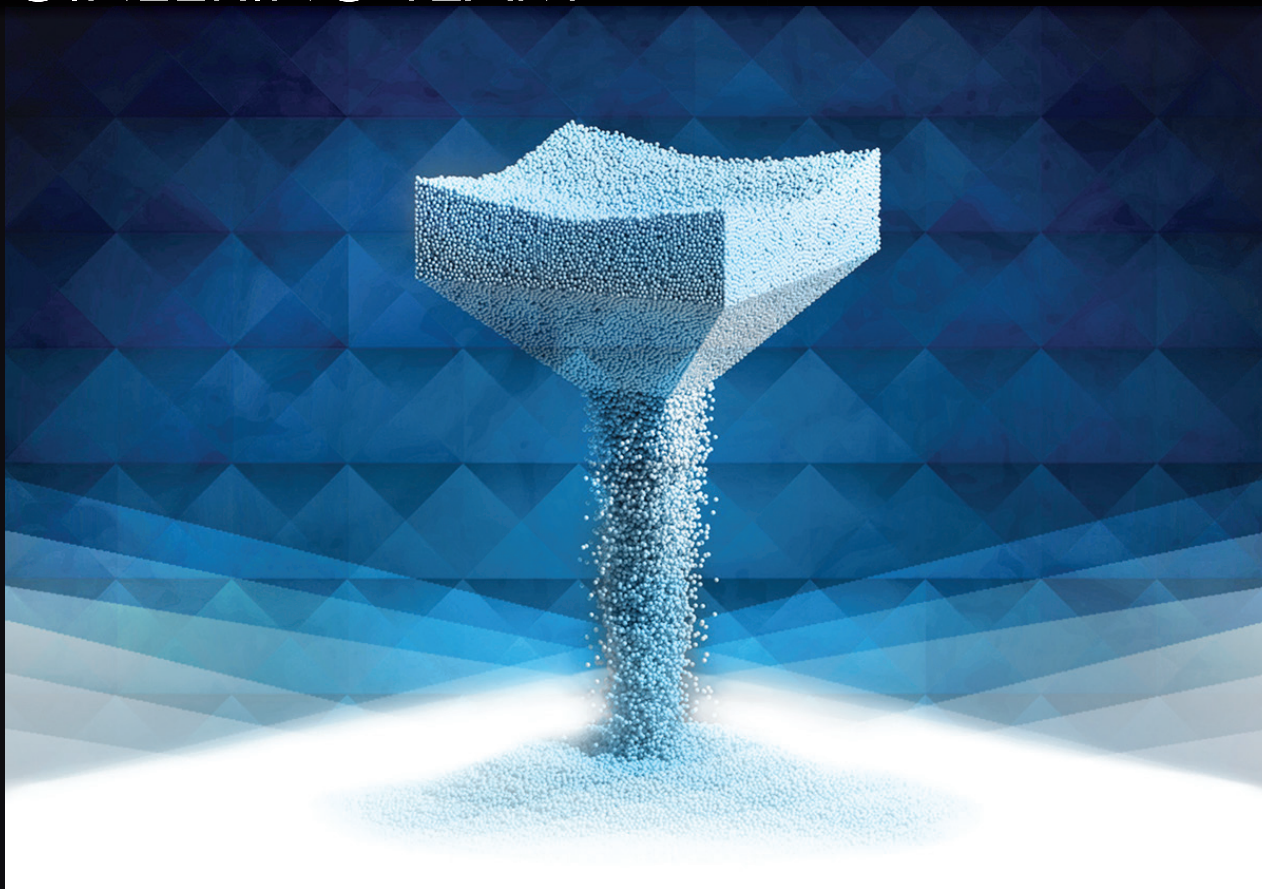
COMPUTATIONAL DEVICE ENGINEERING TEAM



NETL
NATIONAL ENERGY TECHNOLOGY LABORATORY

BACKGROUND

The U.S. Department of Energy's (DOE) National Energy Technology Laboratory's (NETL) Computational Science & Engineering (CSE) Directorate is recognized for its ability to develop science-based simulation models, mathematical methods and algorithms, and software tools to address the technical barriers in the development of next-generation technologies. This competency works in collaboration with other capabilities at NETL to generate information and scientific understanding beyond the reach of experiments alone through the integration of experimental information with computational sciences across different time and length scales. The CSE Directorate is organized into three teams that collectively maintain NETL's computational science and engineering competency: 1) Computational Materials Engineering, 2) Computational Device Engineering, and 3) Data Analytics.

COMPUTATIONAL DEVICE ENGINEERING TEAM

The Computational Device Engineering (CDE) Team at NETL, also known as the Multiphase Flow Science (MFS) Group, provides national laboratory expertise in multiphase flow science through computational and experimental research and development (R&D) coupled with high-performance computing to support DOE's Fossil Energy R&D programs. For more than 30 years, NETL's work in multiphase flow science has served as one of the cornerstones of the Laboratory's research portfolio. Multiphase flow refers to the simultaneous flow of gases, liquids, and solid materials. For example, in fossil fuel combustion and gasification processes encountered in pulverized coal boilers, fluidized bed boilers, entrained flow gasifiers, and coal particles react with and devolve into gases under a wide range of flow conditions and chemistries. Multiphase flow also occurs in other energy system processes, including emissions control units and carbon dioxide (CO_2) capture systems involving gas-phase CO_2 captured by solid-phase sorbents or liquid-phase solvents. Multiphase flow challenges are complex and require sophisticated computational approaches and suitable validation against experimental results to yield robust solutions.

NETL's MFS Group is part of a global community researching multiphase flow in the development of future energy conversion systems that will run more efficiently, delivering reliable energy globally. This work is ongoing as computational science evolves rapidly. Faster and more complex computing systems appear every day to underpin increasingly realistic models/simulations of energy systems.

Supercomputers that broke ground just a few years ago will soon be replaced by systems operating at the exascale (one quintillion floating-point operations each second), representing a thousand-fold increase. This surge of processing power will open the doors to breakthroughs across the scientific community. For example, NETL is involved in DOE's Exascale Computing Project, a multi-year effort to maximize the benefits of high-performance computing for U.S. economic competitiveness, national security, and scientific discovery.

The value of multiphase flow research extends even beyond fossil energy applications. NETL's multiphase flow research promotes capabilities that are marketable in key areas of DOE's research portfolio, including biomass research, nuclear cleanup, and other waste treatment efforts.

CAPABILITIES

MFS GROUP'S SOFTWARE PORTFOLIO

The MFS Group's software portfolio features physics-based modeling tools to guide the design, operation, and troubleshooting of multiphase flow devices, with an emphasis on fossil fuel technologies (e.g., coal gasifiers, CO_2 capture devices, and chemical looping.)

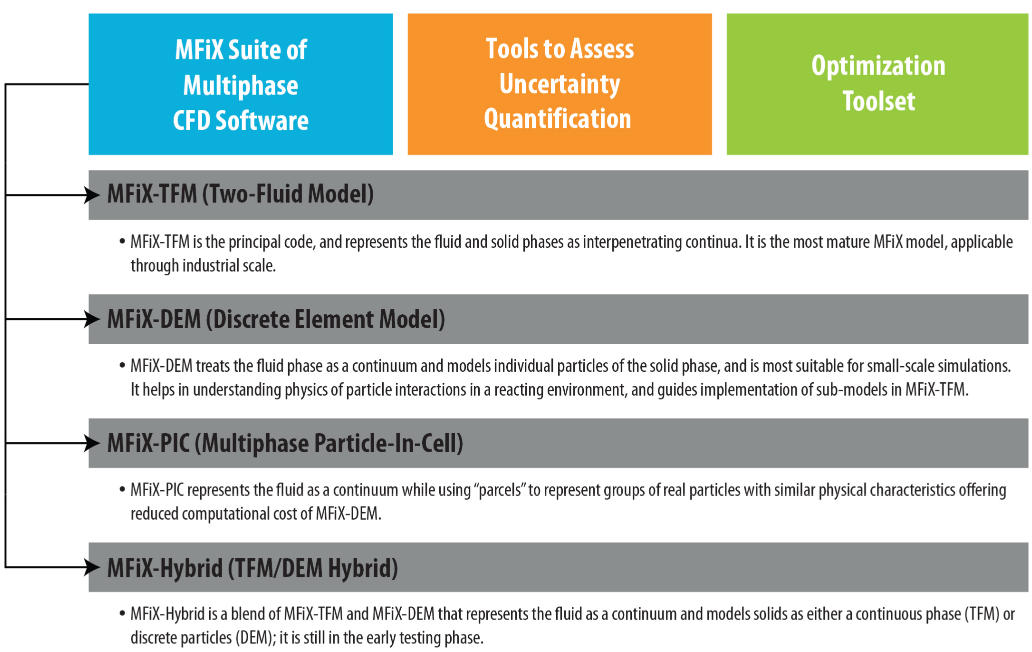


Figure 1. The MFS Group's software portfolio.

MFiX: Open-Source Software for Simulating Multiphase Flow Processes

NETL researchers developed the MFiX (Multiphase Flow with Interphase eXchanges) software as a physics-based model of multiphase reactors to solve scale-up problems for advanced power plants. Advanced power plant technologies require multiphase reactors for processing fossil fuels. For example, coal (solid phase) is reacted with steam and air (gas phase) in a gasifier. The scale-up of such multiphase reactors is notoriously difficult; engineers cannot reliably predict commercial-scale (large) reactor performance merely based on pilot-scale (small) reactor performance.

MFS Experimental Activities

NETL has been performing fluidization research for more than 50 years – studying fluidization technologies applied to coal combustion, gasification, and emissions clean-up. The MFS Group's Multiphase Flow Analysis Laboratory includes several cold-flow and low-temperature reacting experimental units that have varied types of fluidized-bed and fixed-bed conditions in broad size ranges. With these, the NETL MFS program generates well-characterized multiphase flow data at different length and time scales to aid in understanding complex fluidization behavior in reactors, underpinning the development of mathematical models, and validating software code. In these units, construction materials allow the visualization of solids and fluid phases and allow for measurements using a variety of flow diagnostic techniques, such as laser Doppler velocimetry and particle image velocimetry. These methods, combined with standard temperature, transient pressure, and gas composition measurements, provide comprehensive data sets for validation. Additionally, these experiments provide platforms for the development and validation of novel measurement techniques. For example, accurate measurement of the solids circulation rate for circulating fluidized bed application is critical data for model validation. Data from MFS experiments are made available to the research community.

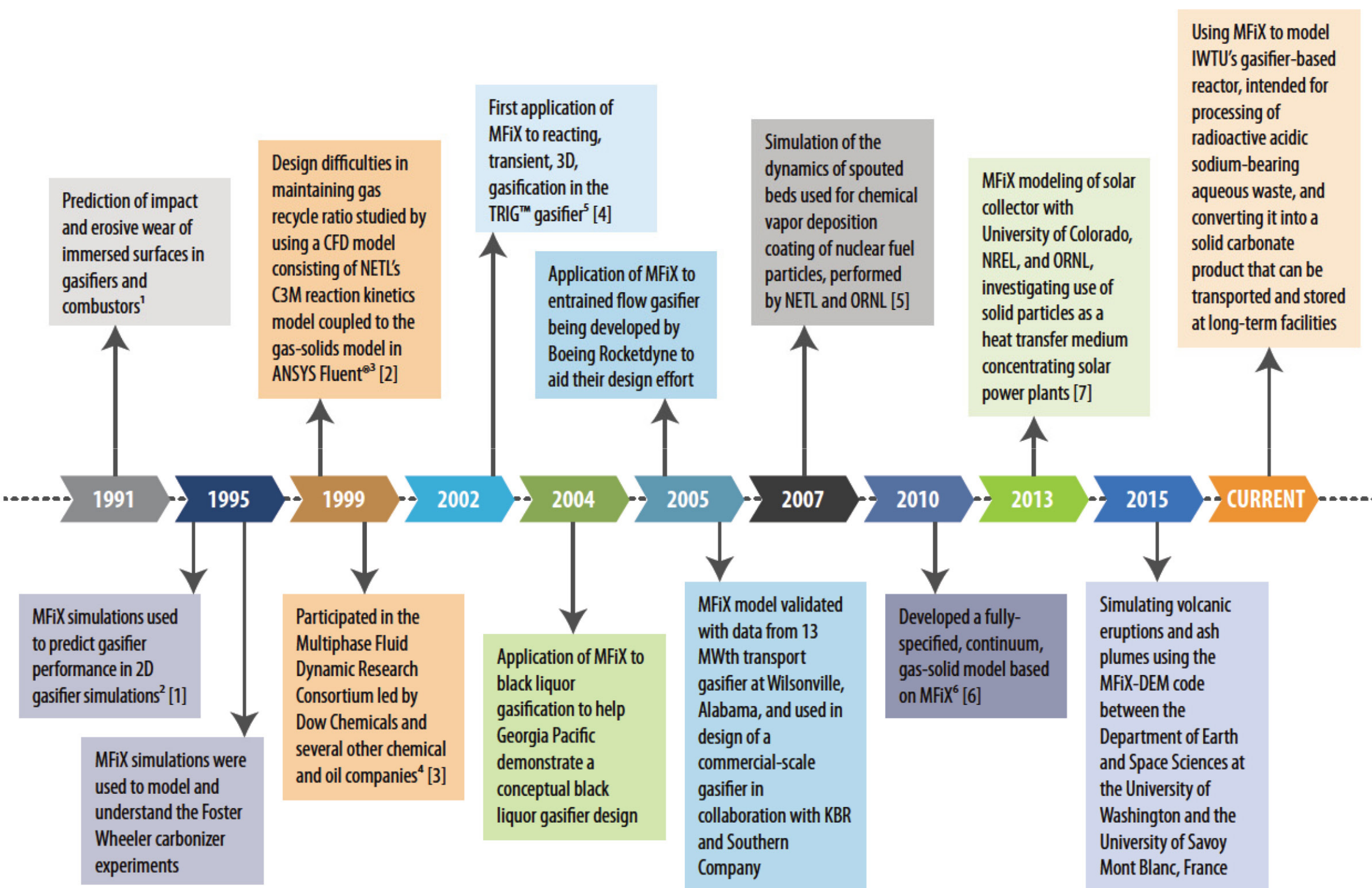


Figure 2. MFiX use timeline.

High Performance Computing

NETL is a leader in applying high-performance computing to computationally demanding multiphase flow science. The MFS Group has considerable expertise in applying high-performance computing to challenging industrial-scale problems.

NETL maintains its own powerful computing and visualization capabilities, which have been invaluable in using the existing portfolio of MFiX codes and computation fluid dynamics (CFD) tools and will be essential in development work moving forward. The Joule supercomputer is the most valuable resource for computationally intensive multiphase CFD simulations performed by the MFS Group.

MFS researchers use high-performance computers provided by DOE's Office of Advanced Scientific Computing Research through Innovative & Novel Computational Impact on Theory & Experiment and ASCR Leadership Computing Challenge awards. Collaborators have conducted large MFiX simulations on high-performance computers at the Oak Ridge Leadership Computing Facility and the Texas Advanced Computing Center.

Notable applications of high-performance computing by the NETL MFS Group range from scale-up efforts for new reactor technology to troubleshooting existing reactors. An example of the former is MFiX modeling of Kellogg, Brown & Root (KBR) and Southern Company's TRIG™ transport gasifier reactor, which underpinned the scale-up of transport gasification technology, leading to successful industrial-scale design.

MFiX Users and Publications

MFS Group scientists and engineers publish and present this work in peer-reviewed journals and at confer¬ences and symposia. The MFS Group monitors published literature for work citing MFiX. Annual MFiX citations have increased steadily over the years; collected data from 2003-17 indicates more than 200 citations per year.

To date, approximately 5,000 MFiX registrations have been made by the user community worldwide. Although the largest subset of the user base is in academia, users from industry and national laboratories also represent significant fractions. MFiX has been applied in a wide range of modeling applications extending beyond the traditional field of combustion and gasification to intriguing examples of uses, such as modeling volcanic eruptions and chemical vapor deposition on nuclear fuel particles. The user base is truly worldwide, with concentrations in North America, Europe, India, and China, but with users found in South America, Africa, Australia, New Zealand, and throughout greater Asia.

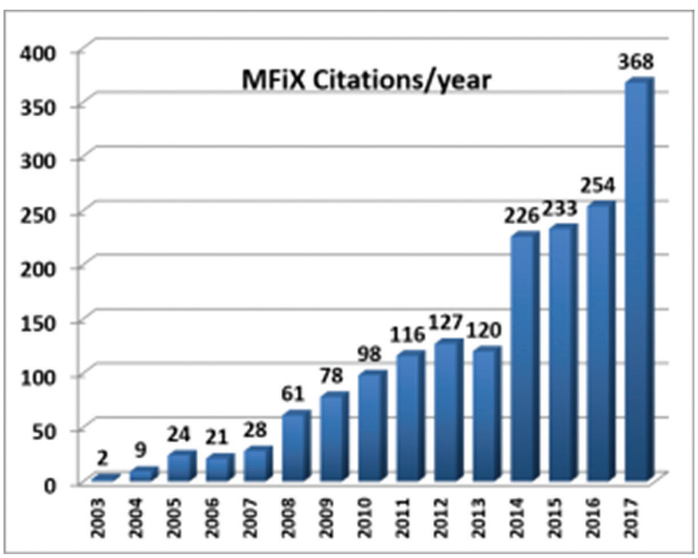


Figure 3. Number of MFiX citations in literature, 2003-17.

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