



the **ENERGY** lab

PROJECT FACTS

Gasification Systems

Low-rank Coal Optimization—TRIG Model Development

Background

Low-rank coals, including lignite and sub-bituminous coal, make up about half of U.S. coal production and reserves. They have lower energy and sulfur contents than bituminous coal, but higher moisture and mineral content. Despite the lower energy content, the cost per British thermal unit is comparable to bituminous coals.

Gasification is a method of obtaining the energy content of fuels including coal and biomass while managing emissions such as carbon dioxide believed to cause global warming. Coal gasification processes, although environmentally superior, raise the cost of electricity by some percentage points. Optimization of gasification processes for use with low-rank coals will increase efficiency and improve reliability, availability, and maintenance (RAM) costs.

Transport Integrated Gasification (TRIG) is a gasification reactor design supported by the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) and the Southern Company. The NETL Office of Research and Development (ORD) is developing a set of computer models for co-feeding of low rank coals and other feedstocks including biomass for the TRIG reactor. Validation of these models will enable reliance on them for design and optimization purposes.

While it is clear that benchmarking and validating computational fluid dynamics (CFD) models on experiments relevant to gas-solids reactors is necessary to gain acceptance of these models as design and optimization tools, there is a growing recognition that validation cannot be complete without explicit accounting of various uncertainties. Coupling uncertainty quantification (UQ) tool kits such as PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) from Lawrence Livermore National Laboratory (LNNL) or DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) from Sandia National Laboratory with a high fidelity suite of multiphase software such as MFIX-DEM (Multiphase Flow with Interphase eXchanges - Discrete Element Model), MFIX continuum, Hybrid MFIX, and MFIX-PIC (Particle-in-Cell) has the potential to achieve for the first time a hierarchy of TRIG co-feed models with uncertainty quantification.

Coupled to these high fidelity gasification models are kinetic sub-models which describe the thermal and chemical transformation of the coal as it travels through the gasifier. Current research addresses the lack of a comprehensive, easily accessible database of kinetic models describing devolatilization (removal of volatile material), secondary tar cracking, soot formation, char gasification, and gas-phase

CONTACTS

Jenny Tennant

Gasification Systems Technology Manager
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4830
Jenny.Tennant@netl.doe.gov

Arun Bose

Project Manager
National Energy Technology Laboratory
626 Cochran's Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4467
arun.bose@netl.doe.gov

Chris Guenther

Project Manager
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4483
chris.guenther@netl.doe.gov

PARTNERS

NETL-Regional University Alliance

PROJECT DURATION

Start Date	End Date
10/01/2010	09/30/2013

COST

Fiscal Year 2013 Project Value
\$1,503,926

PROJECT NUMBER

FWP-2012.03.03 Task 4

NATIONAL ENERGY TECHNOLOGY LABORATORY

Albany, OR • Anchorage, AK • Morgantown, WV • Pittsburgh, PA • Sugar Land, TX

Website: www.netl.doe.gov

Customer Service: 1-800-553-7681



U.S. DEPARTMENT OF
ENERGY

reactions for a wide variety of coals. Such kinetic data exist in a number of commercial software packages (for example, PC Coal Lab [PCCL] and Chemical Percolation Model [CPD]), but these data/models are generally not easily implementable in CFD codes such as MFIX, Fluent, and Barracuda.

The NETL Gasification Team will address these modeling issues using an integrated approach that leverages the expertise of the NETL-Regional University Alliance (NETL-RUA). The approach will combine theory, computational model development, experiments, and industrial input to develop physics-based models to support the development and deployment of advanced gasification-based devices such as the TRIG.

Project Description

The work described is part of an omnibus project in advanced gasification. It comprises several subtasks aimed at provision of model validation data and general multiphase model development. Researchers will conduct statistically designed experiments on gas-solids jets located on the side-wall of NETL's large scale circulating fluidized bed to mimic the flow of coal into an industrial scale transport unit. Smaller-scale, well controlled, and highly instrumented laboratory

experiments will also be conducted to test model expressions for gas solids jets on drag, coefficients of restitution and friction, and polydispersity. While objective statistical methods are routinely available to characterize the uncertainty in experimental data, the bulk of the effort will be to develop a framework that enables quantification of uncertainty associated with CFD characterization of a TRIG unit for co-feeding applications. NETL's open-source suite of multiphase solvers including MFIX-DEM, MFIX-continuum, Hybrid MFIX, and MFIX-PIC will be coupled with the PSUADE UQ package in order to establish confidence levels associated with each CFD simulation by each CFD solver for TRIG co-feed applications.

Researchers will develop kinetic sub-models for devolatilization, secondary tar cracking, and char gasification and continue to develop algorithms to extract the model data from commercial software codes and implement them through the graphical user interface that forms the basis of the Carbonaceous Chemistry for Computational Modeling module (C3M). C3M will also be updated from an experimental program which will identify key parameters affecting soot formation, identify the mechanism of soot formation, and investigate the influence of pressure on the steam reforming mechanism. The team will generate detailed kinetic and product distribution data on the pyrolysis and gasification of low-rank fuels used in the TRIG unit at the National Carbon Capture Center (NCCC).

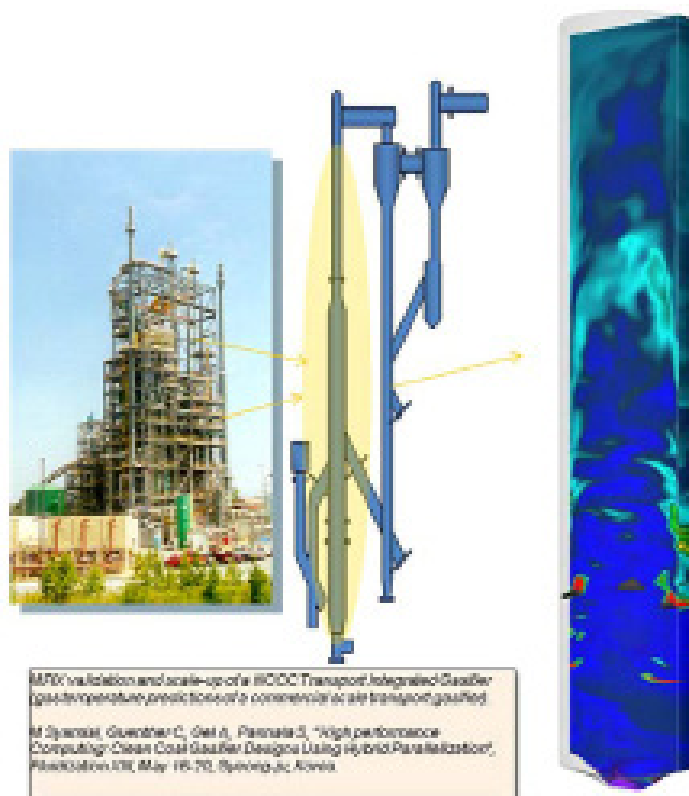


Figure 1. MFIX validation and scale-up of a National Carbon Capture Center Transport Integrated Gasifier.

Goals and Objectives

The goal of this task is to develop a hierarchy of co-feed TRIG models with uncertainty quantification (UQ). The objectives in support of the goal are to (1) develop a hierarchy of Eulerian–Eulerian (EE), Eulerian–Lagrangian, and hybrid co-feed TRIG models; (2) couple NETL’s MFIX model to existing UQ models to determine model parameter sensitivity and perform UQ on large scale NCCC/TRIG; and (3) generate gasification kinetic data and implement into NETL’s C3M kinetic package.

The resulting toolset will be made available to the multi-phase modeling community through MFIX and used to establish a methodology for performing UQ analysis for the hierarchy of co-feed TRIG models to enable confidence-level reporting in simulation results.

Accomplishments

• Uncertainty Quantification (UQ)

Researchers completed coupling LLNL’s software, PSUADE, and NETL’s MFIX model to allow non-intrusive UQ. UQ techniques were applied to small-scale non-reacting DEM study and an oxygen-blown transport gasifier and used in NETL’s C3M to explore uncertainties in kinetic predictions based on temperature, pressure, and heating rate inputs.

• TRIG Model Development

A new MFIX-PIC hydrodynamic model was developed, implemented in MFIX, and validated by comparing it with more accurate DEM simulations. Comparisons were also made with MFIX-EE and Computational Particle Fluid Dynamics’ (CPFD) commercial Multi Phase Particle-in-Cell (MPPIC) solver Barracuda. Documentation and a manuscript are being prepared. The latest version of NETL’s reacting multiphase model was released to the modeling community through the MFIX website (www.mfix.netl.doe.gov).

• Model Validation

The experimental system has been set up to characterize the jetting behavior of a gas-solid mixture continuously injected into the side wall of the mixing zone of a transport reactor. A small scale fluidized bed has been constructed to provide well controlled and highly instrumented laboratory experiments for model development, verification, and validation.

• Cohesive Powder Model

An algorithm that calculates the clusters size was implemented and released in MFIX. Clusters can now be visualized in Paraview and their size calculated along with other local flow properties (such as void fraction and Re number). The effects of cohesive forces on fluidization were shown in several simulations that can capture minimum fluidization and bubbling velocities as well as the hysteresis in the fluidization curves.

• Fundamental Gasification Code Development

The devolatilization subroutines from PCCL, CPD, and Functional-Group, Depolymerization, Vaporization, and Cross-linking (FG-DVC) were implemented in the C3M code and the first round of kinetic data for co-feeding was collected and incorporated. NETL licensed the C3M code for the first time to the Brazilian Associação Beneficente da Indústria Carbonífera de Santa Catarina (Coal Mining Industry Beneficent Corporation of Santa Catarina) (SATC) for the full term of the NETL patent. Negotiations are underway for a second license to KBR, Inc. An R&D 100 application was submitted on the basis of these significant accomplishments and a paper was published in the magazine *Power Engineering*. C3M was also used as a basis for the kinetics in a full-scale TRIG gasifier model for an industrial stakeholder.

Benefits

The validation data sets produced and promulgated through this research will be made available to objectively evaluate, definitively critique, and quantitatively improve design and optimization tools.

It is also expected that the C3M platform will become the “gold standard” for modeling coal chemistry associated with gasification processes. The experimental data obtained are expected to significantly improve and validate the kinetics models in the C3M program for the primary fuels used in the TRIG process, which will enable improvements in fuel flexibility for current and future gasification facilities.

Providing access to a hierarchy of models for numerical simulations of gasifiers with a framework in place to quantify the uncertainty associated with CFD characterization will give stakeholders and researchers the ability to significantly improve gasifier design and performance.



Figure 2. Carbonaceous Chemistry for Computational Modeling.

