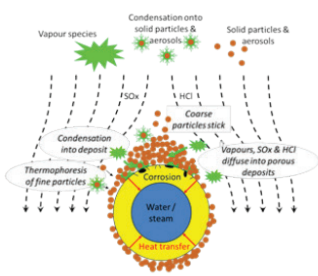
Component Level Modeling of Materials Degradation for Insights into Operational Flexibility of Existing Coal Power Plants

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

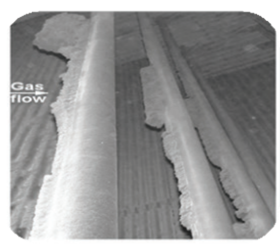
Siemens will develop a computational fluid dynamics/finite element (CFD/FE) modeling toolkit for component-level models of the boilers and low-pressure steam turbines in coal power plants that can tackle multidisciplinary failure mechanisms occurring concurrently for extreme environment materials. The 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

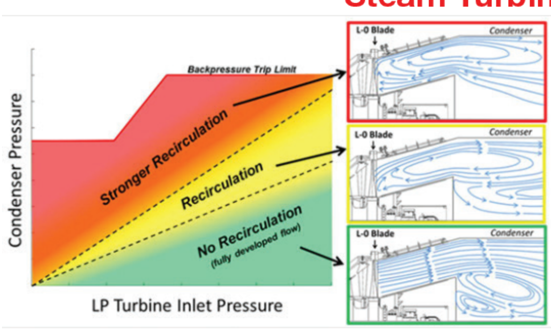


Fouling in heat exchangers

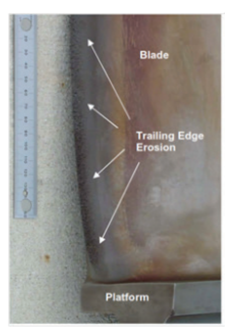


Deposit on real superheater tubes

Steam Turbines



Steam exhaust recirculation causing erosion and cracking



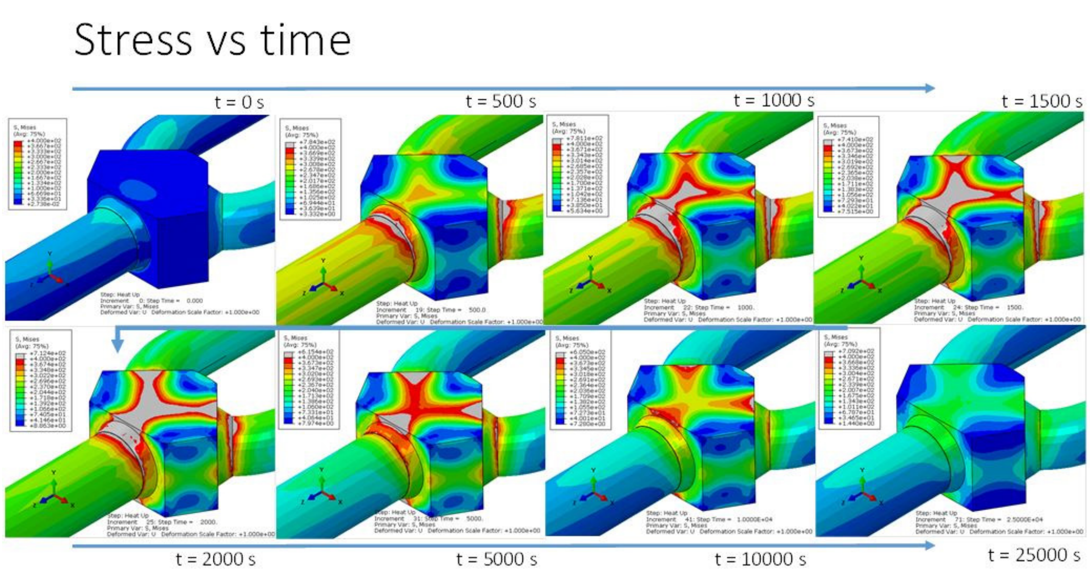
Eroded trailing edge of last row blade

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.

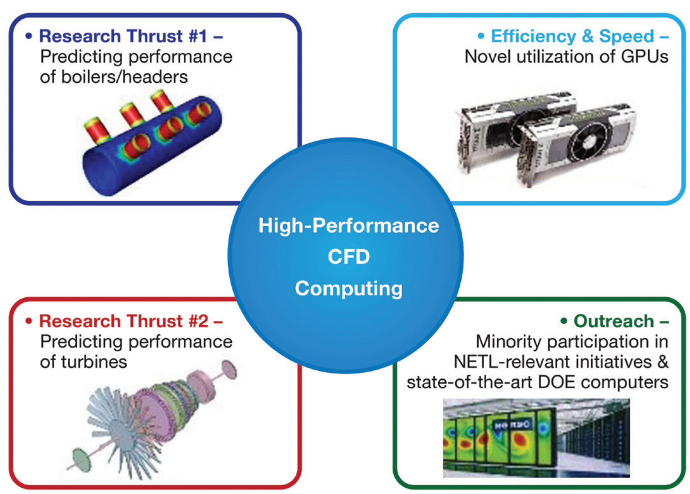


Probing Particle Impingement in Boilers and Steam Turbines Using High-Performance Computing with Parallel and Graphical Processing Units

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 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.



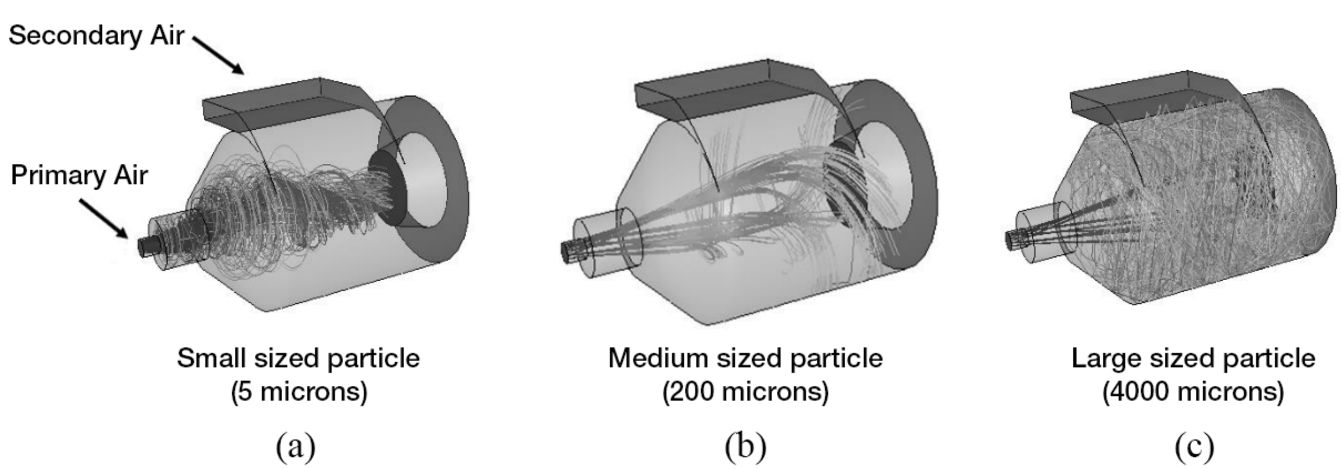
High-performance CFD computing forms a central theme and unifies research thrusts, efficiency, outreach, and technological impact in this HBCU-OMI project.

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.

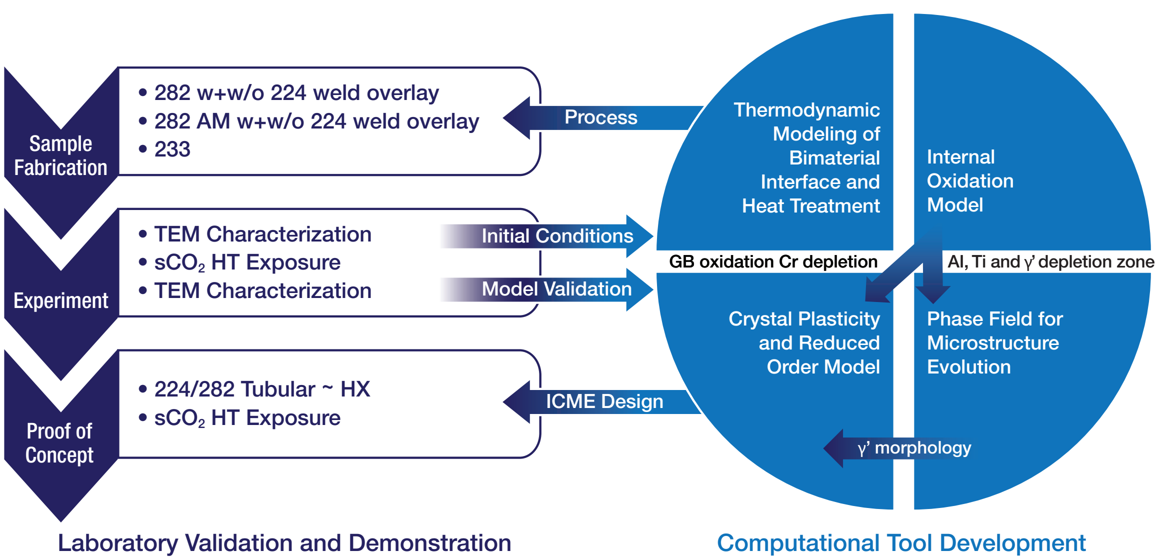
COMPUTATIONAL MATERIALS DESIGN

ICME for Advanced Manufacturing of Nickel Superalloy Heat Exchangers with High Temperature Creep Plus Oxidation Resistance for Supercritical CO_2

Performer	**Det Norske Veritas (DNV) GL USA, Inc.**
Award Number	FE0031631
Project Duration	10/01/2018 – 09/30/2021
Total Project Value	$ 937,500
Collaborator	Ohio State University
Technology Area	Coal Utilization Science

Det Norske Veritas (DNV) GL USA will develop and validate computational design and analysis tools that optimize novel material combinations for fabricating microchannel heat exchangers via additive manufacturing for supercritical CO_2 power cycle technology. Original experiments will be performed for alumina and chromia scale-forming nickel-based superalloys made with conventional and additive manufacturing with simulated compositional grading effects. The project integrates high-temperature oxidation modeling, phase-field modeling of microstructure evolution, and creep performance using crystal plasticity modeling. The three models will be coupled according to an input-output matrix that passes information on solute depletion into microstructure models for gamma-prime (γ') re-distribution and then into the crystal plasticity models for prediction of creep rate and tensile strength reduction. The modeling work will be tightly coupled with experimental high-temperature oxidation and creep testing of advanced alloys and prototype components in supercritical CO_2.

This project could provide the fossil energy industry with new options for materials with property gradients. The integrated computational materials engineering (ICME) approach could improve pre-screening of fabrication techniques and heat treatments, which could reduce design time for materials intended for service in extreme environments.



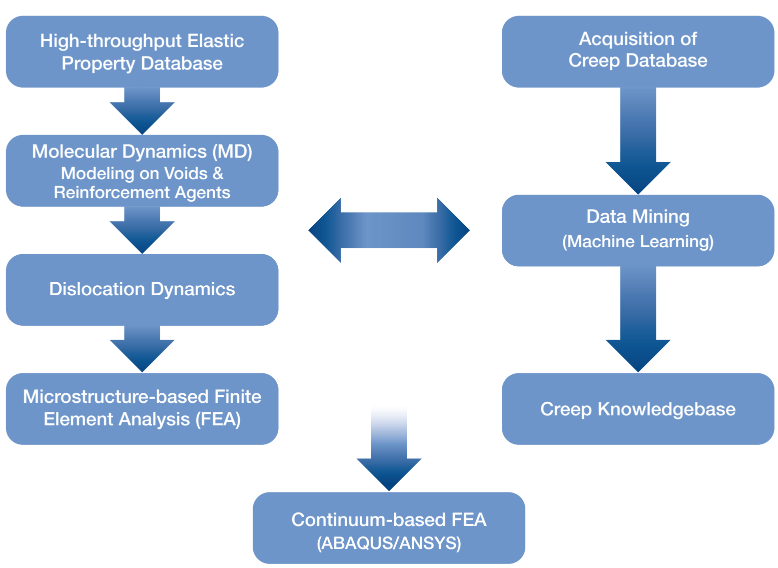
Computational tool development pathway to support multi-material additive manufacturing for high-temperature heat exchange systems.

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

Performer	Missouri State University
Award Number	FE0031554
Project Duration	12/15/2017 – 12/14/2021
Total Project Value	$ 918,370
Collaborators	Missouri University of Science and Technology; University of Missouri–Kansas City
Technology Area	Plant Optimization Technologies

NETL is partnering 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 – 09/30/2021	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	$ 2,065,645	$ 981,000	$ 628,000	$ 590,000	$ 2,063,000	$ 1,604,000	$ 1,090,000
Total Project Value (All)	$ 9,021,645						
Technology Area	Coal Utilization Science						

Affordable, durable, cost effective, heat-resistant alloys are necessary for improving the existing fleet of fossil energy power plants, and enabling advanced fossil energy systems, such as advanced ultrasupercritical Rankine cycles and supercritical carbon dioxide (sCO_2) power cycles. 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.

eXtremeMAT brings together seven of the leading national laboratories to harness the unparalleled breadth of unique capabilities across the DOE complex associated with materials design, high-performance computing power, advanced manufacturing, in-situ characterization, and performance assessment at condition into an integrated, mission-focused team, focused on:

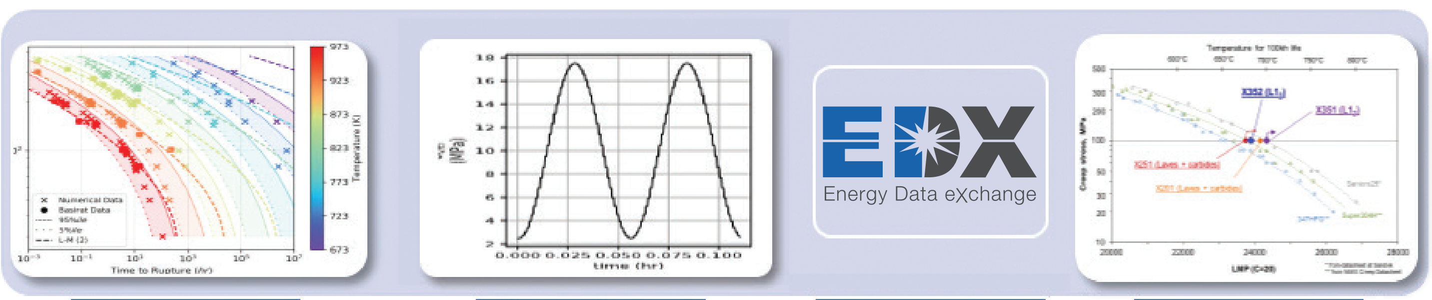
- Developing a suite of improved heat resistant alloys for fossil energy components in existing and future power plants
- Predicting long-term materials performance in existing and future fossil energy power cycles

The objective of eXtremeMAT is to demonstrate how state-of-the-art computational materials modeling and cutting-edge experimental tools can accelerate development and deployment of new heat-resistant alloys for fossil energy applications. In addition, materials modeling and life prediction and the models developed therein can be used to assess the current and remaining life integrity of heat-resistant alloys used in existing plants. It may also be possible to improve the performance envelope of current-generation fossil energy alloys by understanding the relationship between manufacturing, microstructural stability, and mechanical behavior.

Initially, the effort will target enabling sCO_2 technologies through the development of high yield strength, high-temperature austenitic stainless steel alloys. Although nickel (Ni) superalloys can meet the performance objectives of sCO_2 technologies, they are costly and may limit the broad application of these technologies. Improvements in the performance of austenitic stainless steels will enable a wider application of lower-cost alloys, thereby reducing the amount and cost of nickel required in the overall system. The challenge is to increase the yield and creep strength of austenitic steels to enable long-term operation at temperatures above 700 degrees Celsius, while maintaining low costs and manufacturability, using computational tools integrated with experimental characterization. While targeting austenitic alloys, the methodologies developed in this project will be applicable for developing new alloys or for improving the properties and performance of other lower-cost alloys such as 9–12 percent chromium steels and higher-performance alloys such as Ni-based or high-entropy alloys.

In the near term, the project team is working to identify promising candidates for new low-cost iron-based alloys that would perform well in an sCO_2 environment. In the long term, the team aims to develop and demonstrate a new approach to materials discovery and development for future energy applications. This approach would exploit multiscale (molecular-to-continuum) simulation methods to explore the performance of new materials over wide ranges of compositional space, identifying promising formulations for specific service conditions that can subsequently be tested at the bench scale. This requires overcoming major simulation challenges and confidently predicting both the properties of metallic alloys over wide ranges of compositional space and the performance life of these materials. If this can be demonstrated, the current laborious approach to materials discovery can be transformed and the path from materials discovery to commercial deployment can be dramatically accelerated. Lastly, the ability to manufacture these new alloys at scale needs to be demonstrated and matured to a level that would encourage industrial adoption in the commercial application.

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

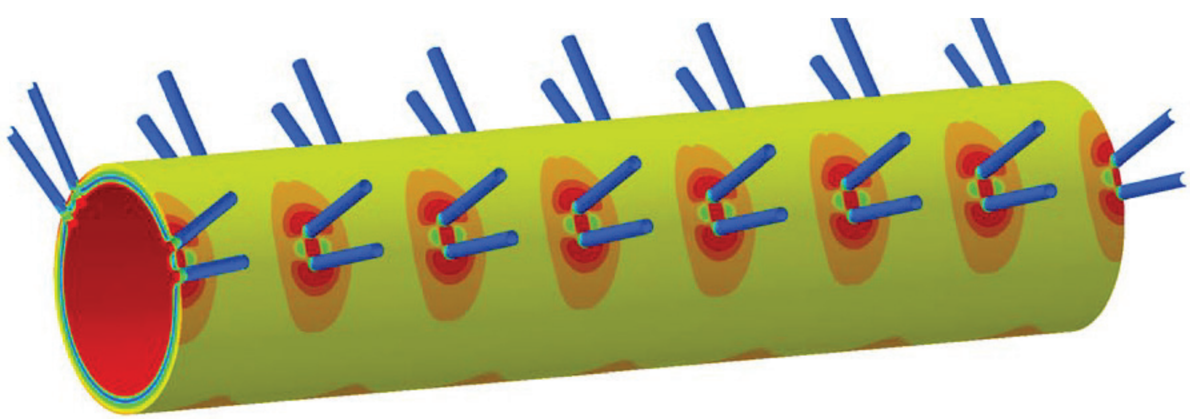
Rapid discovery of new alumina forming alloys

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.



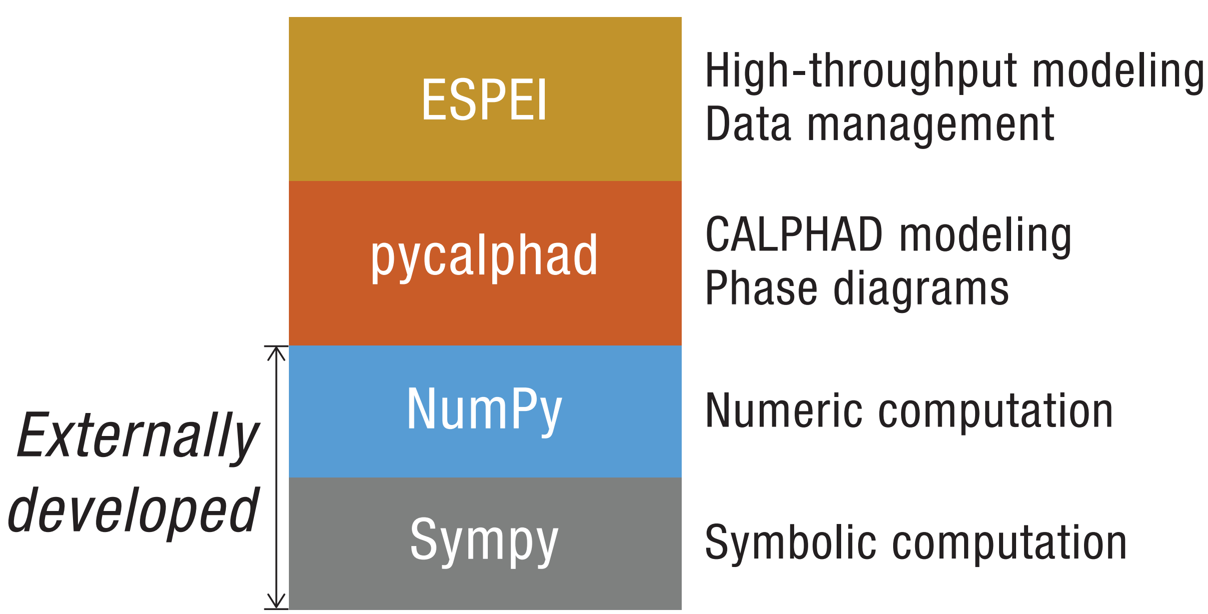
Stress contour plot of a steam header.

High Throughput Computational Framework of Materials Properties for Extreme Environments

Performer	**Pennsylvania State University**
Award Number	FE0031553
Project Duration	12/15/2017 – 12/14/2021
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.



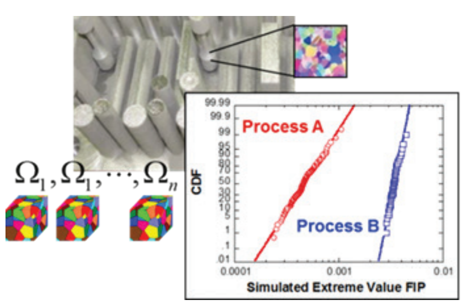
ESPEI-2.0 software stack.

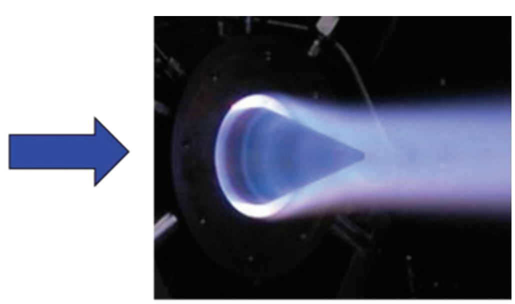
Digital Twin Model for Advanced Manufacture of a Rotating Detonation Engine Injector

Performer	**Southwest Research Institute (SwRI)**
Award Number	FE0031644
Project Duration	10/01/2018 – 09/30/2021
Total Project Value	$ 937,371
Collaborators	Aerojet Rocketdyne, Inc.; Georgia Tech Research Corporation
Technology Area	Coal Utilization Science

Southwest Research Institute (SwRI) will use a digital twin material model (DTMM) to apply advanced manufacturing techniques to advance rotating detonation engine (RDE) injector design. The project will develop both a digital twin model of the injector manufacturing process and an injector that performs in an RDE combustor with a significant reduction in flow loss. This will be accomplished through several subordinate objectives: design of a novel RDE injector that allows for fuel and oxidizer flows to be optimized in ways not possible with conventional manufacturing; comprehensive design of experiments (DofE) focusing on contributing factors that trigger high-cycle fatigue; development of a parametric material model based on actual test coupons from the advanced manufacturing process that allows prediction of mechanical strength properties; and manufacture, test, and post-test destructive evaluation of an RDE injector exposed to a significant high cycle fatigue environment. SwRI is responsible for the material model DofE, producing a portion of the material samples; performing the detailed RDE injector design; performance testing of the RDE injector; and post-test analysis of the injector component. Aerojet Rocketdyne will support the application of this work to the existing RDE; review the DofE for material samples; produce many of the material samples; support the conceptual design of the new RDE injector; manufacture the RDE injector prototypes for testing; and support RDE injector testing, including data capture and post-processing. Georgia Institute of Technology will provide the material model development and application to the design of the RDE injector; review the DofE for completeness; process material samples to extract physical and microstructure qualities; advance the process parameter to microstructure linkage; develop the microstructure-to-fatigue resistance linkage; and support the injector design analysis with process parameter optimization.

The development, implementation, and validation of tools for predicting and verifying microstructural properties, strength, residual stress, and dimensional build characteristics has extremely high relevance for high-temperature high-strength applications that may benefit from additively manufactured parts. Development of a digital twin model of an RDE injector manufacturing process, and an injector that performs in an RDE combustor with a significant reduction in flow loss, will allow the RDE injector to transition to the industrial application of fossil-based power generation.





Modeling of additively manufactured parts leading to low-loss additively manufactured RDE injector.

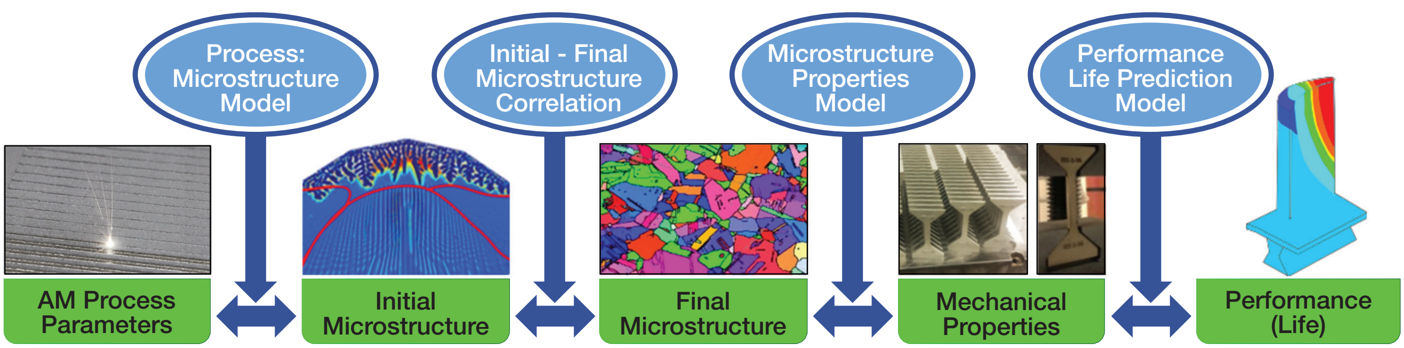
Computation Tools for Additive Manufacture of Tailored Microstructure and Properties

Performer	**Raytheon Technologies Research Center (RTX)**
Award Number	FE0031642
Project Duration	09/01/2018 – 03/31/2021
Total Project Value	$ 950,244
Technology Area	Coal Utilization Science

Raytheon Technologies Research Center (RTX) (formerly United Technologies Research Center) demonstrated the application of computational methods and tools on microstructure evolution and mechanical properties prediction for additively manufactured (AM) nickel-based superalloy parts. Models were developed in three areas: AM process parameters/microstructure correlation models; correlation between initial microstructure and final microstructure after heat treatment; and final microstructure-to-mechanical-properties relationship. The ability to tailor spatially varying mechanical properties in part by appropriately controlling the microstructure evolution during the AM process was demonstrated using these models. An integrated computational materials engineering framework that connects process, structure, properties, and performance was developed and demonstrated.

This project extends computational phase-field models for microstructure evolution—as a function of material processing parameters and crystal plasticity models—fully coupling microstructure, mechanical properties, and service life required for turbine engines.

The tools developed in this project will enable refurbishment of legacy F-Class industrial gas turbines with polycrystalline alloy components built additively by laser powder-bed fusion. These toolsets can be extended to future directionally solidified and single-crystal superalloys produced using AM technology. The time saved by applying validated predictive tools will allow exploration of novel concepts such as tailored property placement based on varying operational requirements within a single part, further unlocking the potential of AM hardware.

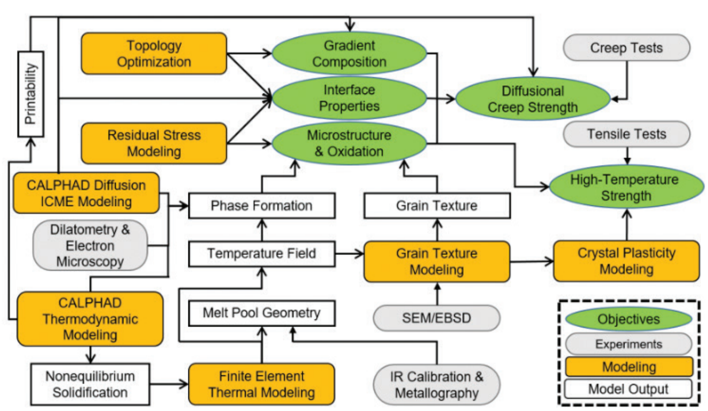


An ICME (Integrated Computational Materials Engineering) framework being developed by Raytheon Technologies Research Center that connects Process – Structure - Properties – Performance by four models.

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 will develop 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 will be 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 will be modeled and employed to design the compositional profile in the interfacial zone using phase transformation modeling and topology optimization techniques. All the models developed will be validated by characterization experiments on both coupon and prototype samples, and their uncertainty will be quantified via sensitivity analysis. Pitt will be responsible for model development and simulation. United Technologies Research Center (UTRC) will perform sample preparation using WAAM, mechanical and tensile strength testing, and high-temperature oxidation and creep tests to support calibration of the structure-property modeling. Both Pitt and UTRC will work on model calibration and verification. Development of a simulation tool that can predict the structure-property relationships of extreme environment materials for fossil energy infrastructure manufacturing will 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.



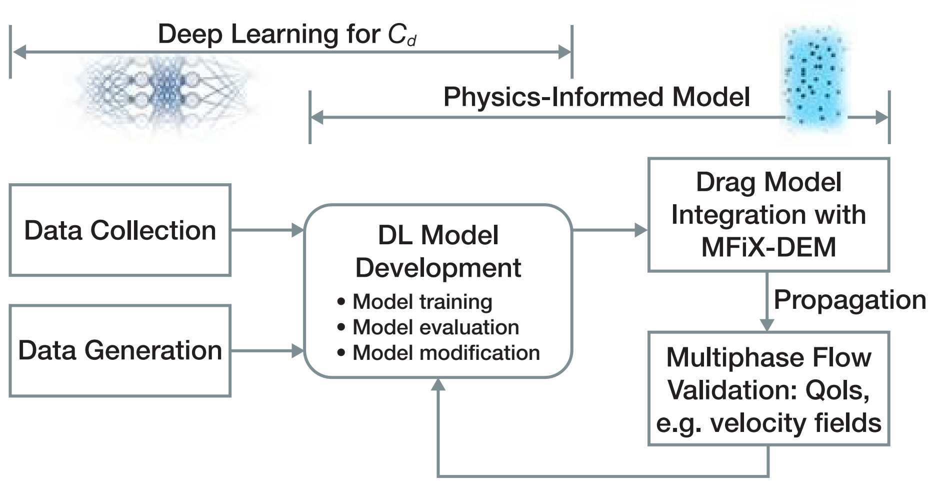
Integrated Computational Materials Engineering model framework for additive manufacturing of alloys with graded structure.

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 proposed 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.

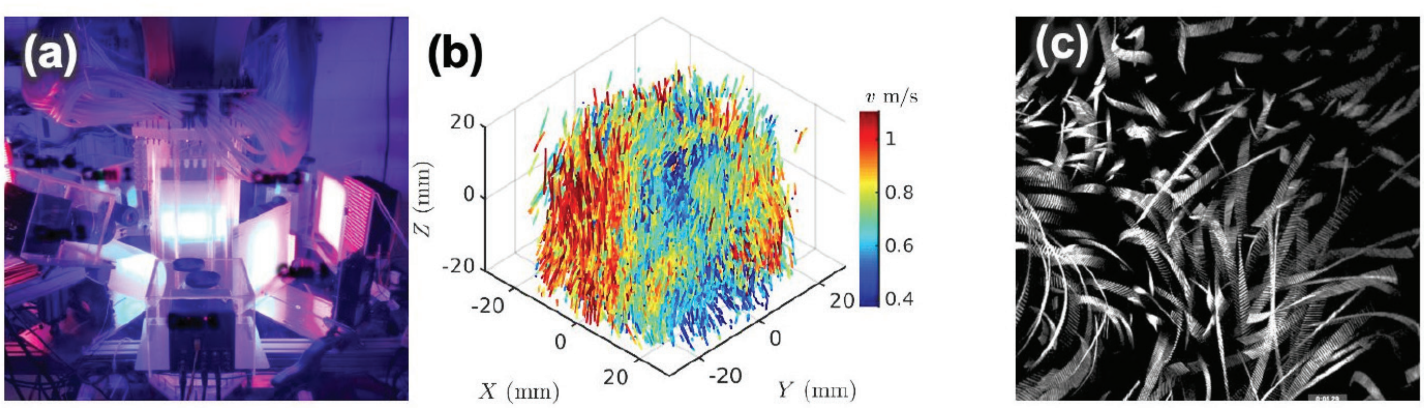


A physics-informed deep learning framework for a drag coefficient model.

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 – 03/31/2022
Total Project Value	$ 6,485,000
Technology Area	Gasification Systems

*EY = Execution Year 2019 (Fiscal Year 2019 funding)

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.

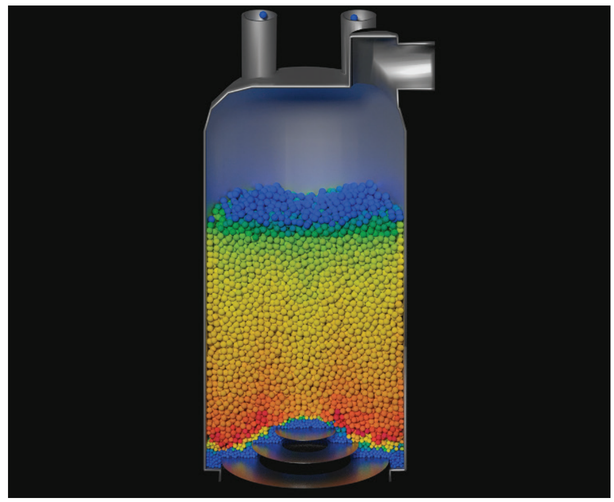
In this research effort, NETL is providing an advanced suite of multiphase flow CFD models that enable the required capability. These models provide detailed predictions of reactor performance including temperature, velocities, chemical composition, reaction rates, and heat transfer for both fluid and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

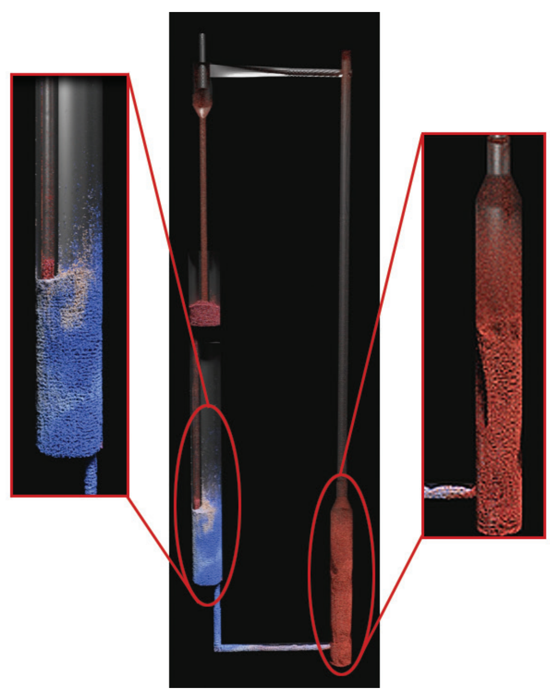
Densely-loaded multiphase flows are very demanding applications for CFD codes. This is made even more challenging in this work due to the need to model

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 – 03/31/2022
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:

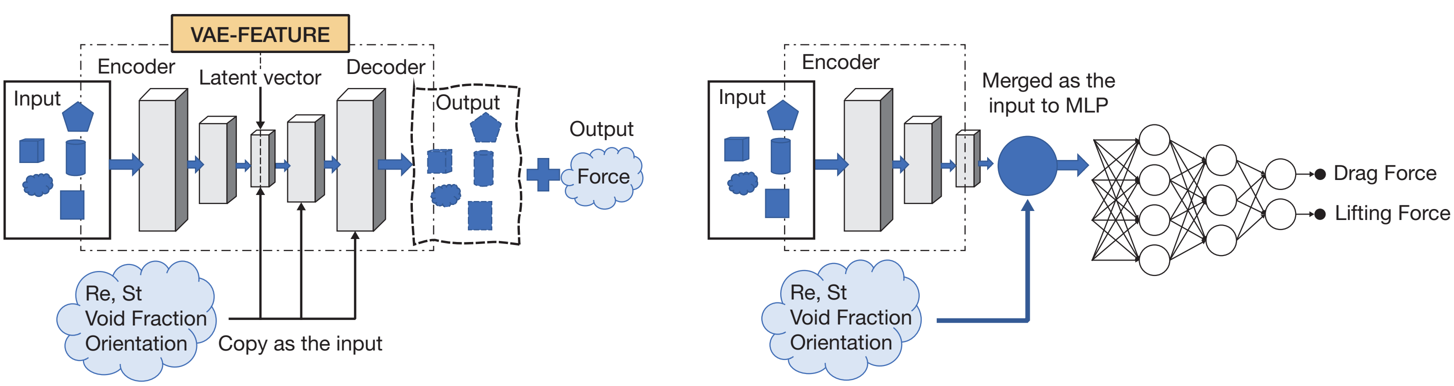
- Develop, validate, apply, publicly distribute, and support the MFiX Suite of multiphase flow modeling software capable of modeling large-scale, reactor systems that include complex chemical reactions and realistic geometry to support the design and optimization of novel reactor systems supporting DOE 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.

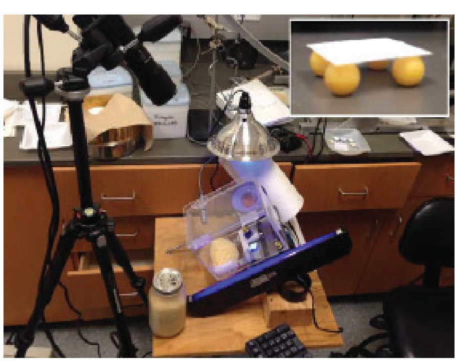
MFIX-DEM Enhancement for Industry-Relevant Flows

Performer	**University of Colorado**	**National Renewable Energy Laboratory**
Award Number	FE0026298	FWP-DOW4659
Project Duration	09/01/2015 – 08/31/2021	10/01/2015 – 08/31/2021
Total Project Value	$ 3,778,002	$ 899,419
Total Value (All)	$ 4,677,421	
Collaborator	Particulate Solid Research, Inc.	
Technology Area	Coal Utilization Science	

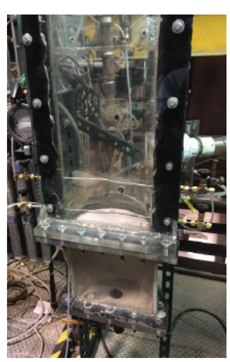
This project will improve performance of the Multiphase Flow with Interphase eXchanges–discrete element method (MFiX-DEM) code to enable a transformative shift for industrial use. The proposed approach will enhance MFiX-DEM by using a state-of-the-art profiling methodology developed by our team members to comprehensively and continuously identify numerical and algorithmic bottlenecks. Both serial and parallelization bottlenecks will be overcome via vectorization, cache utilization, algorithmic improvements, and implementation of hybrid message passing interface/ OpenMP parallelization methods that synergize with current heterogeneous high-performance computing (HPC) architectures and accelerators. Optimizing MFiX-DEM and implementing parallelization for accelerated HPC systems will enable simulations of industrially relevant problems on machines that industry is likely to have in the coming years.

The goal is to achieve an increase in performance of two orders of magnitude; a refined estimate will result from the profiling effort. Over thirty Particulate Solid Research, Inc. consortium member companies were surveyed at the beginning of the project to identify industrial needs. In Phase 2, the focus is on completing simulations for increasingly complex systems involving 109 particles in less than 24 hours. New experiments will be performed involving approximately 107-109 particles in a system of industrial relevance, and these experiments will be used to demonstrate the enhanced MFiX code. Uncertainty quantification (UQ) will also be performed by coupling the freely available UQ toolkit Problem Solving environment for Uncertainty Analysis and Design Exploration (PSUADE) with an enhanced version of MFiX. Uncertainty quantification using the enhanced MFiX code on larger and industrially relevant systems will be demonstrated.

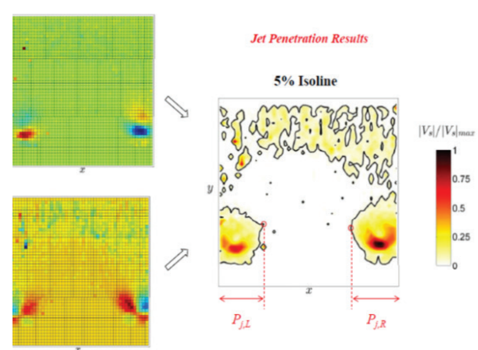
The immediate outcome will be an enhanced DEM tool implemented into the open-source MFiX framework. The enhanced DEM model will be optimized for computational efficiency and will contain parallelization methods that leverage advances in heterogeneous HPC architectures with accelerators.



Horizontal jet experiments particle characterization.



Semi-circular fluidized bed with side jets.

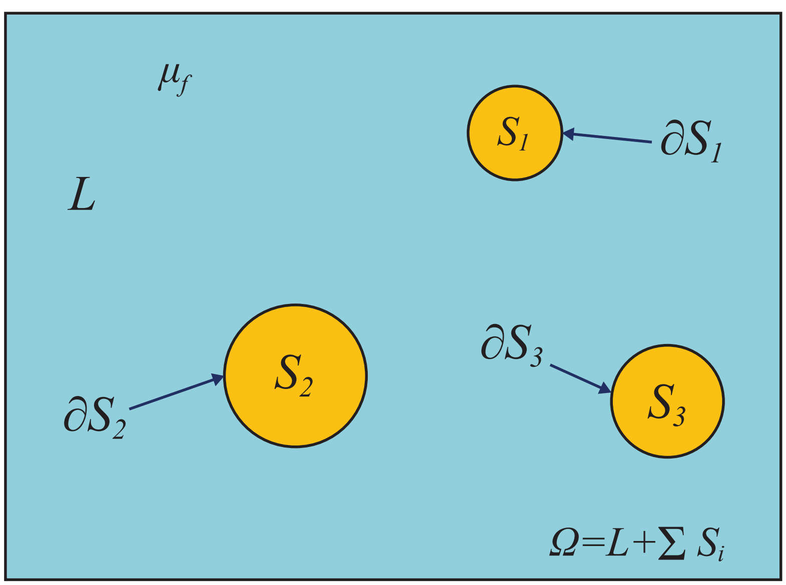


Horizontal jet experiments particle tracking post-processing.

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.



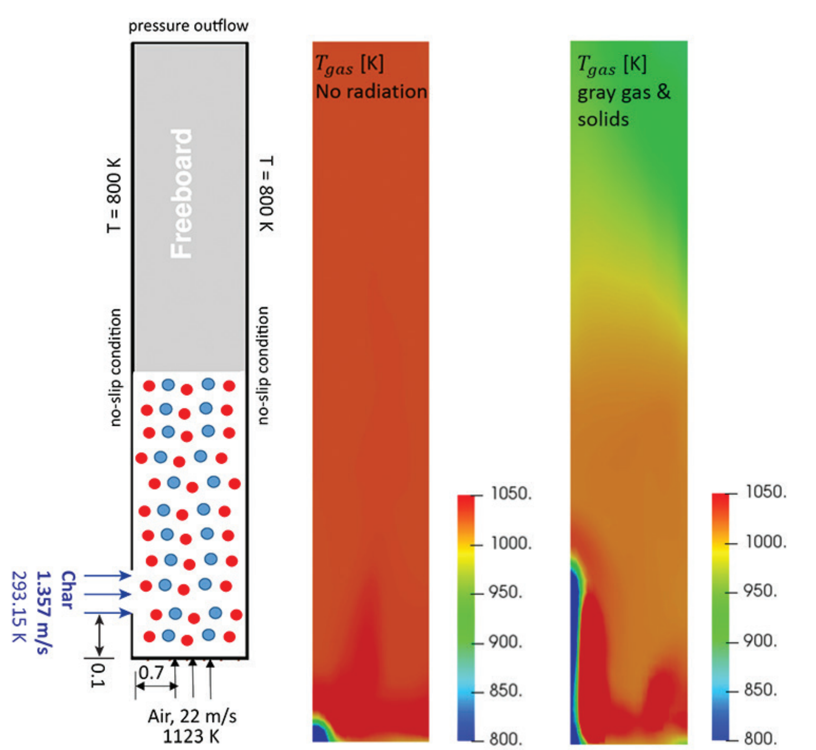
Conceptual model of three particles suspended in a fluid.

Implementing General Framework in MFiX for Radiative Heat Transfer in Gas-Solid Reacting Flows

Performer	**University of Wyoming**
Award Number	FE0030485
Project Duration	08/01/2017 – 07/31/2021
Total Project Value	$ 400,000
Collaborator	University of California, Merced
Technology Area	University Training and Research

The objectives of this research are to (1) develop and implement a general framework to support the integration of modern gas radiation models for gas-solid reacting flows; (2) implement a methodology for developing new multiphase radiation models with accuracy and efficiency commensurate to the different importance in a variety of energy related applications; (3) reduce the computational cost of existing high-fidelity models via systematic optimization; and (4) demonstrate the accuracy and efficiency of the radiation models under typical gas-solids reacting flow conditions.

This project aims to have a significant impact on the development of the National Energy Technology Laboratory's MFiX code and future research of gas-solid reacting flows. Fundamental knowledge of radiation transport and predictive models developed for these processes could shorten design time and reduce design cost of new energy conversion technologies.



Relevance of radiative heat transfer in a lab-scale spouted bed combustor. Simulations performed in 2D with MFiX-TFM and the MFiX-RAD interface.

ABBREVIATIONS

2D .... two-dimensional
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
CSEF .... creep strength enhanced ferrous
Cu .... copper
DEM .... discrete element model
DFT .... density functional theory
DFTB .... density functional tight binding
DOE .... Department of Energy
DofE .... design of experiments
DTMM .... digital twin material model
EY .... execution year
FE .... finite element
Fe .... iron
FECM .... Office of Fossil Energy & Carbon Management
FWP .... Field Work Proposal
FY .... iscal year
GPU .... graphics processing unit
HBCU-OMI .... Historically Black Colleges and Universities-Other Minority Institutions
HEA .... high-entropy alloy
HPC .... high-performance computing
HVOF .... high velocity oxy-fuel
HYPER .... Hybrid Performance
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
MHD .... magnetohydrodynamic
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

PSUADE........................Problem Solving environment for Uncertainty Analysis and Design Exploration

R&D...................................... research and development

RAD .... radiative heat transfer

RDE....................................... rotating detonation engine

SwRI .... Southwest Research Institute

TFM...Two-Fluid Model

UCR ....University Coal Research

UND ....University of North Dakota

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

UQ ....uncertainty quantification

UTRC .... United Technologies Research Center

VAE .... variational auto-encoder

WAAM........................... wire-arc additive manufacturing

γ’ .... gamma prime

η...eta

NOTES

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https://netl.doe.gov/coal/simulation-based-engineering

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