HYDROGEN
with Carbon Management

2023

SIMULATION-BASED ENGINEERING

PROJECT PORTFOLIO

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

DISCLAIMER

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HYDROGEN WITH CARBON MANAGEMENT

As part of the U.S. Department of Energy (DOE) Office of Fossil Energy's Hydrogen with Carbon Management (HCM) program, NETL research focuses on production and evaluation of carbon-neutral hydrogen (i.e., coupled to carbon capture and storage (CCS)) as a fuel and development of technologies to use carbon-neutral hydrogen from any source.

The HCM program's efforts are promoted by the Department of Energy (DOE) Hydrogen Shot, with a goal of reducing clean hydrogen costs by 80% to $1 per 1 kilogram (kg) within 1 decade (1-1-1) while expanding employment of the U.S. energy workforce. Seeking a cost-competitive decarbonized alternative to traditional fossil fuels, HCM has a research and development portfolio consisting of a new generation of carbon neutral or net-negative greenhouse gas emissions technologies. HCM comprises six subprogram activities: (1) Gasification Systems, (2) Advanced Turbines, (3) Reversible Solid Oxide Fuel Cells (R-SOFCs), (4) Advanced Energy Materials, (5) Sensors, Controls, and Other Novel Concepts, and (6) Simulation-Based Engineering.

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

Gasification Systems: The DOE Gasification Systems program is developing innovative modular designs for converting diverse types of carbonaceous feedstocks into clean synthesis gas to enable the low-cost production of clean hydrogen, electricity, transportation fuels, chemicals, and other useful products to suit market needs. Advancements in this area will help enable syngas-based technologies to play a role in economy-wide decarbonization in multiple energy sectors while remaining competitive in both domestic and international markets, and spur on the use of abundant domestic carbon feedstock resources, in turn contributing towards increased energy security and promoting justice through reviving depressed markets in traditional coal-producing regions of the United States.

Advanced Turbines: The NETL Advanced Turbines Program is focused on the development of advanced turbine technologies that will accelerate turbine performance, efficiency, and cost effectiveness beyond the current state of the art. The program will provide tangible benefits to the public in the form of options for eliminating CO_2 emissions, lowering the cost of electricity, and reducing emissions of criteria pollutants. The efficiency of combustion turbines has steadily increased as advanced technologies have provided manufacturers with the ability to produce highly advanced turbines that operate at very high temperatures. Further increases in efficiency are possible through the continued development of advanced components, combustion technologies, material systems, thermal management, and novel turbine-based cycles. The Advanced Turbines Program supports four key technologies that will advance clean, low-cost power production from fossil energy resources while providing options for CO_2 mitigation. These key technologies include: (1) Advanced Combustion Turbines, (2) Pressure Gain Combustion (PGC), (3) Turbomachinery for Supercritical Carbon Dioxide (sCO_2) Power Cycles, and (4) Modular Turbine-Based Hybrid Heat Engines. DOE's research and development in advanced turbines technology develops and facilitates low-cost advanced energy options for carbon-negative energy ecosystems.

Reversible Solid Oxide Fuel Cells (R-SOFCs): The NETL Reversible Solid Oxide Fuel Cell (R-SOFC) program maintains a portfolio of RD&D projects that address the technical issues facing the commercialization of solid-oxide fuel cell (SOFC) and R-SOFC technologies and pilot-scale test projects intended to validate the solutions to those issues. To successfully complete the maturation of these technologies from their present state to the point of commercial readiness, the program's efforts are channeled through three key technology areas, each of which has its respective research focus: (1) Cell Development, (2) Core Technology, and (3) Systems Development.

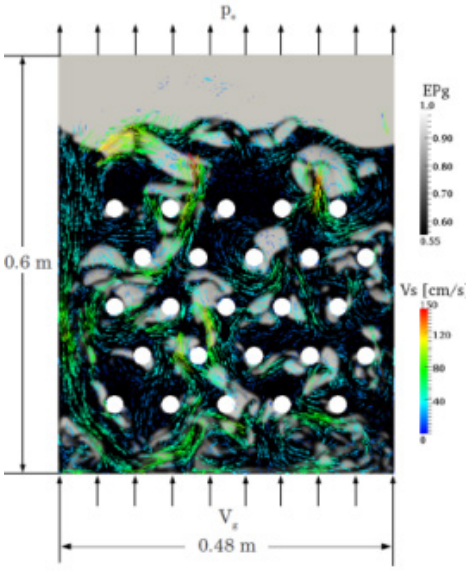
Advanced Energy Materials: The Advanced Energy Materials program drives to characterize, produce, and certify advanced alloys and high-performance materials that are key to realizing dispatchable, reliable, high-efficiency decarbonized power generation from hydrogen. In addition, the program aims to encourage change and stimulate innovation in the high-performance materials value chain to spur U.S. competitiveness and enable achievement of 2050 zero-emission goals. Materials of interest include those that enable components and equipment to perform in the high-temperature, high-pressure, corrosive environments of advanced energy systems with specific emphasis on durability, availability, and cost. The key focus areas of this program include: (1) development of a robust domestic materials supply chain, (2) lifetime prediction and rapid repair critical to manage a flexible fleet of generators that enable high penetration of renewables into the grid, and (3) low-cost, high performance alloy development to enable meeting 2050 zero-emission goals.

Sensors, Controls, and Other Novel Concepts: The NETL Sensors, Controls, and Other Novel Concepts program conducts research and development for technologies that will provide pivotal insights into optimizing performance, reliability, and availability of integrated energy and carbon management systems. NETL develops, tests, and matures novel sensor and control technologies that are operable in next-generation energy systems, including hybrid plants incorporating components such as hydrogen-powered turbines and fuel cells, renewables, and energy storage applications. These sensors enable responsiveness to varying conditions in real time, maintaining high efficiencies and reducing emissions. This research will aid in the achievement of DOE goals, which include net-zero carbon emissions in the energy sector by 2035 and a decarbonized wider economy by 2050.

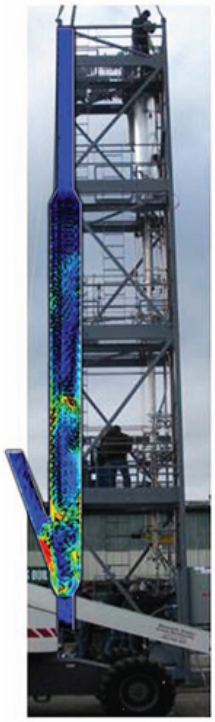
Simulation-Based Engineering: NETL's Simulation-Based Engineering (SBE) program supports the development and application of innovative physics- and chemistry-based models and computational tools at multiple scales (i.e., atomistic, device, process, grid, and market) in order to accelerate development and deployment of clean, advanced fossil fuel technologies. The SBE program combines a multidisciplinary approach comprising technical knowledge, software development, computational power, data repositories, experimental facilities, and unique partnerships to support research into timely and accurate solutions for fossil and sustainable energy and carbon management systems. Analysis and visualization tools are manipulated to gain scientific insights into complex, uncertain, high-dimensional, and high-volume datasets. The information generated is then collected, processed, and used to inform research that combines theory, computational modeling, advanced optimization, physical experiments, and industrial input.

SIMULATION-BASED ENGINEERING

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



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



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

Research through Simulation-Based Engineering develops accurate and timely computational models of complex reacting flows and components relevant to advanced power systems. Model development and refinement is achieved through in-house research and partnerships to utilize expertise throughout the nation, such as NETL's University Training and Research programs. Partnerships have also been formed with other national laboratories through the Institute for the Design of Advanced Energy Systems (IDAES).

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

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

ADVANCED PROCESS SIMULATION

Carbon Solutions, LLC:
Negative CO_2 Emission Transition Roadmap (NECTAR):
A Rapid Decision Support Tool for Negative CO_2 Emission Hybrid Energy System Development and Analysis 9

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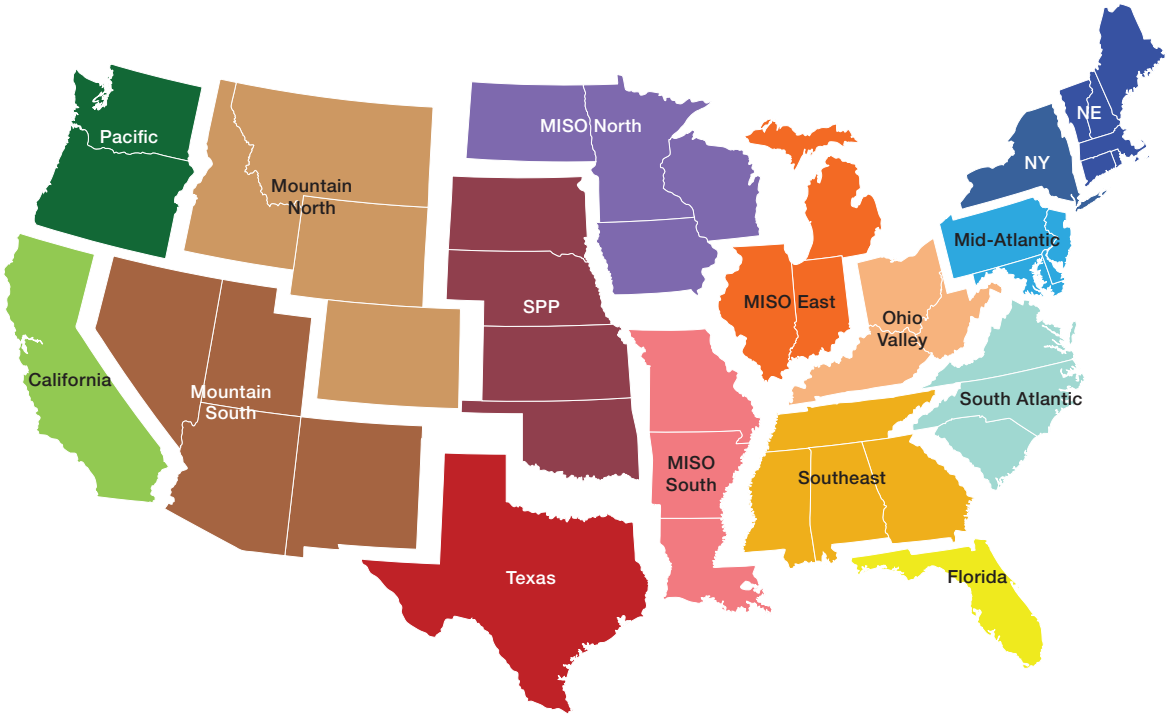
Negative CO_2 Emission Transition Roadmap (NECTAR): A Rapid Decision Support Tool for Negative CO_2 Emission Hybrid Energy System Development and Analysis

Performer	**Carbon Solutions, LLC**
Award Number	SC0022486
Project Duration	02/14/2022 – 02/13/2023
Total Project Value	$ 206,499
Technology Area	Coal Utilization Science

Negative CO_2 Emission Transition Roadmap (NECTAR) will be a decision support tool for expansion planning for decarbonization. NETL's Institute for the Design of Advanced Energy Systems (IDAES) will be used to quantitatively evaluate how direct air capture and carbon storage (DACCS) should be coupled with primary heat sources. Carbon Solutions LLC's SIMCCSPRO™ software will be used to determine CO_2 pipeline networks that optimally connect sources of CO_2 to sequestration locations. The Electric Power Research Institute's U.S. Regional Economy, Greenhouse Gas, and Energy (US-REGEN) Model, an economy-wide expansion planning model, will also be used in NECTAR. A data visualization interface will be developed to allow users to try out and optimize various process-, region-, and systems-level parameters. The target end users are utilities and regulators.

Successful development of NECTAR will enable optimization of DACCS systems in a context of heat sources and CO_2 transport and storage infrastructure on a regional or nationwide basis. This will promote the development and implementation of DACCS systems, a necessary component in the establishment of a net-zero carbon economy.



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

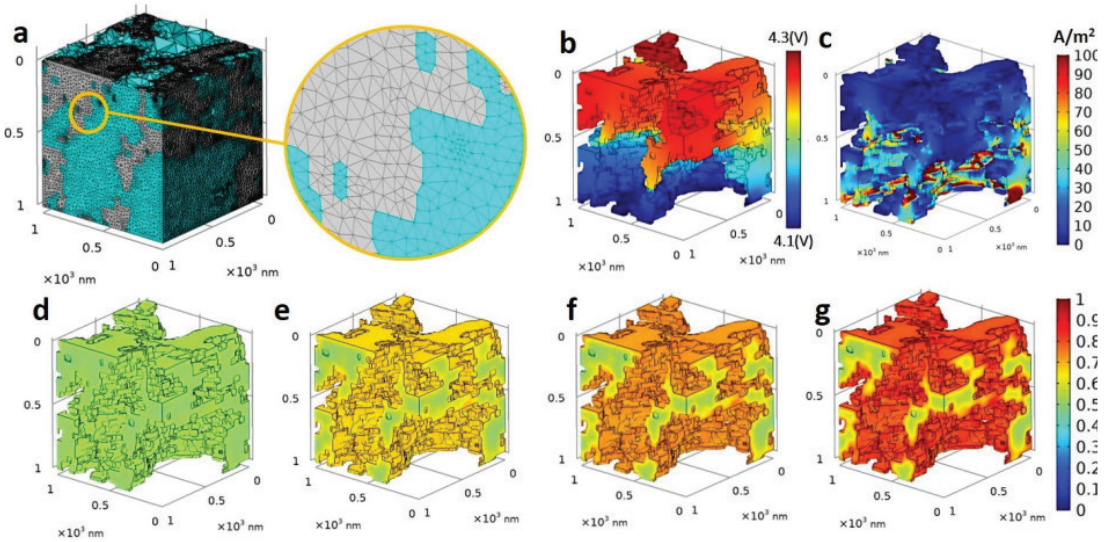
Performer	**Howard University**
Award Number	FE0032092
Project Duration	09/01/2021 – 08/31/2024
Total Project Value	$ 399,935
Technology Area	University Training and Research

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

1. Modeling and simulation methods for coupled multiphysics phenomena involving EM, plasma physics, thermal and fluid dynamics, and quantum chemistry across multiple spatial scales from macro, meso, to microscopic scales and temporal scales from nanoseconds to minutes.
2. Simulation-guided designs for EM energy assisted high-throughput, high-yield, and low-cost hydrogen generation from fossil fuels such as methane and methanol.

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

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



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

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

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022423
Project Duration	01/01/2018 – 03/31/2024
Total Project Value	$ 9,571,881
Collaborator	Carnegie Mellon University; Lawrence Berkeley National Laboratory; Notre Dame; Sandia National Laboratories; West Virginia University
Technology Area	Coal Utilization Science

Over the next decade, hundreds of billions of dollars will be invested in new 21st century energy systems and processes that are more dynamic and interconnected than ever before. The Institute for Design of Advanced Energy Systems Integrated Platform (IDAES) helps companies, technology developers, and researchers to model, design, and optimize these complex systems, potentially resulting in tens of billions of dollars in savings. As an optimization-based, integrated process modeling platform, IDAES enables rigorous analysis of multi-scale, dynamic processes, and operating scenarios to improve efficiency of existing systems and develop next-generation energy systems.

The IDAES Integrated Platform 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 and structured optimization problems. IDAES includes tools for (1) process synthesis and conceptual design, including process intensification; (2) process design, optimization, and 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.

IDAES has an active and growing user community from multiple industries — including power generation and distribution, petrochemical manufacturing, pharmaceuticals, and consumer products — that will increasingly benefit from the capabilities of IDAES. Additional details can be found at https://idaes.org/.

Since its first open-source public release in March 2019, IDAES has demonstrated significant impacts through its unique capabilities, including:

Identifying a process bottleneck at an existing power plant, which enabled the plant to improve its minimum operating load by 44%, significantly reducing fuel cost and CO_2 emissions when demand for electricity is low. IDAES process optimization also identified an opportunity to improve overall efficiency by 2% at the same facility.

Enabling the optimization of an amine-based post-combustion CO_2 process reducing the operating cost by 15-18%. The models were validated against data from the National Carbon Capture Center pilot plant in Wilsonville, Alabama.

Delivering a computationally efficient approach for the design of a post-combustion CO_2 capture process that is inherently robust against uncertainties in the core process thermophysical properties, decreasing technical risk as new and novel systems are scaled up.

Reducing the energy demand of a complex separation system by more than 40% through efficient, automated exploration of 42 million alternatives.

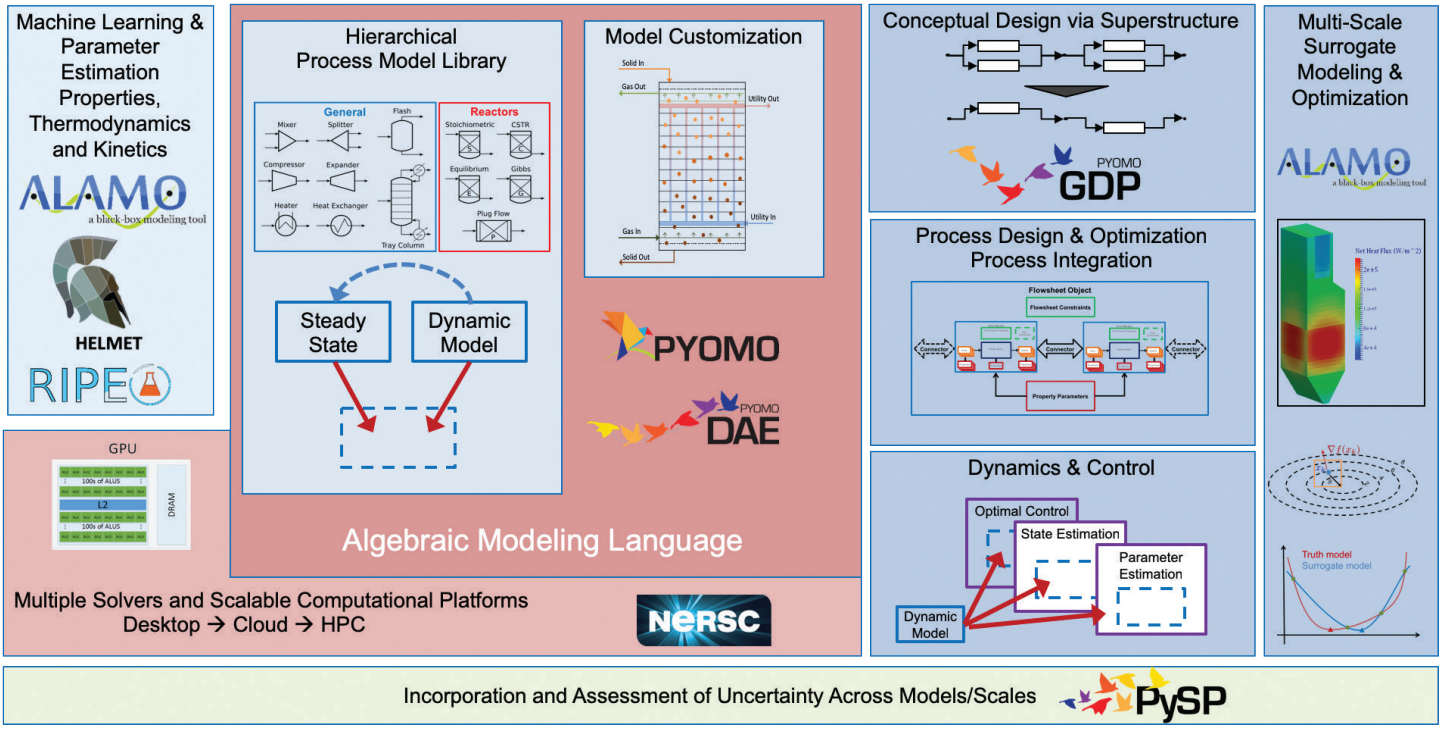
Showing that generator interactions with the bulk power market are more complex than previously thought – a finding with the potential to radically change how new power plants are designed and valued.

Identifying how retrofitting existing generators with energy storage has the potential to reduce equipment wear and tear by 30%.

IDAES

Institute for the Design of Advanced Energy Systems

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



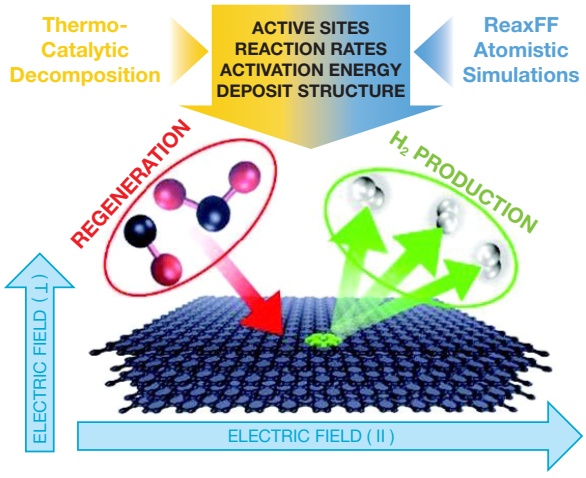
Electric Field Assisted Thermo-Catalytic Decomposition: Comparisons with ReaxFF Atomistic Simulations

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

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

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

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



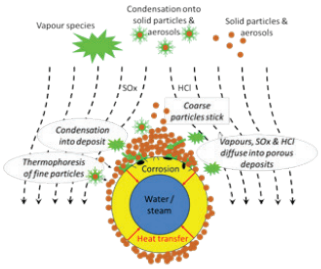
Combined experiment plus modeling for E-field enhanced thermo-catalytic decomposition of methane for hydrogen production.

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

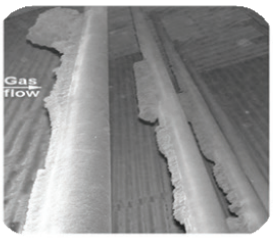
Performer	Siemens Corporation
Award Number	FE0031831
Project Duration	10/15/2019 – 10/14/2022
Total Project Value	$ 952,815
Collaborator	Cranfield University
Technology Area	Coal Utilization Science

Siemens developed 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. A component-level modeling toolkit for materials-based degradation for two key mechanisms that can accelerate with cyclic operations was developed. 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

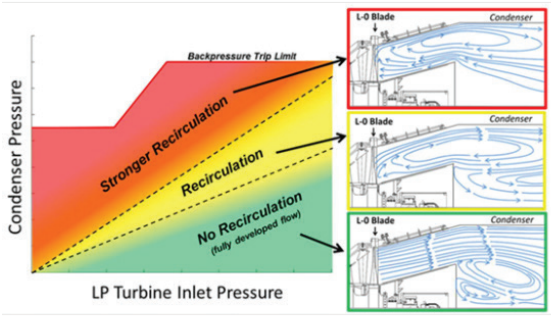


Fouling in heat exchangers

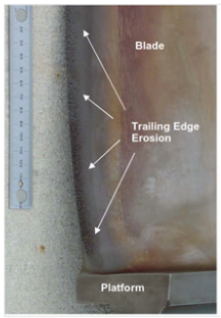


Deposit on real superheater tubes

Steam Turbines



Steam exhaust recirculation causing erosion and cracking



Eroded trailing edge of last row blade

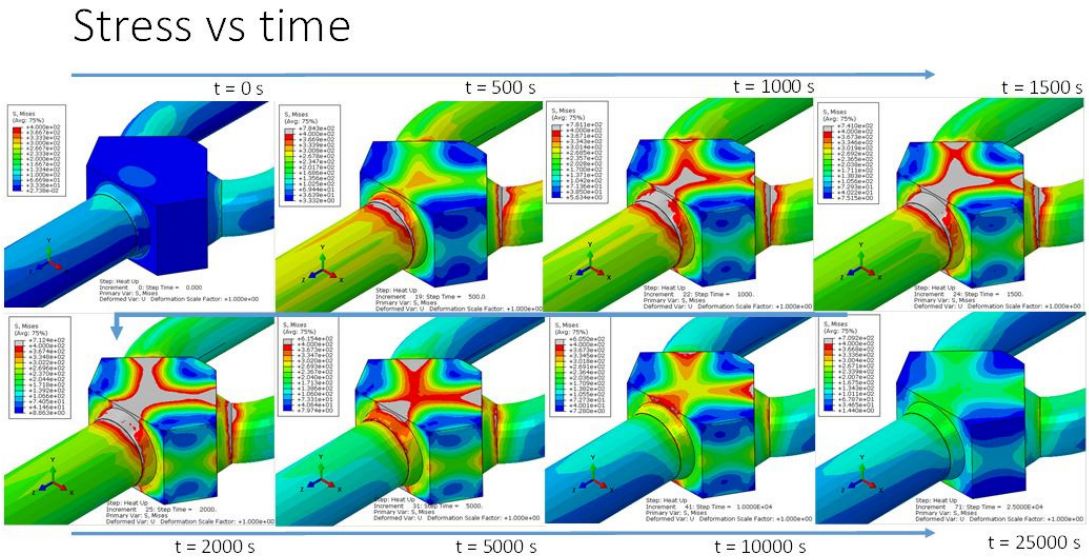
Life Modelling of Critical Steam Cycle Components in Coal-Fueled Power Plants

Performer	**Southern Research Institute**
Award Number	FE0031811
Project Duration	10/01/2019 – 03/31/2023
Total Project Value	$ 862,345
Technology Area	Coal Utilization Science

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

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

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

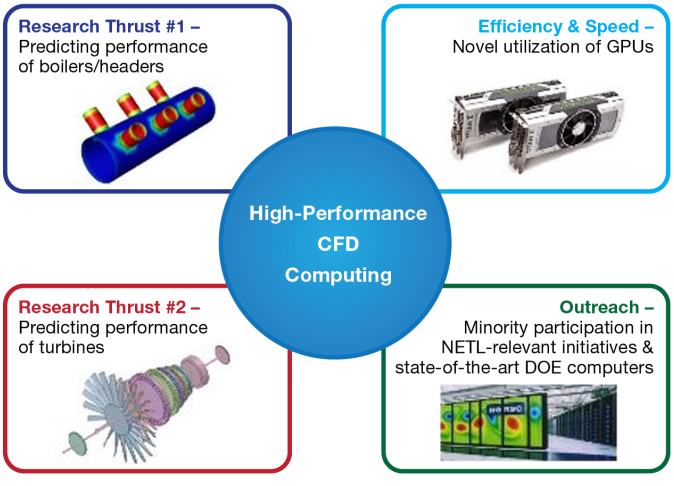


Probing Particle Impingement in Boilers and Steam Turbines Using High-Performance Computing with Parallel and Graphical Processing Units

Performer	**University of California–Riverside**
Award Number	FE0031746
Project Duration	09/01/2019 – 08/31/2023
Total Project Value	$ 400,000
Technology Area	University Training and Research

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

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



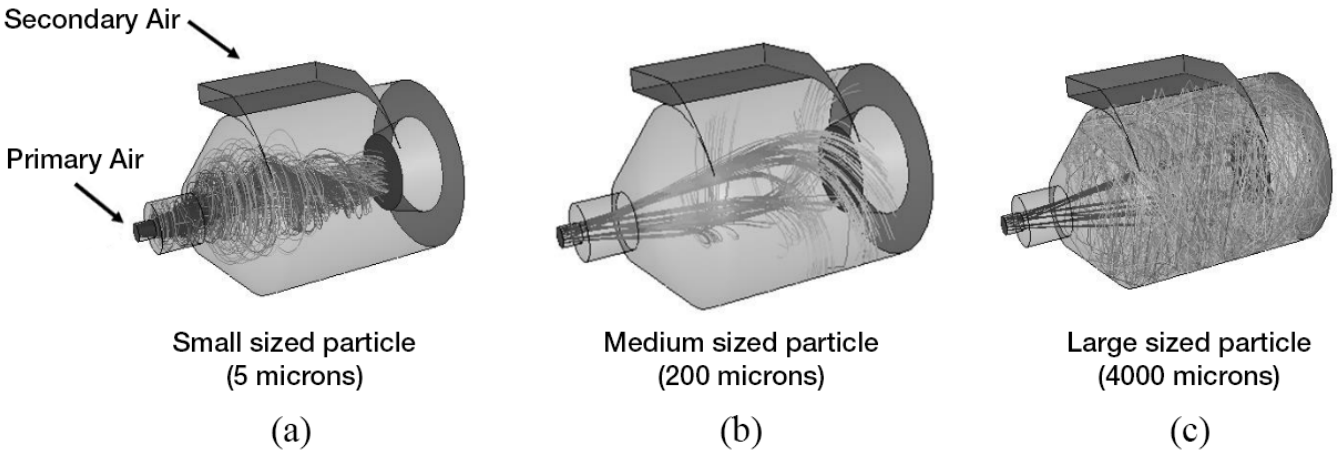
High-performance CFD computing forms a central theme and unifies research thrusts, efficiency, outreach, and technological impact in this HBCU-MSI project.

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 – 07/31/2023
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

Carnegie Mellon University (CMU):
Advanced Modeling and Process-Materials Co-Optimization Strategies for Swing Adsorption Based Gas Separations 19

National Energy Technology Laboratory: eXtremeMAT- Accelerated Design and Manufacture of Next Generation Extreme Environment Materials 20

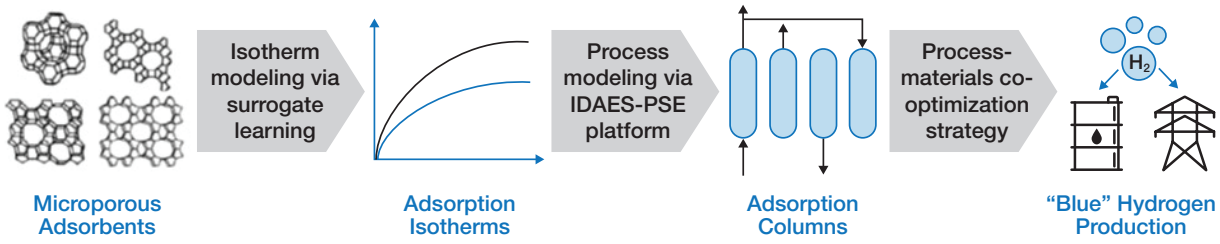
North Carolina Agricultural and Technical State University:
Alloy for Enhancement of Operational Flexibility of Power Plants 22

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

Performer	**Carnegie Mellon University (CMU)**
Award Number	FE0032069
Project Duration	09/13/2021 – 09/12/2024
Total Project Value	$ 400,000
Technology Area	Coal Utilization Science

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

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



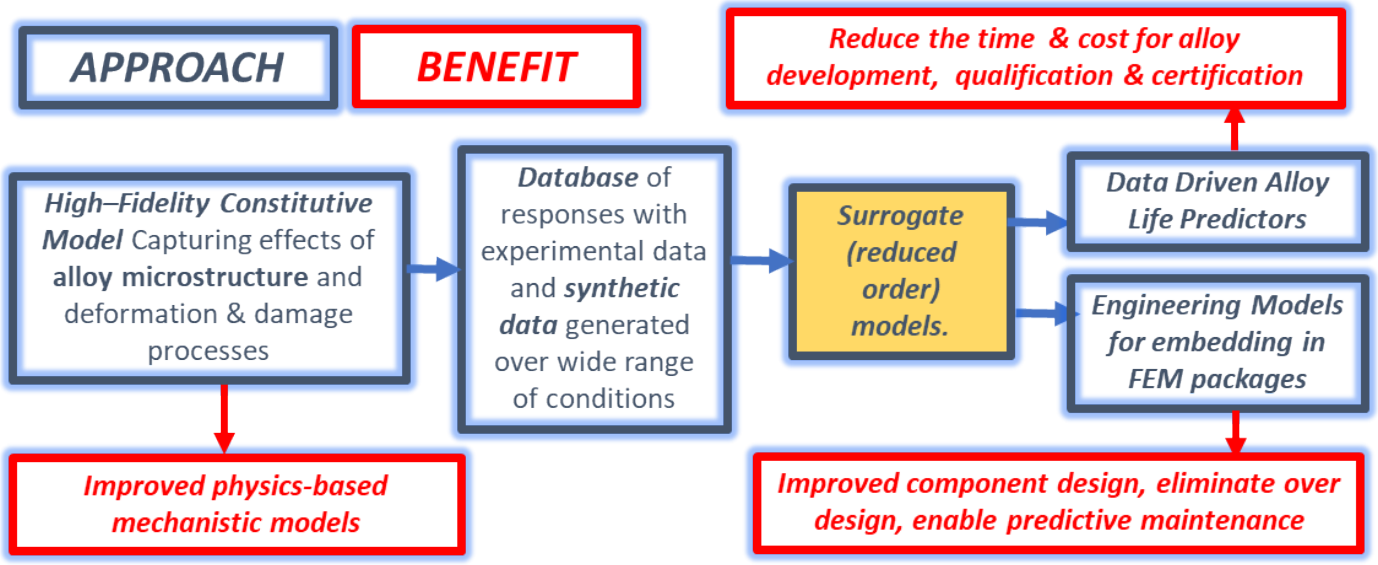
Conceptual workflow of the project.

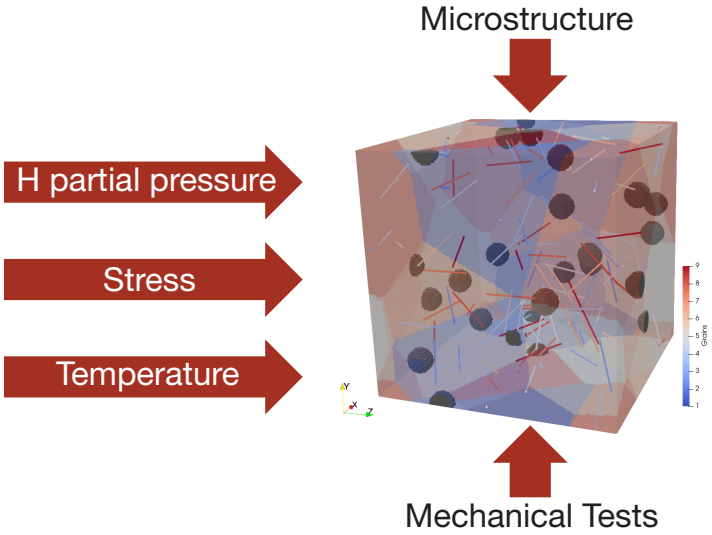
eXtremeMAT- Accelerated Design and Manufacture of Next Generation Extreme Environment Materials

Performer	**National Energy Technology Laboratory**
Award Number	FWP-1022433
Project Duration	10/01/2018 - 09/30/2023
Total Project Value	$ 3,189,921
Technology Area	Coal Utilization Science

The objective of eXtremeMAT is to demonstrate how state-of-the-art computational materials modeling and cutting-edge experimental tools across the National Laboratory (NL) Enterprise, in conjunction with industry partnership, can accelerate the deployment of conventional and additively manufactured alloys for application in extreme environments and are needed to enable technologies to achieve net-zero carbon emissions by mid-century. Hydrogen has become a focal point of attention, as its production and use pave a way towards eliminating carbon emissions. The production of hydrogen from carbonaceous sources with carbon capture via processes, such as gasification and steam methane reforming, will serve as a transition for the use of hydrogen in the power generation and industrial/ manufacturing sectors. These applications (hydrogen production from carbonaceous sources, hydrogen turbines [pre-combustion] for power generation) will impose a harsh constraint on alloys. To improve the reliability and enhance the safety, eXtremeMAT-H_2 aims to study the response of alloys subjected to creep and creep-fatigue under elevated temperatures and in contact with pressurized hydrogen gas. The overall intent is to be able to determine the expected creep-fatigue lifetime of alloys under combined stress, temperature, and hydrogen. This is important, as while the effect of hydrogen on the tensile response of metals has been extensively studied in the literature, little has been investigated on the impact on creep and creep-fatigue scenarios (conditions that are relevant to operating conditions from carbonaceous sources with carbon capture and power generation using hydrogen). In these conditions (elevated temperatures, complex loading states, and long service life), alloy microstructure and moderate changes in composition will have drastic effects on the overall performance of the system. eXtremeMAT developed a framework and a series of toolsets to predict the creep and creep-fatigue behavior of alloys that incorporate the effects of alloy chemistry and microstructural evolution during service. eXtremeMAT-H_2 will expand these tool sets to include materials' lifetime and failure under hydrogen environments. NETL-RIC efforts will focus on four tasks as follows: (i) atomic level calculations to simulate hydrogen-dislocation interactions, (ii) atomic level calculations to simulate hydrogen segregation at interfaces, (iii) quantify the epistemic or model form uncertainty; and (iv) perform as needed creep tests.

XMAT research provides the materials solutions needed to meet the challenges facing fossil energy power generation. Benefits include reducing the cost of alloy development and time-to-deployment; improved fossil energy plant operation performance through condition-based maintenance; eliminating overdesigned components; and enabling new fossil energy-based transformational power generation technologies.





- H effects on creep is poorly studied
- H effects on tensile response is well known (decrease in toughness, embrittlement)
- Creep/ creep fatigue is less studied (increase in creep rate, increase in power law exponent)... Although new studies are poring in

Digital Twin

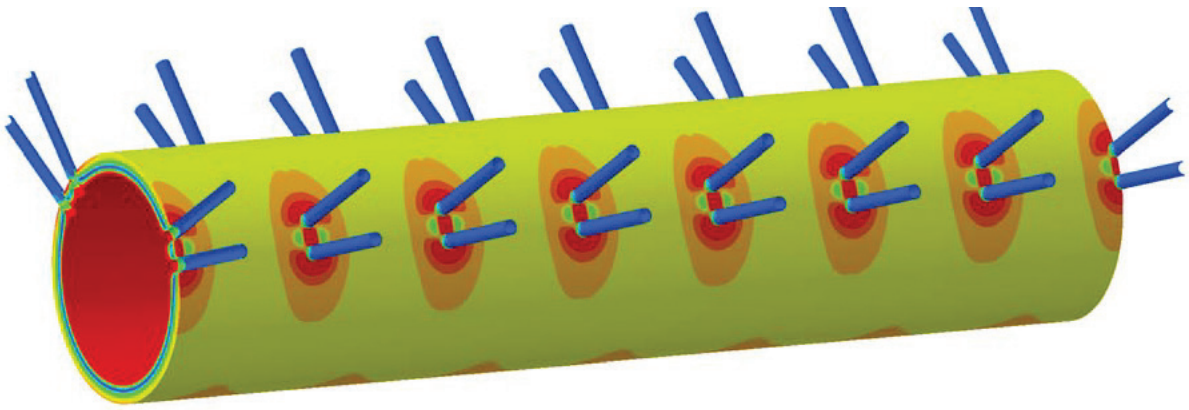
- Local H content at traps as a function of experimental conditions and microstructure?
- Does H increase the likelihood of crack nucleation, does it simply weakens preexisting cracks, does H affect precipitation kinetics?

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 – 08/14/2023
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.

MULTIPHASE FLOW SCIENCE

Florida International University:
Development and Evaluation of a General Drag Model for Gas-Solid Flows Via Physics-Informed Deep Machine Learning 24

Johns Hopkins University:
Developing Drag Models for Non-Spherical Particles through Machine Learning 25

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National Energy Technology Laboratory (NETL):
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Ohio State University:
Unsupervised Learning Based Interaction Force Model for Non-spherical Particles in Incompressible Flows 29

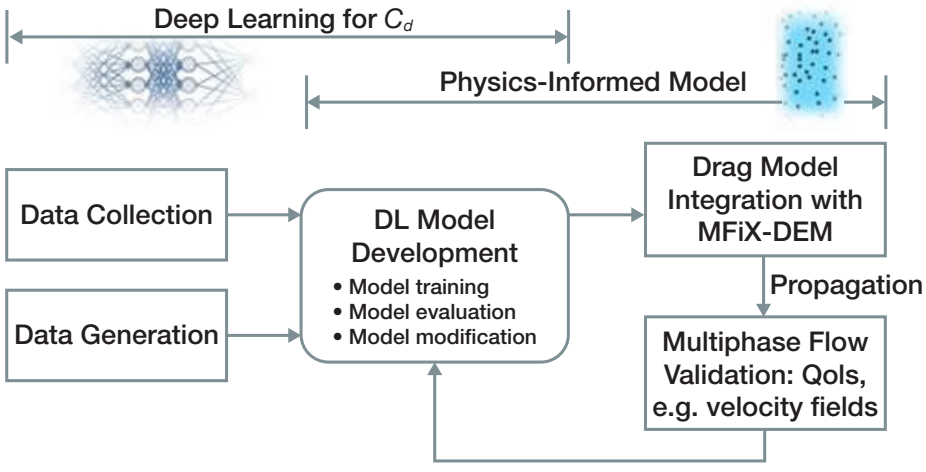
Pennsylvania State University:
Adaptive Depth Neural Networks for Scale-Bridging Modeling of Multiphase Reacting Flows 30

University of Texas at San Antonio:
A General Drag Model for Assemblies of Non-Spherical Particles Created with Artificial Neural Networks 31

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

Performer	**Florida International University**
Award Number	FE0031904
Project Duration	08/01/2020 – 07/31/2023
Total Project Value	$500,000
Technology Area	University Training and Research

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

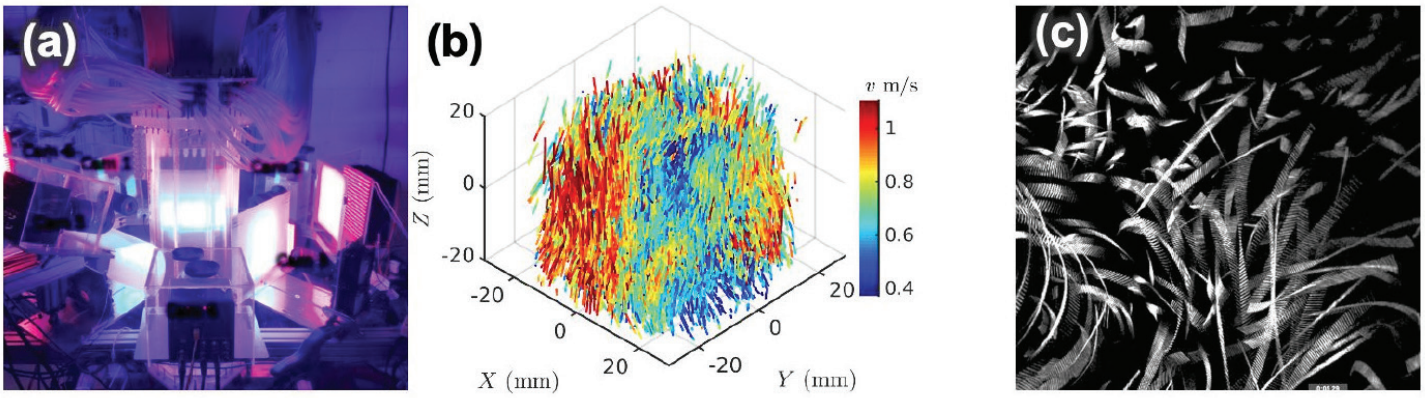


A physics-informed deep learning framework for a drag coefficient model.

Developing Drag Models for Non-Spherical Particles through Machine Learning

Performer	**Johns Hopkins University**
Award Number	FE0031897
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$ 500,000
Technology Area	University Training and Research

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



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

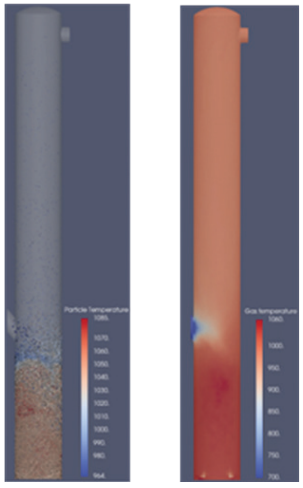
Advanced Reaction Systems

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022405
Project Duration	04/01/2019 – 03/31/2023
Total Project Value	$ 18,423,856
Technology Area	Gasification Systems

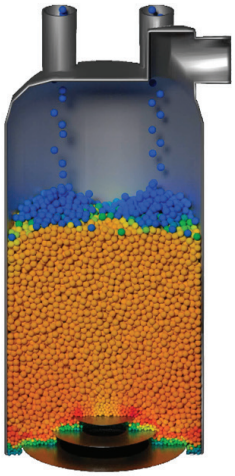
*EY = Execution Year 2019 (Fiscal Year 2019 funding)

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 have been to:

- Analyze novel gasifier technologies to address the FECM H_2 strategy by utilizing NETL's simulation-based engineering tools (MFiX, Optimization Toolset, etc.) to design and optimize novel pyrolysis and gasification reactor designs supporting FECM's mission. Novel oxygen-blown, pilot-scale pyrolysis and gasification reactor designs is being evaluated for use in carbon-negative H_2 production. Simulation-based design and optimization will study both fluidized bed and moving bed reactor configurations operating with mixed feedstocks including biomass, MSW, and waste plastics. Collaborations with the National Renewable Energy Laboratory (NREL) and Oak Ridge National Laboratory (ORNL) projects supported by the NETL gasification program will guide investigation of mixed feedstock gasification for producing precursors that can support production of sustainable aviation fuels and other strategic fuel and chemical feedstocks.
- Develop and validate pyrolysis and gasification models for high density polyethylene feedstock for hydrogen production in a laboratory scale fluidized bed, with the goal of the reactor scale up.



Eucalyptus biomass temperature (L) and gas temperature (R) in a 400-kW fluidized bed gasifier.



Temperature of biomass particles in a 5 MWth moving bed gasifier.

CFD for Advanced Reactor Design (CARD)

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022463
Project Duration	04/01/2020 – 03/31/2023
Total Project Value	$ 6,101,377
Technology Area	Coal Utilization Science

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

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

The Multiphase Flow with Interphase eXchanges (MFiX) suite is a physics-based software for design, optimization and scale-up of multiphase reactors in advanced power plants and the chemical industry. The scale-up of multiphase reactors is notoriously difficult; engineers struggle to predict commercial-scale (large) reactor performance merely based on pilot-scale (small) reactor performance. To that end, the MFiX suite of software provides multiple Eulerian-Eulerian and Eulerian-Lagrangian computational frameworks that can be used to characterize and quantify the performance of multiphase reactors at any scale.

The objectives of MFiX development 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 and Office of Fossil Energy and Carbon Management 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.

MFiX suite of multiphase CFD software.

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

- *MFiX-TFM (Two-Fluid Model)*: An Eulerian-Eulerian model 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 model 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 model 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. The collision between parcels is not directly resolves and is instead represented by a solids stress term. 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.
- *MFiX-CGDEM (Coarse Grain Discrete Element Model)*: An Eulerian-Lagrangian model that treats the fluid phase as a continuum and models solids as discrete groups of particles, called coarse grain particles, with each coarse grain particle representing a group of real particles with the same physical characteristics. The collision between coarse grain particles is fully resolved similarly to MFiX-DEM, but the total number of tracked particles is greatly reduced, which translates into faster simulations with affordable loss of accuracy.

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 FECM 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 7,500 registered users of the MFiX Suite and associated toolsets including industry, academic, and national laboratories.

The CARD portfolio pursues the following primary tasks:

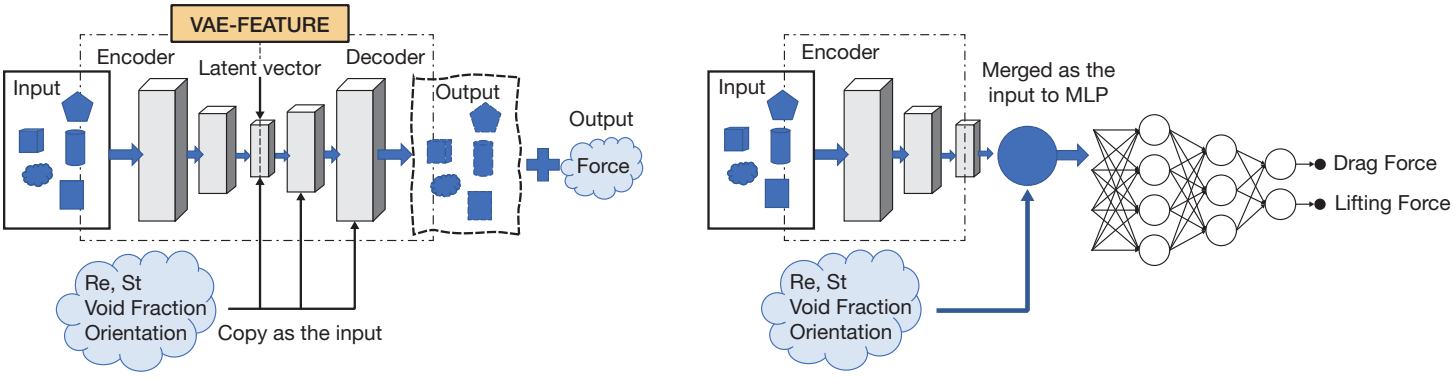
- Develop, validate, apply, publicly distribute, and support the MFiX Suite of multiphase flow modeling software capable of modeling large-scale, reactor systems that include complex chemical reactions and realistic geometry to support the design and optimization of novel reactor systems supporting DOE FECM's programmatic goals.
- Produce an accelerated multi-phase CFD solver that will run on a Wafer Scale Engine.

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

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

Performer	**Ohio State University**
Award Number	FE0031905
Project Duration	08/01/2020 – 07/31/2023
Total Project Value	$ 500,000
Technology Area	University Training and Research

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



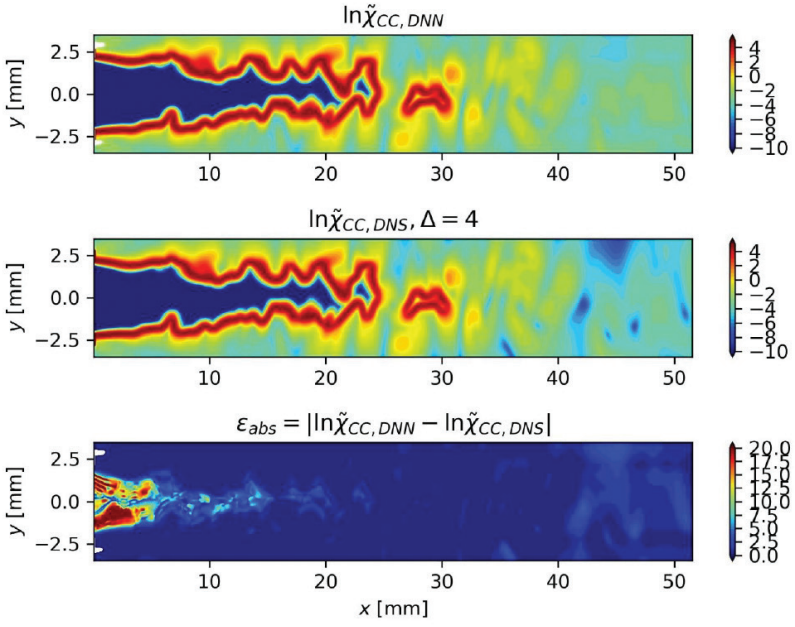
Variational auto-encoder (VAE) will be utilized to extract the primitive geometrical factors of a non-spherical particles. A multi-layer perceptron (MLP) will then be supplied as a regressor for both the drag and lifting force of the non-spherical particles.

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

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

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

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

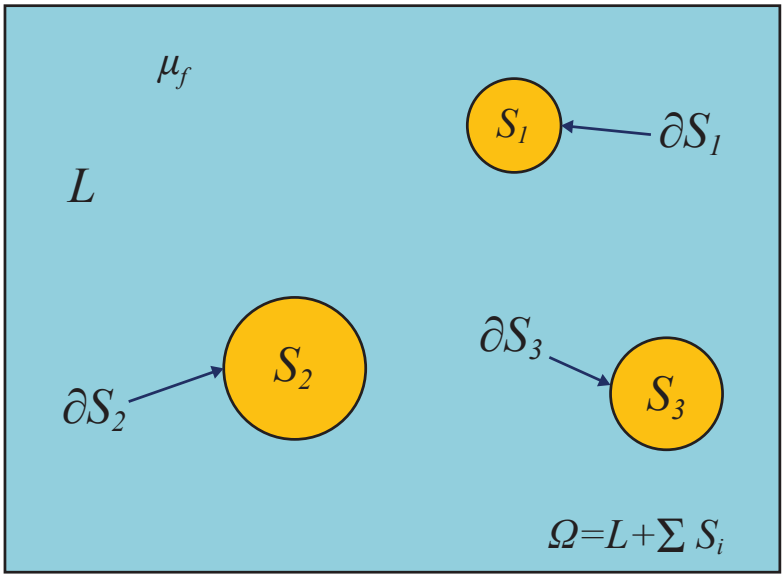


Models of multiphase reacting flows.

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

Performer	**University of Texas at San Antonio**
Award Number	FE0031894
Project Duration	09/01/2020 – 08/31/2023
Total Project Value	$499,982
Technology Area	University Training and Research

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



Conceptual model of three particles suspended in a fluid.

ABBREVIATIONS

ADNN ..... adaptive depth neural networks

AFA ..... alumina-forming alloy

AML .....algebraic modeling language

ANN ..... artificial neural network

ARS.....Advanced Reaction Systems

CALPHAD..... calculation of phase diagrams

CARD .....CFD for Advanced Reactor Design

CCS ..... carbon capture and storage

CFD..... computational fluid dynamics

CO_2 ..... carbon dioxide

Co ..... cobalt

CSEF ..... creep strength enhanced ferrous

DACCS..... Direct Air Capture and Carbon Storage

DEM ..... discrete element model

DNN ..... deep learning neural networks

DOE ..... Department of Energy

E .....electric

EDX .....Energy Data eXchange

EM..... electromagnetic

EY .....execution year

FE.....finite element

Fe..... iron

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

FWP .....field work proposal

FY .....fiscal year

GPU ..... graphics processing unit

HBCU-MSI.....Historically Black Colleges and Universities -Minority Serving Institutions

HCM.....Hydrogen with Carbon Management

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

IN .....Inconel

MFiX.....Multiphase Flow with Interphase Exchanges

MLP ..... multi-layer perceptron

MTI .....Microbeam Technologies Incorporated

NECTAR .....Negative CO_2 Emission Transition Roadmap

NETL..... National Energy Technology Laboratory

Ni .....Nickel

OTP.....Otter Tail Power

PGC .....pressure gain combustion

PI..... principal investigator

PIC ..... particle-in-cell

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

PSE ..... process systems engineering

R-SOFC.....reversible solid oxide fuel cells

R&D.....research and development

ReaxFF.....reaction force field

SBE.....Simulation-Based Engineering

sCO_2..... supercritical carbon dioxide

SOFC ..... solid oxide fuel cell

TCD.....thermo-catalytic decomposition

TFM.....two-fluid model

UCR .....University Carbon Research

UND ..... University of North Dakota

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

US-REGEN.....U.S. Regional Economy, Greenhouse Gas, and Energy

VAE ..... variational auto-encoder

NOTES

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