PROGRAM facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Power Systems Advanced Research

07/2008

COMPUTATIONAL ENERGY SCIENCES PROGRAM

Description

Led by the National Energy Technology Laboratory (NETL), the Advanced Research (AR) Computational Energy Sciences (CES) Program provides high-performance computational modeling and simulation resources to the Office of Fossil Energy (FE) and other programs of the U.S. Department of Energy (DOE). These resources are dedicated to speeding development and reducing costs associated with advanced power system design and performance modeling. CES research is focused on developing a set of complex but flexible computational tools that allow more rapid and efficient scale-up of new subsystems, devices, and components, thereby reducing the need for large and expensive demonstration-scale testing of integrated energy systems, and lowering operational risks associated with commercialization.

In collaboration with industry and academic partners, CES activities support the development of critical and enabling technologies that contribute to the design and operation of advanced, coal-based, near-zero emission power and fuel systems. These systems include the demonstration of multiple commercial-scale Integrated Gasification Combined Cycle (IGCC) or other clean coal power plants with cutting-edge carbon capture and storage (CCS) technology under the Department's restructured FutureGen approach.

The CES Program has established an extensive network of interconnected participants to concentrate talents, resources, and motivations not found in any one organization. NETL serves as the nucleus, due to its extensive background in fossil energy processes and simulation, and its implementation role in the FE research and development (R&D) program. Several other national laboratories have substantial experience in developing complex simulation codes for defense and infrastructure issues. University partners bring extensive theoretical expertise and supply the students who ultimately will carry the expertise into practice in industry. Software firms contribute cutting-edge

Advanced Research — To support coal and power systems development, NETL's Advanced Research Program conducts a range of pre-competitive research focused on breakthroughs in materials and processes, coal utilization science, sensors and controls, computational energy science, and bioprocessing — opening new avenues to gains in power plant efficiency, reliability, and environmental quality. NETL also sponsors cooperative educational initiatives in University Coal Research, Historically Black Colleges and Universities, and Other Minority Institutions.

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expertise in code development that can be applied to the needs of the fossil energy industry. Finally, partnerships with the ultimate industrial users assure that the end goal of establishing simulation and modeling as a principal design and operating tool for new FE systems will be met.

PROGRAM PARTICIPANTS

Carnegie Mellon University
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Duquesne University
Pittsburgh, PA

NASA Independent Verification & Validation (IV&V) Facility
Fairmont, WV

Pittsburgh Supercomputing Center
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Goals

Specific CES Program goals include:

- Developing simulation capabilities that couple fluid flow, chemical reaction, heat generation, heat transfer, electrochemistry, and Reynold stresses for modeling multi-dimensional transient events in fuel cells, heat engines, combustors, gasifiers, chemical reactors, and other crucial unit processes in FutureGen types of plants
- Accessing multiple high-end computing platforms for use in fossil energy simulations
- Developing software for fossil energy systems that can utilize teraflop (one trillion floating-point operations per second) computing resources
- Developing data reduction, data extraction, and data mining techniques for information obtained from simulation studies of advanced FutureGen plants or other systems
- Acquiring high-end visualization capabilities for fossil energy simulation and experimental data display and analysis
- Developing a multi-party laboratory composed of NETL, other national laboratories, and universities that can be quickly mobilized in a cooperative dynamic working environment to provide extensive simulation and modeling expertise
- Training student engineers and scientists to develop and analyze optimal control systems for future fossil energy plants
- Promoting the use of simulation as a principal design, construction, and operating tool for fossil energy equipment suppliers and energy plant owners

Program Areas

The CES Program covers three primary work areas: Multiphase Flow Research and Model Validation, Process and Dynamic Systems Modeling and Device Scale Modeling.

Multiphase Flow Research and Model Validation – The goal of projects in this area is to improve the speed and accuracy of the simulations of complex multiphase flows that are commonly encountered in advanced power and process plants. An example is the Multiphase Flow with Interphase eXchanges (MFIX) tool, as illustrated in Figure 1. In addition, these computational tools will be validated and applied to support development of new fossil energy technologies. Projects include: Advanced Numerical Techniques; Chemical Looping Modeling; Collaboratory for Multiphase Flow Research; Computational Software Development; and Model Development and Validation.

Process and Dynamic Systems Modeling – The objective is to research, develop, and apply advanced steady-state and dynamic process simulation methods and tools to overcome technical barriers associated with the next generation of highly efficient, environmentally acceptable fossil energy systems. R&D activities will utilize NETL's Advanced Process Engineering Co-Simulator (APECS—see Figure 2), commercial steady-state and dynamic process simulators, as well as custom modeling packages. Projects include: APECS R&D and Application to Advanced Power Generation Systems; Dynamic Simulation and Control of Advanced Power Generation Systems; Modeling and Simulation of Fuel Cell/Gas Turbine Hybrid Systems; Systems Optimization, Uncertainty/Risk Analysis, and Cost Estimation; and Continuation of Collaboratory for Process and Dynamic Systems Modeling Activities.

Device Scale Modeling – The objective is to utilize Computational Fluid Dynamic (CFD) techniques to study fossil energy systems, including gas turbine combustors, coal gasifiers, and carbon sequestration. Projects include: Microscale Reactions under Geological Sequestration; Study and Optimization of Mercury (Hg) Capture in Pulverized Coal (PC) Boilers; Liquefied Natural Gas (LNG) Plume Modeling; Device Scale Modeling for APECS; and Gasification Modeling Support.

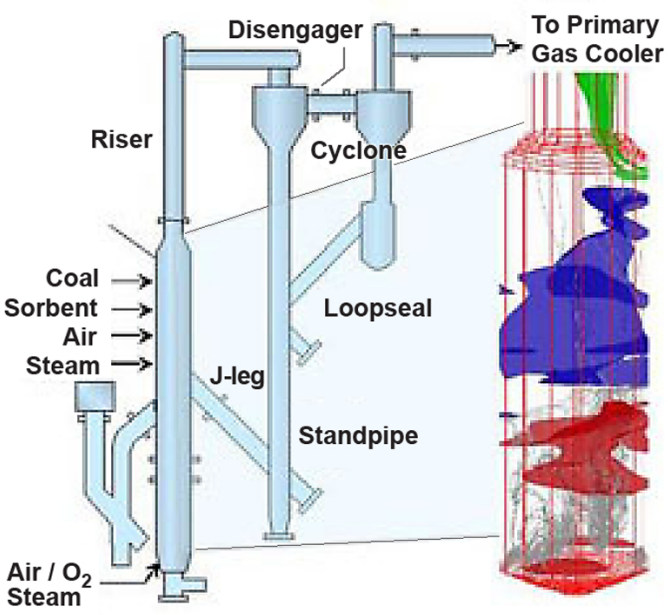

Figure 1. Transport gasifier and MFIX showing particle trajectories and oxygen concentration. MFIX simulations complement testing and development at the DOE demonstration Power System Development Facility (PSDF) in Wilsonville, Alabama (shown above). Coal and recycled materials feed into the lower mixing zone of the plant's circulating fluidized-bed. The validated simulation model is currently being used to design a commercial-scale unit.

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Benefits

The current landscape of the U.S. energy industry — not unlike that in other parts of the world — is undergoing a transformation driven by external changes, such as the deregulation of power generation, more stringent environmental standards and regulations, and climate change concerns. As market, policy, and regulatory forces reshape both the domestic and global energy industries, investments in advanced fossil energy technologies can improve the ability of U.S. industry to be more economically competitive, and provide enhanced energy production and environmental protection. One means of achieving these benefits is through the development of advanced coal technologies that use the Nation's most abundant domestic fossil fuel resources more efficiently and in an environmentally responsible manner. The CES Program plays a vital role in making these advances possible.

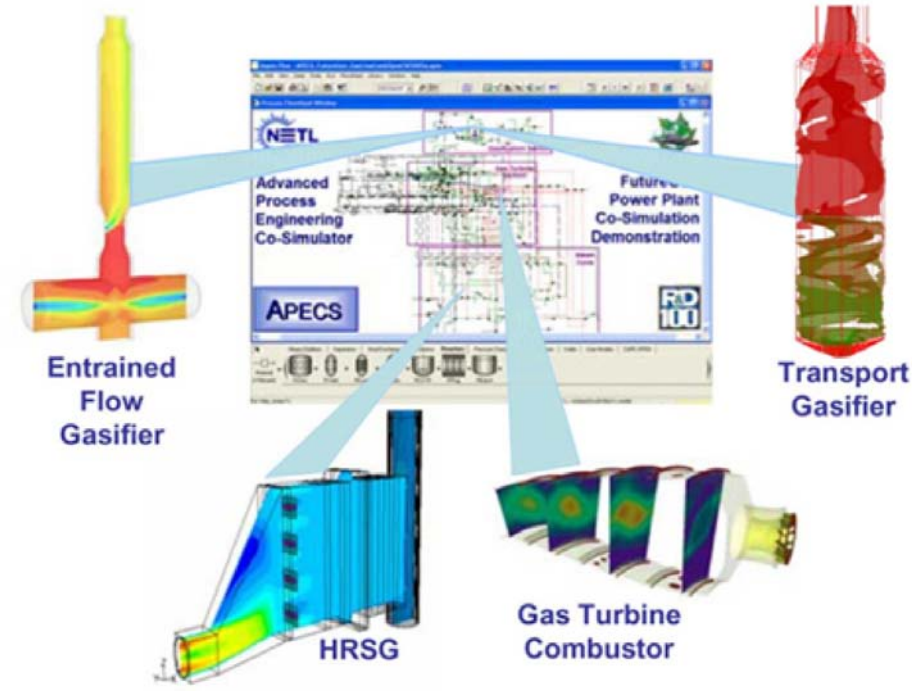

Figure 2. Integrated APECS tools enable system designers to optimize advanced plant performance processes.