CROSSCUTTING RESEARCH

MODELING, SIMULATION AND ANALYSIS PROJECT PORTFOLIO 2019

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

DISCLAIMER

CONTENTS

INTRODUCTION

The Crosscutting Research Program advances and accelerates promising fossil energy technology by serving as a bridge between basic and applied research. The program intersects the core capabilities of the National Energy Technology Laboratory (NETL) and combines researchers' expertise to address the nation's energy priorities. Its primary agenda is to serve as a space which matures and enables commercialization of novel technologies to enhance new and existing coal-fired power plants and reduce water consumption. As the research matures it benefits other Department of Energy (DOE) Office of Fossil Energy (FE) program areas such as those under Advanced Energy Systems. Due to the broad applicability of the Crosscutting portfolio, technologies tend to generate spillover benefits in other sectors, including gas-based power generation, oil and gas infrastructure, and aviation (both commercial and military).

On behalf of FE, NETL facilitates crosscutting research and development (R&D) through collaboration with other government agencies, world-renowned national labs, start-up and established businesses and academic institutions. Through collaboration, the program advances capabilities that accelerate progress toward enabling the next generation of fossil energy. These efforts address both known existing challenges to the coal fleet as well as developing key technologies to benefit the future of coal power. Enhancements to the fleet include improvements to plant efficiency, advancements addressing the challenges of load following and cyber intrusions, and developments in affordable, scalable technical solutions. The program invests in these enhancements to secure flexible, reliable coal power for future generations.

The Crosscutting Research Program sponsors two of the longest-running university training programs, preparing the next generation of scientists and engineers to meet future energy challenges. These are the University Coal Research (UCR) program and the Historically Black Colleges and Universities and Other Minority-Serving Institutions (HBCU-OMI) program. By training at the university level with students excited about technologies on the horizon, several key technology trends will become embedded in coal plants of the future including: advanced manufacturing, cybersecurity, smart data analytics and high-performance computing.

The activities within the five primary research areas target enhanced fossil energy systems with the goal of creating transformational technology, improving plant efficiency, reducing water consumption and reducing costs. To generate transformational technology, the program connects water, sensors, computational simulation, workforce development and materials under a single umbrella.

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

The Crosscutting Research portfolio of programs fosters the development of innovative power systems by conducting research in the following key technology areas:

Sensors and Controls provides pivotal insights into optimizing plant performance, reliability and availability while utilizing and furthering technological megatrends such as advanced manufacturing processes and Industry 4.0 principles.

Sensor research is investigating a range of advanced manufacturing techniques to determine the feasibility of embedding sensors, capable of operation in extreme environments and outfitted with condition-based monitoring algorithms, into turbine blades, boiler walls, piping, and tubing to predict component failure, anticipate maintenance needs and reduce plant downtime.

Controls research is advancing the accuracy of artificial and distributed intelligence systems for process control, automation, and fault detection. The ability to monitor key plant parameters and align results in real-time with self-organizing information networks will enable decision-makers to improve the operational efficiency during challenging transient conditions, increase plant availability and dispatch, tighten cybersecurity and environmental control, and improve plant revenue profiles.

This program is exploring advances within, and the integration of technologies across, three primary platforms: Advanced Sensors, Distributed Intelligent Controls, and Cybersecurity.

High Performance Materials focuses on material discovery and development that will lower the cost and improve the performance of fossil-based power-generation systems.

Materials of interest are those that enable components and equipment to perform in the high-temperature, high-pressure, corrosive environments of an advanced energy system with specific emphasis on durability, availability and cost both within and across each of four primary platforms: Computational Materials Design, Advanced Structural Materials, Functional Materials for Process Performance, and Advanced Manufacturing.

Modeling, Simulation and Analysis applies simulation and modeling capabilities to the full range of maturities and technologies essential to plant operation, from fundamental energy science in reactive and multiphase flows to full-scale virtual and interactive plant performance.

This program supports the development and application of new and innovative physics- and chemistry-based models and computational tools at multiple scales (atomistic, device, process, grid, and market) and investigates the potential positive impact these tools may have in overcoming complexities that confound today's experimental scientists and influencing the discovery of a new generation of advanced fossil-fuel technologies.

Analysis and visualization tools are manipulated to gain scientific insights into complex, noisy, 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, experiments, and industrial input with a focus in three main platforms: Multiphase Flow Science, Advanced Process Simulation, and Innovative Concept Analysis.

Water Management aims to reduce the amount of freshwater used by fossil-fueled power plants and to minimize the potential impacts of plant operations on water quality.

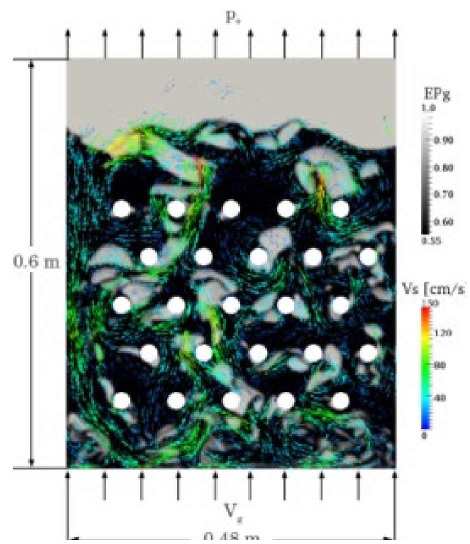
The vision for this program is to develop a 21st century America that can count on our Nation's abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential to our continued economic health and national security.

Thermoelectric power generation accounts for more than 40 percent of freshwater withdrawals (143 billion gallons of water per day) and more than 3 percent of freshwater consumption (4 billion gallons per day) in the United States. As the cost associated with water consumption increases, so will the cost of water treatment, recovery, and reuse.

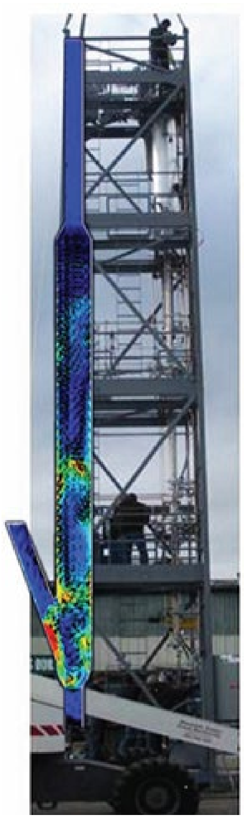
The Water Management Program addresses the competing needs for water consumption through research in three dynamic platforms: Increasing Water Efficiency and Reuse, Treatment of Alternative Sources of Water, and Energy Water Analysis.

MODELING, SIMULATION AND ANALYSIS

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



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



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

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

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

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

ADVANCED PROCESS SIMULATION

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

Performer	**National Energy Technology Laboratory**	**Lawrence Berkeley National Laboratory**	**Sandia National Laboratories**
Award Number	FWP-1022405	FWP-CS IDAES EY19	FWP-19-021286
Project Duration	01/01/2019 – 12/31/2019 (EY19)*	01/01/2019 – 12/31/2019 (EY19)	01/01/2019 – 12/31/2019 (EY19)
Total Project Value	$ 2,892,659 (FY19)	$ 2,014,528 (FY19)	$ 1,595,000 (FY19)
Total Value (All)	$ 6,502,187 (FY19)		
Collaborators	Carnegie Mellon University; West Virginia University		
Technology Area	Coal Utilization Science		

*EY = Execution Year (Fiscal Year 19 funding)

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

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

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

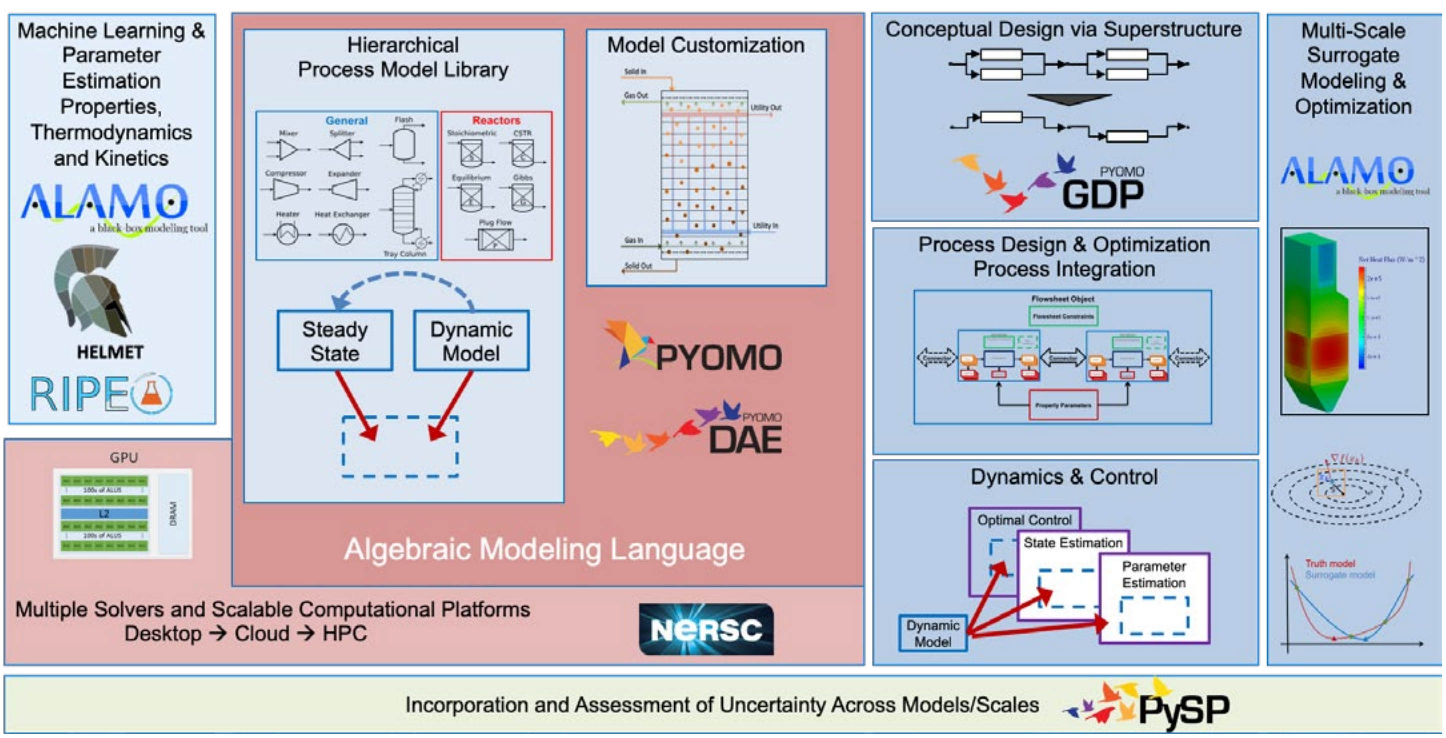
During 2019, the IDAES team anticipates achieving the following milestones:

- Public release of the IDAES framework via github: https://github.com/idaes/idaes-pse
- Public release of general-purpose steady-state power plant modeling library along with example flowsheets.
- Deliver recommendations to partner power plant based on customized and validated optimization models.
- Demonstrate the capabilities of PyoSyn, the IDAES process synthesis tool, on a candidate superstructure for a Coal FIRST plant.
- Public release of the HELmholtz Energy Thermodynamics (HELMET) package that automates thermodynamic property package development in Python.
- Demonstrate market-based nonlinear model predictive control to evaluate short-term operational schedules from the grid dispatch code, Prescient, to demonstrate the potential of co-design and operation of a Coal FIRST thermal plant (see second page following).
- Conduct user workshops and tutorials.

IDAES

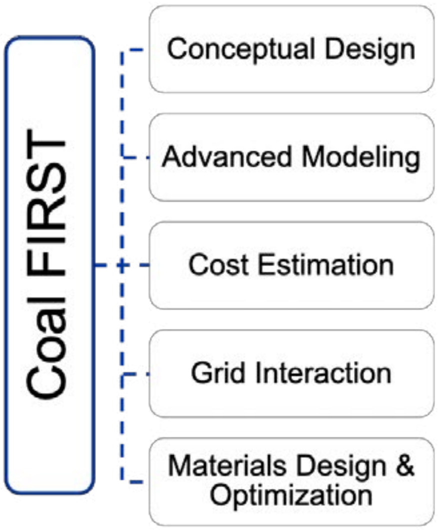
Institute for the Design of Advanced Energy Systems

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



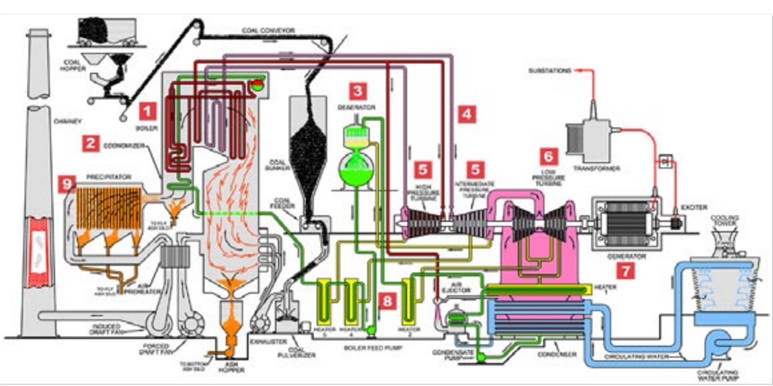
Designing Coal FIRST Power Plants

Flexible, Innovative, Resilient, Small and Transformational



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

Support for the Existing Fleet



Source: Electric Power Research Institute, "Primer on Flexible Operations - 3002000045," EPRI, Palo Alto, Ca, September 2013

- Steady-state power plant optimization model
  - Boiler fire side (combustion, NOx, SOx formation)
  - Boiler water side (vertical tubes, convective superheaters, economizer)
  - Steam cycle (turbines, condenser, feedwater heaters, deaerator)
  - Pollution controls (SCR, FGD)

Key features
  - Hybrid 1-D/3-D zonal model of boiler fire-side
  - Fully EO implementations for remainder of flowsheet
  - Rigorous physical properties calculations
    - Helmholtz-based IAPWS-95 properties for H_2O

Simultaneous optimization
  - System-wide temperatures and pressures
  - Steam extraction splits
  - Flue gas flow into reheater vs. superheater

Direct Power Extraction

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

*EY = Execution Year (Fiscal Year 19 funding)

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

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

The high-level goal of this work is to conclusively determine the viability of MHD power generation for future fossil-derived electrical power generation. To meet this goal, this project is executing the appropriate techno-economic analysis, developing and verifying the required simulation tools, and experimentally validating device-scale simulations. Systems which have utilized DPE are being analyzed and ranked according to efficiency, cost, and various other qualitative factors. Simulations are being developed and utilized to accurately predict MHD generator performance. Experiments are performed to validate those simulations to increase confidence in the performance predictions. Standard and novel materials are being developed, simulated, and tested for use as MHD channel materials. This effort focuses on developing and utilizing fundamentals to be useful in a technology viability assessment, and not focused on demonstrations or detailed optimizations of the technology.

This activity will also define a technology development roadmap, if the technology clears a go/no-go milestone at the end of EY 2019. This roadmap will include consideration of near-term technology spin-offs and efforts toward developing an early commercial application of DPE. Ideas for existing plant retrofits to enhance plant efficiency and remote or temporary power generation applications are under consideration in this activity.

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

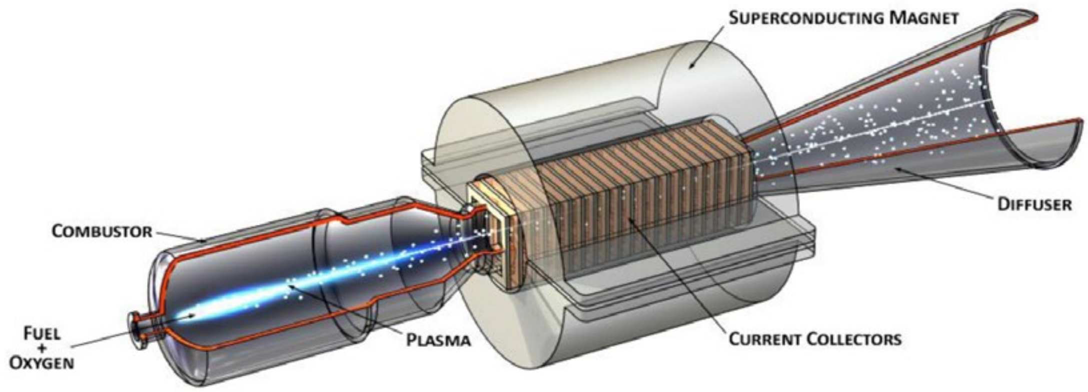


Figure 1: An oxy-fuel fired open cycle MHD power generator. A diffuser is used to slow the flow down prior to it entering a bottoming cycle.

During EY19 progress was made in simulations, validation experiments, materials and systems techno-economic studies for DPE via MHD.

An expanded system scoping study was completed which includes qualitative and semi-quantitative evaluation of a multitude of power systems which use an MHD topping cycle. Several new system concepts with DPE were identified which could work well in cases without carbon dioxide (CO_2) capture (though any system could still add carbon capture). Both closed and open cycle systems were considered. Some of these cases have now been downselected for quantitative assessment. New systems considered include a coal plant retrofit-DPE and dry methane reforming DPE (with CO_2 capture) system.

In the past year, additional techniques were initiated to overcome the technical challenges discovered when trying to measure the plasma conductivity in a seeded oxy-fuel flame. Coincident in-flame atomic potassium concentration, potassium ion concentration, and temperature have now been measured for the first time. The Langmuir probe technique has also been improved. The research team is close to publishing data toward validating our published plasma conductivity model.

Researchers continued time-resolved ion-electron recombination measurements in a laser induced plasma, with additional testing performed using the high velocity oxy-fuel (HVOF) test system. Data were taken over a wider range of conditions than had been taken to date. The team is now exploring discrepancies between the measurements and the model. The fact that our initial simulations did not match the experimental data reinforces the importance of model validation experiments in this project. Efforts were also launched to evaluate a seedless "cold plasma" concept for DPE with SWRI (Southwest Research Institute). The initial analysis shows that high voltage pulses should have a maximum effect on free electrons at some pressure above atmospheric pressure due to cluster formations, which is a phenomenon that is not observed in equilibrium plasma generation.

Simulation codes continue to be refined and were used to support the project. Good progress was made in developing detailed simulations of boundary layer voltage drops. This is an important capability and parameter to understand since this can be a major loss mechanism in smaller utility-scale MHD channels (e.g., 50 MWt). A simple linear MHD Hall channel section has now been designed and built to experimentally validate these simulations. The channel will be tested using the HVOF and a custom hybrid back-power and load tester. Designs for feeding liquid seed compounds into the pressurized combustion chamber were also initiated and will be used in these experiments. Lastly, the team was successful in directly sampling and analyzing gas species in the combustion products using a gas suction enthalpy probe. The system was able to sample gasses up to about 2000 Kelvin. Work is ongoing to further extend the maximum temperature of the probe.

Electrode material efforts continued, though with limited success during dynamic exposure testing using the HVOF system. Additional efforts were made to set-up and conduct static corrosion experiments at Oregon State University, and results will be reported soon. Plans are in place to fabricate and test functionally graded (grading electrical conductivity) ceramics to assess the possibility for a 3D printed MHD channel. A contract was awarded to NEXCERIS to fabricate functionally graded magnesia to doped ceria ceramic discs.

MULTIPHASE FLOW SCIENCE

Advanced Reaction Systems

Performer	**National Energy Technology Laboratory**
Award Number	FWP-1022405
Project Duration	04/01/2019 – 03/31/2020 (EY19)*
Total Project Value	$ 2,260,000 (FY19)
Technology Area	Gasification Systems

*EY = Execution Year (Fiscal Year 19 funding)

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

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

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

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

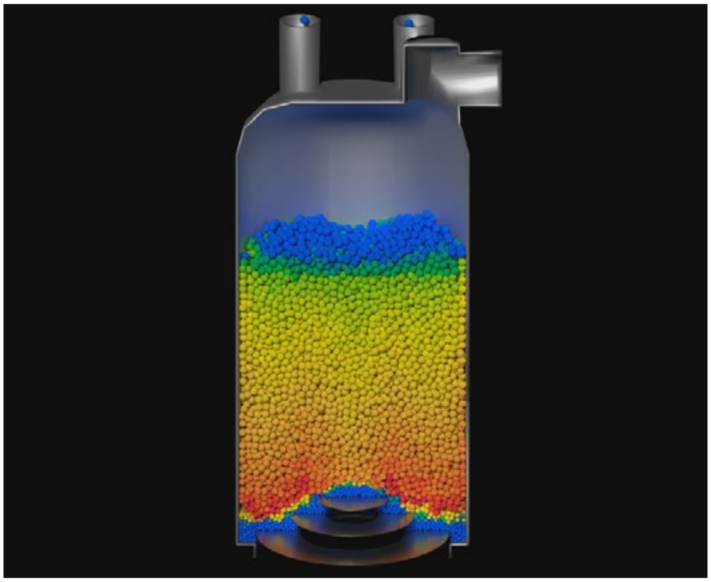
particles, with each parcel representing a group of real particles with the same physical characteristics. This is an emerging capability that will be brought to maturity for use in advanced reactor simulations over the course of the proposed work. The MFiX-MPIC approach greatly reduces the computational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

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

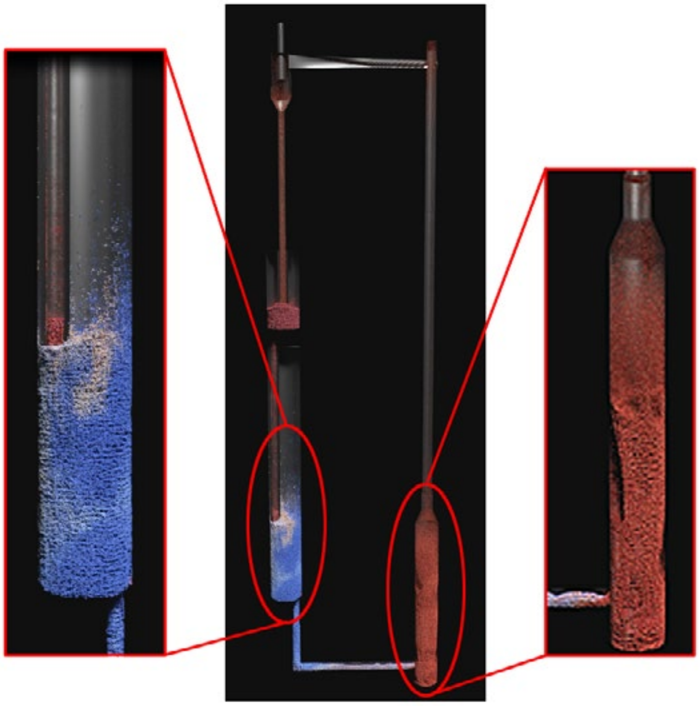
In contrast to expensive, proprietary commercial CFD software, the MFiX suite and associated toolsets are open-source codes that are developed, validated, and supported in-house by NETL's software development and application specialists. As open-source codes, the MFiX suite can be customized for novel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

Densely-loaded, multiphase flows are very demanding applications for CFD codes. This is made even more challenging in this work due to the need to model chemical kinetics and heat transfer in very complex, reacting systems. The systems of interest can span laboratory-scale through pilot- and commercial-scale systems. Multiphase flow CFD requires substantial amounts of computer time so the ability to perform simulations on supercomputing systems is mandatory for larger applications. These codes are quite complex in both quantity of code and complexity of the physics and numerical approaches to obtain a solution. A Quality Assurance Program, including systematic verification, validation, and uncertainty quantification is required to ensure integrity and acceptability of the model predictions.

NETL has maintained a multiphase flow modeling program for over 30 years, starting from when CFD was in its infancy until present day where CFD has become a well-accepted tool for studying reacting flows. NETL's expertise in dense, reacting multiphase flow is unique and continues to be one of NETL's and FE's key capabilities. In the past 5 years, there has been renewed emphasis on the expansion of the MFiX family of codes to include more accurate and capable modeling approaches, such as MFiX-DEM and MFiX-PIC.



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



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

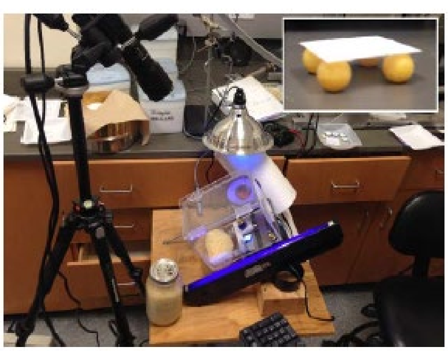
MFiX-DEM Enhancement for Industry-Relevant Flows

Performer	**University of Colorado**	**National Renewable Energy Laboratory**
Award Number	FE0026298	FWP-DOW4659
Project Duration	09/01/2015 – 08/31/2020	10/01/2015 – 08/31/2020
Total Project Value	$ 3,778,002	$ 899,419
Total Value (All)	$ 4,677,421	
Collaborator	Particulate Solid Research, Inc.	
Technology Area	Coal Utilization Science	

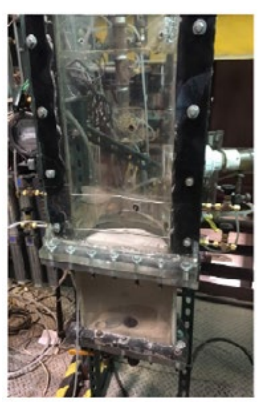
This project will improve performance of the Multiphase Flow with Interphase eXchanges–discrete element method (MFiX-DEM) code to enable a transformative shift for industrial use. The proposed approach will enhance MFiX-DEM by using a state-of-the-art profiling methodology developed by our team members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

The goal is to achieve an increase in performance of two orders of magnitude; a refined estimate will result from the profiling effort. Over thirty Particulate Solid Research Inc. consortium member companies were surveyed at the beginning of the project to identify industrial needs. In Phase 2, the focus is on completing simulations for increasingly complex systems involving 10^9 particles in less than 24 hours. New experiments will be performed involving approximately 10^7-10^9 particles in a system of industrial relevance, and these experiments will be used to demonstrate the enhanced MFiX code. Uncertainty quantification (UQ) will also be performed by coupling the freely available UQ toolkit Problem Solving environment for Uncertainty Analysis and Design Exploration (PSUADE) with an enhanced version of MFiX. Uncertainty quantification using the enhanced MFiX code on larger and industrially relevant systems will be demonstrated.

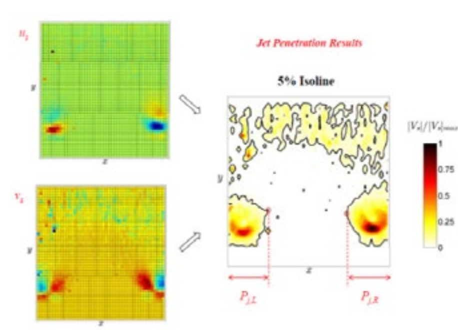
The immediate outcome will be an enhanced DEM tool implemented into the open-source MFiX framework. The enhanced DEM model will be optimized for computational efficiency and will contain parallelization methods that leverage advances in heterogeneous HPC architectures with accelerators.



Horizontal jet experiments particle characterization.



Semi-circular fluidized bed with side jets.



Horizontal jet experiments particle tracking post-processing.

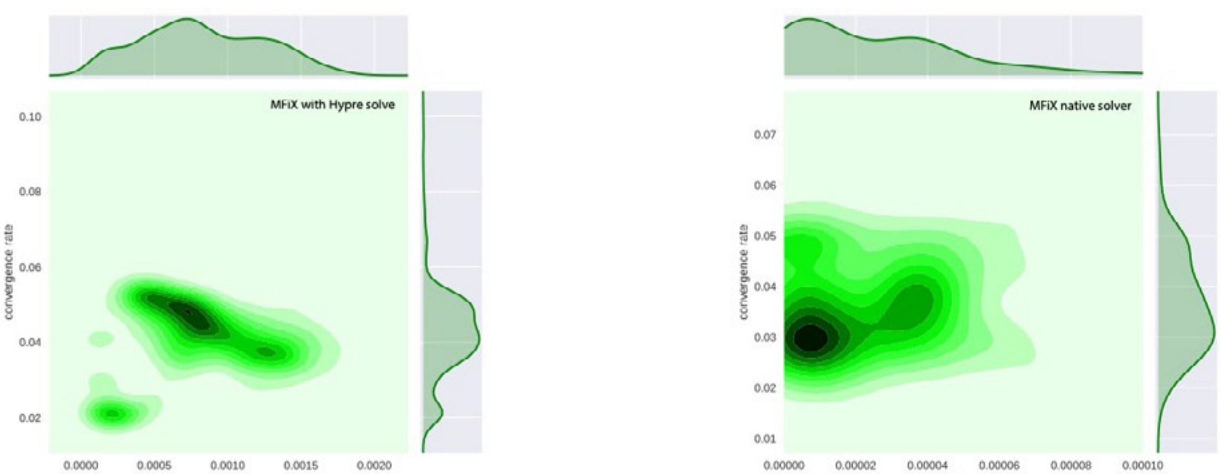
Interfacing MFiX with PETSc and HYPRE Linear Solver Libraries

Performer	University of North Dakota Energy and Environmental Research Center
Award Number	FE0026191
Project Duration	09/01/2015 – 08/31/2019
Total Project Value	$ 400,000
Collaborator	University of Utah
Technology Area	University Training and Research

High computational cost associated with the solution of large, sparse, poorly conditioned matrices is a serious impediment to increasing the utility of computational fluid dynamics models for resolving multiphase flows. This project will interface NETL's MFiX code with Portable Extensible Toolkit for Scientific Computation (PETSc) and High Performance Preconditioners (HYPRE) linear solver libraries with the goal of reducing the time to solution for the large, sparse, and often ill-conditioned matrix equations resulting during the solution process. The lack of robust convergence associated with the current iterative methods in MFiX can be alleviated through appropriate preconditioning techniques to Krylov subspace solvers and multigrid methods accessible from these third-party solver libraries.

The overall objective of this project is to first establish a robust well-abstracted solver interface that will present an extensible back-end enabling MFiX to successfully interface with various solver libraries. Next, this extensibility will be demonstrated by interfacing MFiX with PETSc and HYPRE linear solver libraries with the goal of reducing the time to solution for large, sparse, linearized matrix equations resulting from the discretization of multiphase transport equations.

This project could reduce the time to solution by at least 50 percent when compared to current linear solver options in MFiX. It also could show that near-linear scaling in parallel performance can be achieved to at least 1000 processors, which could translate to achieving good scalability on current high-performance computing systems such as the DOE leadership computing facilities as well as enabling the portability of MFiX with new hardware technologies.



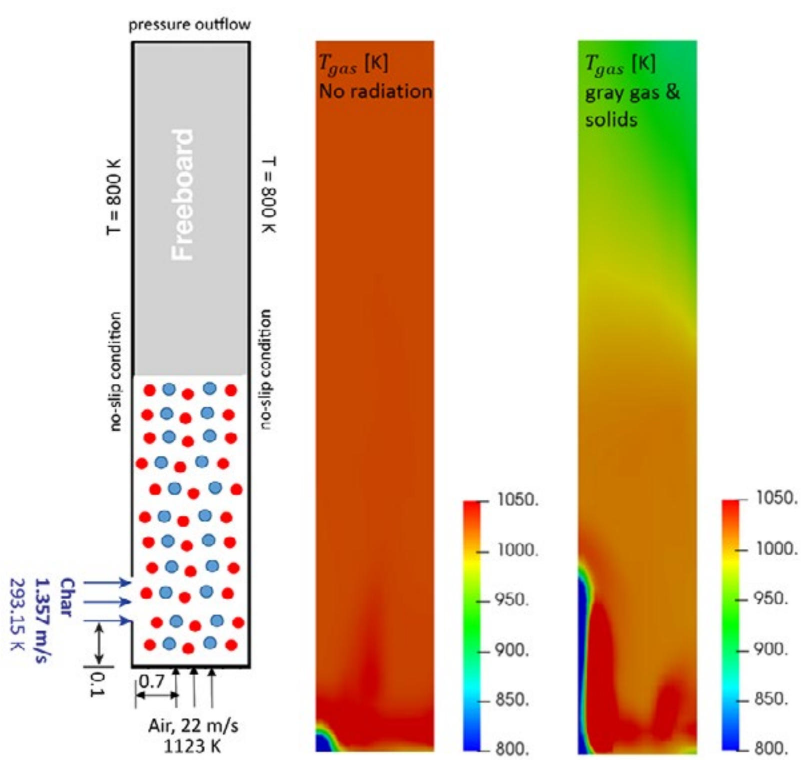
Convergence rate and resulting simulation timestep behavior of the outer solve using (left) HYPRE [biconjugate gradient stabilized method (Bicgstab)/ParFlow multigrid solver] and (right) native MFiX (Bicgstab/diagonal scaling) for the inner gas pressure solve in a fluidized bed problem. The case utilizing the HYPRE solver remained stable over time while the MFiX native solver eventually resulted in divergence.

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

Performer	**University of Wyoming**
Award Number	FE0030485
Project Duration	08/01/2017 – 07/31/2020
Total Project Value	$ 400,000
Technology Area	University Training and Research

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

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



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

ABBREVIATIONS

AML .... algebraic modeling language

ARS.................................. Advanced Reaction Systems

Bicgstab .... biconjugate gradient stabilized method

CFD..................................computational fluid dynamics

CO_2 ....carbon dioxide

DEM ....Discrete Element Model

DOE ....Department of Energy

DPE... direct power extraction

EY .... execution year

FE... Office of Fossil Energy

FWP ....Field Work Proposal

FY .... fiscal year

HBCU...........Historically Black Colleges and Universities

HELMET...................Helmholtz energy thermodynamics

HPC .... high-performance computing

HVOF .... high velocity oxy-fuel

HYPRE .... High Performance Preconditioners

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

MFiX........... Multiphase Flow with Interphase Exchanges

MHD... magnetohydrodynamic

MPIC ....Multiphase Particle-In-Cell

NETL.................National Energy Technology Laboratory

OMI .... Other Minority Institutions

PETSc .... Portable Extensible Toolkit for Scientific Computation

PSE..................................process systems engineering

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

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

RAD ....Radiative Heat Transfer

SWRI .... Southwest Research Institute

TFM...Two-Fluid Model

UCR ....University Coal Research

UQ ....uncertainty quantification

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

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

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