EXCELLENCE IN TECHNOLOGY TRANSFER

National Energy Technology Laboratory

MFIX: Open-Source Software for Simulating Multiphase Flow Processes

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Researchers at the Department of Energy's (DOE) National Energy Technology Laboratory (NETL) 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 (*solids-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. NETL has been conducting research for many years to solve this scale up problem. NETL's effort has resulted in the development of MFIX, which is being transferred through the open-source method (www.mfix.org) and collaborative projects with end users. This has positively impacted not only the primary target, fossil fuel industry, but also the multiphase R&D at universities and national labs.

MFIX simulates heavily-loaded gas-solids flows, commonly encountered in fossil fuel processes and in other industries such as chemical, petrochemical, pharmaceutical, and mineral. MFIX calculates the detailed motion of gas and solids in a general process vessel, allowing for the effects of heat transfer and chemical reactions. In 2001, MFIX was declared open-source software, a novel technology transfer mode increasingly being used by software developers. This has allowed the flow of this technology to universities, national labs and industry as well as enabled a reverse flow of technology into MFIX from external researchers. Now there are around 1000 registered MFIX users from over 250 institutions worldwide. The software is being used by a number of universities to advance multiphase science, which has resulted in numerous publications and 15 graduate theses over the last five years.

A collaborative project between NETL and gasifier developers has resulted in MFIX being used for advanced gasifier design. For the last three years NETL researchers have been using MFIX to simulate the transport gasifier at the Power Systems Development Facility, Wilsonville, Alabama, operated by Southern Company and Kellogg Brown & Root (KBR). The simulations convincingly showed the gasifier developers that the model does not merely reproduce what is already known, but provides insight into unobserved phenomena, which they could later experimentally verify. Also MFIX was used to predict the expected gasifier behavior almost a year before certain design modifications were completed. KBR design engineers are using MFIX simulations to help in the design of a commercial-scale gasifier at Orlando, Florida.

The open-source distribution has led to non-fossil fuel applications as well. For example, Los Alamos National Laboratory is using MFIX to explore multiphase dynamics

(e.g., dust explosions) in the Yucca Mountain Project, Nevada, which is the proposed site for the United States' first permanent geologic repository for high-level radioactive waste.

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