the ENERGY lab

PROJECT FACTS

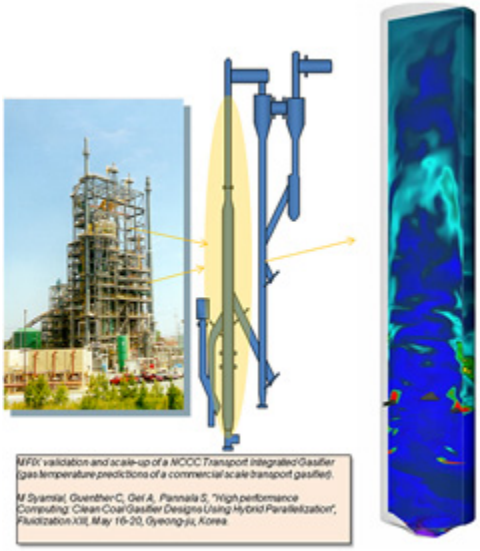
Project No: FWP-2012.03.03 Task 4
Performer: NETL Office of Research and Development

Project Description

NETL's in-house research team is using an integrated approach to combine theory, computational modeling, experiment, and industrial input to develop physics-based methods, models, and tools to support the development and deployment of advanced gasification based devices and systems. The activities in this effort include developing and applying computational and modeling tools to simulate complex flows in applications such as transport or entrained flow gasifiers.

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. TRIG is a pressurized, partially-dried feed, dry ash (non-slagging) discharge and refractory lined gasification that operates under coal ash deformation temperature. 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.

This work will develop a hierarchy of models for numerical simulations of TRIG co-feed conditions that span from fast running reduced order models (ROMs) to high fidelity multiphase computational fluid dynamics (CFD) models. Each model will have uncertainty quantification associated with its predictions to allow a user to choose a model based on the trade-offs between computational speed and uncertainty in the predictions.



MFIX validation and scale-up of a NCCCT

Program Background and Project Benefits

Gasification is used to convert a solid feedstock, such as coal, petcoke, or biomass, into a gaseous form, referred to as synthesis gas or syngas, which is primarily hydrogen and carbon monoxide. With gasification-based technologies, pollutants can be captured and disposed of or converted to useful products. Gasification can generate clean power by adding steam to the syngas in a water-gas-shift reactor to convert the carbon monoxide to carbon dioxide (CO_2) and to produce additional hydrogen. The hydrogen and CO_2 are separated—the hydrogen is used to make power and the CO_2 is sent to storage, converted to useful products or used for EOR. In addition to efficiently producing electric power, a wide range of transportation fuels and chemicals can be produced from the cleaned syngas, thereby providing the flexibility needed to capitalize on the changing economic market. As a result, gasification provides a flexible technology option for using domestically available resources while meeting future environmental emission standards. Polygeneration plants that produce multiple products are uniquely possible with gasification technologies. The Gasification Systems program is developing technologies in three key areas to reduce the cost and increase the efficiency of producing syngas: (1) Feed Systems, (2) Gasifier Optimization and Plant Supporting Systems, and (3) Syngas Processing Systems.

Gasifier Optimization and Plant Supporting System technologies under development are targeted at increasing gasifier availability and efficiency, improving performance, and reducing the capital and operating costs of advanced gasification plants. Ongoing R&D projects are developing more durable refractory materials, creating models to better understand the kinetics and particulate behavior of fuel inside a gasifier, and developing practical solutions to mitigate the plugging and fouling of syngas coolers. Future work will focus on the development of cutting edge gasifier technologies, which will start with multiple competing concepts and continue with support of the most aggressive and successful technologies being developed, both in the Gasification Systems program and other DOE programs, to reduce the cost of coal gasification. Future work will also aim to reduce the amount of water used in gasification plants and integrate technologies throughout the plant and beyond in a holistic approach to increase efficiency and reduce costs (e.g., the optimization of gasification plants to sell CO_2 for EOR applications).

This NETL Office of Research and Development (ORD) project is using an integrated approach to combine theory, computational modeling, experiment, and industrial input to develop physics-based methods, models, and tools to support the development and deployment of advanced gasification-based devices and systems. Project-developed tools will enable simulation of complex flows in applications such as transport or entrained flow gasifiers or chemical looping systems. The results provide for better assessment of gasifier technology risk, with ultimate benefit of capital cost reductions for gasification technology.

Project Scope and Technology Readiness Level

The work described is part of an overall 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 Multiphase Flow with Interphase Exchanges-discrete element method (MFIX-DEM), MFIX-continuum, Hybrid MFIX, MFIX-PIC (particle-in-cell) will be coupled with the Problem Solving environment for Uncertainty Analysis and Design Exploration uncertainty qualification (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).

The Technology Readiness Level (TRL) assessment identifies the current state of readiness of the key technologies being developed under the DOE's Clean Coal Research Program. In FY 12, this project was assessed a TRL of 3.

The TRL assessment process and its results including definition and description of the levels may be found in the "2012 Technology Readiness Assessment-Analysis of Active Research Portfolio".

Accomplishments

- Uncertainty Quantification (UQ)
  Researchers completed coupling Lawrence Livermore National Lab (LLNL) PSUADE software and NETL's MFIX model to allow non-intrusive UQ. UQ techniques were applied to small-scale non-reacting discrete element model (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 (Eulerian-Eulerian) and Computational Particle Fluid Dynamics' 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 cluster 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 Reynolds 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 devolatization subroutines from PC Coal Lab (PCCL), Chemical Percolation Model for Coal Devolatilization (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 Carbonifera 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.

Contacts, Duration, and Cost

Contacts

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Duration
Award Date: 10/01/2011
Project Date: 09/30/2014

Cost
Total 2013 Project Value: $1,503,926

Presentations, Papers, and Publications

- Energy & Fuels, "Computational Fluid Dynamic Simulations of a Pilot-Scale Transport Coal Gasifier: Evaluation of Reaction Kinetics," (2013), Tingwen Li, Kiran Chaudhari, Dirk VanEssendelft, Richard Turton, Philip Nicoletti, Mehrdad Shahnam, and Chris Guenther
- Research Efforts at the National Energy Technology Laboratory to Improve Gasifier Performance Presented by James Bennett, U.S. Department of Energy, National Energy Technology Laboratory, Gasification Technologies Conference, October 13-16, 2013, Colorado Springs, CO.
- Gasification Modeling Activities at the National Energy Technology Laboratory (Oct 2012) Presented by Chris Guenther, Gasification Technologies Conference, October 28-21, 2012, Washington DC.

- Recent Developments in Carbonaceous Chemistry for Computational Modeling (C3M) with Uncertainty Quantifications (UQ) (Oct 2012)
  Presented by Kiran Chaudhari, AICHE 2012, October 31, 2012, Pittsburgh, PA.
- Power Engineering®, "Gasification Modeling in the 21st Century" (June 2012), Chris Guenther, Dirk VanEssendelft, Kiran Chaudhari, Phil Nicoletti, Mehrdad Shahnam, Tingwen Li, Richard Turton, Nathan Weiland, and Ping Wang, U.S. Department of Energy National Energy Technology Laboratory

Performer website: NETL Office of Research and Development

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