CROSSCUTTING RESEARCH

SIMULATION-BASED ENGINEERING

CROSSCUTTING SIMULATION-BASED ENGINEERING

Simulation-Based Engineering research applies simulation and modeling capabilities to represent the full range of energy science from reactive and multiphase flows up to a full-scale virtual and interactive power plant.

Computational tools focus on developing and applying models at multiple scales: atomistic, device, process, and grid and market that accelerates the development and deployment of fossil fuel technologies.

Research in this technology focuses on three main platforms:

- **MULTIPHASE FLOW SCIENCE**
- **ADVANCED PROCESS SIMULATION**
- **COMPUTATIONAL MODELING OF MATERIALS**

Physics- and chemistry-based models and tools are needed to accelerate development and deployment of advanced fossil-fuel technologies that confound the ability of experimental scientists.

The programs apply analysis and visualization tools to gain scientific insights into complex, noisy, high-dimensional, and high-volume datasets.

MULTIPHASE FLOW SCIENCE

NETL is the world-leader in multiphase flow modeling that simulates complex energy processes, deploying state-of-the-art computational modeling to accelerate the commercialization and ultimately widespread deployment of technologies for advanced power generation. NETL has developed the **Multiphase Flow with Interphase eXchanges** (**MFiX**) software suite which is the world's leading open-source design software. Device scale simulations provide significant time and cost savings compared to traditional build and test methods.

ADVANCED PROCESS SIMULATION

The newly initiated **Institute for the Design of Advanced Energy Systems** (**IDAES**) identifies, synthesizes, optimizes, and analyzes advanced energy systems at scales ranging from process to system to market. IDAES accelerates innovation by identifying and optimizing systems in the context of full energy portfolios.

COMPUTATIONAL MATERIALS MODELING

Provides a conceptual framework for integrating models at different scales. The approach allows for evaluation of new hardware concepts and virtual exploration of systems. The national laboratory consortium, **Extreme Environment Materials** allows for development of new materials and demonstrates predictive materials behavior.

SIMULATION-BASED ENGINEERING SOLVES PROBLEMS OF NATIONAL IMPORTANCE BY ACCESSING KNOWLEDGE BEYOND THE REACH OF EXPERIMENTS AND HAS THE FOLLOWING IMPACTS:

- Accurate, high-fidelity, fast models will reduce the time of development of advanced technologies critical for the U.S. Department of Energy to meet its low-cost and high-efficiency goals.
- Models developed will reduce the risk of modifications, enabling fuel and product flexibility based on market drivers.
- MFiX Software Suite has over 4,500 registered users and is the national leading platform for computational fluid dynamics code.
- IDAES optimizes and enhances energy platforms while increasing grid reliability.

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