HYDROGEN
with Carbon Management

2024

SIMULATION-BASED ENGINEERING

PROJECT PORTFOLIO

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

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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 carbon-neutral hydrogen (i.e., coupled to carbon capture and storage (CCS)) as a fuel and developments technologies to use carbon-neutral hydrogen from any source.

The HCM program's efforts are promoted by the Department of Energy's (DOE) Hydrogen Shot, with a goal of reducing clean hydrogen costs by 80% to $1 per 1 kilogram 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 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 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.

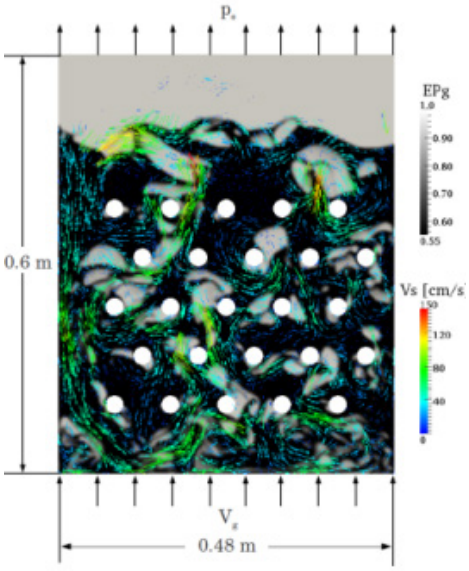
Advanced Energy Materials: The Advanced Energy Materials program drives to characterize, produce, and certify advanced alloys and high-performance materials that are key to realizing dispatchable, reliable, high-efficiency decarbonized power generation from hydrogen. In addition, the program aims to 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.

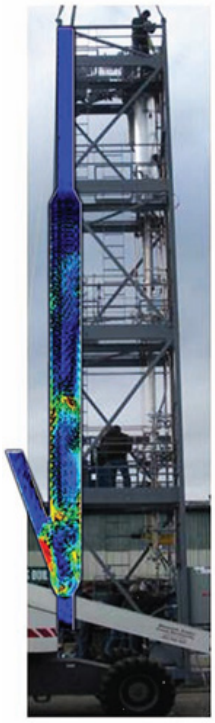
Simulation-Based Engineering: NETL's Simulation-Based Engineering (SBE) program supports the development and application of innovative physics- and chemistry-based models and computational tools at multiple scales (i.e., atomistic, device, process, grid, and market) in order to accelerate development 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.

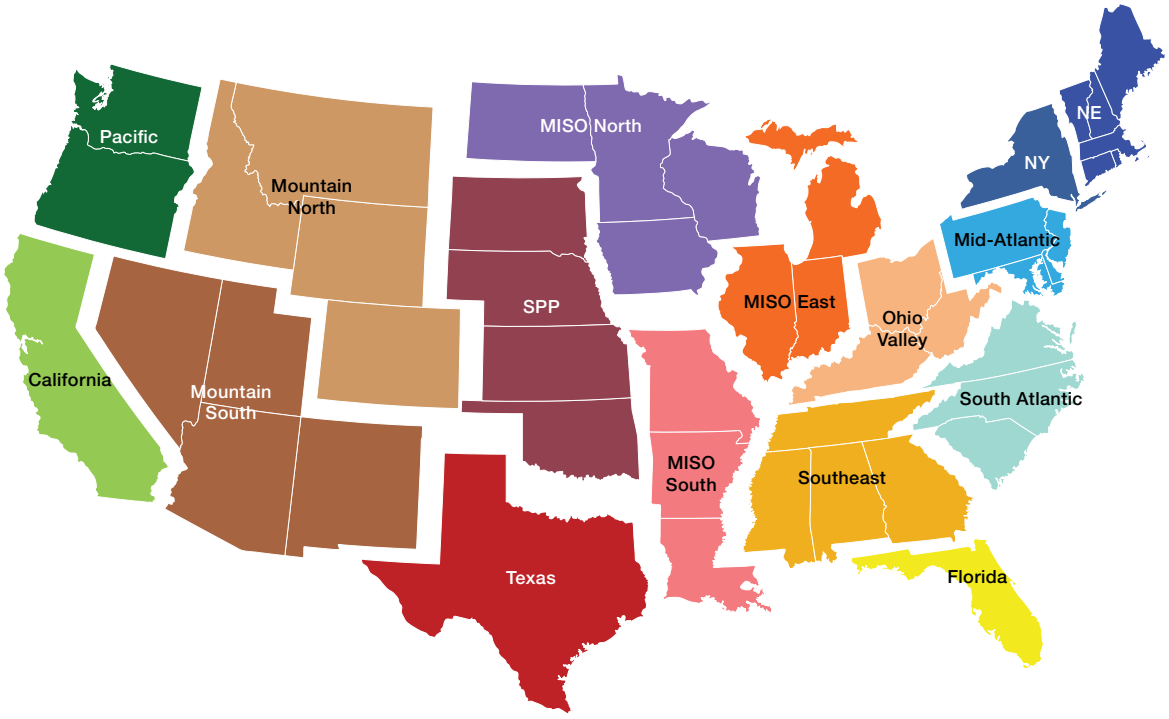
ADVANCED PROCESS SIMULATION

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 – 02/13/2024
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.



Web-based Decision Support Software for Hybrid Energy Systems Based on the IDEAS Framework

Performer	**Reaction Engineering International**
Award Number	SC0022426
Project Duration	02/14/2022 – 04/02/2025
Total Project Value	$ 1,349,056
Technology Area	Coal Utilization Science

Significant commercial scale deployment of carbon capture and sequestration (CCS) technologies are necessary to achieve the climate change mitigation goal of greatly reducing the global CO_2 emissions, while allowing for the utilization of fossil fuels as a transitional power source to continue. There is a diverse portfolio of enabling technologies for global climate change mitigation available for large-scale CO_2 emissions reductions and CCS will play a critical role in meeting the international goal of limiting the global warming to 2° C. To achieve this goal, significant investments in new technologies will be required over the next 20 years. Hybrid energy systems combine energy sources, energy storage and carbon capture to provide the potential of greater flexibility and lower costs for various decarbonization scenarios. Reaction Engineering International will deliver a novel, cloud-based hybrid energy decision-making software tool for modeling hybrid power systems with Carbon Capture and Storage (CCS). The software will take advantage of significant investments by DOE in hybrid systems modeling and economic analysis, while allowing non-expert users to evaluate various decarbonization scenarios. The IDAES-based software will be wrapped with a web-based user interface and will be sold using a software-as-a-service (SaaS) model, where users pay for access to the website and corresponding simulation engine.

The competitive advantage of our product will be its ease-of-access, ease-of-use, as well as enhanced modeling capabilities that will be phased in by the team. The result will be a cloud-deployed modeling capability that will provide a vital link in the chain to make hybrid energy with CCS achievable at large-scale. The proposed software's powerful simulation capabilities will be made available to decision-makers that do not have dedicated modeling, simulation, and financial experts on staff.

This decision support tool will help enable the widespread use of models and simulations for expansion planning to inform future investments for decarbonization. The software is expected to be of interest to the numerous stakeholders involved in hybrid energy and CCS projects, including power utilities, investors, landowners, DOE and regulatory entities and capital investors.

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

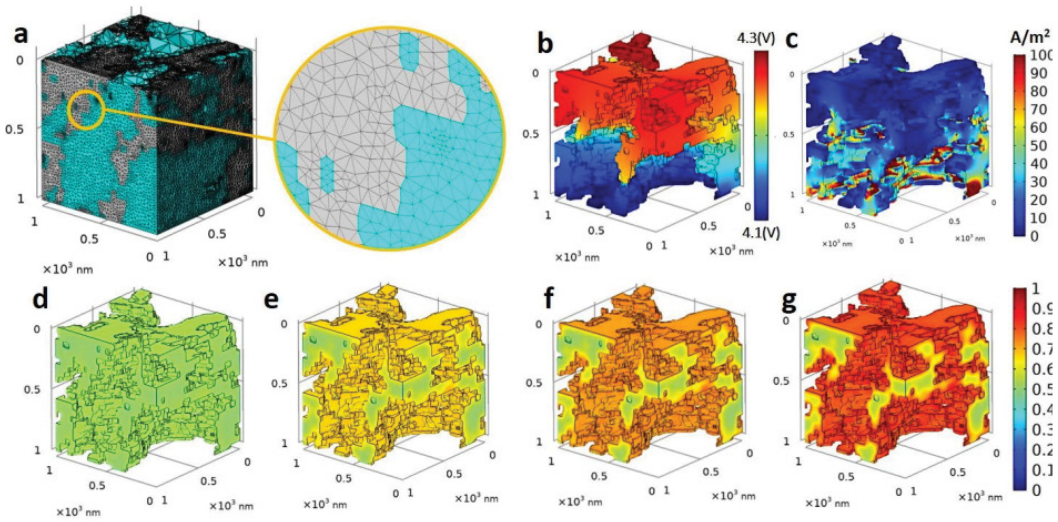
Performer	**Howard University**
Award Number	FE0032092
Project Duration	09/01/2021 – 08/31/2024
Total Project Value	$ 399,935
Technology Area	University Training and Research

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 hydrogengeneration 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.

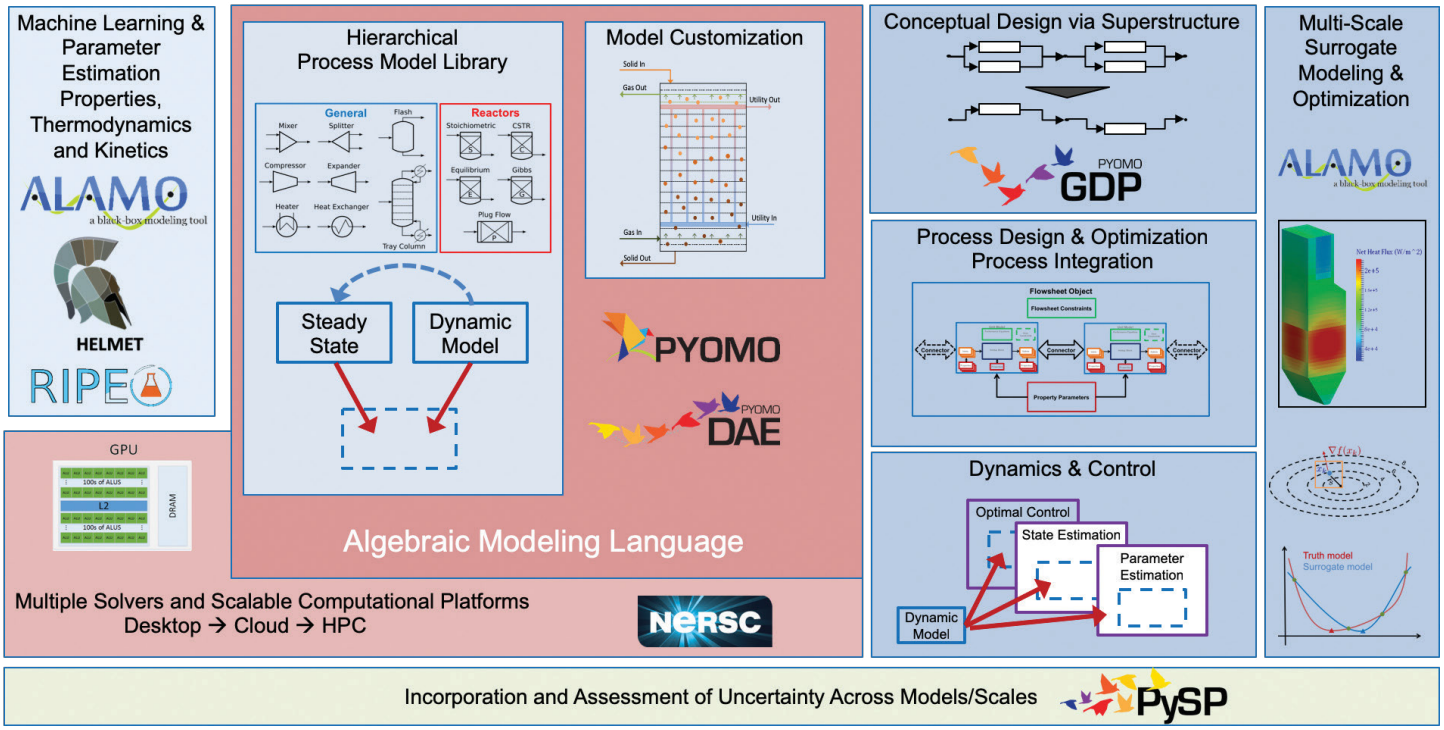
Reducing the energy demand of a complex separation system by more than 40% through efficient, automated exploration of 42 million alternatives.

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.

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



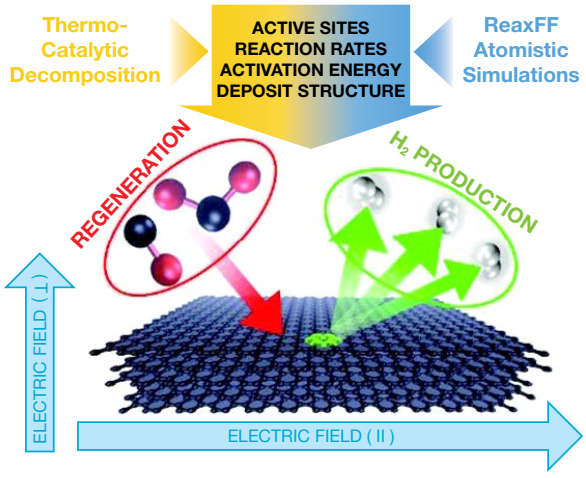
Electric Field Assisted Thermo-Catalytic Decomposition: Comparisons with ReaxFF Atomistic Simulations

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.

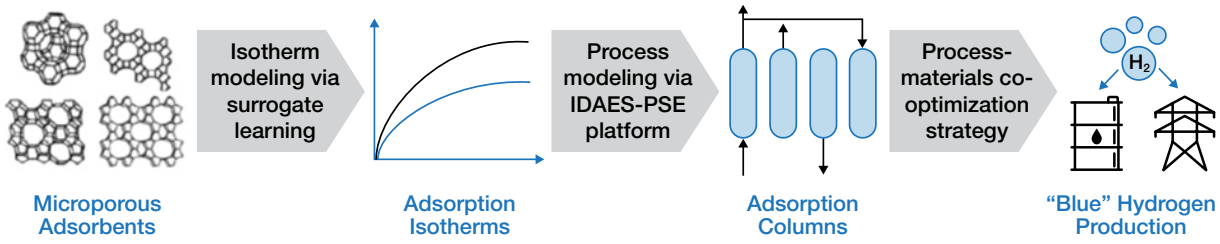
COMPUTATIONAL MATERIALS DESIGN

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

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

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.



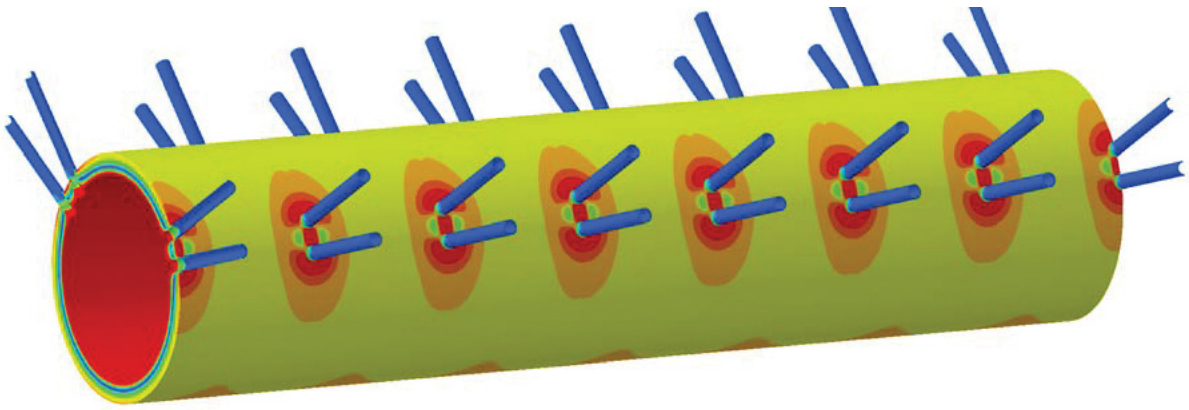
Conceptual workflow of the project.

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 – 12/31/2023
Total Project Value	$ 400,000
Collaborator	University of North Carolina Charlotte
Technology Area	University Training and Research

North Carolina Agricultural and Technical State University employed 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 was 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 used 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 was conducted. This analysis considered the higher cost of IN740H with respect to CSEF steels and the lower maintenance cost of IN740H during operation of the power plant.



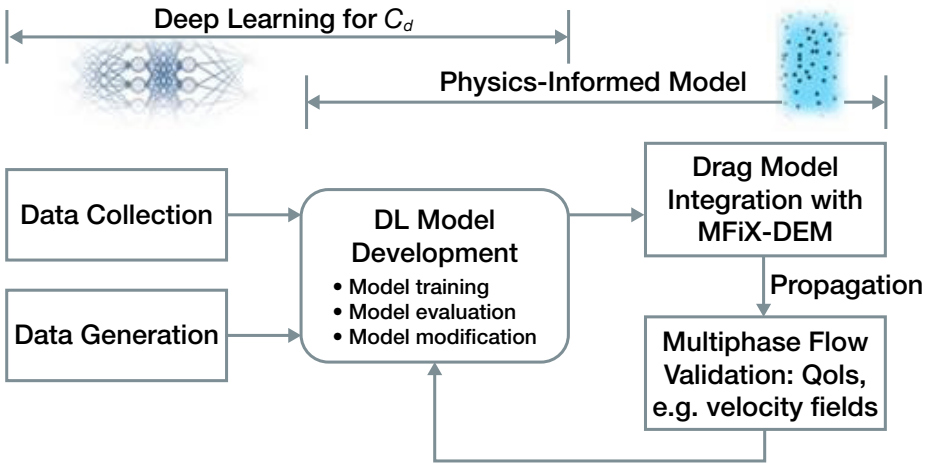
Stress contour plot of a steam header.

MULTIPHASE FLOW SCIENCE

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 – 07/31/2024
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.

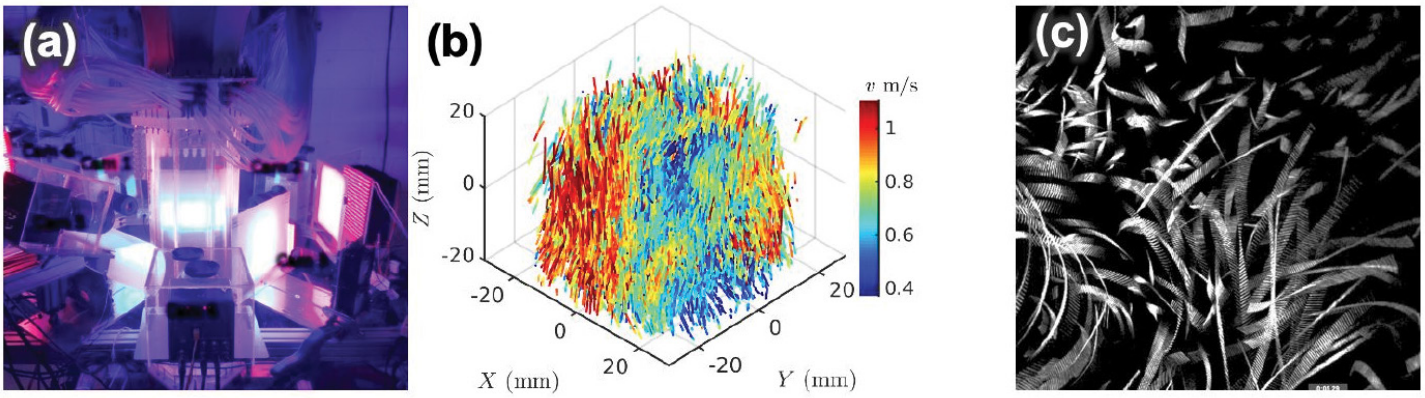


A physics-informed deep learning framework for a drag coefficient model.

Developing Drag Models for Non-Spherical Particles through Machine Learning

Performer	**Johns Hopkins University**
Award Number	FE0031897
Project Duration	09/01/2020 – 08/31/2024
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.

CFD for Advanced Reactor Design (CARD)

Performer	**National Energy Technology Laboratory (NETL)**
Award Number	FWP-1022463
Project Duration	04/01/2020 – 03/31/2024
Total Project Value	$ 10,959,514
Technology Area	Coal Utilization Science

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

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

In contrast to expensive, proprietary commercial CFD software, the MFiX Suite, and associated toolsets are open-source codes that are developed, validated, and supported in-house by NETL's software development and application specialists. These specialists are experts in application of CFD tools to FE technologies. As an open-source code, the MFiX Suite can be customized for novel applications. The MFiX Suite is available on NETL's Joule 2.0 supercomputer, enabling advanced, large-scale, challenging, computer-intensive applications. There are over 8,900 registered users of the MFiX Suite and associated toolsets including industry, academic, and national laboratories.

The CARD portfolio pursues the following primary tasks:

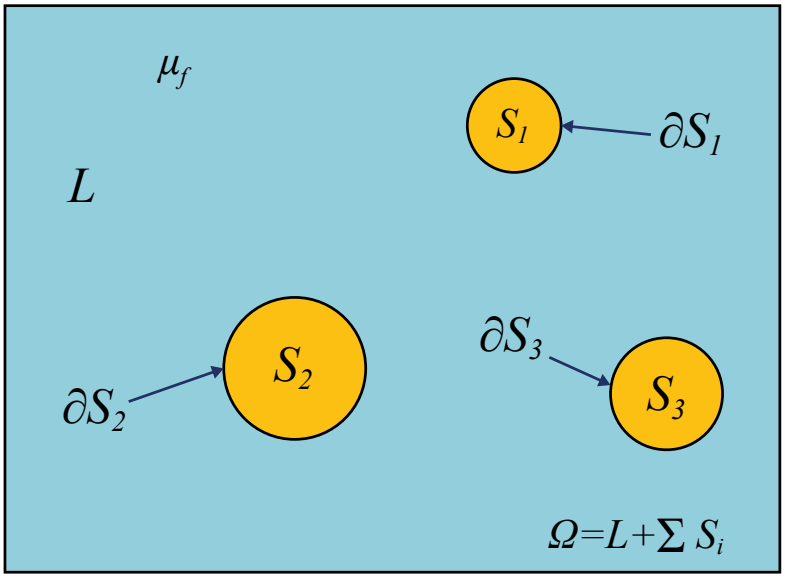
- Develop, validate, apply, publicly distribute, and support the MFiX Suite of multiphase flow modeling software capable of modeling large-scale, reactor systems that include complex chemical reactions and realistic geometry to support the design and optimization of novel reactor systems supporting DOE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

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

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 – 08/31/2024
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

AML ..... algebraic modeling language

ANN ..... artificial neural network

C ..... celsius

CARD ..... CFD for Advanced Reactor Design

CCS ..... carbon capture and storage

CFD ..... computational fluid dynamics

CO_2 ..... carbon dioxide

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

EM ..... electromagnetic

FE ..... finite element

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

FWP ..... field work proposal

H_2 ..... hydrogen

H_2O ..... water

HCM ..... Hydrogen with Carbon Managament

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

IN ..... Inconel

MFiX ..... Multiphase Flow with Interphase Exchanges

NECTAR ..... Negative CO_2 Emission Transition Roadmap

NETL ..... National Energy Technology Laboratory

Ni ..... Nickel

PGC ..... pressure gain combustion

PI ..... principal investigator

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

R&D ..... research and development

ReaxFF ..... reaction force field

SaaS ..... software-as-a-service

SBE ..... Simulation-Based Engineering

sCO_2 ..... supercritical carbon dioxide

SOFC ..... solid oxide fuel cell

TCD ..... thermo-catalytic decomposition

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

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

CONTACTS

John Crane
Technology Manager
Simulation-Based Engineering

412-386-9215

john.crane@netl.doe.gov

Jason Hissam
Technical Project Coordinator
Integrated Carbon Management Team

304-285-0286

jason.hissam@netl.doe.gov

Seth Lawson
Team Supervisor
Integrated Carbon Management Team

304-285-0578

seth.lawson@netl.doe.gov

WEBSITES:

https://netl.doe.gov/carbon-management/simulation-based-engineering

https://mfix.netl.doe.gov/

https://idaes.org/

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NATIONAL ENERGY TECHNOLOGY LABORATORY

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochran Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

Program staff are also located in
Houston, TX and **Anchorage, AK**.

Visit us: **www.NETL.DOE.gov**

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