PROJECT facts

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

Gasification Technologies

8/2006

CONTACTS

Gary J. Stiegel
Gasification Technology Manager
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236
412-386-4499
gary.stiegel@netl.doe.gov

Madhava Syamlal
Computational Science Division
National Energy Technology Laboratory
3610 Collins Ferry Road
P. O. Box 880
Morgantown, MV 26507
304-285-4685
madhava.syamlal@netl.doe.gov

Multiphase Flow

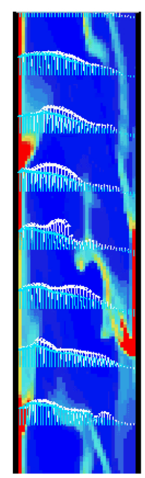
Background

Advanced gasifiers in which carbonaceous fuels (solids phase) are reacted with steam and air (gas-phase) are typical multiphase reactors. The scale-up of multiphase reactors is notoriously difficult; engineers cannot reliably predict the performance of commercial-scale (large) gasifiers merely based on the data from pilot-scale (small) gasifiers. Furthermore, the complex gas-solids flow patterns and the harsh environment in the gasifier makes detailed measurements impractical. So the data available from pilot-scale units are usually limited to product gas composition and pressure drop. However, multiphase flow simulations provide detailed information on the flow patterns, species, and temperature distribution and thereby offer a way to reduce the uncertainty in scale-up. NETL has an ongoing research program to solve this scale-up problem by developing physics-based multiphase flow simulations. This technology will reduce the time and cost for developing advanced gasifiers.

Accomplishments

- Multiphase Flow with Interphase eXchange (MFIX): MFIX is a result of the research work done at NETL over the last fifteen years. It gives the underlying framework for developing high-fidelity gasifier models. It is being distributed as open-source software, which registered users can download from the web site www.mfix.org. 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 1000 researchers from 250 institutions worldwide have registered at the web site. Some of the significant features are as follows:
  - Continuum model for gas-solids flow
  - Discrete element model (DEM) and hybrid continuum-DEM capability
  - Subgrid scale models for improving the accuracy of coarse-grid simulations
  - Direct Quadrature Method of Moments (DQMOM) for modeling particle size changes because of agglomeration and breakage
  - In Situ Adaptive Tabulation (ISAT) method for increasing the speed of chemistry calculation

MFIX
www.mfix.org



Periodic channel flow:
Solids volume fraction (red - high, blue - low) and velocity vectors (white - gas, light blue - solids).
Benyahia, Syamlal and O'Brien, 2005

ADDRESS

National Energy Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South
Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

One West Third Street, Suite 1400
Tulsa, OK 74103-3519
918-699-2000

CUSTOMER SERVICE

1-800-553-7681

WEBSITE

www.netl.doe.gov

- Gasifier chemistry model. Gas-solids reactions account for coal gasification and combustion reactions. Homogeneous reactions account for devolitization, tar cracking, water-gas shift reaction, and gas phase combustion. The gas phase consists of eight species: O_2, CO, CO_2, CH_4, H_2, H_2O, N_2, and tar. The solids phase consists of four species: carbon, volatile matter, ash, and moisture.

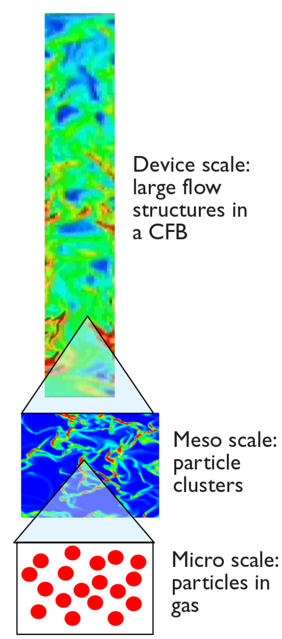
- MFIX-NG: A "next generation" version of MFIX is under development. A prototype is expected to be completed by October 2006. The goal of the project is to improve the speed and accuracy of the simulations of dilute-to-dense, diabatic, chemically reactive multiphase flows. The software will incorporate both continuum and discrete representations of particle motion and will operate within a framework to achieve scalable performance on large-scale parallel computing platforms. It will be composed of best-in-class software components developed at national laboratories, universities, and other open-source software organizations. The software will include a scripting-front end that would enable scientists and engineers to focus on model, algorithm development, and validation rather than on code development and debugging, thereby providing a substantially advanced research capability for computational multiphase flow.

- Chemical Looping: This promises to become a technology for the efficient conversion of fossil fuels with the ability to reduce NO_x, to allow in-bed sulfur capture, and to enable CO_2 separation. The success of the process depends upon solving critical issues such as the dense-solids flow, gas-particle contacting, and solids mixing and segregation in the reduction unit, which multiphase flow simulations are ideally suited to address. Development of a chemical-looping fuels-reactor model was started.

- Transport Gasifer: MFIX was used to conduct transient three-dimensional simulations of an industrial-scale Kellogg, Brown & Root (KBR) Transport Gasifier in operation at the Power Systems Development Facility (PSDF) in Wilsonville, Alabama. MFIX simulation results include time-dependent distribution of pressure, temperature, composition, void fraction, and velocity inside the gasifier. Simulation results of a western sub-bituminous and a western bituminous coal showed excellent agreement with experimental data.

Benefits

This 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 to not only make incremental improvements to an existing design but also to discover and explore new designs. As this is an emerging technology, actual cost savings figures are not available. It has been estimated that the use of such technology in commercial-scale gasifier design will result in savings of the order of $10 million.



Levels of averaging: discrete particles to continuum to filtered-continuum models