R & D facts

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National Energy Technology Laboratory

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Computational Energy Science

Description

The Computational Energy Science focus area within the National Energy Technology Laboratory (NETL) aims to use advanced, science-based computational tools to design of clean, highly-efficient energy plants of the future. These "virtual power plant" models will have the capability to simulate dynamic responses to design changes and options, and to indicate interactions of major components, such as turbines, fuel cells, combustors, and environmental control systems.

The work of the Computational Energy Science focus area will take advantage of and incorporate the expanding capabilities of high-speed computing. Science-based predictive models, device and system-scale simulations, and visualization of large databases will ultimately reduce the number of actual experimental studies. This will result in a substantial savings in program costs, and at the same time, compress development times for new technologies.

There is a revolution occurring in science as significant as the development of modern experimental science to our current technological society. Advances in high-speed computing and in our basic understanding of the non-linear nature of physics and chemistry is leading to the use of simulation and modeling as basic predictive and design methods for advancing technology. The aircraft, automobile, electronic, pharmaceutical, and petrochemical industries are already beginning to use simulation, modeling, and three-dimensional visualization to aid and speed designs of complex systems. High-speed computing allows natural processes to be simulated in a virtual space, where they are easily explored, understood, and manipulated to achieve desired outcomes.

The fossil energy industry has historically been slow to incorporate new technology into its approach to research, engineering, and design. Past efforts in modeling of fossil processes have, however, laid the groundwork for moving quickly towards this new approach to technology. These efforts have developed fundamental multi-phase codes to describe fluidized bed combustors, gasifiers and other multi-phase systems. Single-phase fluid flow codes have also been developed to describe flows in gas turbines and combustion systems. Process simulators have been developed to describe heat and material balances, codes for geological studies of oil and gas fields, and other codes to address specific system issues. Advanced simulation and modeling methods will be developed for Vision 21 technologies, such as gas turbines, fuel cells, gasifiers, combustors, gas cleanup processes, separation devices, and heat exchangers, and for the coupling of these devices in clean, efficient energy plants.

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NETL

Computational Energy Science

Benefits

- Simulation will reduce the need for experimental development by 20%.
- Simulation will allow the scale up of new processes at twice the current scaling ratio.
- Simulation models will be available for most Vision 21 plant components.
- Fossil Energy developed codes will be accepted and used by utility and industrial companies.
- Extensive computational and visualization resources will be available for use by NETL, Fossil Energy Headquarters, and NETL partners through the co-laboratory network.

Goal

Our goal is to have the focus area Computational Energy Science provide simulation and computational resources to the Fossil Energy programs to speed development and reduce costs for developing new technologies. Specific objectives for the Focus Area include:

- Develop simulation capabilities that couple fluid flows, chemical reactions, heat generation, heat transfer, electrochemistry, and Reynolds stresses for modeling multi-dimensional transients in fuel cell, heat engines, combustors, gasifiers, chemical reactors, and other crucial unit processes in Vision 21 plants.
- Develop data reduction, data extraction and data mining techniques to utilize the extensive information made available from simulation studies of advanced Vision 21 systems.
- Develop a co-laboratory between NETL, multiple national laboratories, and universities, to provide extensive simulation and modeling expertise for Vision 21 systems.
- Train student engineers and scientists to develop and analyze optimal control systems for future fossil energy plants.
- Promote the use of simulation as a principle design, construction, and operating tool for fossil energy equipment suppliers and energy plant owners.
- Develop software for fossil energy systems which can utilize teraflop computing resources.

Milestones:

- In FY2001 - Implement computational and visualization laboratory.
- In FY 2002 – Implement complementary computational study for device-level experimental investigations of critical Vision 21 components.
- In FY 2003 – Complete initial visualization of key Vision 21 plant components.
- In FY 2004 - Develop accurate, science-based, scalable simulations of key devices in advanced energy systems.
- In FY 2005 - Develop and validate integrated dynamic simulation tools.