MODELING, SIMULATION, AND ANALYSIS



NATIONAL ENERGY TECHNOLOGY LABORATORY

The Modeling, Simulation and Analysis¹ program within the Crosscutting Research Portfolio applies simulation and modeling capabilities to the full range of maturities and technologies essential to plant operation, from fundamental energy science in reactive and multiphase flows to full-scale virtual and interactive plant performance.

This program supports the development and application of new and innovative physics- and chemistry-based models and computational tools at multiple scales (atomistic, device, process, grid and market). This program also investigates the potential positive impact these tools may have in overcoming complexities that confound today's experimental scientists and influencing the discovery of a new generation of advanced fossil-fuel technologies.

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NETL implements this effort as part of DOE's Crosscutting Research Program.

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Analysis and visualization tools are manipulated to gain scientific insights into complex, noisy, high-dimensional and highvolume datasets. The information generated is then collected, processed and used to inform research that combines theory, computational modeling, advanced optimization, experiments and industrial input with a focus in the following three main platforms:

- Multiphase Flow Science
- Advanced Process Simulation
- Innovative Concept Analysis

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 considerable 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.

INNOVATIVE CONCEPT ANALYSIS — NETL provides analytical research on innovative concepts such as Direct Power Extraction (also known as Magneto Hydrodynamics). Analytical work focused on techno-economics of various component integration schemes to calculate performance, cost, and benefits. The results guide data-informed investments in these early-stage, high-risk, high-reward concepts to effectively steward government funding and efficiently mature technology.

MODELING, SIMULATION AND ANALYSIS 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 DOE to meet its low-cost, 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 5,000 registered users and is the national leading platform for computational fluid dynamics code.
- IDAES optimizes and enhances energy platforms while increasing grid reliability.
- Guide research and develop investment decisions with structured analytical results.

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