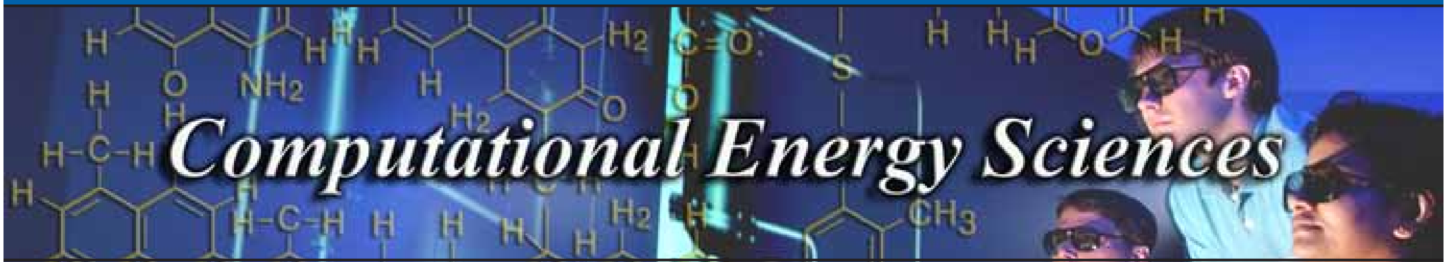
U.S. Department of Energy • Office of Fossil Energy
National Energy Technology Laboratory



Successes

Multiphase Flow with Interphase eXchanges Modeling Software

Advanced Research

To support coal and power systems development, NETL's Advanced Research Program conducts a range of pre-competitive research focused on breakthroughs in materials and processes, coal utilization science, sensors and controls, computational energy science, and bioprocessing—opening new avenues to gains in power plant efficiency, reliability, and environmental quality. NETL also sponsors cooperative educational initiatives in University Coal Research, Historically Black Colleges and Universities, and Other Minority Institutions.

Accomplishments

- ✓ Process improvement
- ✓ Cost reduction
- ✓ Greater efficiency
- ✓ Design optimization

Computational Fluid Dynamics

Research, development, and demonstration initiatives by the National Energy Technology Laboratory (NETL) are leading to improved operations of coal-based power systems, and to future power supplies that are environmentally clean and economically affordable. One method NETL researchers are using is advanced computational and experimental research, which is helping to develop novel technologies, including transport gasifiers, circulating fluidized-bed combustors, and hot gas desulfurization. Enhanced computational capabilities are leading to major improvements in power plant efficiency, and therefore to reduced emissions.

Computational fluid dynamics (CFD) has become an important tool for achieving scientific and engineering advances in combustion —and the more efficient the combustion, the cleaner the process becomes, with fewer emissions. Advanced power plant technologies require multiphase reactors for processing fossil fuels; in a gasifier, for example, coal (solids phase) is reacted with steam and air (gas phase). The scaling up of such multiphase reactors is notoriously difficult, in that engineers cannot reliably predict commercial-scale (large) reactor performance merely based on pilot-scale (small) reactor performance. NETL's Advanced Research Program has been conducting research for many years to solve this problem, with support from Aeolus Research, Inc., Dunbar, PA; Parsons Brinckerhoff (PB), Morgantown, WV; and Oak Ridge National Laboratory, Oak Ridge, TN, among others. These efforts have resulted in the development of the award-winning **MFIX (Multiphase Flow with Interphase eXchanges)** physics-based modeling software that is used to simulate the flows inside combustion reactors, among other useful applications. This technology reduces the time and cost for developing advanced gasifiers, for example.

MFIX Description

The MFIX tool helps researchers and plant designers understand how fluid-bed combustion systems work by describing their inherent fluid dynamics, heat transfer, and chemical reactions. MFIX calculations allow researchers to visualize the distribution of pressure, velocity, temperature, and behavior of the fuel and its by-products in three-dimensional models. The vast amounts of data generated by the detailed models then can be rendered, through NETL's "virtual reality" environment, into a readily understandable form that allows scientists to visualize the inner workings of fluidized beds. Using MFIX, NETL researchers now have a tool to scale up concepts and designs from pilot scale to commercial scale at minimal risk, and to reduce time-consuming, costly testing at intermediate scales.

Project Duration

Start Date

01/01/01

End Date

12/31/08

Cost

Total Project Value

$2,225,000

DOE/Non-DOE Share

$1,750,000 / $475,000

Industrial Partners

Aeolus Research, Inc.
Dunbar, PA
www.aeolusresearch.com

ANSYS/Fluent
Lebanon, NH
www.fluent.com

Iowa State University
Ames, IA
www.iastate.edu

KBR
Houston, TX
www.halliburton.com/kbr

Oak Ridge National Laboratory
Oak Ridge, TN
www.ornl.gov

Parsons Brinckerhoff (PB)
Morgantown, WV
www.pbworld.com

Princeton University
Princeton, NJ
www.princeton.edu

Southern Company
Atlanta, GA
www.southerncompany.com

MFIX Uses and Capabilities

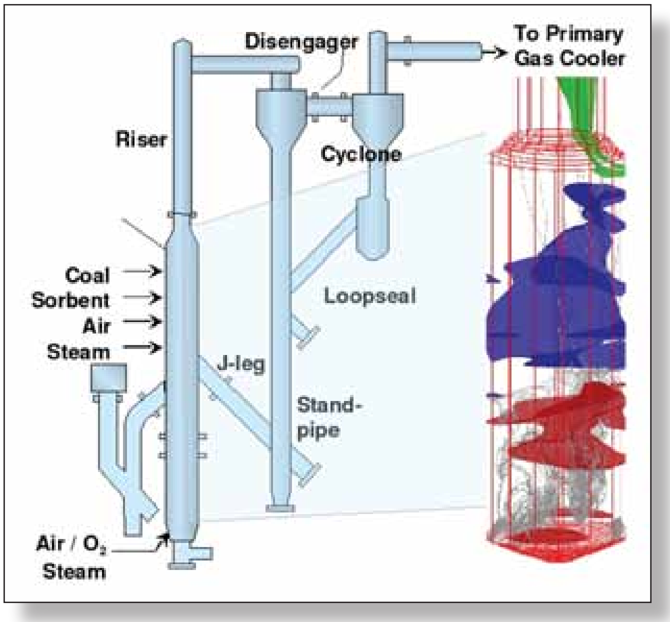
MFIX is being used by researchers around the world to model a variety of flow processes ranging from coal gasification to volcanic eruptions. Partners include academia, private research and development (R&D) groups, and other national laboratories. The MFIX program has been developed as "open-source" code, distributed to registered users through the web page www.mfix.org. When technology developers contribute to the improvement of MFIX, all modifications are documented using "version control" and tested against a suite of control cases. MFIX has been used to develop and validate multiphase flow theory (transport equations and constitutive relations) and to develop numerical techniques for solving these equations efficiently and accurately. Over 1,000 researchers from 250 institutions worldwide have registered at the website. Computational models and methods used by MFIX include the following:

- Continuum model for gas-solids flow;
- Discrete element method (DEM) and hybrid continuum-DEM capability for modeling particle flows;
- Subgrid-scale models for improving the accuracy of coarse-grid simulations;
- Direct Quadrature Method of Moments for modeling particle size changes due to agglomeration and breakage;
- In-Situ Adaptive Tabulation method for increasing the speed of chemistry calculations; and
- Gasifier chemistry model for gas-solids reactions, including coal gasification and combustion; and for homogeneous reactions, including devolitization, tar cracking, water-gas shift, and gas phase combustion.

MFIX Accomplishments

The latest version of MFIX was recognized in 2007 as one of three NETL-originated technologies selected by an independent judging panel and the editors of *R&D Magazine* as being among the 100 most significant products introduced into the marketplace that year. Additionally, the Federal Laboratory Consortium, Mid-Atlantic Region, presented a 2006 Excellence in Technology Transfer Award to NETL for innovative efforts in transferring the MFIX software to universities and to industry. Two technology transfer processes were used, as discussed below.

First, through a collaborative project, NETL researchers have used MFIX to simulate the transport gasifier at the Power Systems Development Facility (PSDF), Wilsonville, AL, operated by Southern Company and Kellogg Brown & Root (KBR). The gasifier is part of a Clean Coal Power Initiative project managed by NETL. The simulations convincingly showed that the model does not merely reproduce what is already known, but provides insight into unobserved phenomena, which the engineers could later experimentally verify. MFIX



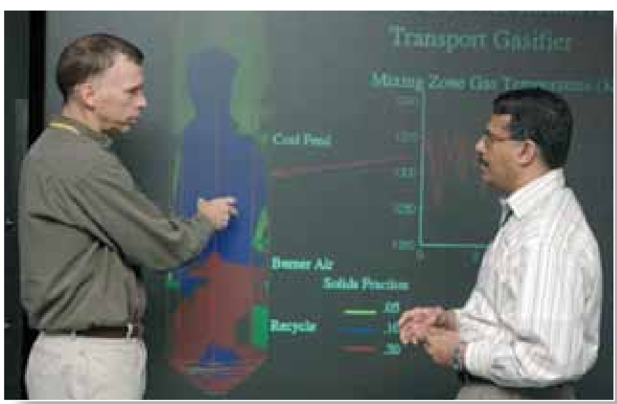
Transport gasifier and MFIX display showing particle trajectories and oxygen concentration. MFIX simulations complement testing and development at the DOE demonstration PSDF in Wilsonville, AL (shown above). Coal and recycled materials feed into the lower mixing zone of the plant's circulating fluidized-bed. The validated simulation model currently is being used to design a commercial-scale unit.

simulation results included time-dependent distribution of pressure, temperature, composition, void fraction, and velocity inside the gasifier. Simulation results on western bituminous and subbituminous coals showed excellent agreement with experimental data. Also, MFIX was used to predict the expected gasifier behavior almost a year before certain design modifications were completed.

MFIX simulations also are being used to help in the design of commercial-scale transport gasifiers. NETL is taking advantage of supercomputer time allocated by the U.S. Department of Energy (DOE) Undersecretary for Science on the CRAY XT4 system at the National Center for Computational Science to run the software on thousands of processors, a 50-fold increase in the number of processors used over previous simulations conducted on computer clusters at NETL and at the Pittsburgh Supercomputing Center. Also, a factor-of-three improvement in the parallel efficiency of MFIX was achieved on the CRAY computer. Specifically, using massively parallel computations to enable higher resolutions, the more recent work has allowed gasifier simulations to be conducted using 10 million computational cells running on 2,048 processors. Results from these high-resolution simulations will be shared with industrial stakeholders using this information in the design of their commercial-scale transport gasifiers.

As a second means of technology transfer, MFIX was made available as open-source software for registered users. Many users have viewed and participated in the development of the software, greatly strengthening the capabilities and quality of MFIX, and promoting research and graduate student training by disseminating information on computational multiphase flow. For example, a numerical technique developed by Iowa State University using MFIX has been transferred to commercial software and was used for a commercial polyethylene reactor simulation. Additionally, MFIX availability has promoted the use of computational multiphase flow in non-fossil fuel applications such as for the Yucca Mountain Project and for nuclear fuel particle coating reactor modeling. The open-source technology transfer has made it possible for some of the brightest people working in the multiphase field in power production and other industries to shape the code for specific purposes; as a result, the value of the MFIX code has been recognized and the software utilized by a broad field of researchers from academia and industry.

A next-generation version of MFIX now being developed is aimed at further improving the speed and accuracy of multiphase flow simulations, using enhanced representations of particle motion and best-in-class software components to achieve scalable performance on large-scale computing platforms. Developed at national laboratories, universities, and other open-source software organizations, these software enhancements allow scientists and engineers to focus on model algorithm development and validation rather than on code development and debugging, thereby providing a substantially advanced computational research capability by which to simulate multiphase flows.



Chris Guenther, left, and Madhava Syamlal discuss the results of a transport gasifier simulation produced by MFIX.

Benefits

The MFIX development effort has led to the use of this technology in the design of commercial-scale gasifiers. The simulations of the PSDF gasifier showed that the model does not merely reproduce what is already known, but provides insight into unobserved phenomena. Such insights enable engineers not only to make incremental improvements to an existing design but also to discover and explore new designs. Due to its versatility, the use of MFIX has gone beyond its originally intended applications, primarily fluidization, to others, such as the simulation of industrial and natural processes. As this is still an emerging technology, actual cost savings figures are not available; however, it has been estimated that the use of such technology in commercial-scale gasifier design is likely to result in substantial cost savings.

"...MFIX is being used by researchers around the world to model a variety of flow processes ranging from coal gasification to volcanic eruptions. Partners include academia, private research and development groups, and other national laboratories."

States and Localities Impacted

Wilsonville, AL

Orlando, FL

Atlanta, GA

Ames, IA

Lebanon, NH

Princeton, NJ

Dunbar, PA

Pittsburgh, PA

Oak Ridge, TN

Houston, TX

Morgantown, WV

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U.S. Department of Energy
Office of Fossil Energy

Printed in the United States on recycled paper

June 2008

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