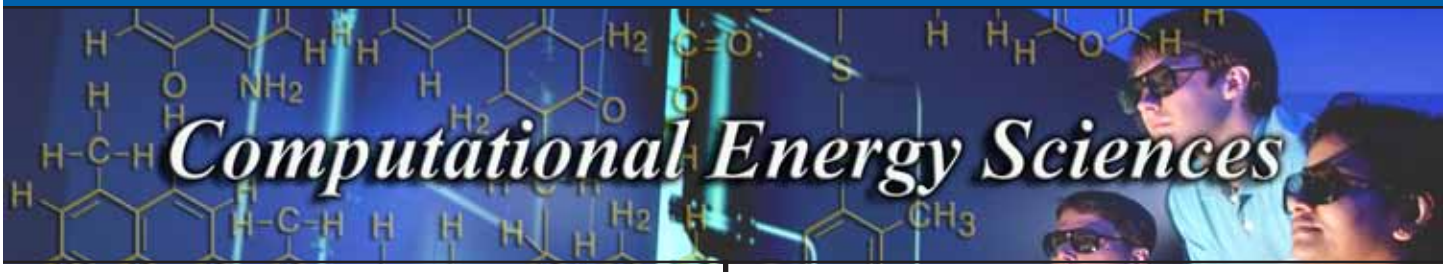


Successes

Integrated Process Engineering and Computational Fluid Dynamics Simulation System

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.

Accomplishments

- ✓ Process improvement
- ✓ Cost reduction
- ✓ Greater efficiency
- ✓ Design optimization

Description

Through the National Energy Technology Laboratory (NETL), the U.S. Department of Energy's (DOE) Office of Fossil Energy has developed a powerful suite of computational and analytical tools for modeling and simulating advanced energy and power generation system processes. Known as the Advanced Process Engineering Co-Simulator (APECS), this innovative software enables engineers to better understand and optimize power plant performance with respect to coupled fluid flow, heat and mass transfer, and chemical reactions. APECS also has applicability to other process industries such as petroleum, chemicals, and pharmaceuticals. To date, engineers and researchers in more than a dozen organizations worldwide use APECS to address challenges of designing next-generation plants to operate with unprecedented efficiency and near-zero emissions, while operating profitably amid cost fluctuations for raw materials, finished products, and energy.

A 2004 R&D 100 award-winner, APECS provides a highly sophisticated co-simulation capability by facilitating, for the first time, the efficient and systematic integration of process simulation with computational fluid dynamics (CFD) models of key plant equipment, such as combustors, gasifiers, synthesis gas (syngas) coolers, steam and gas turbines, heat recovery steam generators, and fuel cells. By coupling process/CFD co-simulations with advanced visualization and high-performance computing, APECS also offers opportunities for using virtual plant simulation to reduce the time, cost, and technical risk of developing high-efficiency, zero-emissions power plants such as DOE's FutureGen project, the world's first coal-based, electricity and hydrogen generation plant that integrates carbon capture and storage (sequestration).

In 2007, NETL won a national Excellence in Technology Transfer Award from the Federal Laboratory Consortium for innovative efforts in transferring APECS to the private sector. The approach used to transfer the APECS software includes a DOE-funded cooperative R&D project and agreement among NETL; ANSYS/Fluent, the world's leading supplier of CFD software and services; Aspen Technology, a major supplier of process simulation software; Carnegie Mellon University; Iowa State University; West Virginia University; and ALSTOM Power, a major worldwide industrial supplier of power generation equipment and services. The cooperative agreement assigned the commercialization rights to ANSYS/Fluent to position APECS for rapid market acceptance. ANSYS/Fluent offers the APECS product and corresponding consulting services commercially to the process and energy industries, as well as to universities, national laboratories, and other research entities.

Project Duration

Start Date
10/01/05

End Date
09/30/08

Cost

Total Project Value
$1,883,320

DOE/Non-DOE Share
$1,883,320 / $0

Industrial Partners

ANSYS, Inc. /Fluent
Lebanon, NH
www.fluent.com

Aspen Technology, Inc.
Cambridge, MA
www.aspentech.com

ALSTOM Power
Windsor, CT
www.alstom.com

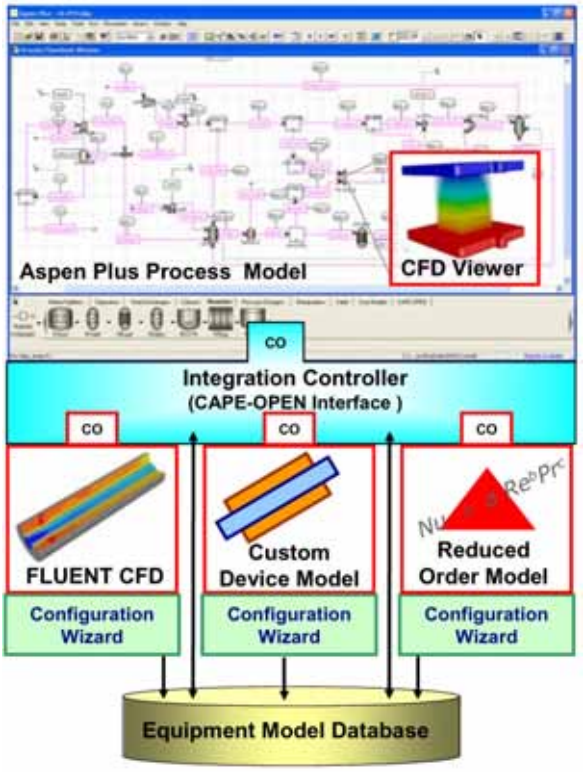
Carnegie Mellon University
Pittsburgh, PA
www.cmu.edu

Iowa State University
Ames, IA
www.iastate.edu

West Virginia University
Morgantown, WV
www.wvu.edu

NETL research engineers review APECS results

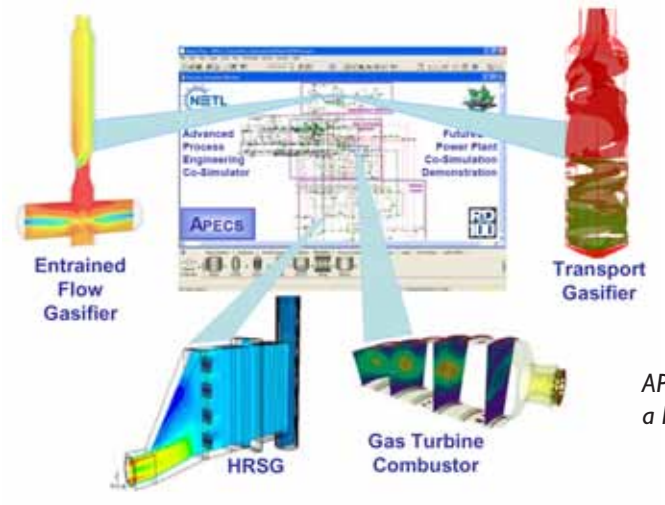
APECS builds on the advanced computational framework developed in 2000–2004 by NETL's Advanced Research program, and implemented by NETL's Office of Research and Development. This project integrated Aspen Technology's commercial Aspen Plus® process flowsheet simulation software with FLUENT®, the joint ANSYS, Inc./Fluent CFD software for detailed plant equipment modeling. APECS uses the process industry-standard CAPE-OPEN software interfaces for plug-and-play interoperability between process simulation and equipment models. The hierarchy of models used by APECS ranges from high-fidelity CFD models, to custom engineering models (CEMs), to fast reduced-order models (ROMs). The CFD models provide detailed and accurate representations of a wide variety of process equipment items, while CEMs are typically engineering models that calculate mass and energy balances, phase and chemical equilibrium, and reaction kinetics. ROMs are a class of equipment models based on pre-computed CFD solutions over a range of values, but are much faster than CFD models.



APECS integrates process simulators and equipment models using open software interfaces

APECS Applications

Systems analysts at NETL are applying APECS to a wide variety of advanced power generation systems and configurations. For example, APECS is playing a key role in the design of the FutureGen project. When operational, FutureGen will be the cleanest fossil fuel-fired power plant in the world and a prototype for co-production of coal-fired power, and multiple fuels and chemicals. In a recent demonstration case, the FutureGen co-simulation combined a plant-wide simulation with two CFD-based equipment models. The first model was for the entrained-flow gasifier where fluid dynamics strongly affect syngas quality and carbon conversion, and the other for the gas turbine combustor where the blending of air and fuel is vital to gas turbine combustion performance and efficiency. Turnaround time for the co-simulation was improved by running the computationally intensive CFD models in parallel on multiple computers at NETL and the Pittsburgh Supercomputing Center. Ongoing work on the FutureGen co-simulation is focused on the integration of additional equipment models, including FLUENT®CFD models of a heat recovery steam generator (HRSG) and a solid oxide fuel cell stack, as well as a ROM that is based on time-averaged transient CFD results from a commercial-scale transport gasifier simulation.



APECS Co-Simulation of a FutureGen power plant

Other work on advanced systems using APECS has ranged from small fuel cell systems to commercial-scale power plants. The overall performance of solid oxide fuel cell auxiliary power units for transportation applications was optimized with respect to the local fluid flow, heat and mass transfer, electrochemical reactions, current flow, and potential field in simulated fuel cell stacks. The process/CFD co-simulations were performed over a range of fuel cell currents to map out a voltage-current curve, and to analyze the effect of current on fuel utilization, power density, and overall system efficiency.

In the chemical industry, process engineers are using APECS to optimize plant performance by analyzing the impact of complex reactor mixing and fluid flow phenomena on overall plant product quality and yield. In the power industry, ALSTOM Power cycle engineers are routinely employing the APECS technology to design and optimize commercial-scale power plants, including conventional pulverized coal-fired steam plants and natural gas-fired, combined-cycle power plants.

Participants in the United Kingdom's Virtual Plant Demonstration Model program are leveraging APECS to integrate high-fidelity CFD equipment models into overall power plant models developed with the Process Systems Enterprises gPROMS® simulator. In the research community, APECS is used by Carnegie Mellon University for developing optimization-based ROMs based on CFD results. Iowa State University and Ames National Laboratory are coupling process/CFD co-simulation to immersive 3-D virtual engineering software, and the Vishwamitra Research Institute, Westmont, IL, is using stochastic analysis and multiobjective optimization capabilities for process/CFD co-simulation.

Benefits

The process and energy industries manage some of the most complex and expensive plants in the world, spending nearly $600 billion annually in plant design, operation, and maintenance. The development, transfer, and commercialization of the APECS co-simulation technology, through NETL's leadership and innovation efforts, are helping these industries to accelerate technology development and reduce associated uncertainties and risks. Specifically, APECS offers the following advantages:

- Helps engineers to better understand and visualize fluid flow behavior, which impacts process design and operation;
- Considers detailed equipment models in the context of plant-wide simulations, with recycle loops, heat integration, and water management;
- Enables rigorous analysis and optimization of entire plants with respect to CFD-related equipment model parameters;
- Eliminates the potential for design incompatibilities by using the same physical properties and reaction kinetics in the underlying equipment and process models;
- Speeds technology development by reducing pilot/demonstration-scale facility design time and operating campaigns; and
- Offers opportunities to achieve the aggressive performance, environmental, and economic goals for high-efficiency, zero-emission power plants.

"...This innovative software enables engineers to better understand and optimize power plant performance with respect to coupled fluid flow, heat and mass transfer, and chemical reactions. APECS also has applicability to other process industries...."

States and Localities Impacted

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Pittsburgh, PA
Ames, IA
Morgantown, WV

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