the ENERGY lab

PROGRAM FACTS

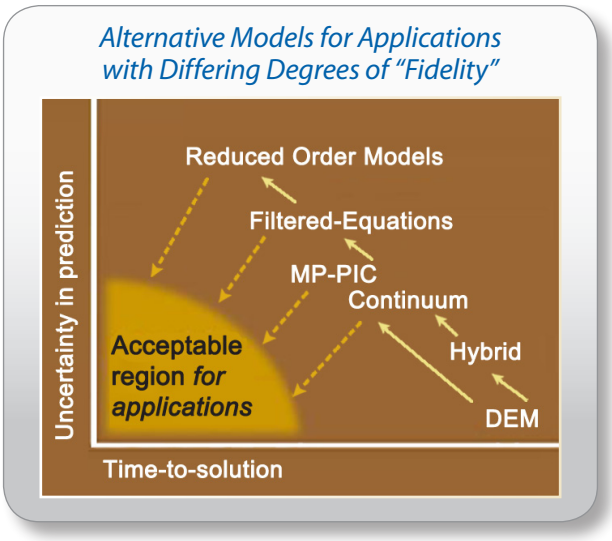
Strategic Center for Coal

Crosscutting Technology Research Program Simulation-Based Engineering Summary

Simulation-Based Engineering (SBE) 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 phenomenon occurring in fossil fuel conversion processes and development of multi-scale, multi-physics simulation capabilities are just some of the tools and capabilities. Activities include: developing a framework to quantify uncertainties and assess the impact of their propagation in the models; providing quantitative error-bars on simulation data; creating simplified models to balance the needs of accuracy and time-to-solution; and validating models. The simulation based engineering is comprised of two main subtasks, each with its own goals and objectives.

- **Physics- and Science-Based Modeling** predicts the behavior of complex multiphase flow reactors used in fossil energy technologies. This combines theory, computational modeling, experiments, and industrial input. Physics-based computational models and tools are being funded to support the development and deployment of advanced fossil fuel energy devices such as gasifiers and carbon capture reactors.

- **Consortium for Advanced Energy System Simulation and Optimization (CAESSO)** is working to advance current integrated computational tools to revolutionize the ability to use simulation to reduce the risks and time required to scale-up new advanced energy system technologies, such as co-generation and energy storage.



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U.S. DEPARTMENT OF ENERGY

In addition to the two subtasks, collaborator efforts have been developed through the Crosscutting Technology Research Program to accelerate novel carbon management technologies and techniques. The **Carbon Capture Simulation Initiative** (CCSI) was developed to provide technology developers and plant operators with a validated suite of integrated models and simulation tools to enable the rapid development and deployment of new carbon capture technologies. The toolset developed in the **National Risk Assessment Partnership** (NRAP) through the Crosscutting Technology Research Program that has transitioned to the Storage Program uses computational tools for quantifying potential risks and associated uncertainties for long-term CO_2 storage over time.

Impacts and Benefits

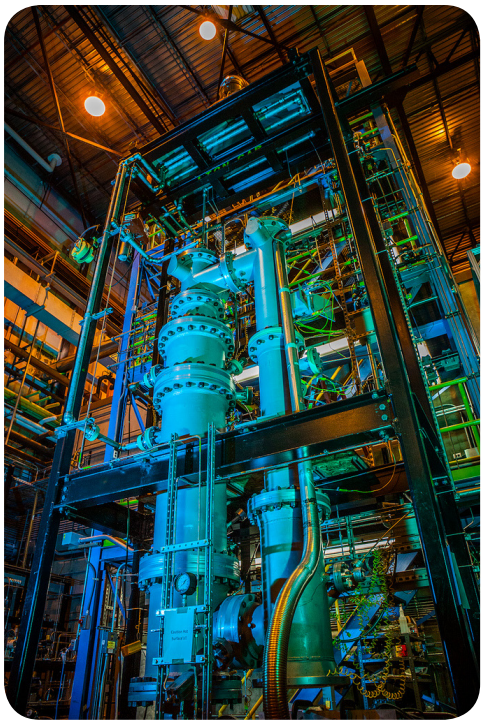
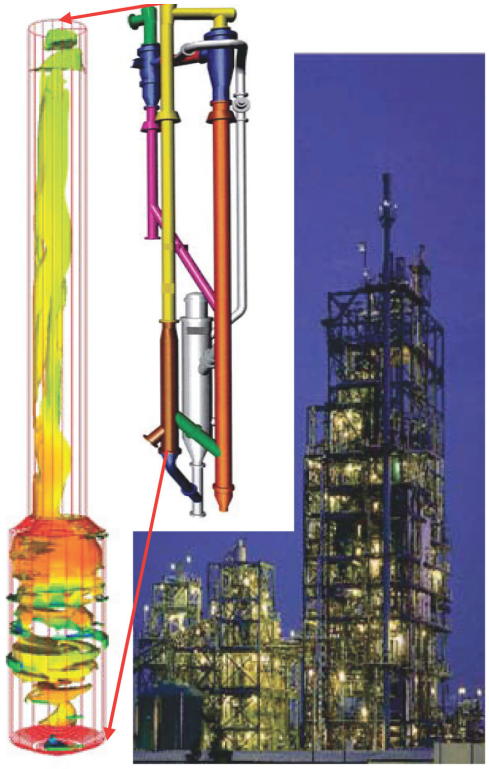
The following impacts are possible through this proposed research:

- The efficient and reliable operation of fossil energy plants depends upon reactors that contact multiple phases: gas, liquid, or solids. These multiphase reactors are difficult to scale-up, especially when solids are present in the system; however, the development of new, advanced technologies is critical for DOE to meet its low-cost, small carbon footprint power goals. Accurate, high-fidelity, and fast models will reduced the time of development of these new technologies.

- By positioning modeling as a common and trusted tool for design and operation decisions, costs will be reduced. The primary driver of cost reduction will be the shortened time required to validate advanced technologies for industrial use. These models will also reduce the risk of modifications, enabling fuel and product flexibility based on market drivers. Risk can also be reduced when using known technologies for slightly different applications, or integrated in new ways with advanced technologies.

- These efforts will provide industry and academia across the world with a hierarchy of well-characterized computational tools. Development of these tools will be used to reduce the cost of coal-conversion technologies, improve operations, and speed the design of advanced technologies to help reduce global carbon emissions.

Chemical Looping Hot Testing Pilot Unit



MFIX Simulation of Pilot Scale KBR/ Southern Transport Gasifier