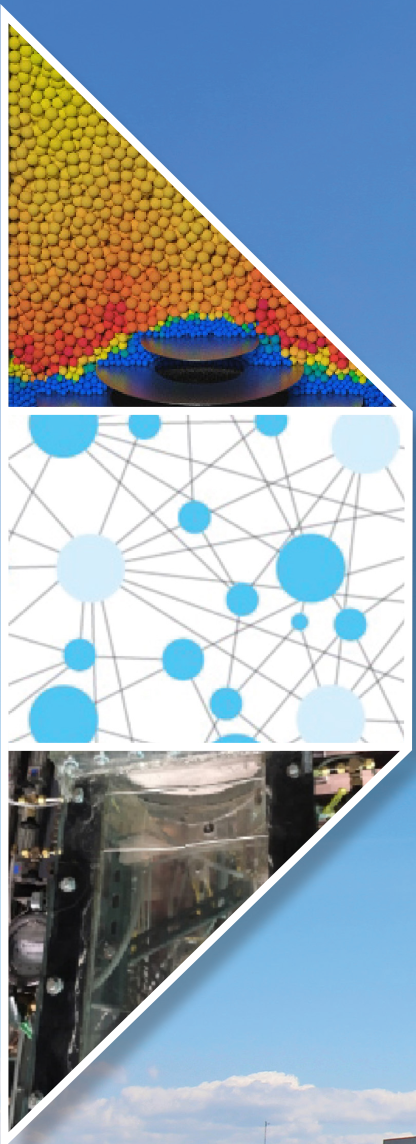
CROSSCUTTING RESEARCH

MODELING, SIMULATION AND ANALYSIS PROJECT PORTFOLIO 2020



U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

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INTRODUCTION

NETL's Crosscutting Research Program matures novel technologies for commercialization that can enhance new and existing fossil-fired power plants. Six research and development (R&D) programs target enhanced fossil energy systems: High Performance Materials; Sensors, Controls, and Cybersecurity; Modeling, Simulation and Analysis; Water Management; Energy Storage; and University Training and Research.

The goals are to create transformational technologies that improve plant efficiency and security, reduce water consumption, and reduce costs, all under a single research umbrella. The research is leading to enhancements to the fleet such as improved plant efficiency, 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 Program's portfolio, its technologies often have applicability to other energy sectors such as oil and natural gas infrastructure and aviation (both commercial and military).

On behalf of the U.S. Department of Energy's Office of Fossil Energy, NETL pursues crosscutting R&D by collaborating with other government agencies, world-renowned national labs, entrepreneurs, industry, and academic institutions. 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 fossil energy infrastructure, and enable the adoption of cutting-edge data technologies for plant owners and operators.

Sensors and Controls: The Sensors and Controls 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 coal-fired power plants, capable of real-time measurements, improve overall plant efficiencies, and allow for more effective ramp rates. Given the crosscutting nature of sensors and controls, these technologies will also benefit natural gas power generation and other harsh-environment applications.

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

High Performance Materials: High Performance Materials 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 and supports the existing fossil fleet with materials solutions that enhance flexibility and reliability.

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, and Computational Materials Design.

Modeling, Simulation and Analysis: Modeling, Simulation and Analysis (MSA) 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 MSA 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 analyses that are essential in informing and deciding between priority technology choices. 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.

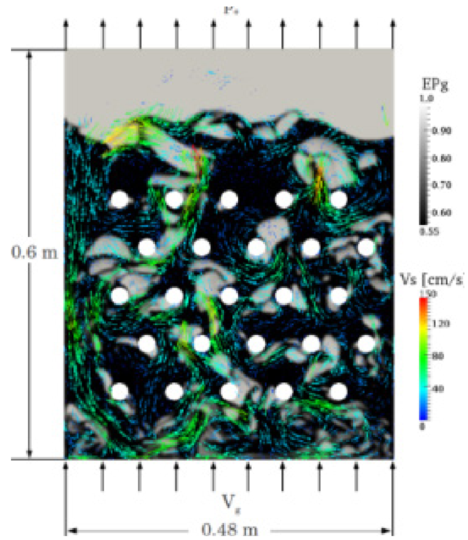
The program leads a critical national effort directed at removing barriers to sustainable, efficient water and energy use; developing technology solutions; and enhancing the understanding of the intimate relationship between energy and water resources. Water Management R&D focuses its research in three 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: FE's Advanced Energy Storage program aims to address the needs and challenges of fossil assets through the integration of energy storage technologies. As the penetration of variable renewable energy increases, energy storage at the generation site will be essential to a resilient and flexible electricity network. Energy storage also benefits the environment through optimization of fossil generation and by enabling additional renewables on the grid to reliably transmit their energy to end users. Program activities include plant- and system-level analyses, conceptual and detailed engineering designs, breakthrough R&D on innovative energy storage concepts, and targeted R&D on component and system-integrated energy storage technologies.

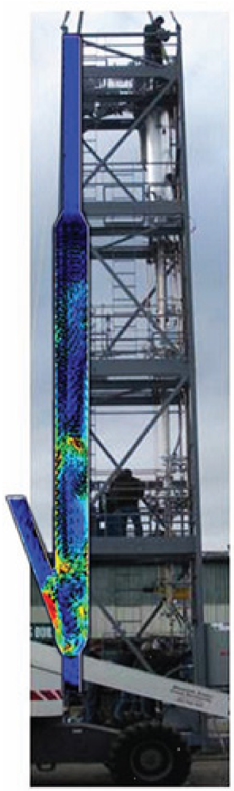
University Training and Research: University Training and Research supports two of the longest-running university training programs, the Historically Black Colleges and Universities (HBCU) and Other Minority Institutions (OMI) and the University Coal Research (UCR) programs, to support the education of students in the area of coal science is promoted through grants to U.S. colleges and universities that emphasize FE 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. The Outreach Initiative provides opportunities for qualified students and post-doctoral researchers to hone their research skills with NETL's in-house scientists.

MODELING, SIMULATION AND ANALYSIS

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 Modeling, Simulation and Analysis 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 Modeling, Simulation and Analysis 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. Modeling, Simulation and Analysis 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.

Modeling, Simulation and Analysis 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 Modeling, Simulation and Analysis are Advanced Process Simulation, Computational Materials Design (with High Performance Computing), and Multiphase Flow Science.

ADVANCED PROCESS SIMULATION

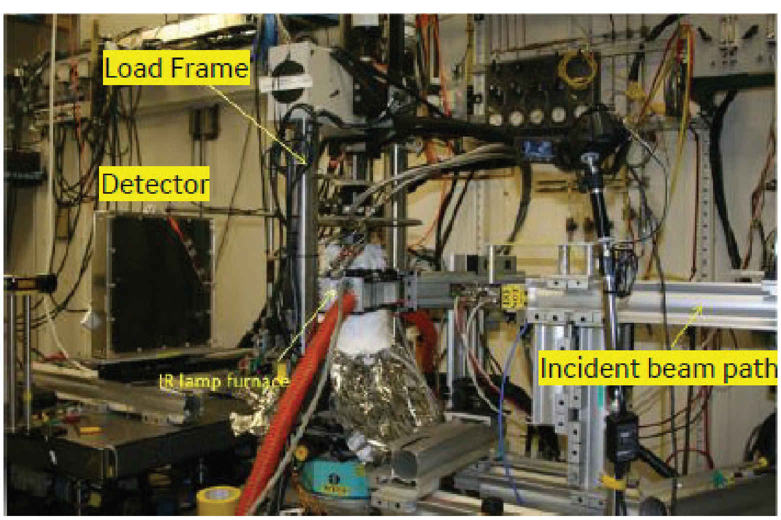
Damage Accumulations Predictions for Boiler Components Via Macrostructurally Informed Material Models

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 Value (All)	$ 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.

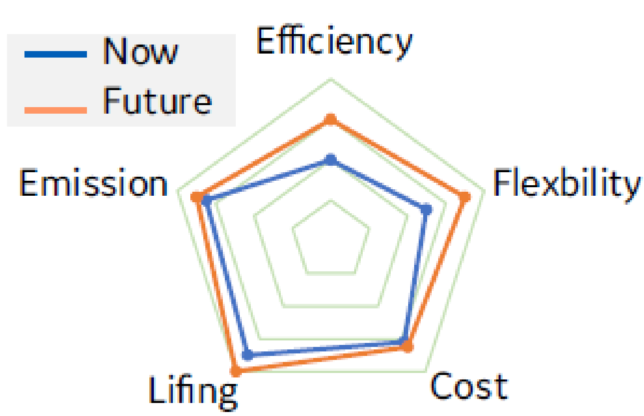
Investigation of Cycling Coal Fired Power Plants Using High-Fidelity Models

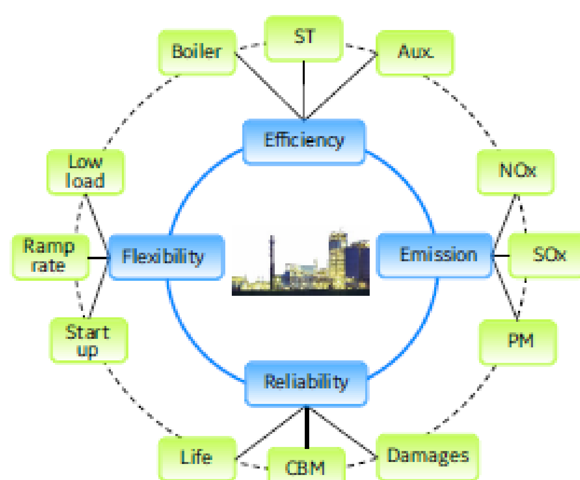
Performer	General Electric (GE) Company
Award Number	FE0031822
Project Duration	10/01/2019 – 03/31/2021
Total Project Value	$ 937,429
Technology Area	Coal Utilization Science

Using General Electric (GE) Company's existing process models (both transient and steady state) and mechanical integrity models, an integrated high-fidelity simulation platform will be built to enable critical component analysis. An automated data processing and model calibration tool will be developed to allow easy adaption of the models built under this program to other units, thereby saving future engineering project costs. An economics model will be 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 will be generated. The primary focus of this program will be 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 will be 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.



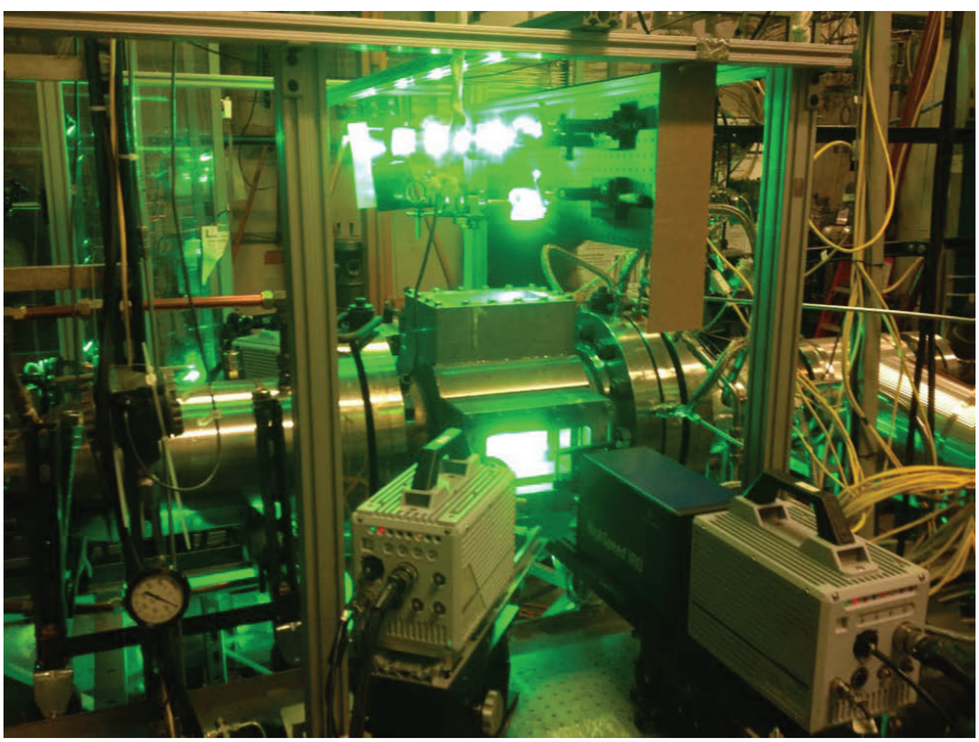


Multi-dimensional analysis for critical components.

Real-Time Health Monitoring for Gas Turbine Components using Online Learning and High Dimensional Data

Performer	**Georgia Tech Research Corporation**
Award Number	FE0031288
Project Duration	10/01/2017 – 09/30/2021
Total Project Value	$ 750,297
Technology Area	Plant Optimization Technologies

The Georgia Tech Research Corporation will use two industry-class gas turbine component test rigs to generate first-of-its-kind data for critical gas turbine faults with varying severity levels. Combustor and turbine tests will generate data to support predictive algorithm development; the test conditions will include common critical events that occur in the operation of power plants. The data will be correlated with physics-based models and first-principle relationships to improve component life predictions. Additionally, a comprehensive big data analytics methodology will be developed, guided by the generated experimental data, industrial data from collaborators, and physics-based models with engineering domain knowledge. The effort will leverage existing research facilities that will generate the first publicly available data with simulated combustor and turbine faults.



Over-instrumented blowout experiment in optically accessible combustion test rig at Georgia Tech.

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

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022423
Project Duration	01/01/2020 – 12/31/2020 (EY20)*
Total Project Value	$ 7,306,316 (FY20)
Collaborator	Carnegie Mellon University; Lawrence Berkeley National Laboratory; Notre Dame; Sandia National Laboratories; West Virginia University
Technology Area	Coal Utilization Science

*EY = Execution Year (Fiscal Year 2020 funding)

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 chemical looping combustion 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, flow-sheet/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

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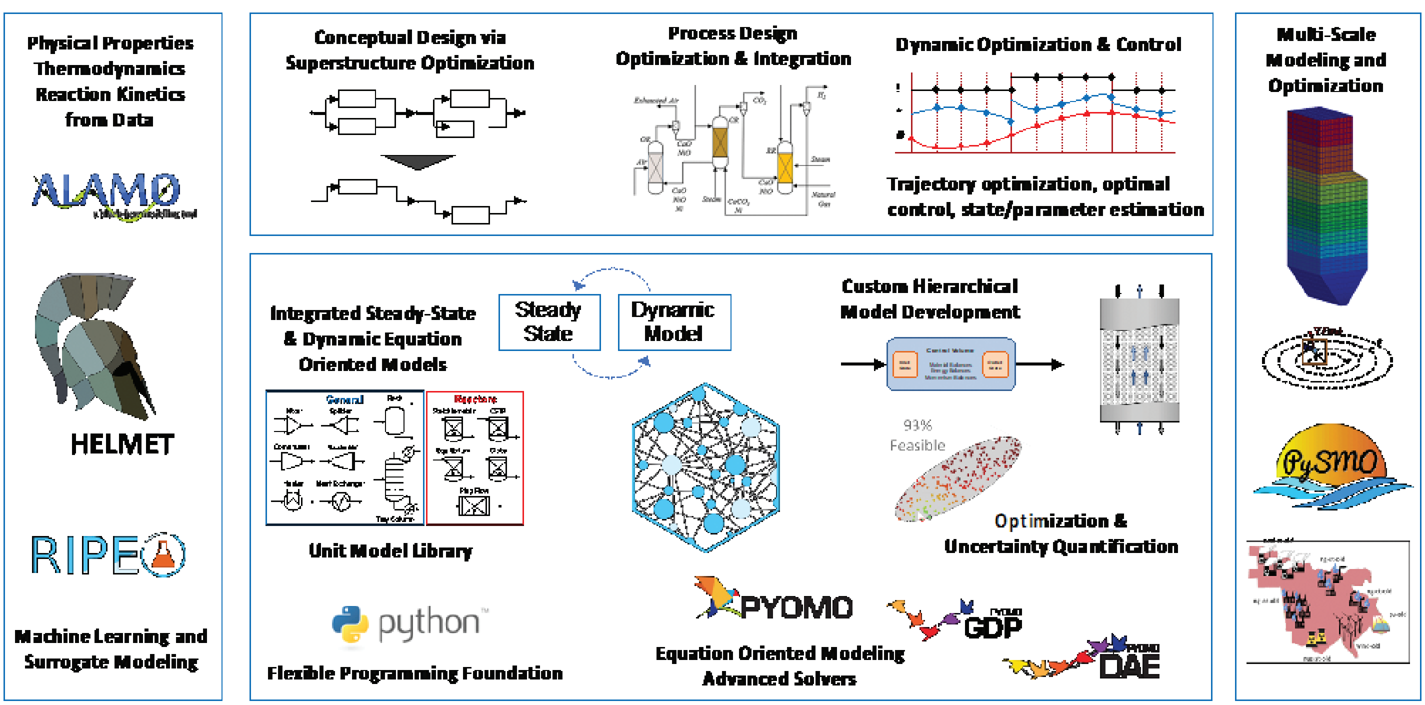
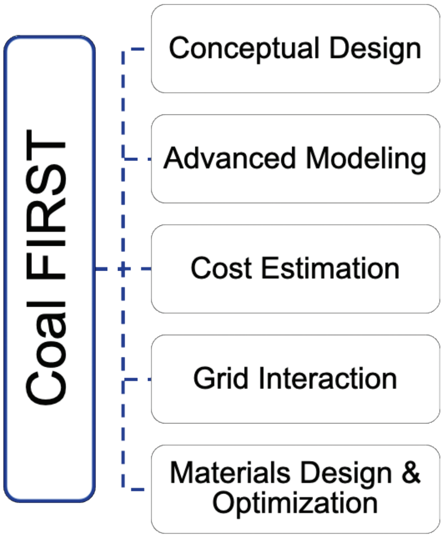


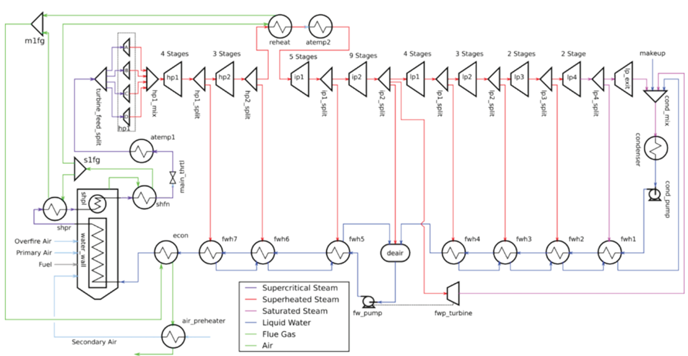
Designing Coal FIRST Power Plants

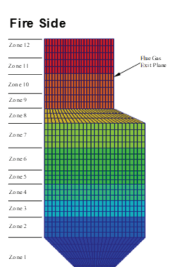
Flexible, **I**nnovative, **R**esilient, **S**mall and **T**ransformational

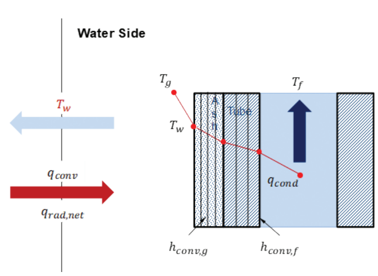


- Synergistic advantages when producing power + synthetic chemicals + fuels + storage
- Develop robust conceptual design tools to identify the flexible design (< 400 MW)
- Create advanced models for transformational technologies (Chemical Looping, Carbon Capture) that enable optimal design and analysis
- 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

Direct Power Extraction

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022401
Project Duration	04/01/2019 – 03/31/2020 (EY19)*
Total Project Value	$ 1,450,000 (FY19)
Technology Area	Advanced Combustion Systems

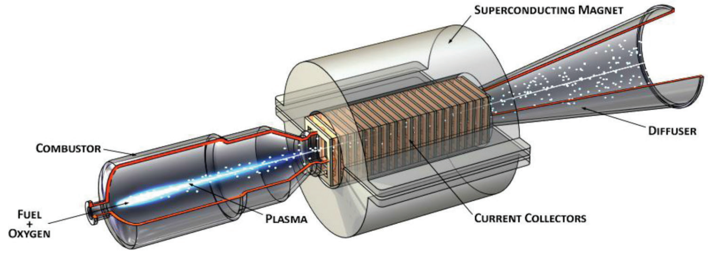
*EY = Execution Year (Fiscal Year 19 funding)

This early-stage R&D project is investigating and testing magnetohydrodynamic (MHD) power generation concepts for future fossil-derived electrical power generation with and without carbon capture. An MHD power generator directly converts the kinetic energy of a working fluid into electrical power, and is shown in Figure 1. MHD replaces the concept of conventional mechanical conversion steps (e.g., momentum transfer in a turbine) with direct power extraction (DPE). Consequently, the maximum efficiencies are inherently higher than those of conventional turbine-based fossil conversion systems. A combined cycle system with fossil-based MHD power generators could in theory exceed 60 percent higher heating value thermal efficiency, and constructed MHD power generators have yielded expected power performance. It is now apparent that MHD-derived power complements the oxy-fuel approach for carbon capture. It is generally clear that material durability and overall systems costs were key issues that hampered commercialization following past U.S. Department of Energy research into MHD power generation.

Advantageous technology improvements related to magnets and other key technologies have been developed, and oxy-fuel products can yield about twice the MHD power density compared to legacy pre-heated air or enriched-air open cycle systems. A devoted and focused technical effort allows the Office of Fossil Energy to critically evaluate the promise of this potentially high-efficiency technology. Technology development is focused on the establishment of the theoretical and practical performance of MHD energy conversion systems and experimental validation of the performance and reliability of key components for those systems.

The high-level goal of this work is to improve the viability of MHD power generation for future fossil-derived electrical power generation. To meet this goal, this project is executing techno-economic analysis, developing and verifying the required simulation tools, and experimentally validating device-scale simulations to increase confidence in the performance predictions. Systems which have utilized DPE are being analyzed and ranked according to efficiency, cost, and various other qualitative factors. Standard and novel materials are being developed, simulated, and tested for use as MHD channel materials. This effort focuses on improving fundamentals for technology viability assessments, rather than on demonstrations or detailed optimizations of the technology.

In addition to improving the technical viability of direct power extraction, the project will produce and transfer significant research on fossil energy-relevant topics including mass and thermal flow modeling in aggressive operating environments, functional material development for aggressive applications, and in situ measurement techniques for reactive flow streams, among others.



An oxy-fuel fired open cycle MHD power generator. A diffuser is used to slow the flow down prior to it entering a bottoming cycle.

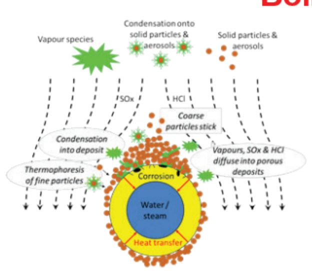
Component Level Modeling of Materials Degradation for Insights into Operational Flexibility of Existing Coal Power Plants

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

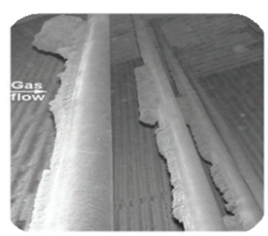
Siemens will develop a computational fluid dynamics/finite element (CFD/FE) modeling toolkit for component-level models of the boilers and low-pressure steam turbines in coal power plants that can tackle multidisciplinary failure mechanisms occurring concurrently for extreme environment materials. The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

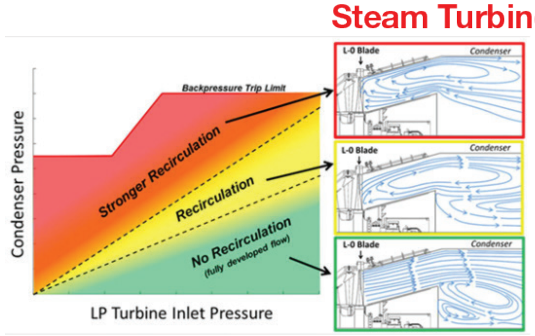


Fouling in heat exchangers

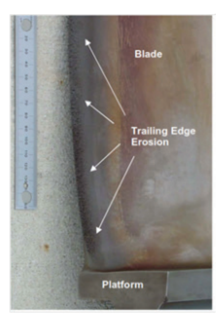


Deposit on real superheater tubes

Steam Turbines



Steam exhaust recirculation causing erosion and cracking



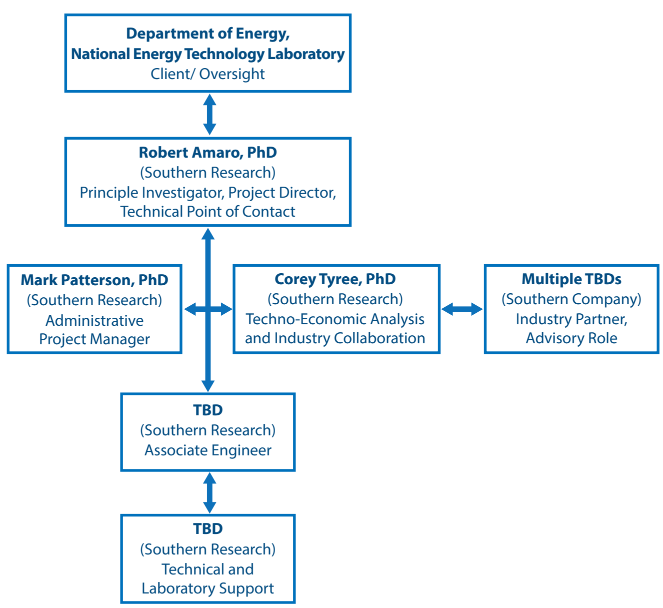
Eroded trailing edge of last row blade

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

Southern Research Institute will 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 that will be calibrated accounts for coupled thermomechanical damage accumulation, material microstructural evolution, and material or component erosion or 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 particular input data such as inelastic strain, hydrostatic stress, temperature-time waveforms, initial microstructure, etc., from a component-specific finite element analysis, to predict component lifetime. The work will be performed in conjunction with Southern Company, an industry partner and owner of a coal-fueled power plant. The project will include four primary tasks: (1) project management and planning, (2) materials characterization, (3) damage model calibration, and (4) component life model calibration and verification. The primary goal is to provide calibrated life estimation models for a DR22 steel Y-block and a Jethete stainless steel turbine blade.

The tool developed will enable lifetime prediction as a function of historical plant steam-cycle operational data as well as any potential proposed future operational cycling. Consequently, existing coal-fueled power plants will be able to operate safely for longer periods of time and at higher efficiencies, thereby reducing the economic and environmental impact of the existing coal power plant fleet.



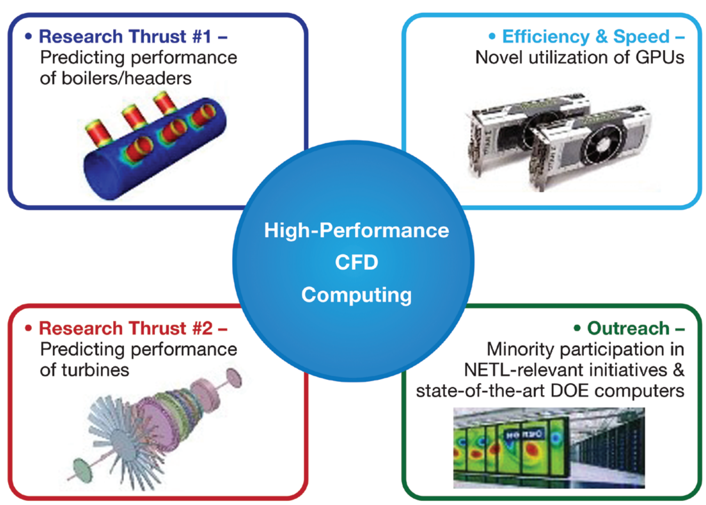
Project Organizational Chart.

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 Ansys, Inc. Fluent computational fluid dynamics (CFD) code used in this project. A sizeable portion of operational damage in fossil fuel power plants occurs in the boiler's superheater/reheater headers; therefore, Objective 2 will be to make use of these GPU-parallelized simulations to understand the durability of and damage mechanisms to these header structures under various cycling and operational modes. Objective 3 will be to assess subsequent damage mechanisms by quantifying and calculating the effects of particulates within "steam in" boilers as a function of both boiler geometry and operating conditions. Objective 4 will combine the results of the previous three objectives to create a holistic, comprehensive, and systems-level assessment of damage rates under different cycling modes.

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



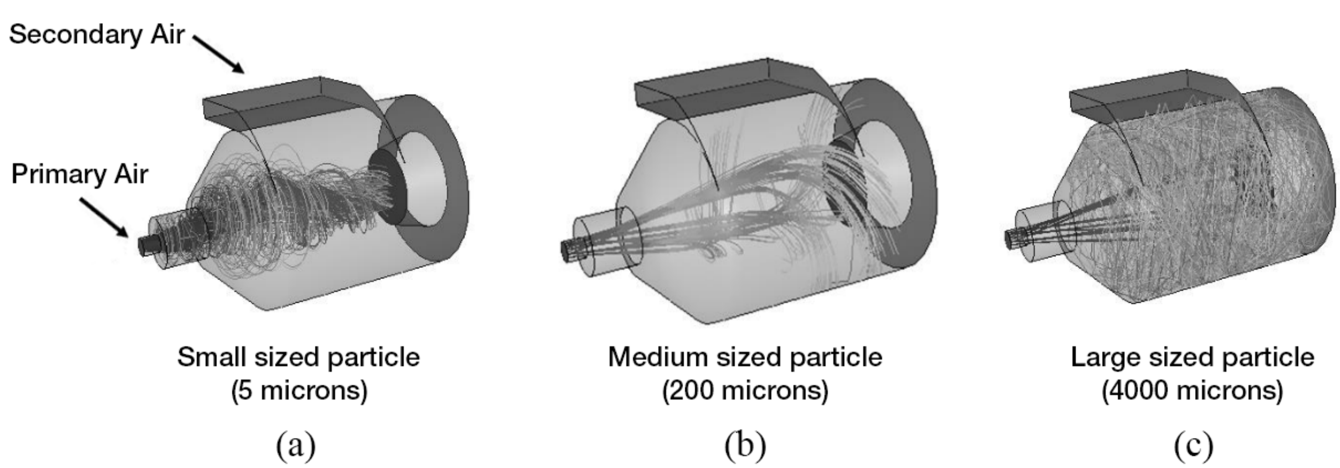
High-performance CFD computing forms a central theme and unifies research thrusts, efficiency, outreach, and technological impact in this HBCU-OMI project.

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.

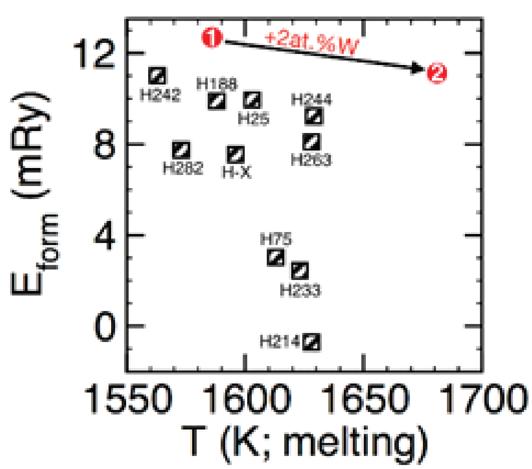
COMPUTATIONAL MATERIALS DESIGN

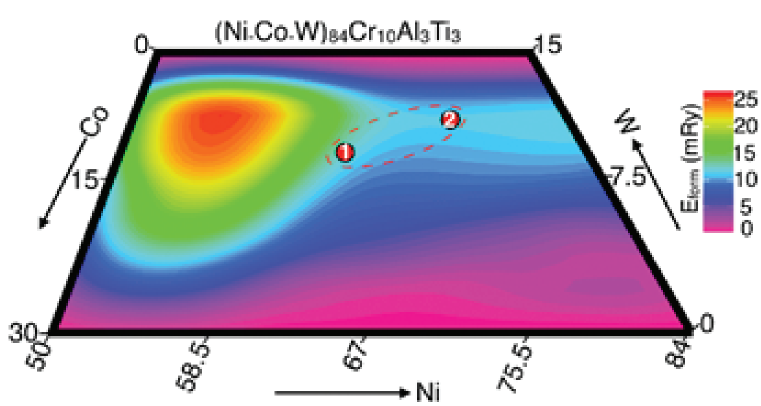
Predictive Design of Novel Ni-based Alloys

Performer	**Ames National Laboratory**
Award Number	FWP-AL-19-510-097
Project Duration	04/08/2019 – 09/30/2021
Total Project Value	$ 750,000
Technology Area	Plant Optimization Technologies

Ames Lab proposes to increase operating temperatures of the Ni-based superalloys through controlled alloying additions. Additions will be chosen using a three-pronged approach to computational design and optimization of the alloys: (i) alloying additions aimed at preventing the formation of topologically close-packed (TCP) phases, (ii) improving the liquidus temperature of the gamma phase, and (iii) preventing microstructural coarsening by improving the microstructural stability of the gamma prime phase. Beyond the effect of alloying additions and processing on the melting temperatures, Ames will investigate the effect of alloying additions on the alloy's high-temperature oxidation resistance. Differing from a number of traditional approaches to high-temperature oxidation, recession rates rather than parabolic kinetics will be employed to ascertain the oxidation resistance. Once precipitation and coarsening kinetics are established for given chemistries and temperature, a regression-decision approach will be developed for creating an optimization "surface" of alloy design parameters (chemistry, processing parameters, and desired melting/liquidus temperatures and oxidation resistance) enabling optimization of the Ni-based alloys.

Thus, Ames proposes a novel alloy design and optimization strategy for Ni-based alloy systems that establishes the interrelation between alloying additions, processing conditions, and performance metrics. The approach is based on destabilization of deleterious phases through alloying additions, while controlling the microstructure and near-surface chemistries to design an oxidation-resistant high-temperature alloy.





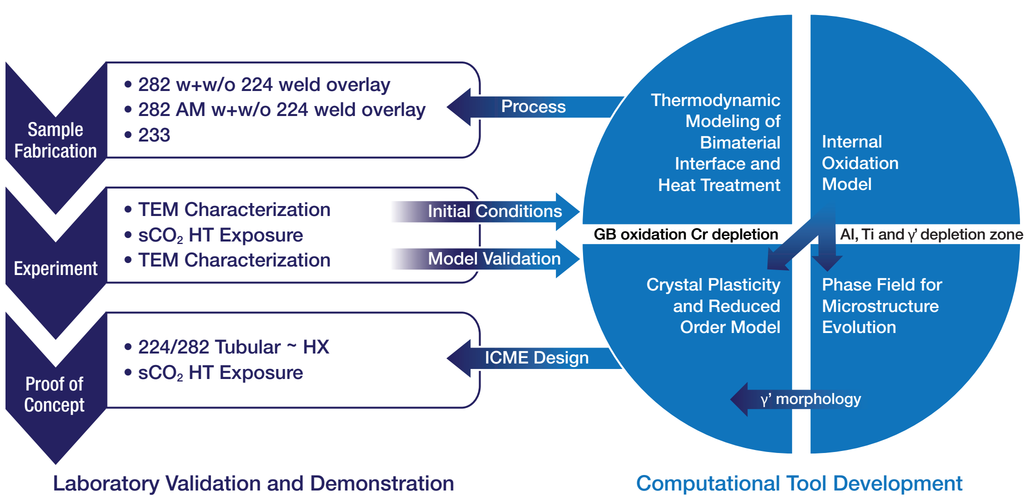
Left chart shows how Eform varies with experimentally determined Tm for common Haynes alloys. Right graphic shows (on a reduced pseudo-quaternary plot) how Eform varies with content of the refractory element; W, with Ni and Co.

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 – 09/30/2020
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.



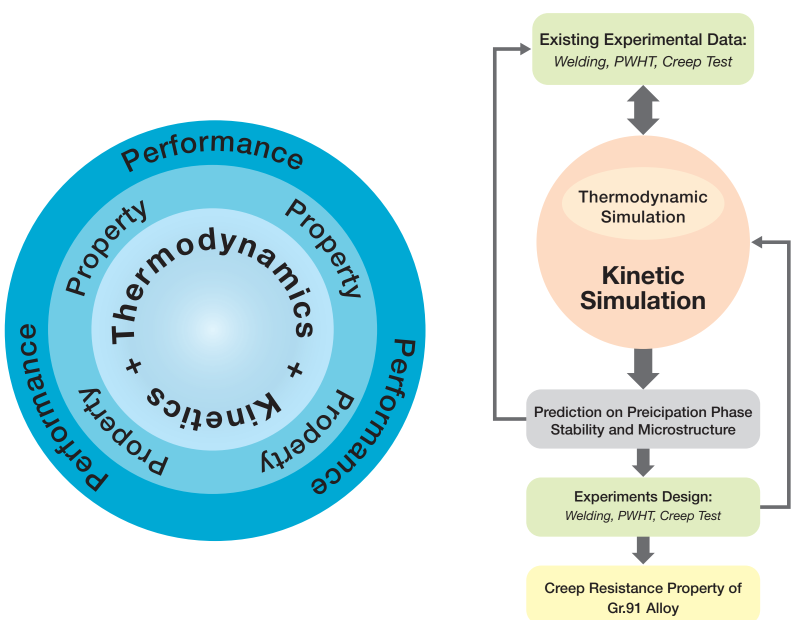
Computational tool development pathway to support multi-material additive manufacturing for high-temperature heat exchange systems.

The Fundamental Creep Behavior Model of GR.91 Alloy by Integrated Computational Materials Engineering (ICME) Approach

Performer	**Florida International University**
Award Number	FE0027800
Project Duration	08/01/2016 – 01/31/2021
Total Project Value	$ 250,000
Collaborator	Ohio State University
Technology Area	University Training and Research

NETL is partnering with Florida International University to investigate the fundamental creep cracking mechanism of the Grade 91 alloy under advanced power generation operating conditions to establish links among composition, processing parameters, phase stability, microstructure, and creep resistance using the ICME approach. Specifically, the project team will predict the phase stability and microstructure of Grade 91 base alloy and weldment with the computational thermodynamics and kinetics–calculation of phase diagrams (CALPHAD) approach; perform welding, heat treatment, and creep testing of the Grade 91 alloy; develop a model that will provide an excellent match with experimental data from current and previous work on Grade 91 alloy; and predict how to improve the long-term creep resistance for the Grade 91 family of alloys.

The model will improve the creep resistance of Grade 91 alloys for use in advanced fossil-fueled power generation systems and other applications, thus increasing fossil-fueled power generation efficiency and reducing emissions.



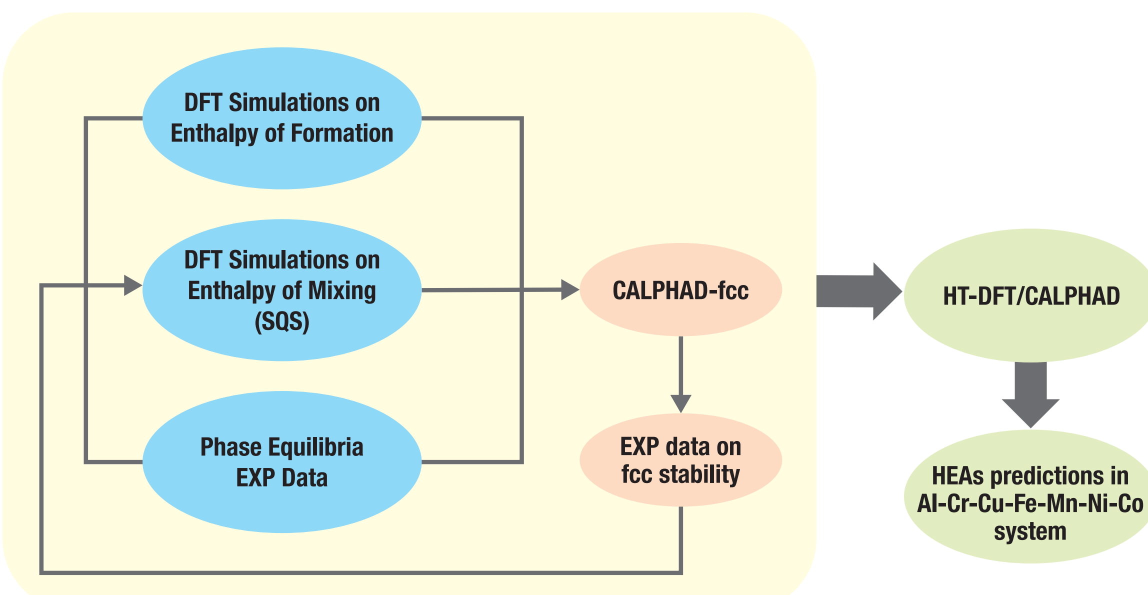
Materials design using ICME approach.

The Novel Hybrid Start-off Model of High Performance Structural Alloys Design for Fossil Energy Power Plants

Performer	Florida International University
Award Number	FE0030585
Project Duration	08/01/2017 – 07/31/2020
Total Project Value	$ 250,000
Technology Area	University Training and Research

The project team will develop an ab initio approach to quickly design new high-performance structural alloys for use in fossil energy power plants. The specific project objectives are to (1) conduct density functional theory (DFT) simulations for the selected Fe-Co-Cr-Ni quaternary system; (2) develop a thermodynamic database specifically for the face-centered cubic (FCC) phase of the selected system; (3) predict the compositions of new alloys in the selected system and compare them to experimental observations; (4) develop a hybrid high-throughput DFT/CALPHAD model capable of efficiently predicting the compositions of new alloys for multicomponent systems; and (5) apply the approach to make predictions on high-entropy alloys in an Al-Cr-Cu-Fe-Mn-Ni-Co multicomponent system.

The project will culminate in the development of a hybrid model based on high-throughput DFT simulations and computational thermodynamics to provide guidance on how to identify new multicomponent, high-performance structural alloys with much less computational effort. The model will address the extensive computational time needed for DFT when designing new alloys.



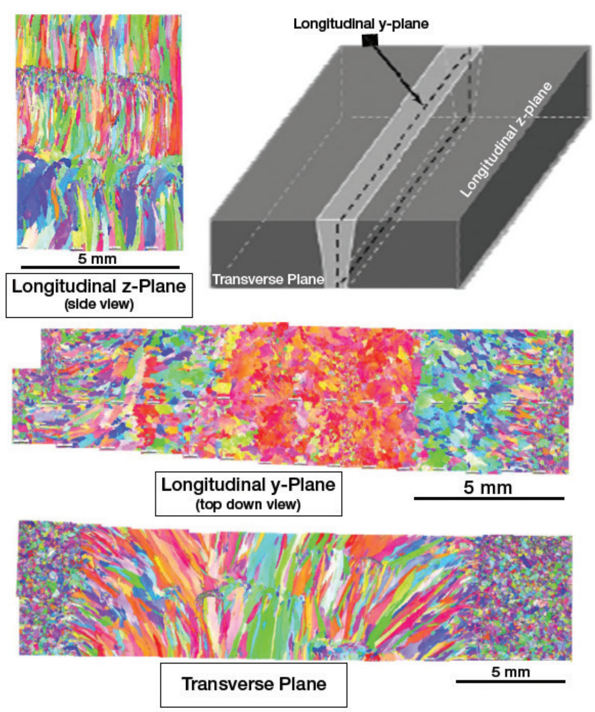
Development of the hybrid ab initio/CALPHAD approach.

Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications

Performer	**Idaho National Laboratory (INL)**
Award Number	FWP-B000-14029
Project Duration	06/01/2015 – 03/31/2020
Total Project Value	$ 955,000
Technology Area	Coal Utilization Science

Idaho National Laboratory (INL) will improve the capability to perform accurate and rapid computational modeling of the long-term mechanical behavior of nickel superalloy weldments that will be used in advanced fossil energy power cycles. An improved capability to predict the long-term behavior of weldments will allow materials scientists and structural component designers to optimize the use of advanced materials in advanced fossil energy applications. In this project INL will develop a microstructure-based creep model for nickel superalloys and add it to a computational platform, Multiphysics Object-Oriented Simulation Environment (MOOSE), that INL has developed for multi-scale simulation of the behavior of high-temperature materials in nuclear power plant applications.

This project will develop improved computational methods to predict the long-term behavior of advanced materials and structural components in fossil energy power plants that will reduce the time and expense of developing and qualifying new materials and enable a more cost-effective use of advanced materials at higher operating temperatures and pressures, which will result in higher-efficiency fossil fuel based power systems.



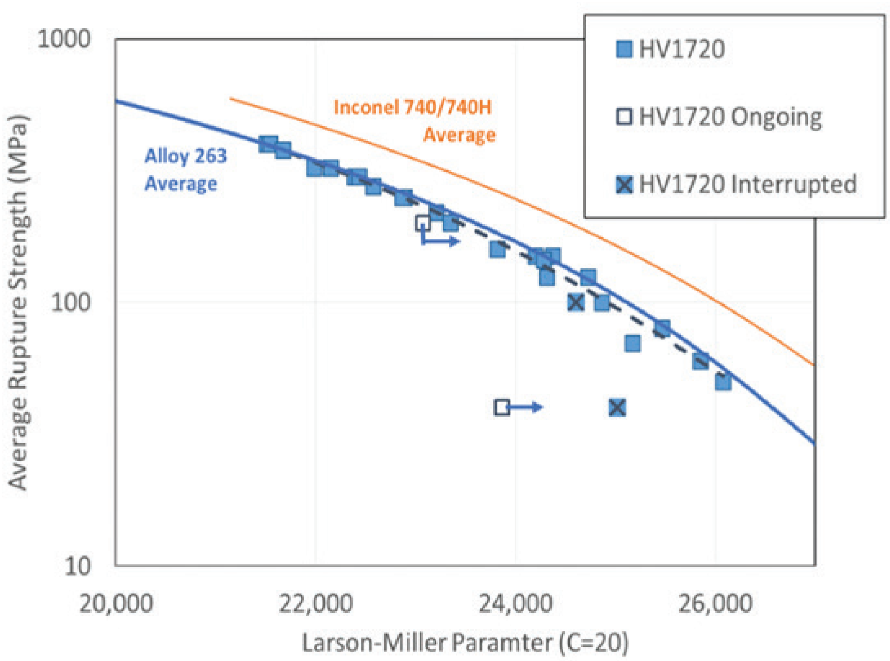
Microstructure of base metal, heat affected zone, and weld metal.

Development of a Physically-Based Creep Model Incorporating Eta Phase Evolution for Nickel-Base Superalloys

Performer	**Michigan Technological University**
Award Number	FE0027822
Project Duration	08/15/2016 – 08/14/2020
Total Project Value	$ 399,996
Technology Area	University Training and Research

NETL is partnering with the Michigan Technological University to develop a physically based creep model for Nimonic 263 that synthesizes known creep behavior based on gamma prime (γ') strengthening to gain a new understanding of the effects of eta (η) phase on creep performance at long service times in fossil energy power plants. This project team will develop heat treatments for commercial Nimonic 263 to obtain a mixture of both eta and gamma prime phases prior to creep testing, with the γ' distribution being as close to commercial Nimonic 263 as possible; conduct creep tests on these materials at the Electric Power Research Institute; fully characterize microstructures and deformation mechanisms during creep for all three alloys (standard Nimonic 263, Nimonic 263 heat-treated to contain η + γ', and the Michigan Tech-modified Nimonic 263 alloy that contains only η); and use the knowledge gained to develop and validate a physically-based creep model that synthesizes known gamma prime creep behavior to gain a new understanding of the effects of eta phase on creep performance.

The results will enhance life prediction, component design, and alloy selection for advanced fossil energy power plant systems.



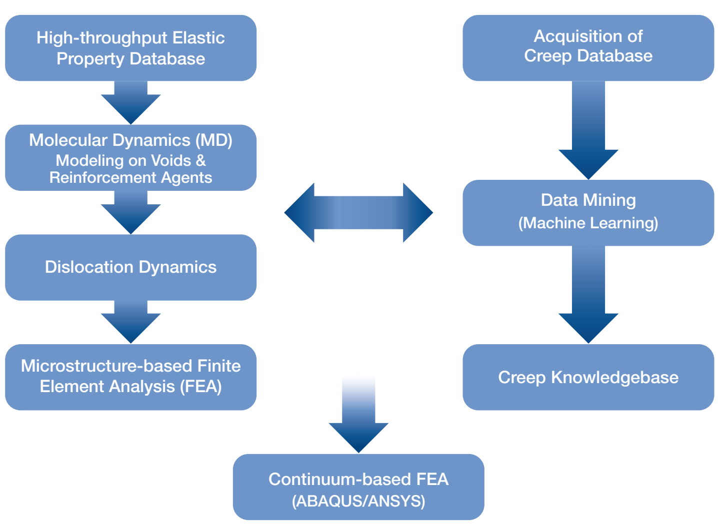
Alloy 20, Widmanstätten microstructure, creep.

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	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2020	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2020	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2023	09/01/2017 – 09/30/2023
Funding to Date 09/01/2017-9/30/2021	$ 2,074,000	$ 981,000	$ 997,000	$ 590,000	$ 3,448,000	$ 2.604,000	$ 1,520,000
Total Value (All)	$ 9,610,000						
Technology Area	Coal Utilization Science						

Affordable, durable, heat-resistant alloys are necessary for improving the existing fleet of fossil energy (FE) 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 FE 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, 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:

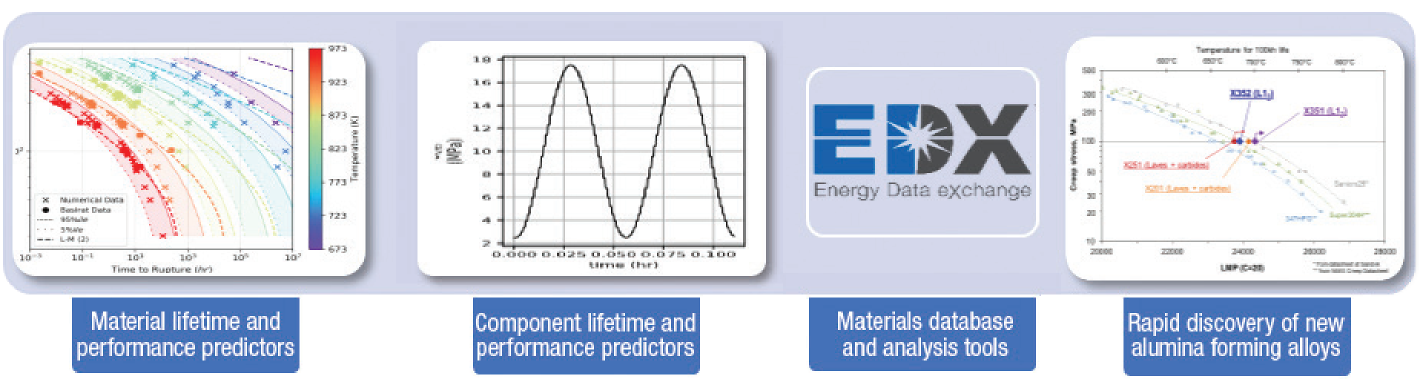
- A suite of eXtremeMAT models was developed to predict creep rupture life using a minimum of short-term creep tests. This model has been extended to multi-axial stresses and cyclic loading (i.e., ratcheting) conditions.

- 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 the 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/

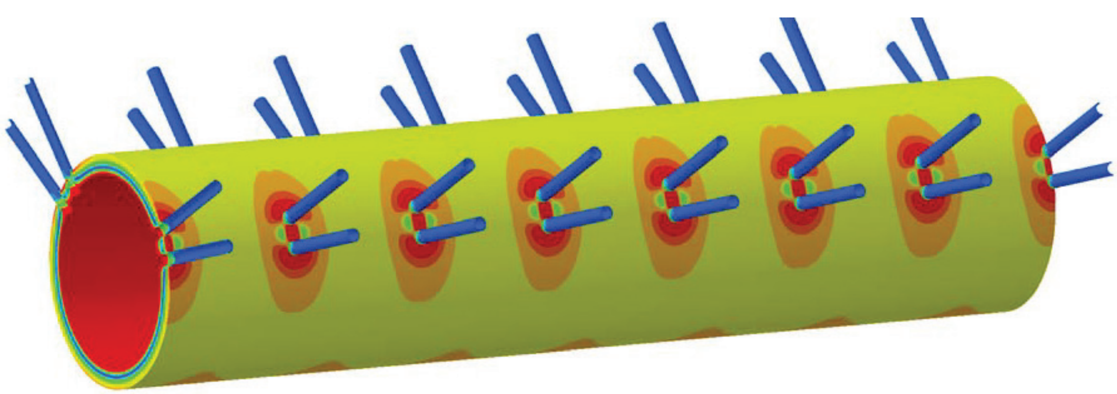


Alloy for Enhancement of Operational Flexibility of Power Plants

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.



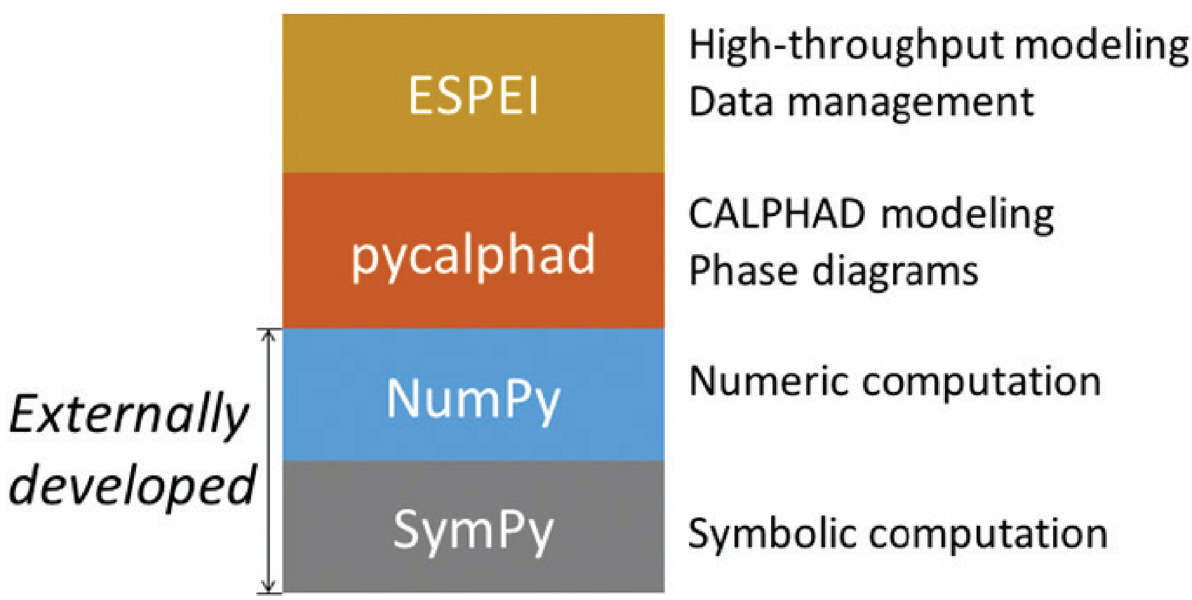
Stress contour plot of a steam header.

High Throughput Computational Framework of Materials Properties for Extreme Environments

Performer	**Pennsylvania State University**
Award Number	FE0031553
Project Duration	12/15/2017 – 12/14/2020
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.

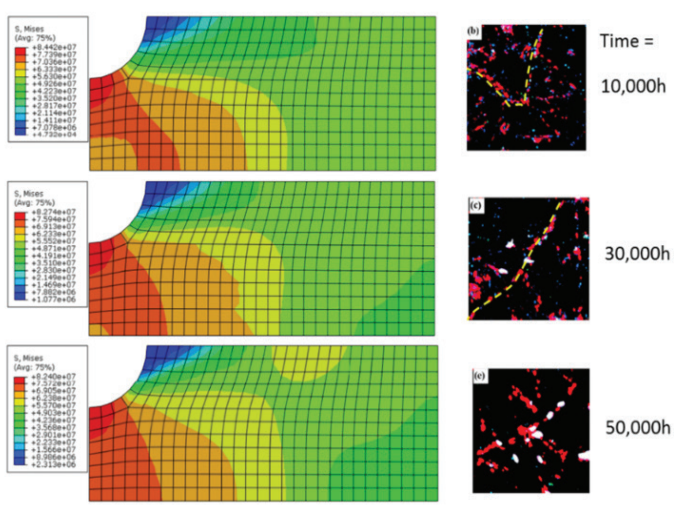


ESPEI-2.0 software stack.

Improved Models of Long-Term Creep Behavior of High Performance Structural Alloys for Existing and Advanced Technologies Fossil Energy Power Plants

Performer	**QuesTek Innovations, LLC**
Award Number	SC0015922
Project Duration	06/13/2016 – 01/31/2020
Total Project Value	$ 1,164,586
Technology Area	Plant Optimization Technologies

NETL is partnering with QuesTek Innovations LLC to develop a robust creep modeling toolkit to predict the long-term creep performance of materials for base alloys and weldments in fossil energy systems under wide thermal and mechanical conditions. Precipitation modeling using thermodynamic databases will provide fundamental quantities that will be used as inputs for upscaling strategies and methods. The goal is to establish microstructure-sensitive models that capture the different creep mechanisms observed in ferritic steels and integrate the models into QuesTek's Defense Advanced Research Projects Agency–Accelerated Insertion of Materials (DARPA–AIM) efforts to predict the variability of the creep strength as a function of the microstructure and service conditions. In the Phase I effort, the methods proposed have been demonstrated to predict creep life near 100,000 hours for P91 ferritic steels with microstructure inputs obtained from the National Institute of Material Science. In Phase II, the tools will be expanded and exercised in wider operating conditions including different temperatures and applied stresses in order to predict creep behaviors with over 300,000 hours creep life. Integration of precipitate evolution schemes into the long-term material behavior (i.e., stability of microstructure and the different phases over long periods), along with a refined uncertainty quantification of various material and process parameters, will be assessed and calibrated in Phase II. Additionally, the methodology that is developed would be applicable to alternative material systems and microstructures through additional modules that capture the relevant mechanisms of creep. Accurate and efficient quantification of material properties for advanced ultrasupercritical (AUSC) boilers will directly enhance the success of DOE's crosscutting research and new alloy development program and provide significant public benefits.



Model prediction with microstructure evolution.

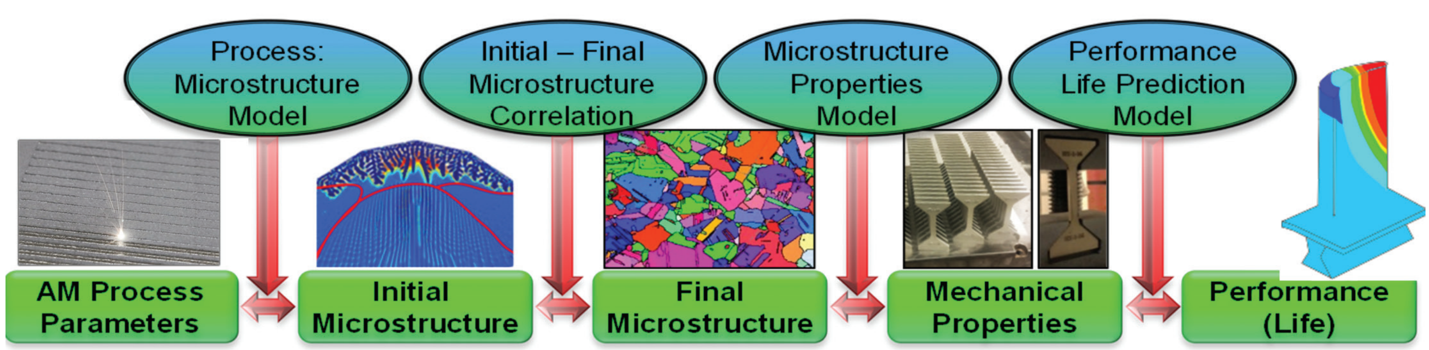
Computation Tools for Additive Manufacture of Tailored Microstructure and Properties

Performer	**Raytheon Technologies Research Center**
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 (formerly United Technologies Research Center) is demonstrating the application of computational methods and tools on microstructure evolution and mechanical properties prediction for additively manufactured (AM) nickel-based superalloy parts. Models is being 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 is being demonstrated using these models. An integrated computational materials engineering framework that connects process, structure, properties, and performance is being 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.



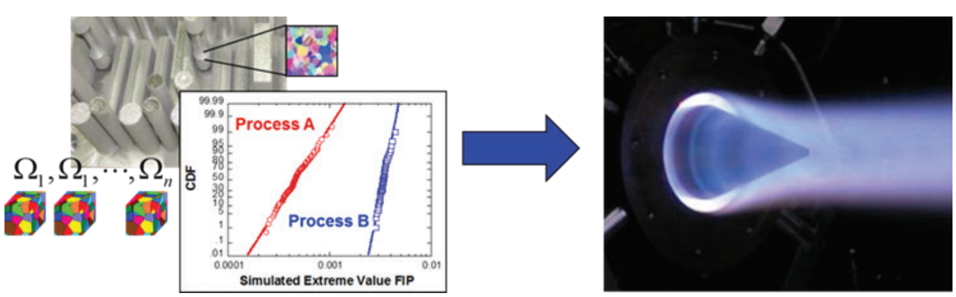
An ICME (Integrated Computational Materials Engineering) framework being developed by Raytheon Technologies Research Center that connects Process – Structure - Properties – Performance by four models

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.



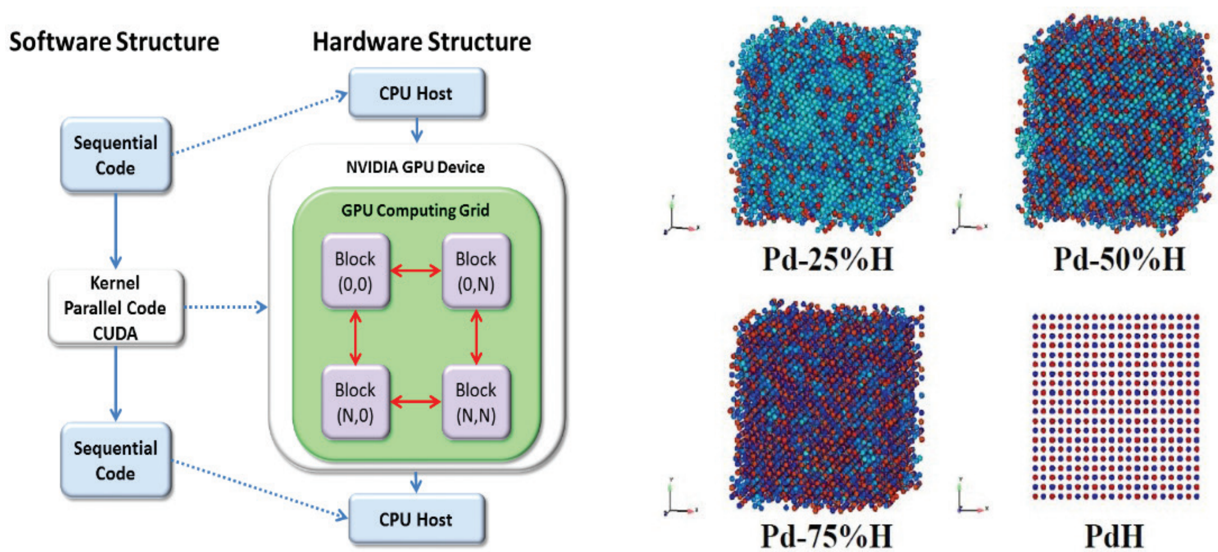
Modeling of additively manufactured parts leading to low-loss additively manufactured RDE injector.

Large-Scale, Graphics Processing Unit (GPU)-Enhanced Density Functional Tight Binding (DFTB) Approaches for Probing Multi-Component Alloys

Performer	**University of California - Riverside**
Award Number	FE0030582
Project Duration	08/01/2017 – 06/30/2021
Total Project Value	$ 250,000
Technology Area	Coal Utilization Science

The objectives of this project are to develop, analyze, and introduce (1) accurate intermolecular potentials and (2) graphics processing unit enhancements to the density functional tight binding approach for high-throughput ab initio molecular dynamics calculations of multi-component alloys at elevated temperatures. Specifically, this transformative approach utilizes two complementary pathways that will employ a high degree of coordination and communication between them to realize a final rigorously sound and validated computational capability upon completion.

The capabilities developed in this project will provide accurate, efficient, and reduced-cost assessment of alloy structural performance at elevated temperature and pressure operational conditions in advanced fossil energy power plants.



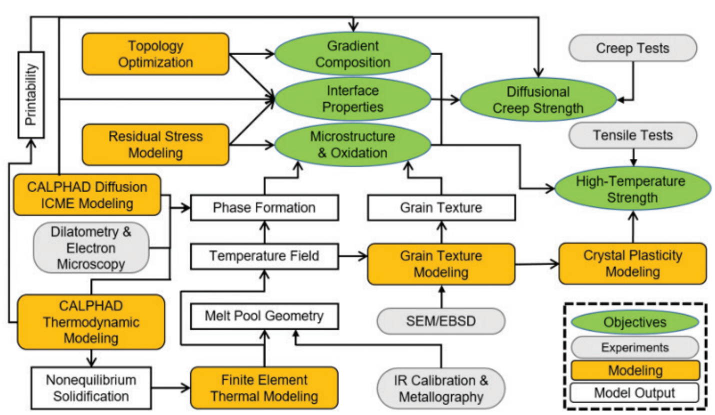
Large-scale simulations of alloy systems.

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

Advanced Reaction Systems

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022405
Project Duration	04/01/2019 – 03/31/2020 (EY 2019)*
Total Project Value	$ 2,260,000 (FY19)
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 Fossil Energy 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.

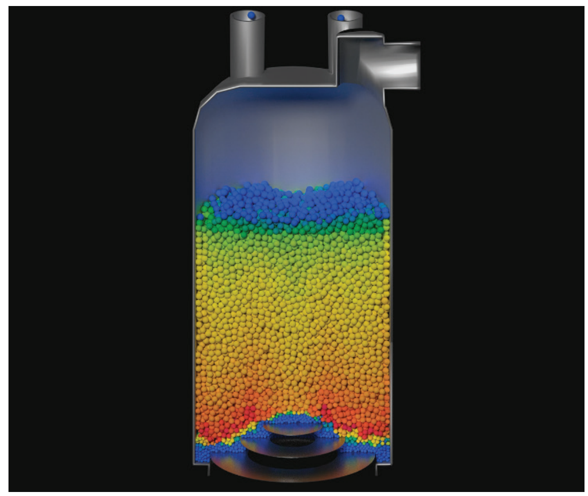
- *MFiX-PIC (Particle-In-Cell):* An Eulerian-Lagrangian code that treats the fluid phase as a continuum and models solids as discrete "parcels" of particles, with each parcel representing a group of real particles with the same physical characteristics. This is an emerging capability that will be brought to maturity for use in advanced reactor simulations over the course of 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.

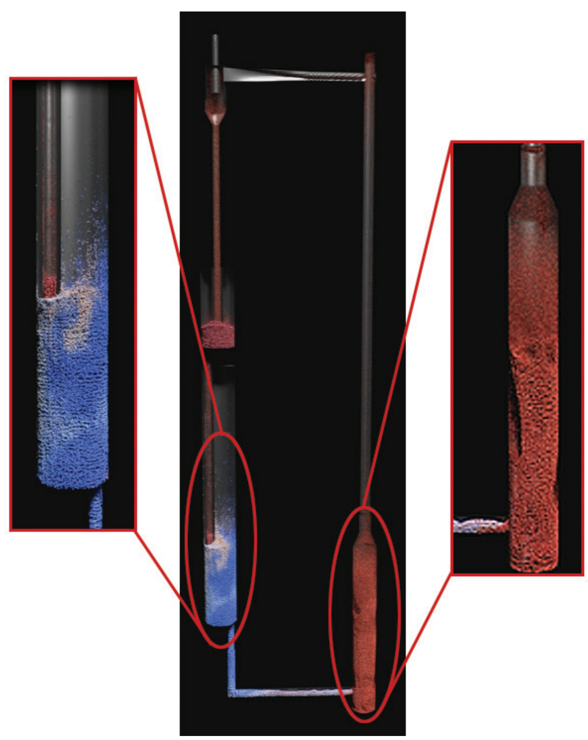
In contrast to expensive, proprietary commercial CFD software, the MFiX suite and associated toolsets are open-source codes that are developed, validated, and supported in-house by NETL's software development and application specialists. As open-source codes, the MFiX suite can be customized for novel applications. The MFiX 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 when CFD was in its infancy until the present day where 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'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 – 03/31/2021
Total Project Value	$ 2,643,000
Technology Area	Coal Utilization Science

The computational fluid dynamics (CFD) for advanced reactor design (CARD) efforts continue the development, enhancement, and application of the National Energy Technology Laboratory's (NETL's) suite of multiphase computational fluid dynamics software tools based on the NETL Multiphase Flow with Interphase eXchange (MFiX) Software Suite that are used for design and analysis of novel reactors and devices for fossil energy (FE) applications.

Science-based models are critical tools for reducing the risk, cost, and time required for development of novel FE 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 6,300 registered users of the MFiX Suite and associated toolsets including industry, academic, and national laboratories.

The CARD portfolio includes 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 FE programmatic goals.
- In collaboration with industry partners, apply computational tools and FE/NETL supercomputing resources to aid in understanding and optimizing circulating fluidized bed (CFB) boiler performance under challenging operating conditions of interest to operators.
- Google's TensorFlow™, 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 (MFS) web portal (https://mfix.netl.doe.gov).

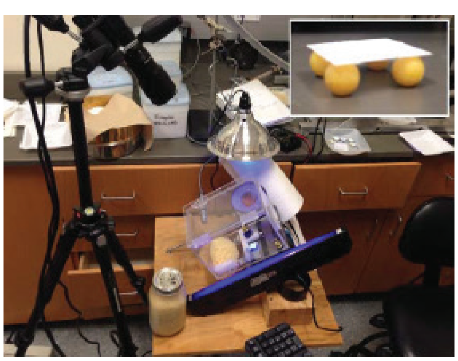
MFIX-DEM Enhancement for Industry-Relevant Flows

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.

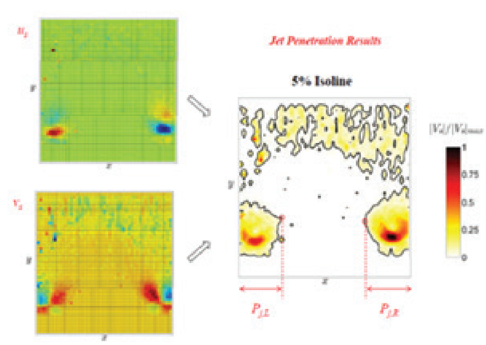
The goal is to achieve an increase in performance of two orders of magnitude; a refined estimate will result from the profiling effort. Over thirty Particulate Solid Research, Inc. consortium member companies were surveyed at the beginning of the project to identify industrial needs. In Phase 2, the 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



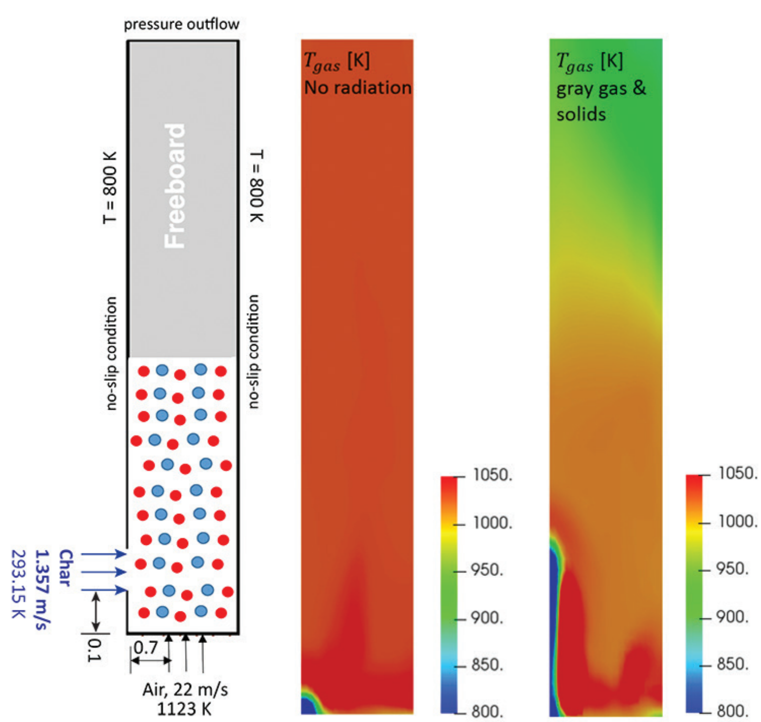
Horizontal jet experiments particle tracking post-processing.

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
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
DARPA-AIM .... Defense Advanced Research Projects Agency—Accelerated Insertion of Materials
DEM .... discrete element model
DFT .... density functional theory
DFTB .... density functional tight binding
DOE .... Department of Energy
DofE .... design of experiments
DPE .... direct power extraction
DTMM .... digital twin material model
EY .... execution year
FCC .... face-centered cubic
FE .... Office of Fossil Energy
Fe .... iron
FWP .... Field Work Proposal
FY .... fiscal 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
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
MOOSE .... Multiphysics Object Oriented Simulation Environment
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

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

WAAM .... wire-arc additive manufacturing

γ' .... gamma prime

η .... eta

NOTES

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WEBSITES:

https://netl.doe.gov/coal/program134

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https://www.energy.gov/fe/science-innovation/clean-coal-research/crosscutting-research/coal-utilization-science

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

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