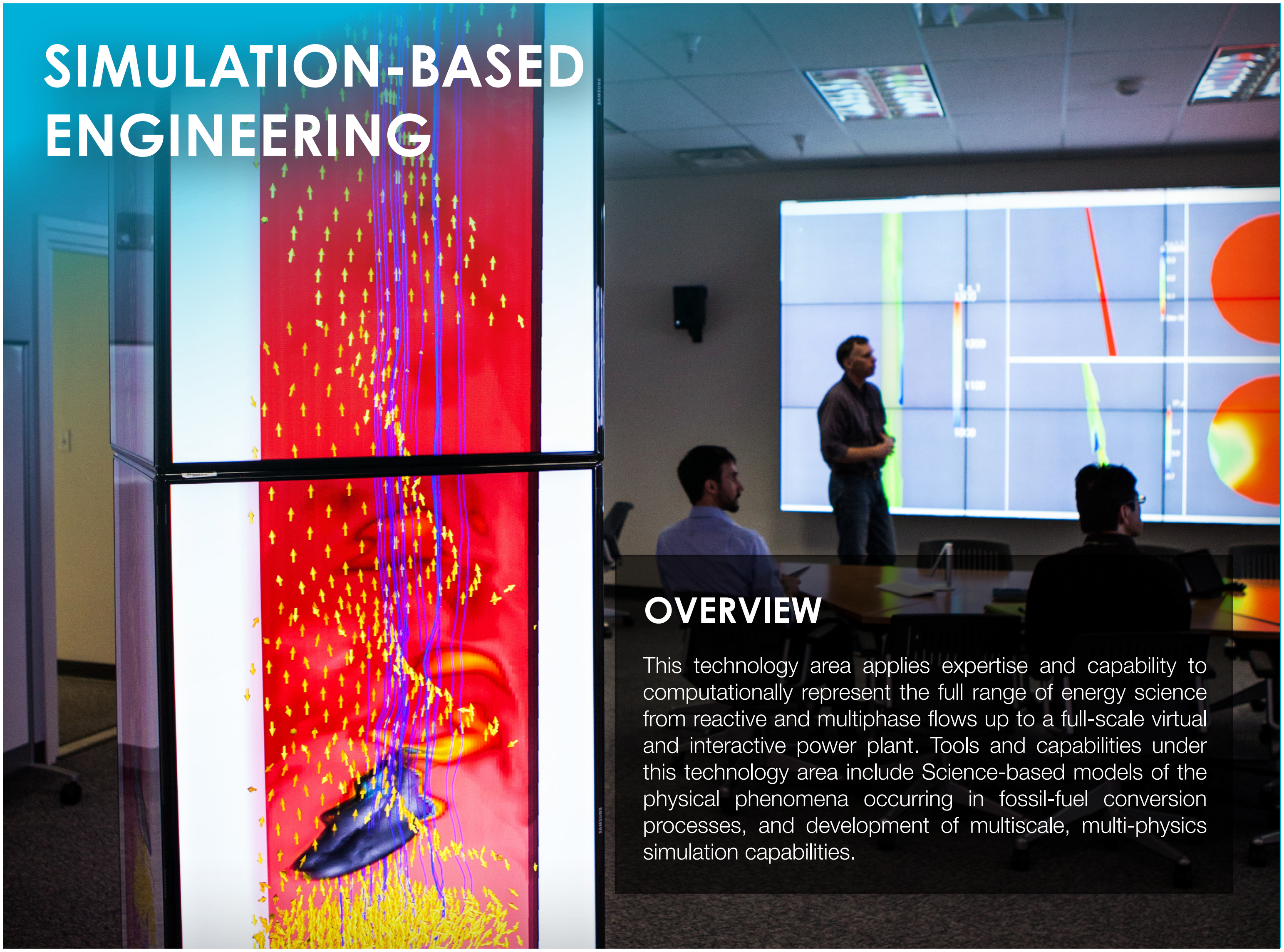
SIMULATION-BASED ENGINEERING



OVERVIEW

This technology area applies 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. Tools and capabilities under this technology area include Science-based models of the physical phenomena occurring in fossil-fuel conversion processes, and development of multiscale, multi-physics simulation capabilities.

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Modeling efforts stem from the motivation to reduce costs and shorten time delays resulting from the use of expensive lab set-ups in research and physical prototypes in projects' design and engineering phases. Improvements are being sought in all aspects of modeling from algorithms to software engineering. NETL's Simulation-Based Engineering area combines the technical knowledge, software development, computational power, data repository, experimental facilities, and unique partnerships to support research to provide timely and accurate solutions for complex power systems. Understanding the performance of complex flows and components used in advanced power systems and having the means to impact their design early in the development process provides significant advantages in product design. Computational models can be used to simulate a device and understand its performance before the design is finalized. In addition, during new technology development—e.g., the development of sorbent adsorber/desorber reactors for carbon dioxide capture—empirical scale-up information is not available because reactors have not yet been built at the scales required. Traditional scale-up methods do not work well for many of the components present in complex power systems. Therefore, science-based models with quantified uncertainty are important tools for reducing the cost and time required to develop these components.

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MULTIPHASE FLOW WITH INTERPHASE EXCHANGES

The vast computational resources available to NETL ensure timely solutions to the most complex problems. The NETL supercomputer is one of the world's fastest, most energy-efficient supercomputers, intended to help energy researchers discover new materials, optimize designs, and better predict operational characteristics. Speed-up is also achieved through research in modern graphical processing unit computing as well as the implementation of reduced order models when appropriate. Simulation-based Engineering exploits onsite, highly instrumented experimental facilities to validate model enhancements. Models are made available to the public through the Laboratory's computational fluid dynamics code Multiphase Flow with Interphase eXchanges (MFiX), developed specifically for modeling reacting multiphase systems.

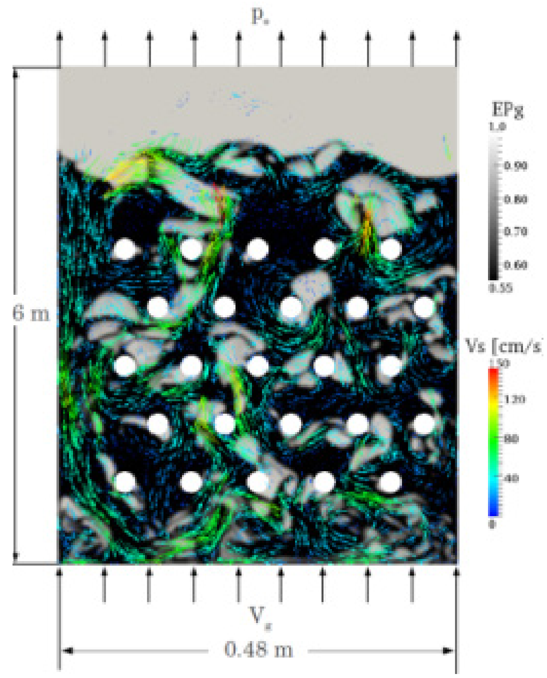
The development of data integration software packages such as the R&D 100 Award-winning VE-Suite provides a mechanism whereby commercial modeling and simulation code can be exchanged seamlessly across scales. NETL's unique capabilities in multiphase flow science coupled with its extensive knowledge of carbonaceous fuel reactions resulted in the development of the Carbonaceous Chemistry for Computational Modeling (C3M) platform to perform virtual kinetics experiments that elucidate the effect of operating conditions (e.g., heating rate, temperature, pressure, fuel type) on output variables such as conversion rates and yield.

IMPACTS AND BENEFITS

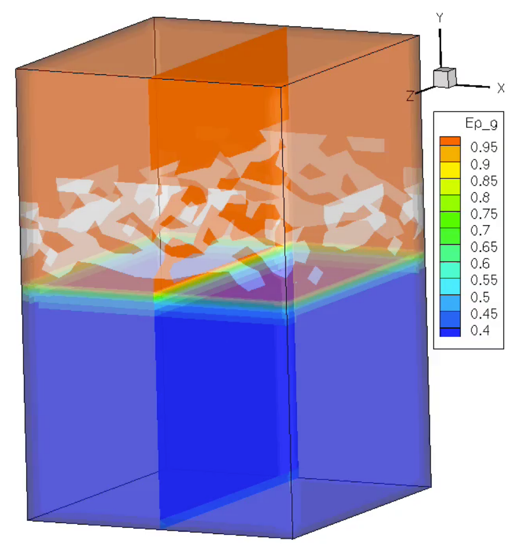
- Accurate, high-fidelity, fast models will reduce the time of development of advanced technologies critical for the U.S. Department of Energy to meet its low-cost, small carbon footprint power generation goals.

- Models developed will reduce the risk of modifications, enabling fuel and product flexibility based on market drivers.

- Tools developed 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.



The simulation of a bubbling fluidized bed with heat transfer tubes used for model validation



Reduced-order model

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