the ENERGY lab

PROJECT FACTS

Advanced Research

Package Equivalent Reactor Networks as Reduced Order Models for Use with CAPE-Open Compliant Simulations

Description

The Department of Energy's (DOE) National Energy Technology Laboratory (NETL) supports research leading to more environmentally responsible uses of domestic fossil-based fuels. The Nation's electric power industry widely uses coal combustion. To reduce toxic emissions, coal gasification was developed as an alternative to traditional coal combustion methods. Coal gasification converts coal into carbon monoxide and hydrogen by reacting it at high temperatures with oxygen or steam. The resulting gas mixture is synthesis gas (syngas), which can be used as a fuel or separated into its component gases. Optimization of the coal gasification process will facilitate the DOE's energy security goals.

The use of simulation software to explore options for improving gasification processes can facilitate innovation, reduce risk, speed development, and improve testing plans. Reaction Design, a San Diego-based software developer, is producing gasification and reaction kinetics simulation software to help solve critical engineering and operating problems that arise throughout the lifecycle of a gasification power plant. For this project, Reaction Design will research and develop software simulation capabilities to enhance the performance of next-generation fossil energy power systems. The software will be used in the development, implementation, and operation of highly efficient coal-based power generation technologies that reduce emissions.

Goals and Objectives

The goal of this project is to support the development of gasification technology improvements that minimize emissions and maximize efficiency. The main objective of the project is to develop simulation modeling software using reduced-order models and computer-aided process engineering (CAPE)-open architecture to provide the power plant industry with an efficient and accurate alternative to using existing high-fidelity fluid-dynamics models, which can become computationally expensive for the development of gasification plants.

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PERIOD OF PERFORMANCE

10/01/2009 to 09/30/2012

COST

Total Project Value
$1,045,838

DOE/Non-DOE Share
$818,026/ $227,812

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U.S. DEPARTMENT OF ENERGY

Technological Approach

Simulation software has already been established for gas-turbine combustors. This project will extend the same kind of simulation programming to include the complex kinetics found in gasifiers. Reaction Design will also incorporate these capabilities into a CAPE-open compliant package. CAPE-open software allows plug-and-play interoperability of unit operation models, physical properties, and reaction kinetics. This new model will provide state-of-the-art kinetics modeling within flow-sheet type simulations and will be the basis for developing accurate models for combined gasification and combustor processes.

Reaction Design's technology focuses on the gasification of condensed-phase material into combustible gas and the combustion of resulting gases in gas-turbine combustors. Reaction Design will derive reduced-order models from computational fluid dynamics models and package these as equivalent reactor networks to incorporate with the CAPE-open interface. This process will be expanded and applied to models of gasifiers and combustors. The developers will then create more realistic kinetics descriptions of the gasification and combustion processes in the reduced-order models, which will allow for more accurate and efficient simulations of these components. The result will be faster and more accurate simulations of entire systems.

Benefits

This research will develop gasification simulation software that will enable more cost-effective exploration of options to improve the gasification processes in integrated gasification combined cycle power plants. Ultimately, the use of this software may lead to faster implementation of improvements to the gasification process, increasing the benefits of gasification power plants and further decreasing the negative effects of electricity production on the environment. Optimization of the coal gasification process will lead to more efficient use of domestic fuel sources with lower emissions and support DOE's energy security mission.

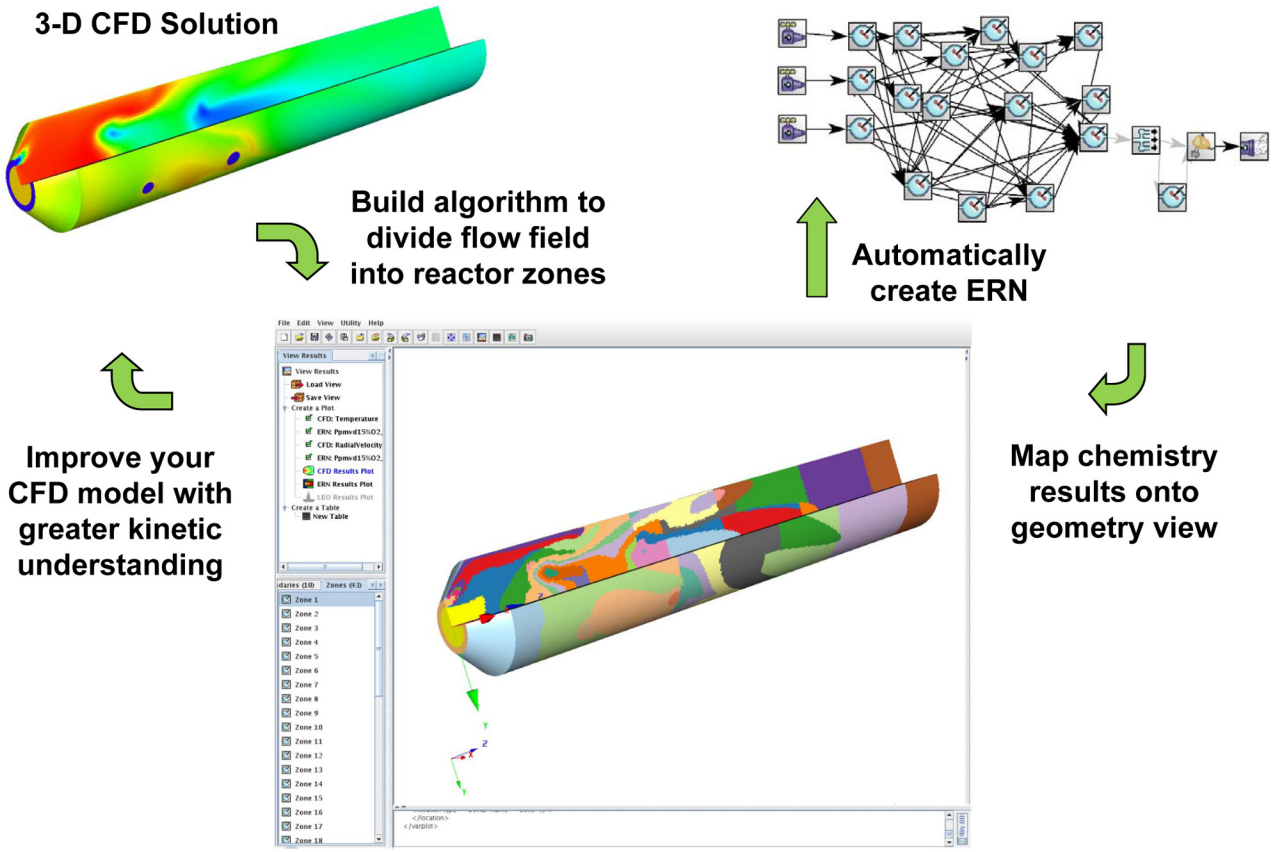

Figure 1. Equivalent reactor networks represent complex systems while allowing detailed kinetics.