MULTIPHASE MODELING

OVERVIEW

Understanding the performance of energy, environmental, and chemical process devices based on multiphase flow physics is very challenging. Having the means to impact their design early in the development process is critically important to control costs and reduce the risk of not meeting performance standards. About 75 percent of the manufacturing cost of any product is committed at the conceptual design stage, even when the incurred cost might be very small. Using computational models to simulate a multiphase device can provide insight to its performance before the design is finalized, thereby reducing cost. Computational models are valuable when empirical scale-up information is not available and when reactors at the appropriate scale have not been built. Furthermore, it is well known that traditional scale-up methods do not work well for multiphase flow reactors. A critical need exists for science-based models with quantified uncertainty that reduce the cost and time required for development of multiphase flow devices. NETL’s Multiphase Flow Science (MFS) research program is a strategic combination of computational and physical models of reacting multiphase flows that provide validated science-based modeling tools.
MFS research at NETL is performed by a crosscutting team of engineers and scientists who are skilled in development and application of multiphase computational fluid dynamics software and multiphase experimentation. The Multiphase Flow Team consists of 30 U.S. Department of Energy (DOE) and contractor researchers from U.S. and international multiphase flow academic and industry research programs.

MFS research and development (R&D) at NETL is funded by DOE programs, primarily from the Office of Fossil Energy. The work emphasizes energy and environmental applications including gasification, carbon capture using solid sorbents or liquid solvents, and chemical-looping combustion of gaseous and solid fuels. MFS research also supports DOE’s Office of Environmental Management for analysis of thermochemical processes for environmental remediation of radioactive wastes. Details about the various research programs and projects in the Multiphase Flow Science portfolio can be found at https://mfix.netl.doe.gov/research/.

MFS R&D combines development and application of multiphase computational fluid dynamic (CFD) models with small-scale, well-resolved experiments to develop accurate models and provide validated computational tools. These tools and experimental data are made available to the multiphase flow science community as open-source software and public domain datasets.

The Laboratory’s suite of multiphase CFD code, called Multiphase Flow with Interphase eXchanges (MFIX) is central to NETL’s multiphase flow reactor modeling effort. MFIX has been developed specifically for modeling reacting multiphase systems. This open-source suite of software tools has more than three decades of development history and 3,500 registered users worldwide. This software has become the standard test bed for comparing, implementing, and evaluating multiphase flow constitutive models and has been applied to an extremely diverse range of applications involving multiphase flows. The successes achieved in modeling complex problems have led to new and improved models that are now available to the modeling community, which feature greatly improved simulations of key attributes within multiphase flow systems such as complex heterogeneous chemical reactions, interphase drag, polydispersity, particle attrition, particle agglomeration, and other significant advances.