Crosscutting Technology Research Simulation-Based Engineering Project Portfolio

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U.S. DEPARTMENT OF ENERGY

the ENERGY lab

NATIONAL ENERGY TECHNOLOGY LABORATORY

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Contents

Introduction

The Crosscutting Technology Research Program develops a range of innovative and enabling technologies that are key to improving existing power systems and essential for accelerating the development of a new generation of highly efficient environmentally benign fossil fuel-based power systems. The mission space is focused on bridging the gap between fundamental and applied research and development (R&D) efforts. Technologies that successfully bridge this gap are intended to offer viable step-change improvements in power system efficiency, reliability, costs, and environmental impacts.

The Crosscutting Technology Research Program executes the R&D efforts by partnering and collaborating with research institutions and the power generation industry throughout the United States and in select international collaborations. The Crosscutting Technology Research Program also sponsors one of the longest running and most important university training and research programs to reinforce the research-based education of students at U.S. universities and colleges with emphasis on fossil energy science. The major objective for this program is to produce tools, techniques, and technologies that map to the Clean Coal Research Program efforts.

The Program comprises three technology areas: Coal Utilization Sciences, Plant Optimization Technologies, and University Training and Research. A general description of each of these technology areas is detailed below:

Coal Utilization Sciences: The Coal Utilization Sciences technology area research effort is conducted to develop modeling and simulation technologies leading to a suite of products capable of designing and simulating the operation of next-generation near-zero-emissions power systems such as gasification and oxy-combustion. These products are based on validated models and highly detailed representations of equipment and processes. Multinational laboratory efforts are being coordinated through the National Risk Assessment Partnership (NRAP) and Carbon Capture Simulation Initiative (CCSI) to focus on post-combustion capture of carbon, risk assessment, and integrated multiscale physics-based simulations.

Plant Optimization Technologies: The Plant Optimization Technologies technology area exists to develop advanced sensors and controls, materials, and water- and emissions-related technologies. Projects within this funding area enable novel control systems to optimize operations where harsh environmental conditions are present in both current and future applications in power plants and industrial facilities.

University Training and Research: The University Training and Research (UTR) program awards research-based educational grants to U.S. universities and colleges in areas that benefit the Office of Fossil Energy and the Crosscutting Technology Research Program. UTR is the umbrella program under which the University Coal Research (UCR) and Historical Black Colleges and Universities (HBCU) and Other Minority Institutions (OMI) initiatives operate. These grant programs address the scientific and technical issues key to achieving Fossil Energy's goals, and build our nation's capabilities in energy science and engineering by providing hands-on research experience to future generations of scientists and engineers.

In addition to the Crosscutting Technology Research funding programs listed above, NETL uses its participation in the U.S. Department of Energy's (DOE) Office of **Science Small Business Innovation Research (SBIR) Program** to leverage funding, enhance the research portfolio, and most importantly, facilitate a pathway to commercialization. SBIR is a highly competitive program that encourages small businesses to explore technological potential and provides the incentive to profit from commercialization. By including qualified small businesses in the nation's

R&D arena, high-tech innovation is stimulated and the United States gains entrepreneurial spirit to meet specific research and development needs. SBIR targets the entrepreneurial sector because that is where most innovation and innovators thrive. By reserving a specific percentage of Federal R&D funds for small business, SBIR protects the small business and enables competition on the same level as larger businesses. SBIR funds the critical startup and development stages and it encourages the commercialization of the technology, product, or service, which, in turn, stimulates the U.S. economy. Since its inception in 1982 as part of the Small Business Innovation Development Act, SBIR has helped thousands of small businesses to compete for Federal research and development awards. These contributions have enhanced the nation's defense, protected the environment, advanced health care, and improved our ability to manage information and manipulate data.

The Crosscutting Technology Research program comprises these key technology areas:

Sensors and Controls: The basis for this research area is to make available new classes of sensors and measurement tools that manage complexity, permit low cost, robust monitoring, and enable real-time optimization of fully integrated, highly efficient power-generation systems. Controls research centers around self-organizing information networks and distributed intelligence for process control and decision making.

High Performance Materials: Materials development under the Crosscutting Technology Research Program focuses on structural materials that will lower the cost and improve the performance of fossil-based power-generation systems. Computational tools in predictive performance, failure mechanisms, and molecular design of materials are also under development to support highly focused efforts in material development.

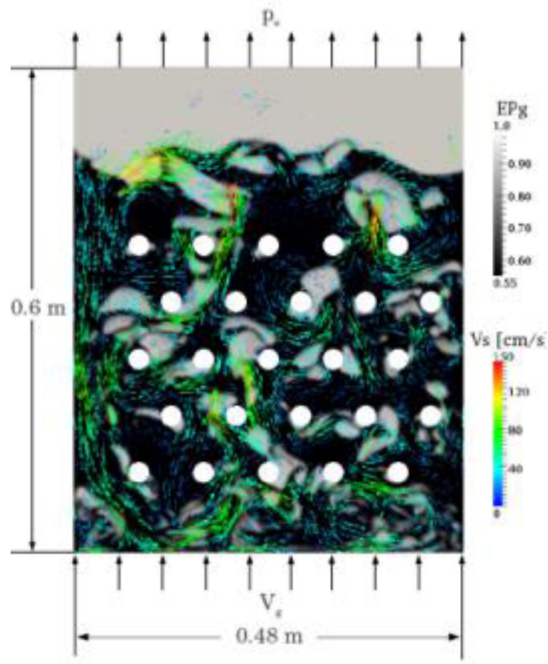
Simulation-based Engineering: This technology area represents a vast amount of expertise and capability to computationally represent the full range of energy science from reactive and multiphase flows up to a full-scale virtual and interactive power plant. Science-based models of the physical phenomena occurring in fossil fuel conversion processes and development of multiscale, multi-physics simulation capabilities are just some of the tools and capabilities under this technology area.

Innovative Energy Concepts: Innovative Energy Concepts is concerned with the development of novel cost-effective technologies that promote efficiency, environmental performance, availability of advanced energy systems, and the development of computational tools that shorten development timelines of advanced energy systems. This area provides for fundamental and applied research in innovative concepts with a 10–25 year horizon that offers the potential for technical breakthroughs and step-change improvements in power generation and the removal of any environmental impacts from fossil energy-based power system.

Water Management Research and Development: Water research encompasses the need to reduce the amount of freshwater used by power plants and to minimize any potential impacts of plant operations on water quality. The vision for this program area is to develop a 21st-century America that can count on abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential for continued security and economic health. To accomplish this, crosscutting research is needed to lead a critical national effort directed at removing barriers to sustainable, efficient water and energy use, developing technology solutions, and enhancing understanding of the intimate relationship between energy and water resources.

Simulation-Based Engineering

Modeling efforts stem from the motivation to reduce costs and time delays resulting from the use of expensive lab set-ups in research and physical prototypes in the design and engineering phase of projects. Improvements are sought 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 in providing 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 developmental 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. Additionally, during new technology development—for example, the development of sorbent adsorber/desorber reactors for CO_2 capture—empirical scale-up information is not available because reactors at the required large scales have not been built. Traditional scale-up methods do not work well for many of the components that are present in complex power systems. Therefore, science-based models with quantified uncertainty are important tools for reducing the cost and time required for development of such components.



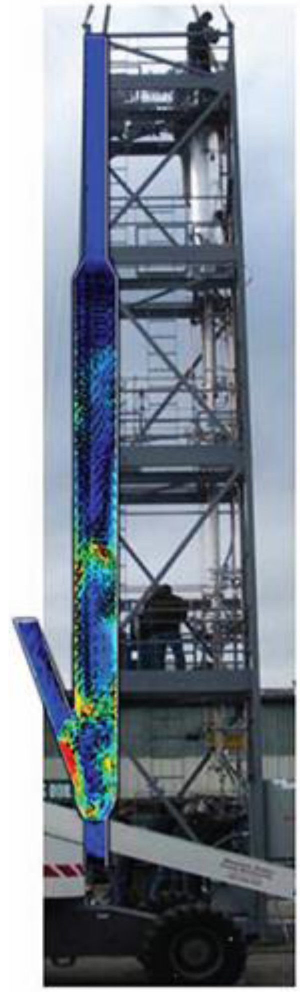
The simulation of a bubbling fluidized bed with heat transfer tubes used for model validation.

The 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 country, such as NETL's University Training and Research programs. Partnerships have also been formed with other national laboratories through the Carbon Capture Simulation Initiative (CCSI) and National Risk Assessment Partnership (NRAP) to resolve the complexities associated with carbon capture and storage.

The vast computational resources available to NETL ensure timely solutions to the most complex problems. The NETL supercomputer is one of the world's fastest, most energy-efficient supercomputers, intended to help energy researchers discover new materials, optimize designs, and better predict operational characteristics. Speed-up is also achieved through research in the areas of modern graphical processing unit (GPU) computing as well as the implementation of reduced order models (ROMs) 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.

The development of data integration software packages such as the R&D 100 award-winning VE-Suite provides a mechanism whereby commercial modeling and simulation code can be exchanged seamlessly across scales. NETL's unique capabilities in multiphase flow science coupled with its extensive knowledge of carbonaceous fuel reactions resulted in the development of the Carbonaceous Chemistry for Computational Modeling (C3M) platform to perform virtual kinetics experiments that elucidate the effect of operating conditions (e.g., heating rate, temperature, pressure, fuel type) on output variables such as conversion rates and yield.

The Simulation-Based Engineering area works closely with stakeholders and partners to outline issues, emerging trends, and areas of need. NETL has sponsored multiphase flow workshops in 2006 and 2009-14 to bring together industry and academia for the identification of and identify R&D priorities to ensure that key technologies will be available to meet the demands of future advanced power systems. NETL, in collaboration with a scientific advisory committee, has also released multiphase flow simulation challenge problems in 2010 and 2013 to improve the reliability of computational modeling of multiphase flows by validation with accurate and well-defined experimental data.



CFD model of a pilot-scale CO_2 adsorber (shown in the background).

Engineering of Complex Systems

Performer: Ames National Laboratory

Award Number: FWP-AL-14-450-011

Project Duration: 10/1/2014 – 9/30/2015

Total Project Value: $250,000

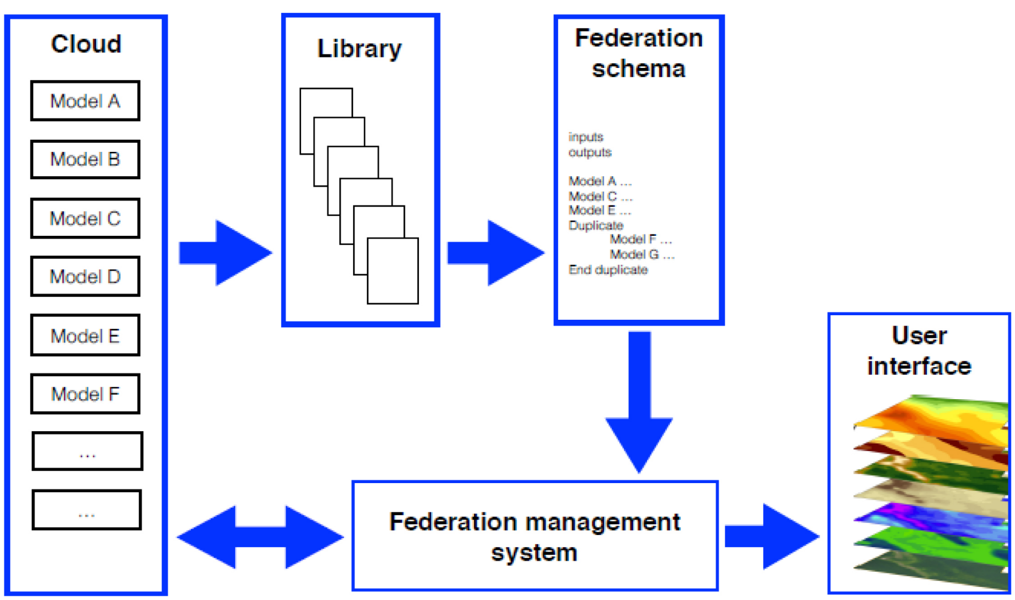
Technology Area: Coal Utilization Sciences

NETL is partnering with Ames National Laboratory to develop the framework and tools needed to create the holistic, complex models that enable policy, engineering, and operational decisions for these energy systems. Specifically, this project is focused on (1) the development of federated model sets as a decentralized approach to coordinating the exchange of information between these independently developed autonomous models and (2) user interaction tools that support assembly, decision making, exploration, design, engineering, and other critical tasks with these federated model sets.

This project seeks to develop a decentralized approach to the coordinated sharing and exchange of information between autonomous models. This architecture provides for decentralized model development and maintenance without a global ontology or schema. Rather, a peer-to-peer ontology and brokered information exchange between models is used to create constituency within a federation of models. The key aspects of this approach are:

- Peer-to-peer ontology
- Development of collaborative communities based on shared interfaces
- Decentralized development of models and model federations

This project can help provide a path forward for integrating models in a number of areas including the design of various power systems; integrating materials design and components (atoms to devices); developing large-scale, granular models of energy components such as gas turbines; modeling the interaction between the grid, consumers, and energy sources; and developing the detailed models needed for the energy-water nexus.



Components and information flow in a federated model architecture.

High Density Sensor Network Development

Performer: Ames National Laboratory

Award Number: FWP-AL-14-450-002

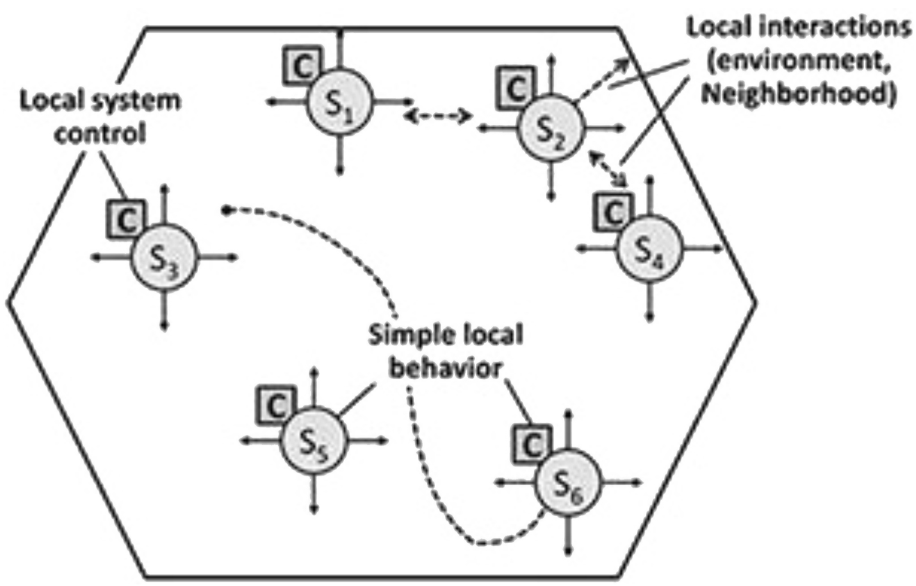
Project Duration: 10/1/2013 – 9/30/2014

Total Project Value: $450,000

Technology Area: Coal Utilization Sciences

NETL partnered with Ames National Laboratory to develop the understanding, algorithms, and control strategies needed to utilize large-scale, high-density sensor networks in advanced power plants. The cost of various sensors is dramatically dropping, the capability of sensors is increasing, and the demands for control and sensing in advanced power plants are significant. Based on this, future power plant sensor development will be based on implementing large-scale, high-density sensor networks. These networks will include a large variety of different kinds of sensors ranging from simple temperature and pressure measurement with little on-board processing capability to those with advanced lab-on-a-chip capabilities. Because of the size and complexity of these sensor networks, sensors will need to be synchronized and orchestrated to provide the significantly improved power plant control and engineering capability needed to achieve the efficiency and near-zero emissions goals of the Department of Energy.

The goal of the project is to develop the mathematics, algorithms, and understanding needed for the implementation of these networks. The expected impact of this technology is reduced operating costs and emissions, and increased efficiency of energy systems such as coal-fired furnaces, fluidized beds, gasifiers, fuel cells, and advanced hybrid power plants.



Management and control in self-organizing systems.

Kinetic Theory Modeling of Turbulent Multiphase Flow

Performer: Ames National Laboratory

Award Number: FWP-AL-14-330-058

Project Duration: 10/1/2013 – 9/30/2015

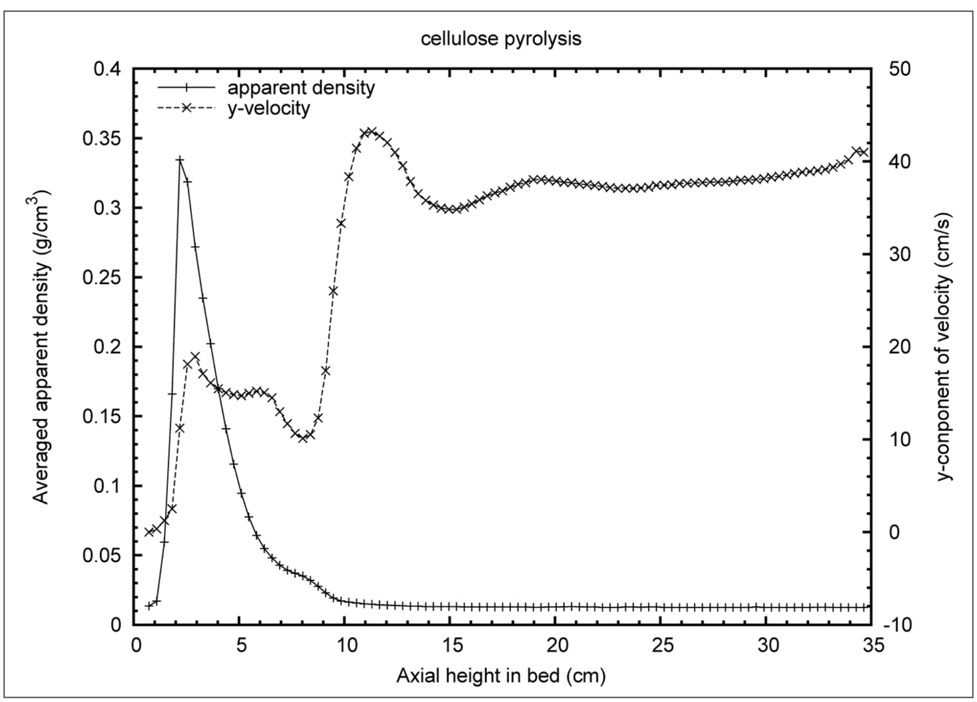
Total Project Value: $580,000

Technology Area: Coal Utilization Sciences

NETL is partnering with Ames National Laboratory to contribute directly to improving the continuum computational models used by the gasification group at NETL for system design and analysis to handle variable-density, variable-size reacting particles in turbulent flow using state-of-the-art mathematical modeling tools. Objectives include (1) implementation of a variable-size reacting particle Computational Flow Dynamics (CFD) model in Multiphase Flow with Interphase eXchanges (MFIX), (2) coupling of a reacting particle CFD model with a detailed gasification kinetic model in MFIX to model coal/biomass gasification, and (3) implementation of a gas-solid turbulence model developed for collisional riser flows in MFIX.

The project will further the present understanding of circulating fluidized beds from the conceptual standpoint of kinetic theory. The primary purpose is to provide a theoretical underpinning for the construction of computer codes to better understand and predict multiphase flow behavior in circulating fluidized beds and, in particular, to provide theoretical estimates for the transport coefficient analogues that parameterize the computer simulations.

This project will reduce design time for gasification combustion systems and supporting systems which will result in lower capital costs for future facilities.



Time-averaged apparent density and y-component of velocity of biomass.

Development of Reduced Order Model for Reacting Gas-Solids Flow Using Proper Orthogonal Decomposition

Performer: Florida International University

Collaborator(s): Texas A&M University

Award Number: FE0023114

Project Duration: 9/1/2014 – 8/31/2017

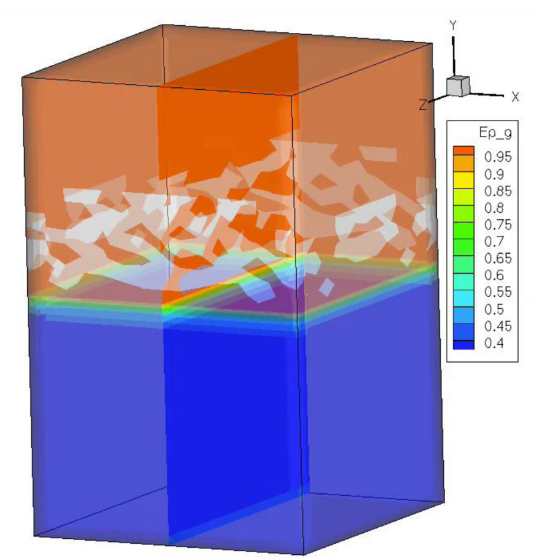
Total Project Value: $279,305

Technology Area: University Training and Research

NETL is partnering with Florida International University to (1) apply advanced computational techniques in order to develop reduced-order models in the case of reacting multiphase flows, based on high fidelity numerical simulation of gas-solids flow structures in risers and vertical columns obtained by the MFIX software; (2) generate numerical data necessary for validation of the models for multiple fluidization regimes; (3) expose minority students to scientific research in the field of fluid dynamics of gas-solids flow systems; and (4) maintain and upgrade the educational, training and research capabilities of Florida International University.

The proposed research will include the numerical investigation of a reacting and non-reacting gas-solids flow system and computational analysis that will involve model development to accelerate the scale-up process for the design of fluidization systems by providing accurate solutions that match the full scale models. The computational work will result in the development of a methodology for obtaining reduced-order models that is applicable to the system of gas-solid flows. Finally, the validity of the developed reduced-order models will be evaluated by comparing the results against those obtained using the MFIX code.

The robustness of existing proper orthogonal decomposition (POD)-based reduced-order model (ROM) for multiphase flows will be improved by avoiding non-physical solutions of the gas void fraction and ensuring that the reduced kinetics models used for reactive flows in fluidized beds are thermodynamically consistent.



Reduced-order model.

Computational Fluid Dynamic Simulations of a Regenerative Process for Carbon Dioxide Capture in Advanced Gasification Based Power Systems

Performer: Illinois Institute of Technology

Award Number: FE0003997

Project Duration: 8/1/2010 – 7/31/2014

Total Project Value: $431,975

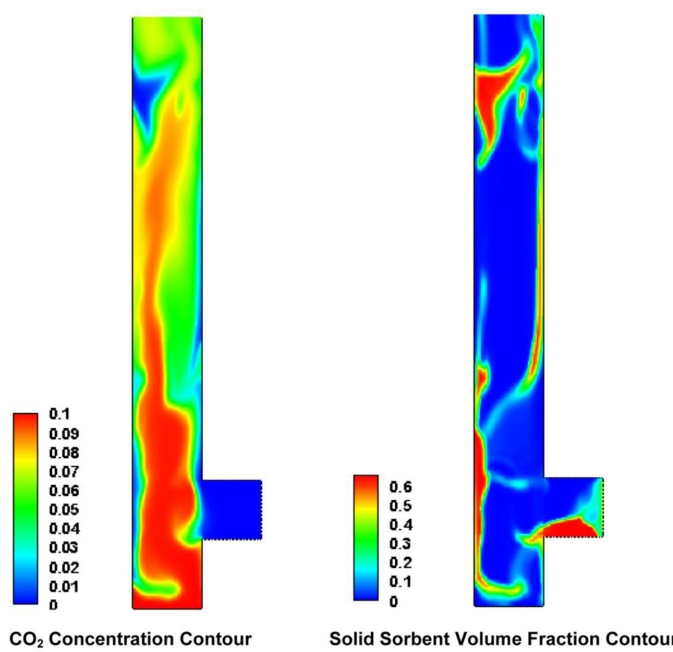
Technology Area: University Training and Research

NETL partnered with Illinois Institute of Technology in a project to model and perform simulations for a regenerative magnesium oxide-based (MgO-based) process for simultaneous removal of carbon dioxide (CO_2) and enhancement of hydrogen (H_2) production in coal gasification. If successful, this process would improve CO_2 absorption capacity and allow for fast and complete regeneration.

The team is focusing on a process that consists of a two-reactor system (absorber and regenerator) containing a mixture of MgO-based sorbents and a commercially available water-gas-shift (WGS) reaction catalyst. The sorbents are characterized by a particle porosity distribution (PPD) whose evolution during the process can strongly affect both the reaction rates of absorption/ regeneration and the particle phase fluid dynamics. To account for such effects, a multiphase computational fluid dynamics (CFD) model is being developed which will include a population balance equation (PBE) governing the PPD evolution.

The project is obtaining the experimental data necessary to determine the key parameters for the CO_2 absorption/ regeneration and the WGS reactions. These parameters will be used to describe the variation of the density and gas compositions due to the reactions. The model will be solved and simulations of the regenerative CO_2 removal process will be performed. The simulation results will be used to determine the optimum reactor configuration and geometry as well as operating conditions for the CO_2 removal and H_2 production.

The project will advance the understanding of the MgO catalyst for use in coal gasification processes. The knowledge gained and CFD/ PBE model and simulations developed will be applied to simulate and aid in design of the advanced gasification-based power systems. Development of this technology is a key element in achieving near-zero emissions while meeting system performance and cost goals.



Carbon dioxide (CO_2) and sorbent concentrations in the riser section of the fluidized bed CO_2 absorber.

Development of a Two-Fluid Drag Law for Clustered Particles using Direct Numerical Simulation and Validation through Experiments

Performer: Florida International University (Applied Research Center)

Collaborator(s): Iowa State University

Award Number: FE0007260

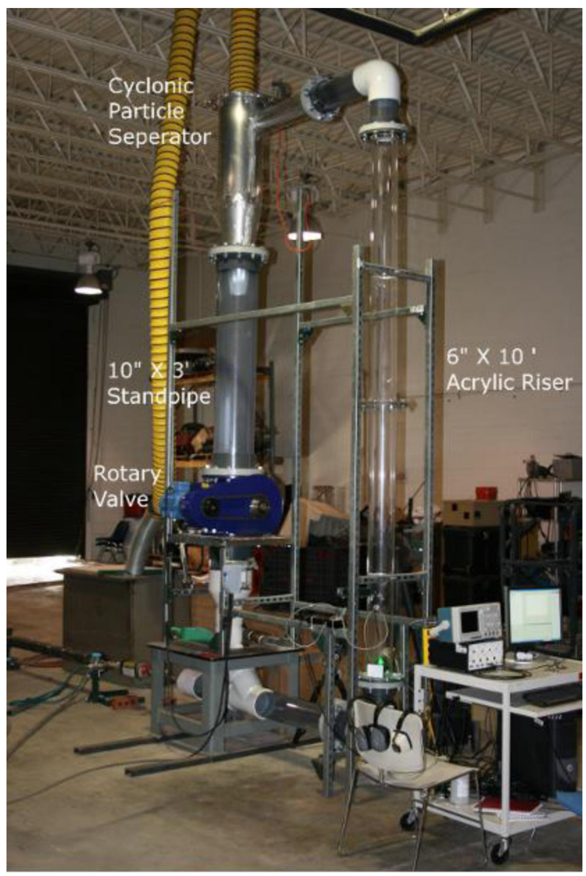
Project Duration: 10/1/2011 – 12/31/2014

Total Project Value: $221,629

Technology Area: University Training and Research

NETL partnered with Florida International University and Iowa State University to develop an accurate drag correlation for gas-solid multiphase flow that includes the effect of clustered particles. The experiments will utilize high-speed imaging to capture instantaneous solid volume fraction and particle velocities in a large laboratory-scale gas solid riser column. Images of the clustered particle structures will be converted into a computational model where the detailed flow field around the particles will be resolved using direct numerical simulation (DNS). The drag force correlation will then be tested in the NETL open-source multiphase gas-solids flow and reactions simulator MFIX (Multiphase Flow with Interphase eXchanges) by comparing the simulation results against experimental data (pressure loss) obtained in the vertical riser.

The goal of the project is to develop a two-fluid drag law for clustered particles using DNS. Computational fluid dynamics (CFD) has become a valuable tool in assisting the design and optimization of gasifiers, combustors, and chemical reactors using fossil fuels. Accurate closure laws are needed to capture the interaction of gas and solid phases in CFD simulation of multiphase reactors such as coal gasifiers and fluidized bed boilers. Interphase drag between the gas and the solids plays a key role in the accurate prediction of the hydrodynamics in CFD simulation of multiphase reactors. The project will develop and validate a new drag law which accounts for particle clustering effects inside the reactor. This will allow scientists and engineers to more realistically simulate the hydrodynamics, gasification kinetics, and thermal behavior of complex gas-particle flow systems. With more realistic simulation capability, more efficient and less costly advanced fossil energy based power generation systems can be designed and built.



Circulating Fluidized Bed Set-up at FIU.

Multiphase Flow Research-Uncertainty Quantification Tools for Multiphase Gas-Solid Flow Simulations using MFIX

Performer: Iowa State University

Award Number: FE0006946

Project Duration: 10/1/2011 – 9/30/2015

Total Project Value: $322,198

Technology Area: University Training and Research

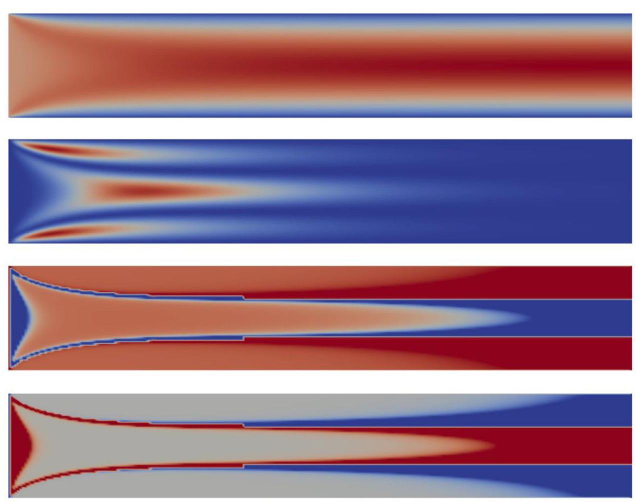
NETL is partnering with Iowa State University to develop uncertainty quantification (UQ) tools for multiphase gas-solid flow simulations using the open source code Multiphase Flow with Interphase eXchanges (MFIX) developed by NETL. Uncertainty quantification (UQ) in complex multiphase computational fluid dynamics (CFD) codes is needed to determine the effect of uncertainty in input parameters, boundary conditions, and theoretical sub-models on the numerical results provided by these codes. One of the most often applied and successful methods to quantify uncertainty from a probabilistic point of view is the polynomial chaos (PC) method.

Polynomial chaos methods have been developed both by reformulating a set of equations in order to obtain a system of coupled equations to evaluate the strength of the PC modes (the so-called intrusive approach), and by using deterministic or random sampling of the original deterministic model to evaluate the PC modes from the outputs of an existing numerical implementation of the model (the non-intrusive approach). However, the application of intrusive UQ to multiphase codes such as MFIX (Multiphase Flow with Interphase eXchanges) for gas-solids flows is prohibitive due to the complexity of the underlying model equations and the time-dependent nature of the output.

This project will develop a non-intrusive PC approach to implement UQ in MFIX. This methodology will generate a set of samples from the output results of the original model. For each sample, a PC expansion as a function of the uncertain parameter is determined.

The overall objective of the project is to develop a non-intrusive UQ approach based on the PC methodology together with reconstruction of the multivariate probability density function required by the approach, and to apply it to the uncertainty quantification in multiphase gas-solids flow simulations.

Multiphase flow is prevalent in fossil-fuel processes such as coal gasifiers and reactors used for sorbent-based carbon dioxide (CO_2) capture. In spite of widespread use and success of computer simulation for design and optimization of multiphase reactors, the current state of the art in computer simulation approaches usually falls short in the crucial aspect of providing objective or statistically meaningful confidence levels for the predicted results. This project will develop and implement an efficient non-intrusive UQ method for gas-solids flow simulations, allowing for error estimation and sampling requirements for UQ analysis. These studies and the new UQ procedure will contribute to the design and deployment of more efficient and environmentally benign power generation systems, by reducing the amount of uncertainty that must currently be factored into the design of multiphase coal fired power generation equipment and systems. Lowering design uncertainty factors will result in lower equipment and operating costs of these systems.



Example application of the quadrature-based UQ procedure to a computer simulation of laminar flow of a fluid between two parallel plates, where the fluid viscosity is uncertain.

Carbon Capture Simulation Initiative (CCSI)

Performer: National Energy Technology Laboratory – ORD

Collaborator(s): Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Pacific Northwest National Laboratory (PNNL), Carnegie Mellon University, the University of Pittsburgh, Virginia Tech, Penn State, Princeton University, West Virginia University, ADA Environmental Solutions (ADA-ES), Alstom Power, Ameren, Babcock Power, Babcock & Wilcox, Chevron, the Electric Power Research Institute (EPRI), Eastman, Fluor, General Electric, Ramgen Power Systems, and Southern Company

Award Number: FWP-2012.04.02

Project Duration: 10/1/2011 – 1/31/2016

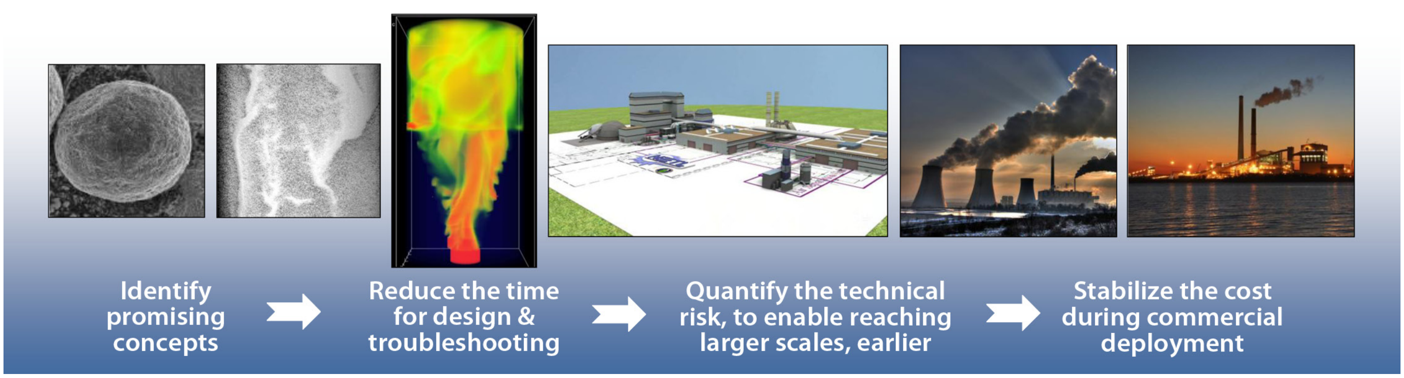
Total Project Value: $42,246,093

Technology Area: Coal Utilization Sciences

The Carbon Capture Simulation Initiative (CCSI) project is led by the National Energy Technology Laboratory (NETL) and leverages the DOE national laboratories' core strengths in modeling and simulation. CCSI's industrial partners provide representation from the power generation industry and the power equipment manufacturers. The initial industrial partners are ADA Environmental Solutions (ADA-ES), Alstom Power, Ameren, Babcock Power, Babcock & Wilcox, Chevron, the Electric Power Research Institute (EPRI), Eastman, Fluor, General Electric, Ramgen Power Systems, and Southern Company. CCSI's academic participants bring unparalleled expertise in multiphase flow reactors, combustion, process synthesis and optimization, planning and scheduling, and process control techniques for energy processes.

CCSI will develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon-capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. By developing the CCSI Toolset, a comprehensive, integrated suite of validated science-based computational models, this initiative will provide simulation tools that will increase confidence in designs, thereby reducing the risk associated with incorporating multiple innovative technologies into new carbon-capture solutions. The scientific underpinnings encoded into the suite of models will also ensure that learning will be maximized from successive technology generations.

The CCSI Toolset will provide end users in industry with a comprehensive, integrated suite of scientifically validated models, with uncertainty quantification, optimization, risk analysis, and decision making capabilities. The CCSI Toolset will incorporate commercial and open-source software currently in use by industry and will also develop new software tools as necessary to fill technology gaps identified during execution of the project. The CCSI Toolset will (1) enable promising concepts to be more quickly identified through rapid computational screening of devices and processes; (2) reduce the time to design and troubleshoot new devices and processes; (3) quantify the technical risk in taking technology from laboratory scale to commercial scale; and (4) stabilize deployment costs more quickly by replacing some of the physical operational tests with virtual power plant simulations.

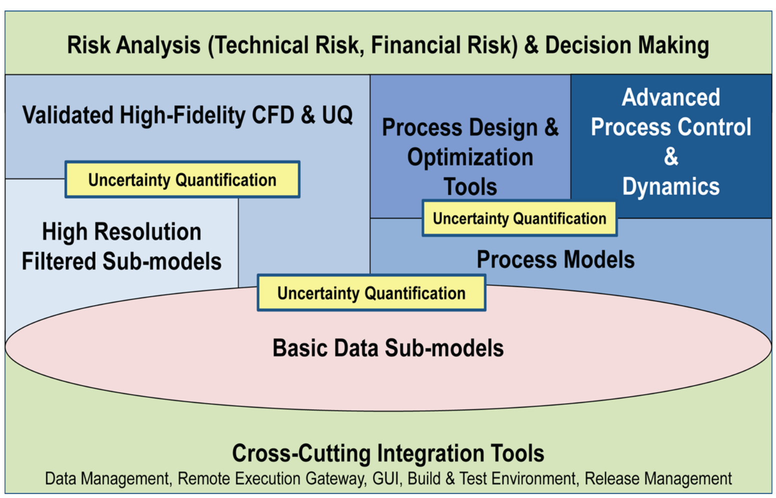


Framework around which the toolset can be developed and demonstrated.

While the ultimate goal of the CCSI is to deliver a toolset that can simulate scale-up of a broad set of new carbon-capture technologies from laboratory scale to full commercial scale, the project scope during the first five years will be limited to the development of capabilities applicable to three industrial challenges: that is, to make deployment of carbon capture and sequestration widespread, safe, and cost-effective. Among possible carbon-capture technologies, post-combustion capture by solid sorbents and by advanced solvents and combustion in an oxygen atmosphere (oxy-combustion) are expected to have the most significant impact on U.S. pulverized coal (PC) power plants, which currently generate nearly half of the nation's electricity and will emit 95 percent of the coal-based CO_2 between 2010 and 2030.

The CCSI toolset will include validated models of carbon-capture equipment and processes as well as new design and analysis tools and methodologies. Industry utilizing the CCSI toolset will be able to reduce the time and expense of new technology development, from discovery to demonstration to widespread deployment, by a minimum of five years. The total cost savings that could be realized by using the CCSI toolset to scale up and widely deploy just one carbon-capture technology is estimated to be approximately $500 million (net present value basis). Another objective of CCSI is to use information from science-based models with quantified uncertainty to inform investors. Validating the models at different scales, quantifying the uncertainty of model predictions, and estimating the technical risk will enable smarter demonstrations and ultimately could accelerate demonstrations by several years.

Ultimately, the entire nation benefits from this successful collaboration. As laboratory breakthroughs move more quickly into the commercial marketplace, industry can accelerate the deployment of successful carbon-capture technologies—and America's abundant fossil resources will provide cleaner energy well into the future.



The 8 product categories of the CCSI Toolset.

Innovative Process Technology Field Work Proposal/ Task 6: Multiphase Flow

Performer: National Energy Technology Laboratory – ORD

Collaborator(s): Carnegie Mellon University (CMU), University of Pittsburgh (Pitt), Pennsylvania State University (Penn State), West Virginia University (WVU), and Virginia Polytechnic Institute and State University (Virginia Tech)

Award Number: FWP-2012.04.01

Project Duration: 10/1/2011 – 9/30/2015

Total Project Value: $2,515,961

Technology Area: Plant Optimization Technologies

NETL will focus on developing an improved physics-based computational fluid dynamics (CFD) capability for simulating reacting multiphase flows. This effort will focus on (1) the reduction of time to solution of multiphase CFD simulations through porting Multiphase Flow with Interphase eXchanges (MFIX) to graphics processing unit architecture and extension of the multiphase reduced order models to reacting flows; (2) improving the fidelity of multiphase CFD simulations by accounting for particle size and density distribution in reacting multiphase flows, and developing predictive capability at the porous microstructure scale of solid sorbent particles used in carbon dioxide (CO_2) capture; and (3) including uncertainty quantification as an integral part of simulations, with incorporation of stochastic analysis with minimal sampling technique to reduce the data sampling required.

Gas-solids multiphase flows occur in fossil energy devices such as gasifiers and solid-sorbent based CO_2 adsorbers/regenerators. In order to reduce time to solution of multiphase reacting flow simulations, it is proposed to accelerate MFIX-DEM using general purpose graphics processing units (GPU) and extend the current multiphase reduced order models (ROMs) to chemically reacting flows. The reduction in data sampling for uncertainty quantification will be achieved by stochastic analysis with minimal sampling. Improvements to the MFIX reacting capabilities will be made by incorporating a variable density model along with a variable size model.

GPU Acceleration of MFIX: Beginning with the dominant grid-based neighbor search routine, NETL will perform an analysis of alternatives to neighbor search algorithms for general purpose GPUs (GPGPUs) and consider their impact on MFIX-DEM data structures. Concurrently, researchers will re-assess strategies and technologies (e.g., CUDA, compiler directive-based approaches, and source-to-CUDA translation) for implementing MFIX-DEM on GPGPUs.

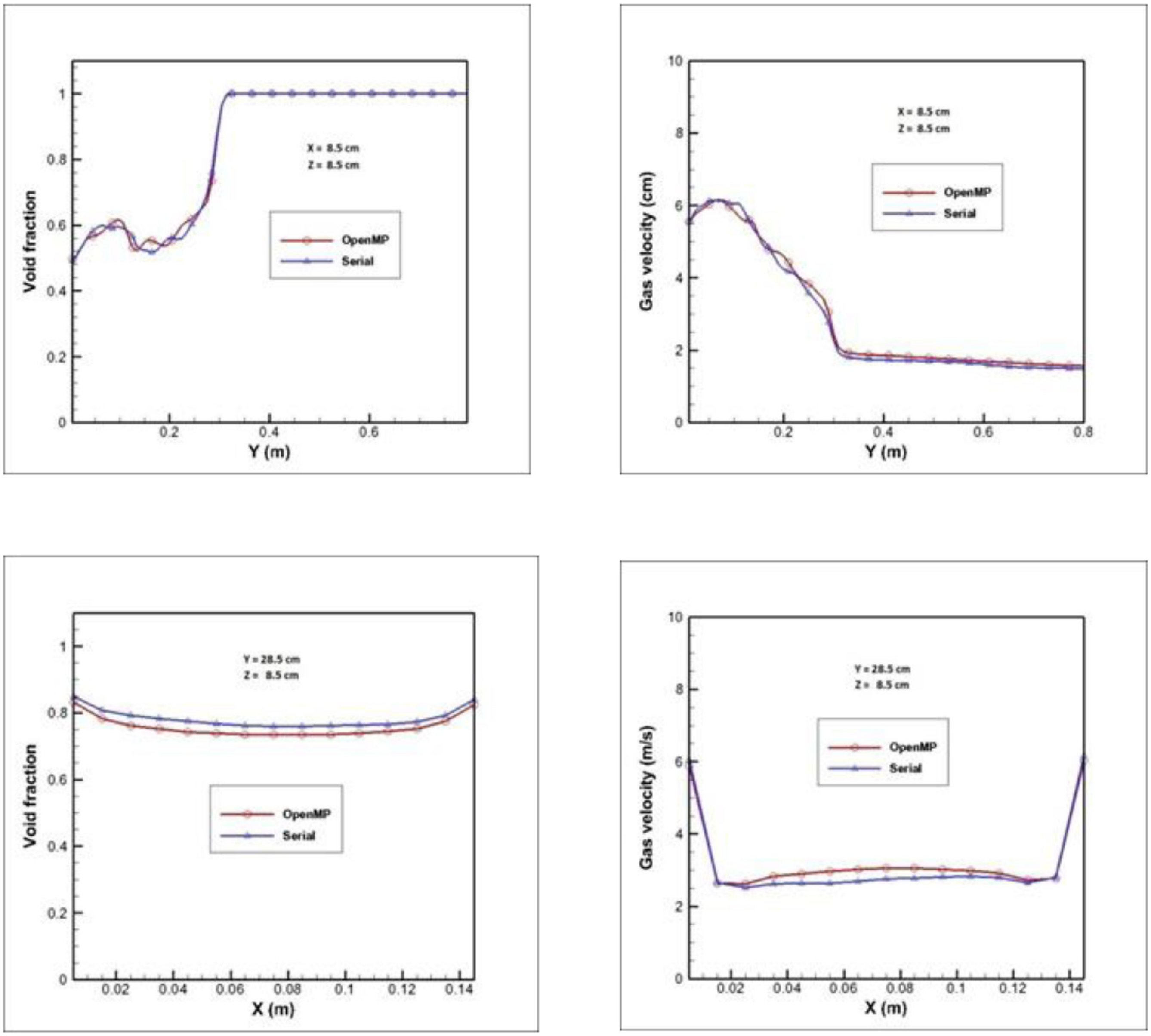
Reacting Multiphase ROM: This research will expand on existing proper orthogonal decomposition (POD) multiphase ROM software to incorporate the framework necessary for chemically reacting multiphase flow modeling and allow for examination of other multiphase systems. Specifically, the current POD Multiphase ROM software is only capable of handling a single species each of gas and solid matter. The proposed work will first build in the supporting framework for multiple species and phase handling. Secondly, thermal transport capabilities will be incorporated into the software.

Heat and Mass Transfer in Porous Sorbent Particles: This effort will develop predictive capability at the porous microstructure scale of solid sorbent particles used in CO_2 capture. The diffusion of heat and species mass through the porous microstructure control the rate of absorption and desorption of CO_2 and hence are important to quantify for a fundamental understanding and control of the process. Transmission electron microscopy (TEM) will be used to characterize the porosity of typical sorbent particles; this characterization will be used to construct a porous microstructure based on stochastic procedures. The constructed microstructure will be used within the framework of the immersed boundary method to calculate the flow, heat, and species mass transfer.

MFIX Model for Polydisperse Particles: By developing MFIX-based models for polydisperse, reacting, variable-density solid particles with strong coupling to the gas phase, this project will facilitate the numerical simulation and scale-up of energy systems such as gasifiers.

Stochastic Analysis with Minimal Sampling (SAMS): Towards addressing the challenges associated with uncertainty quantification in computationally intensive physical simulations, an innovative method called Stochastic Analysis with Minimal Sampling (SAMS) will be used to approximate output distributions of MFIX, where some or all of the input data could be uncertain.

It is expected that the GPU acceleration of MFIX will yield a 2- to 8-fold reduction in time to solution. Along with improvements in reacting gas-solid models in MFIX, the reacting multiphase ROM, and a reduction in the number of data sampling requirements for uncertainty quantification, the simulation capabilities put in place at the successful completion of these projects will enhance NETL's predictive capabilities to design and optimize reactors used in fossil energy systems.



Comparisons between the parallel implementation using Open-MP and serial version of MFIX-DEM, for a bubbling fluidized bed.

National Risk Assessment Partnership (NRAP)

Performer: National Energy Technology Laboratory – ORD

Collaborator(s): Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), and Pacific Northwest National Laboratory (PNNL)

Award Number: FWP-2012.04.03

Project Duration: 10/1/2011 – 9/30/2015

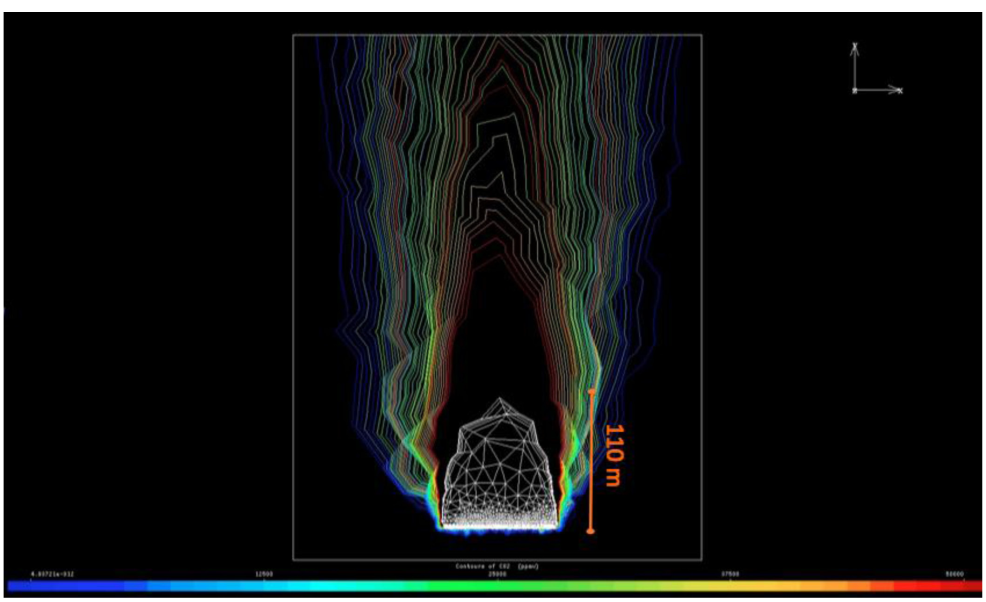
Total Project Value: $40,677,000

Technology Area: Coal Utilization Sciences

The U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) is conducting research to advance the science and engineering knowledge base for technologies that will accelerate the business case for carbon dioxide (CO_2) capture and storage, including prediction and quantification of risks that may relate to potential liabilities. As part of this effort, NETL, through its Office of Research and Development (ORD), is leading a multi-laboratory effort that leverages broad technical capabilities across the DOE complex. NRAP involves five DOE national laboratories. This team is working together to develop a science-based method for quantifying the likelihood of risks (and associated potential liabilities) for CO_2 storage sites.

The primary objective of NRAP is to develop a defensible, generalized, and science-based methodology and platform for quantifying risk profiles at CO_2 storage sites. The methodology must incorporate and define the scientific basis for assessing residual risks associated with long-term stewardship and help guide site operational decision-making and risk management. Development of an integrated, strategic, risk-based monitoring and mitigation protocol is part of the NRAP objective; this protocol will help to minimize uncertainty in the predicted long-term behavior of the site and thereby increase confidence in storage integrity.

NRAP will address innate characteristics of environmental risks by focusing on probabilistic quantification of site-specific risk profiles. In general, risk profiles (risk over time) should describe the time-dependent components of risk as the engineered natural system evolves and eventually equilibrates with the regional subsurface environment. The site-specific nature of the assessment methodology will allow for spatially varying components of risk. The probabilistic approach will be designed to capture uncertainties associated with site heterogeneity and complexity, which will be incorporated with other factors in the uncertainty quantification (UQ) conducted by NRAP.

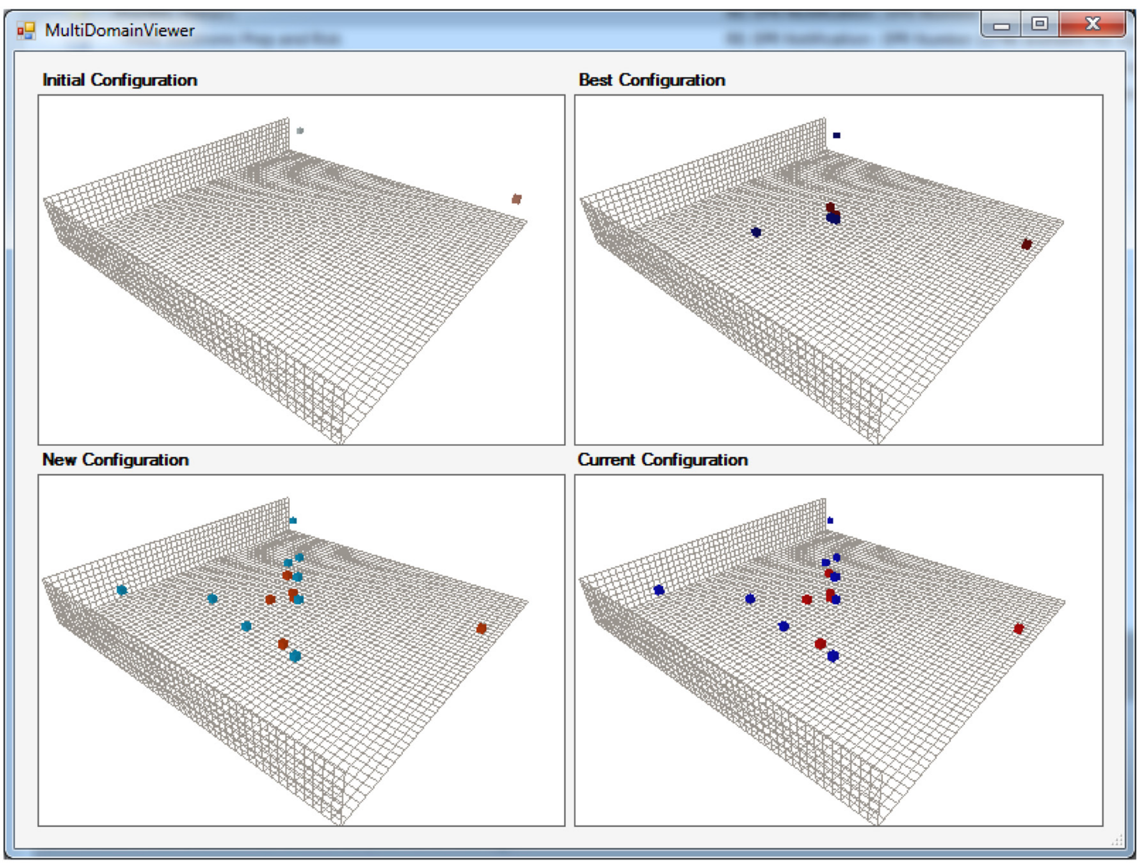


Carbon Dioxide (CO_2) isoconcentration lines after three hours of atmospheric dispersion of CO_2 following constant leakage up the fault (line source) at the bottom of the image.

The overall NRAP effort is divided into four general technical components, plus an additional component that captures issues with large stationary sources other than power plants. The four main components are:

- Development of a methodology and computational platform for quantifying risk profiles based on integrated assessment models (IAMs) and uncertainty quantification (UQ).
- Targeted scientific investigations at the laboratory and field scales to reduce uncertainties in the predicted risk profiles.
- Integration of risk-based monitoring and mitigation strategies to reduce both uncertainty and overall risk.
- Field-scale tests of specific processes to validate predicted behaviors of natural systems.

The tools and improved science base generated by NRAP will aid operators in the design and application of monitoring and mitigation strategies. These tools can also be used by regulators or their agents to help identify and quantify risks associated with geologic carbon storage and perform appropriate cost-benefit analysis for specific storage projects. Additionally, costs of long-term liability can be much more easily estimated and with less uncertainty, thereby providing greater confidence to investors regarding CCS projects and to regulators in approving them.



MVA Optimization Model.

Implementation and Refinement of a Comprehensive Model for Dense Granular Flows

Performer: Princeton University

Award Number: FE0006932

Project Duration: 10/1/2011 – 9/30/2015

Total Project Value: $420,366

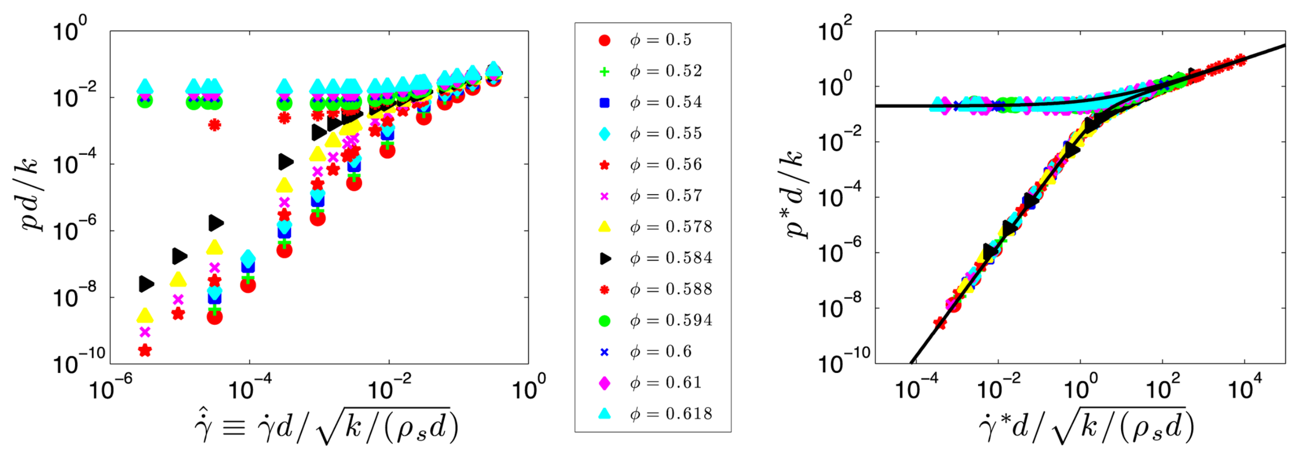
Technology Area: University Training and Research

NETL is partnering with Princeton University to utilize a combination of continuum simulations for model validation and discrete particle simulations for model refinement. The overall thrust of this project is to implement and test a new rheological model for dense granular phase in MFIX while continuing to improve it to capture more complex flow behavior. Specific objectives accomplished to date include:

- Implementation of the steady-shear rheological model for dense granular assemblies in MFIX and testing using boundary conditions already available in MFIX
- Generalization of the steady-shear rheological model for dense granular assemblies to account for cohesive interactions
- Development of a modified kinetic theory for dynamic evolution of the stresses
- Development improved wall boundary conditions for the particle phase

Implementation of the modified kinetic theory and the wall boundary conditions into MFIX, and their testing will be completed in the remaining period of the project.

The continuum model developed at Princeton predicts stresses in a wide range of granular flow conditions, and is a promising candidate for predicting flow behaviors in industrially relevant flows. It will enhance the ability to interrogate both dense and moderately dilute flow behavior in large-scale processes. This research in combination with other modeling efforts is targeting improved accuracy and predictive capability of system and flow behavior, which will lead to better process design and reduced cost associated with scale-up of advanced technologies that include complex flow regimes.



Regime map displaying dimensionless pressure vs. dimensionless shear rate at various particle volume fractions, as determined from DEM simulations. The figure on the left shows pressure, made dimensionless using particle diameter (d), and the contact stiffness (k) as a function of scaled shear rate. The figure on the right shows that all the results could be collapsed nicely by rescaling the pressure and shear rate. $p^* = \hat{p}/|\phi-\phi_c|^{2/3}; \dot{\gamma}^* = \hat{\dot{\gamma}}/|\phi-\phi_c|^{4/3}$. Here ϕ_c refers to the critical (jamming) volume fraction, which is a function of particle friction coefficient (= 0.5 in these figures).

Coal Combustion and Gasification Science

Performer: Sandia National Laboratory (SNL)

Award Number: FWP-14-017206

Project Duration: 10/1/2014 – 9/30/2015

Total Project Value: $300,000

Technology Area: Coal Utilization Sciences

NETL is partnering with Sandia National Laboratory to provide experimental measurements of the reaction kinetics of coal char at high temperatures and elevated pressures. This research will utilize Sandia's pressurized combustion and gasification reactor to quantify the kinetics of oxidation and gasification under conditions relevant to pressurized circulating fluidized bed reactors and coal gasifiers. This project includes oxidation and gasification kinetics of chars, as well as the influence of pressure on devolatilization and char formation.

Pressurized entrained flow reactor.

This project will incorporate kinetic models and data into the Carbonaceous Chemistry for Computational Modeling (C3M) package. The objectives of this research are to generate the validation data necessary for the Sandia kinetic model for oxy-combustion of coal char and a report detailing the incorporation of this kinetic model into C3M.

This information is needed to improve both the phenomenological understanding and the comprehensive computational fluid dynamic (CFD) modeling of many technologies including pressurized circulating fluidized bed combustors (PCFBCs), entrained flow gasifiers (e.g., Shell, Destec, and Texaco/GE designs), and transported bed gasifiers (KBR design).

Study of Particle Rotation Effect in Gas-Solid Flows Using Direct Numerical Simulation with a Lattice Boltzmann Method

Performer: Tuskegee University

Collaborator(s): Ohio State University

Award Number: FE0007520

Project Duration: 10/1/2011 – 9/30/2014

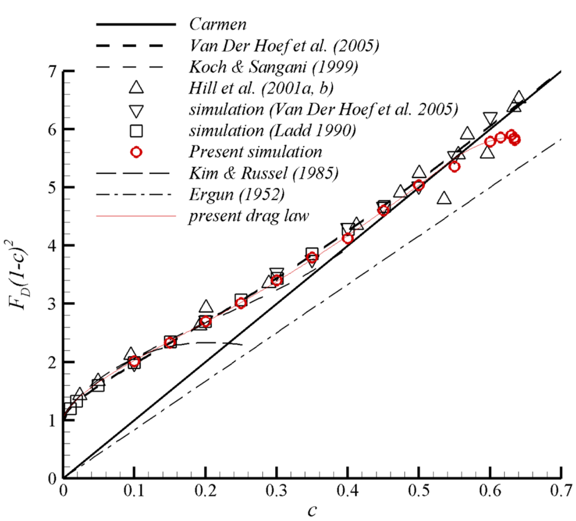
Total Project Value: $200,000

Technology Area: University Training and Research

NETL partnered with Tuskegee University and Ohio State University to investigate the drag force between solid particles and gas phases using the DNS method. The advanced lattice Boltzmann method (LBM) will be used to carry out simulations for microscopic model systems in which the particle surface is directly resolved. The immersed boundary (IB) technique will be included in the LBM to accurately represent particle shapes in the simulation, allowing for straightforward accounting of poly-dispersed and non-spherical particles. Effects of particle rotation and of hydrodynamic interactions and direct contacts between particles will be included in the simulation. Particle motion and forces will be recorded and compared to experimental results obtained using high-speed particle imaging methods developed by NETL. The particle-fluid drag force data acquired from fine-scale simulations will be used to generate a database to help formulate an improved drag correlation that explicitly includes information on microstructures of particles and fluid flows as well as particle and fluid properties. Finally, the new drag correlation will be tested in the NETL open-source multiphase gas-solids flow and reactions simulator MFIX (Multiphase Flow with Interphase eXchanges) by comparing simulation results using the new drag correlation with simulation results using existing drag models, and comparing the simulation results with published experimental data. The project team will also conduct studies to compare the new model with other traditional drag models to predict gas-solid flow interactions at mesoscopic scales.

The goal of this project is to address the effects of particle rotation in gas-solid flows. Specific objectives to be studied include (1) the direct impact of particle rotation on the average particle-fluid drag force of a particle suspension at various Reynolds numbers (i.e., ratios of inertial to viscous forces); (2) the indirect impact of particle rotation on the drag force through the change in particle concentration distribution or the microstructure of a flow; and (3) the role of particle rotation in energy dissipation of a particle-fluid system.

At completion, this project will provide a new drag model that accounts for particle rotation effects and quantitative insights into fundamental gas-solid particle interactions in flow regimes of interest to fossil energy power generation systems. The database resulting from this study will help to fill a data gap and formulate the constitutive equations necessary for more accurate Eulerian-Lagrangian multiphase flow models. These studies will eventually contribute to the design of more efficient and environmentally benign power generation systems.



The normalized Stokes-flow drag force FD [multiplied by the porosity squared $(1-c)^2$] on the non-rotational spheres in random arrays as a function of the solid volume fraction. The simulation result of Ladd (1990), Hill et al. (2001a,b) and Van Der Hoef et al. (2005) are represented by symbols. The fit proposed by Van Der Hoef et al. (2005) is represented by a dashed line. The results from the theories of Carmen and Koch & Sangani (1999) are also shown. The present fit based on our simulation data is consistent with previous studies at solid volume fractions c less than 0.55. For close-packed solid volume fractions, the present fit is closer to the most commonly adopted drag relation by Ergun (1952).

Quantifying the Uncertainty of Kinetic-theory Predictions of Clustering

Performer: University of Colorado

Collaborator(s): Extremadura, Colorado School of Mines

Award Number: FE0007450

Project Duration: 9/21/2011– 9/20/2014

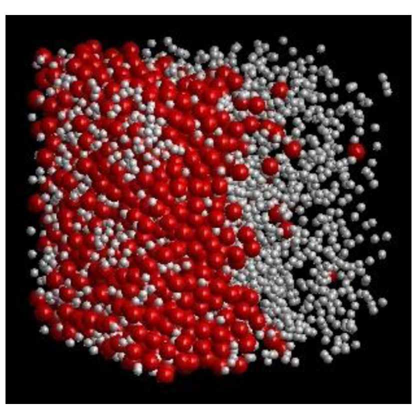
Total Project Value: $300,000

Technology Area: University Training and Research

NETL partnered with the University of Colorado to quantify the uncertainty of kinetic-theory predictions of particle clustering. Processes involving the flow of solid particles are ubiquitous in both industry and nature, though a predictive understanding of their behavior has not been achieved. One area of interest is a better understanding of high-velocity gas-solids flows such as those found in circulating fluidized beds used in coal gasification. Of particular interest are instabilities, often referred to as clusters, which are commonplace in the riser section of circulating fluidized beds and are known to have a significant impact on system performance. Clusters are loose collections of particles that join and disperse due to collisions between the particles within the flow. Contributors to clusters include inelasticity, friction, viscous dissipation, and mean drag. Clustering causes instabilities that affect the flow behavior of the system. A predictive knowledge of the instabilities observed in high-velocity flows is critical to the design, scale-up, and optimization of systems used for the production of energy from coal.

Streamers and clusters observed in high-velocity gas-solid risers strongly influence the lateral mixing of particles and the associated gas-solid contact efficiency, which ultimately impacts reactor efficiency (i.e., the amount of energy obtained per unit of coal). Reactor efficiency, in turn, is directly related to the environmental impact of the energy production process. A number of systems will be examined to quantify the type, onset, evolution, and steady-state characteristics of instabilities and to isolate the mechanisms leading to them.

Successful translation to quantitative predictions is uncertain since cluster interfaces are known to have a high Knudsen number (a ratio relating the molecular mean free path length to a representative physical length scale), which is counter to the assumption used in the derivation of kinetic-theory models. However, previous work indicates that kinetic-theory models often perform well outside their expected range of validity. The research team expects that these models will provide sound quantitative predictions for the instabilities. The team will generate a range of benchmark simulation data in which particles are treated discretely, and compare results to transient, three-dimensional predictions from the kinetic-theory-based model. In order to quantify the type, onset, evolution, and steady-state characteristics of the instabilities and to effectively isolate the mechanisms leading to such instabilities, a number of systems will be examined, including those exhibiting homogeneous cooling, simple shear, and infinite settling.



Molecular dynamics (MD) simulations are used to understand particulate flows.

The main goal of the project is to quantify the uncertainty associated with kinetic-theory predictions of the clustering instabilities present in high-velocity gas-solid flows. There are two major objectives. The first is to generate benchmark data with an eye toward determining the relative importance of the physical mechanisms that give rise to the instabilities. Although it has been established previously that inelastic collisions and gas-phase effects can independently lead to instabilities in granular and gas-solid flows, their relative importance has not been examined, nor has the expected important effect of friction. The second objective is to apply kinetic-theory (continuum) models, with no adjustable parameters, to the same flow geometries used for the benchmark data. Kinetic-theory models have been shown to predict such instabilities, though previous validation work, such as snapshots and/or movies of particle clusters, is largely qualitative in nature.

The project is the first study to identify the relative importance of each contributor to the particle clusters present in high-velocity gas-solid flows. It also represents the first attempt to quantify the uncertainty associated with the kinetic-theory predictions of clustering instability. Such knowledge is critical for accurate prediction of industrial systems, and the results are expected to provide critical information for improving reactor efficiency in energy production systems. Greater efficiency of power systems will allow the nation to produce more power using less fuel, leading to decreased emissions of greenhouse gases and toxic substances from power plants.

Use of an Accurate DNS Method to Derive, Validate and Supply Constitutive Equations for the MFIX Code

Performer: University of Texas at San Antonio

Award Number: FE0011453

Project Duration: 7/1/2013 – 6/30/2016

Total Project Value: $189,825

Technology Area: University Training and Research

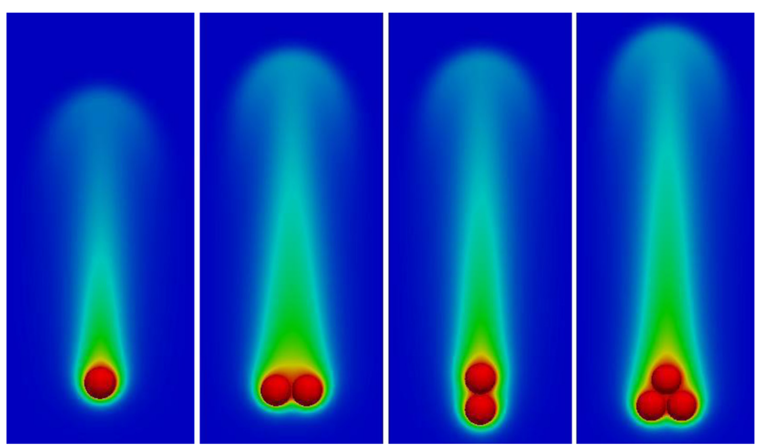
NETL is partnering with University of Texas at San Antonio by selecting several categories of non-spherical particles at various solid fractions to perform appropriate numerical computations under different flow conditions and particle properties. The project team will use their direct numerical simulation immersed boundary (DNS-IB) model (Feng and Michaelides, 2005, 2008, 2009a; Davis et al., 2011), which has been validated in several projects, in order to produce meaningful and accurate constitutive heat and mass transfer equations for non-spherical particles and clusters. The constitutive equations on heat transfer of solid and fluid phases will substitute the currently used expressions in the MFIX code. The main advantage of using the DNS-IB code is that it requires the least amount of empirical input.

The DNS-IB code will then be used to further achieve the following objectives: (a) to obtain the heat transfer coefficients (or Nusselt numbers) for several classes of non-spherical particles and clusters, (b) to determine the influence to the heat transfer from particles of different shapes in the presence of neighboring particles and to discover an explicit functional relationship between the Nusselt numbers and the solid fractions; (c) and to provide meaningful correlations for these coefficients that may be used directly in the MFIX code. It must be pointed out that, in order to achieve these objectives, particles of commonly encountered shapes such as ellipsoidal (glass bead), cubic (sugar, calcite), angular (crushed minerals), platelet (clays, graphite), and irregular particles formed as aggregates of spheres will be considered, and extensive simulations will be performed to cover a large range of solid fractions. These correlation equations will be ready for use with the MFIX code and will significantly improve its predictive capabilities.

The overall goal of this project is to improve the performance and accuracy of the MFIX code frequently used in multiphase flow simulations. The specific objective of the project is to use a novel and validated direct numerical simulation particulate flow program combined with the immersed boundary method (DNS-IB) to establish, modify, and validate needed constitutive equations for the heat and mass transfer from non-spherical particles and clusters of particles to be used in the MFIX code.

The results of the computations will be used to derive accurate constitutive equations for the solids-fluid heat and mass transfer. In addition, constitutive equations will be also derived for clusters of particles.

The equations will be ready to be used in the MFIX code and will significantly improve its predictive capabilities.



Comparing Natural convection from an isolated sphere, bi-spheres in contact, and triangular cluster for Pr=0.72 and Gr=100 on each sphere – temperature contour slices at time 3s.

Abbreviations

AARA ..... American Recovery and Reinvestment Act

C3M .... Carbonaceous Chemistry for Computational Modeling

CCS .... carbon capture and storage

CCSI .... Carbon Capture Simulation Initiative

CCUS .... carbon capture, utilization, and storage

CES .... Computational Energy Sciences

CFB .... circulating fluidized bed

CFD .... computational fluid dynamics

CO_2 .... carbon dioxide

CUS .... Coal Utilization Science

DEM .... discrete element method

DNS .... direct numerical simulation

DOE .... Department of Energy

EPRI .... Electric Power Research Institute

GPU .... graphic processing unit

H_2 .... hydrogen

HBUC ...... historically Black colleges and universities

IAM .... integrated assessment model

IB .... immersed boundary

LAMMPS .... Large Scale Atomic/Molecular Massively Parallel Simulator

LANL .... Los Alamos National Lab

LBNL .... Lawrence Berkeley National Lab

LLNL .... Lawrence Livermore National Lab

LMB .... Lattice Boltzmann Method

MD .... molecular dynamics

MFIX .... Multiphase Flow with Interphase eXchanges

NETL .... National Energy Technology Lab

NO_x .... nitrogen oxides

NRAP .... National Risk Assessment Partnership

ORD .... Office of Research and Development

PBE .... population based equation

PC .... polynomial chaos

PC .... pulverized coal

PCFBC .... pressurized circulating fluidized bed combustor

PCGR .... pressurized combustion and gasification reactor

PPD .... porosity distribution

PIV .... particle image velocimetry

POD .... proper orthogonal decomposition

R&D .... research and development

ROM .... reduced-order model

RTE .... radiative transfer equation

RUA .... Regional University Alliance

SAMS .... stochastic analysis with minimal sampling

SBIR .... Small Business Innovation Research

SCC .... Strategic Center for Coal

SBEUC ...... Simulation-Based Engineering User Center

TEM .... transmission electron microscopy

UCR .... University Coal Research

UQ .... uncertainty quantification

WGS .... water gas shift

3-D .... three-dimensional

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Websites:

http://energy.gov/fe/coal-utilization-science

http://www.netl.doe.gov/research/coal/crosscutting/simulation-Based-engineering

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