Gasification CFD Modeling for Advanced Power Plant Simulations

Stephen E. Zitney and Chris Guenther

National Energy Technology Laboratory, Morgantown, WV 26507-0880, USA

ABSTRACT

We describe here our progress toward developing high-fidelity computational fluid dynamics (CFD) models of commercial-scale gasifiers for use in advanced power plant simulations. The first gasifier is a two-stage, coal slurry-fed, oxygen-blown, pressurized, entrained-flow gasifier modeled using the commercial FLUENT® CFD software. The Eulerian-Lagrangian modeling approach is applied whereby the gas phase is treated as continuous and the coal particles are handled using the discrete phase model (DPM). The second gasifier is a scaled-up design of the transport gasifier at the Power Systems Development Facility (PSDF) located near Wilsonville, Alabama. The transient Eulerian-Eulerian MFIX multiphase CFD code from the National Energy Technology Laboratory (NETL) is used to model the gas-solids hydrodynamic conditions and the complex gasification processes that take place in the transport gasifier.

In this paper we also highlight recent NETL efforts to integrate CFD-based gasifier models into advanced power plant simulations using NETL's Advanced Process Engineering Co-Simulator (APECS). In one case study, the entrained-flow gasifier CFD model is coupled into an Aspen Plus® steady-state process simulation of a potential coal-fired, gasification-based power and hydrogen production plant for the U.S. Department of Energy's (DOE) FutureGen project. The APECS results illustrate that the co-simulation technology offers the potential to optimize overall power plant performance with respect to gasifier fluid dynamics, which strongly affect carbon conversion and synthesis gas quality.

Depending on initial solution estimates, the APECS co-simulations for the FutureGen typically require several hours of CPU time to converge on a single-CPU workstation. The turnaround times are improved by running the computationally-intensive gasifier CFD model remotely and in parallel on the Linux clusters at NETL and/or Pittsburgh Supercomputing Center. The APECS system also enables NETL engineers to speed up co-simulations by generating fast, reduced-order models (ROMs) based on previously-computed results from higher-order CFD models. For the transport gasifier, we discuss the MFIX simulations performed to generate a CFD results database for use in developing a ROM for integration into a FutureGen plant simulation. To cover the wide range of potential FutureGen operating conditions and to generate a more accurate ROM, parametric runs are required for both air-blown and oxygen-blown gasifier cases and for different feed stocks, operating pressures, and recycled char and synthesis gas flow rates. The seamless integration of CFD-based ROMs with process simulation will provide an efficient capability to investigate the effect of transport gasifier fluid mechanics on overall FutureGen plant performance and efficiency.

INTRODUCTION

Gasification technology is a key component of today's Integrated Gasification Combined Cycle (IGCC) power plants and is expected to be the centerpiece of tomorrow's high-efficiency, zero-emission systems. The gasifier provides a means for converting coal to a hydrogen-rich synthesis gas, ideally suited for power generation, refining, and chemical applications. In order to realize the full potential of this promising new technology, NETL researchers are using CFD modeling to better understand the complex physical and chemical phenomena, including fluid flow, heat and mass transfer, and chemical reactions, that impact gasifier performance and efficiency. These high-fidelity CFD models are also used within overall process simulations for improving the design, analysis, and optimization of gasification-based power plants.

The DOE's $1 billion, 10-year, FutureGen Research Initiative is aimed at creating the world's first coal-fired, gasification-based, near-zero emissions electricity and hydrogen production power plant (DOE, 2004). The FutureGen plant will employ advanced coal gasification technology integrated with combined cycle electricity generation, hydrogen production, and capture and sequestration of carbon dioxide (CO_2). Figure 1 provides a simplified flow diagram of the FutureGen plant. The plant gasifies a coal slurry using oxygen from an air separation unit (ASU) to produce a hydrogen-rich synthesis gas (syngas). After exiting the gasifier, the syngas is cleaned and shifted to produce a concentrated gas stream of hydrogen, steam, and CO_2. Following separation of these three species, the generated hydrogen is used to power a gas turbine and/or delivered as a product for use in fuel cells, as well as in applications other than power generation, for example, transportation and refineries. The FutureGen plant will be the cleanest fossil fuel-fired power plant in the world, capturing and sequestering at least 90% of the CO_2 with potential for 100% sequestration. The reference design plant efficiency is projected at 50% for hydrogen and power production with CO_2 sequestration. The actual plant efficiency and cost will depend on the hydrogen and electricity product ratio.

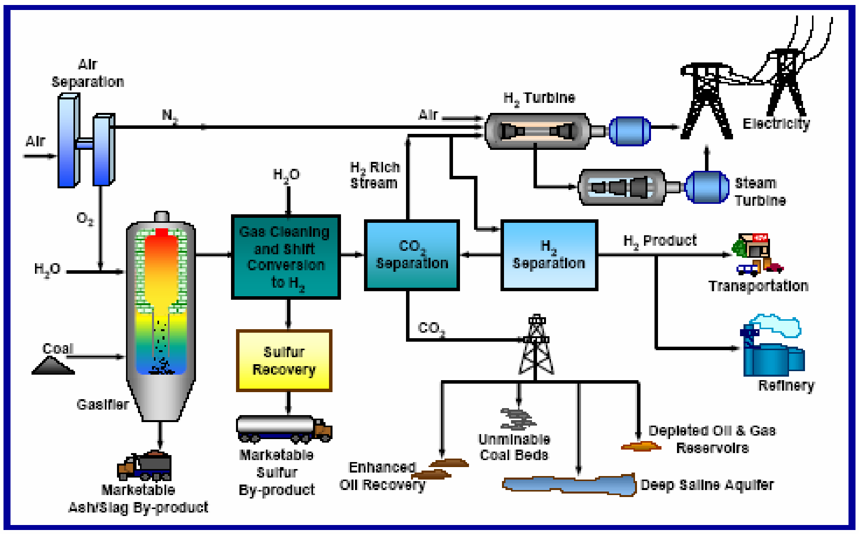


Figure 1. Simplified Flow Diagram of the FutureGen Plant

To help achieve the aggressive integration, environmental, and performance goals for the FutureGen plant, NETL computational scientists and engineers are building on strong collaborations with R&D technology partners (e.g., Syamlal *et al.*, 2001; Sloan *et al.*, 2002; Bockelie *et al.*, 2005; McCorkle *et al.*, 2003) to develop the Advanced Process Engineering Co-Simulator (APECS) (Zitney, 2004a). APECS is an integration framework that combines process simulation with high-fidelity equipment models, for example those based on computational fluid dynamics (CFD). Process simulation and CFD are highly complementary technologies and coupling the two offers significant opportunities to analyze overall system performance with respect to fluid flow, mass and heat transfer, chemical reactions, and related phenomena. In APECS, NETL design engineers are able to run the widely-used, steady-state process simulator, Aspen Plus® (Aspen Technology, 2003) with various equipment models, including CFD models based on FLUENT® (Fluent, 2004), a leading software package for detailed flow analysis of process equipment. Integrated Aspen Plus and FLUENT simulations have been applied to various chemical process (Zitney and Syamlal, 2002) and power generation applications (Syamlal *et al.*, 2003; Sloan *et al.*, 2004, 2005; Zitney *et al.*, 2004, 2005).

In NETL's APECS system shown in Figure 2, plug-and-play interoperability is achieved by using the international standard CAPE-OPEN (CO) interfaces for unit operations, physical properties, and reaction kinetics (Osawe *et al.*, 2002; Syamlal *et al.*, 2004; Zitney, 2004b, 2005). The CO standard for process simulation is managed by the CAPE-OPEN Laboratories Network (CO-LaN, www.colan.org) and supported by over forty leading process-industry companies, software suppliers, and academic and government research institutions (Braunschweig and Gani, 2002). The interfaces are open, multi-platform, available free of charge, and supported by many of the leading commercial process simulators. A recent review of industrial applications of the CO standard, including a brief discussion of the integrated Aspen Plus and FLUENT solution used in APECS, can be found in Pons (2003).

The APECS technology addresses the performance issue that equipment simulations based on high-fidelity CFD models require much more computational time than the process simulations based on simplified models. The design engineer often needs to run many process simulations in a short period of time and detailed equipment models may lead to unacceptable turnaround times. APECS overcomes this potential barrier by providing solutions on both ends of the performance spectrum, including parallel execution of the CFD models on high-performance computers (Zitney, 2004a) and use of fast reduced-order models based on CFD results (Syamlal and Osawe, 2004).

The APECS system also provides a wide variety of analysis tools for optimizing overall plant performance with respect to mixing and fluid flow behavior (Zitney, 2004a). Advanced 2D and 3D visualization tools enable the design engineer to display, within the process simulator, the results of a CFD simulation conducted as a part of an integrated simulation. Other analysis tools include design specifications to calculate operating conditions or equipment parameters to meet specified performance targets; case studies to run multiple simulations with different input for comparison and study; sensitivity analysis to show how process performance varies with changes to selected equipment specifications and operating conditions; and optimization for maximizing an objective function, including plant efficiency, energy production, and process economics.

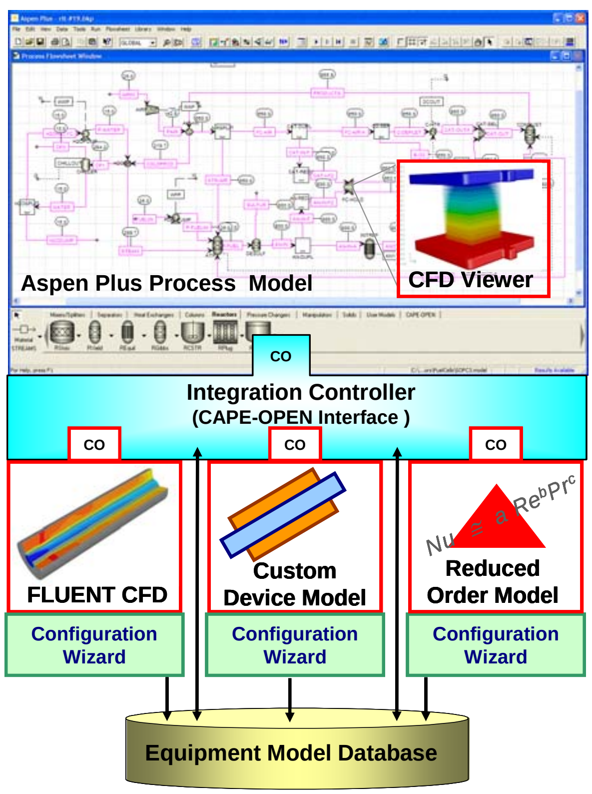


Figure 2. APECS Integration Framework

ENTRAINED-FLOW GASIFIER

The entrained-flow, coal-slurry gasifier considered here is a two-stage, up-flow gasifier consisting of a horizontal first stage and a vertical second stage as shown in Figure 3. All of the oxidant and 78% of the coal slurry are evenly divided between the left- and right-hand inlets of the first stage. This horizontal stage is mainly a coal combustor and provides hot gases through the connection to the second stage in which the remaining 22% of the coal slurry is injected. Most of the coal gasification process occurs in the second stage. The total volume of the gasifier is 45.5 m^3. The particle volume fraction is estimated to be around 4% and the average particle residence time is estimated to be 10 seconds. The operating pressure is 28 atm. The coal slurry and the oxygen are fed into the gasifier at temperatures of 450 K and 411.4 K, respectively. It is important to note here that this is a prototype gasifier design which is not intended to represent any existing gasifier designs, commercial or otherwise.

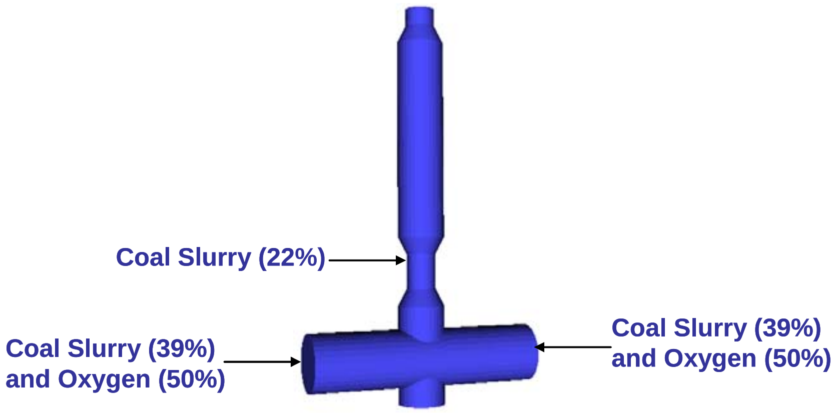


Figure 3. Entrained-Flow Gasifier with Coal Slurry and Oxidant Feed Streams

CFD Model of Entrained-Flow Gasifier

The entrained-flow gasifier is modeled using the steady-state, three-dimensional CFD model described by Shi *et al.* (2004, 2005b). The continuous gas phase conservation equations include the continuity equation, momentum equations, energy equation, turbulence equations, species transport equations, and radiation transfer equation. The gas phase reactions are modeled using the eddy dissipation model along with an Arrhenius rate law. The discrete phase model (DPM) is used to simulate the coal slurry flow as two separate particle types, namely water droplets and coal particles, which are injected into the gasifier through the carrying gas with a particle diameter distribution of Rosin-Rammler (Fluent, 2005). The assumption of two particle types is reasonable given that the water evaporates quickly after the slurry enters the gasifier. Using DPM, the particle trajectories, along with mass and energy transfer to/from the particles, are computed with a Lagrangian formulation. The physical and chemical processing of the coal slurry is implemented by using user-defined functions (UDFs) in which the coal particles undergo moisture release, vaporization, devolatilization, char oxidation, and gasification. The coal gasification model evolved from earlier models developed at NETL for fixed bed gasifiers (Syamlal and Bissett, 1992), and dilute (Shahnam *et al.*, 2000) and dense (Syamlal *et al.*, 1996; Guenther *et al.*, 2002, 2003) transport gasifiers. The coupling between the continuous phase (gas) and the discrete phase (particle) is solved by tracking the exchange of mass, momentum, and energy (Figure 4).

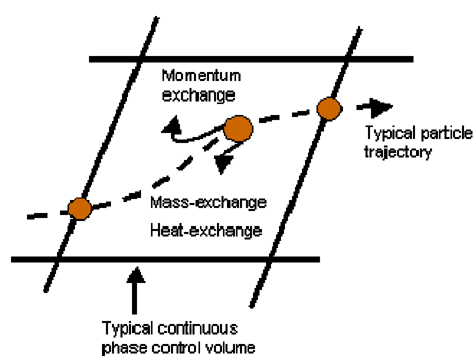


Figure 4. Heat, mass, and momentum transfer between discrete and continue phases

The gasifier CFD simulation with over 12,000 hexahedral computational cells was converged using approximately 50,000 gas phase iterations in FLUENT (Version 6.1.22). Convergence was achieved when the residuals were less than their specified maximum values and the DPM mass and energy were balanced. A temperature of 2500 K was patched in the gasifier to initialize the combustion reaction. The DPM calculations were performed at every 50th iteration of the fluid phase calculation. The continuous phase and discrete phase equations are calculated alternatively until a converged coupled solution is achieved. During the continuous phase iterations, accumulated sources from the particles remain unchanged, and vice versa.

APECS Integration of Entrained-Flow Gasifier CFD Model and FutureGen Plant Simulation

The converged entrained-flow gasifier CFD simulation described above was then coupled into a FutureGen plant simulation using the APECS integration framework. The entrained-flow gasifier model is instantiated on the process flowsheet via the CFD block in the CAPE-OPEN Model Library. The two-stage gasifier CFD model replaces two restricted equilibrium reactor models (REquil) from the Aspen Plus Model Library. The gasifier CFD model is coupled to the Aspen Plus process flowsheet by a total of twelve material streams—nine inlets and three outlets (Figure 5). Typically, an equipment item represented by a CFD model has "material stream ports" corresponding to the standard inlet and outlet boundaries of the computational domain. When the CFD model is instantiated on the flowsheet, Aspen Plus "material streams" are connected to the "material stream ports". For the gasifier, the oxidant inlet streams and tail gas recycle in Aspen Plus are linked to standard "material stream ports" corresponding to mass-flow-inlet boundaries in FLUENT. Similarly, the syngas outlet stream is linked to a pressure-outlet boundary. However, a CFD model may also contain physical sub-models, such as DPM and/or a heat exchanger, which have stream connectivity requirements. In this case, a "physical model port" capability is provided. For the coal slurry-fed gasifier, separate coal and water "material streams" are connected to the CFD block via "physical model ports" representing DPM injections for coal particles and water droplets. The solid particles exiting the top and bottom of the gasifier are calculated in the FLUENT UDF and passed back to Aspen Plus using "physical model ports".

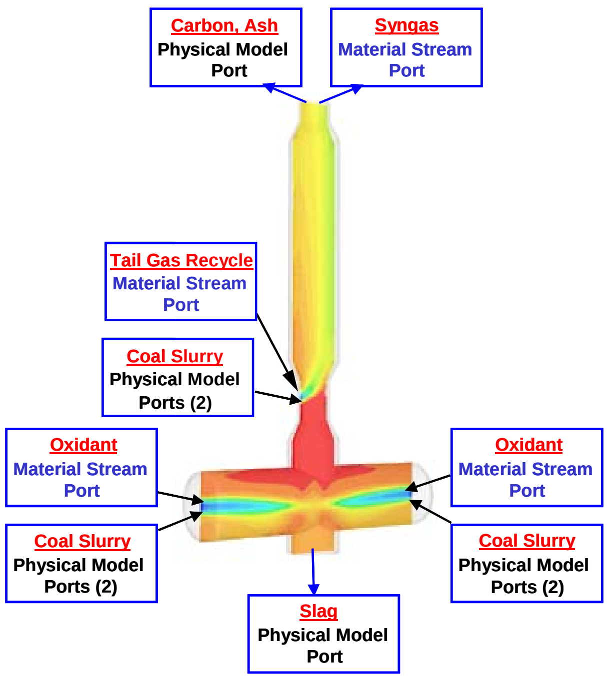


Figure 5. Gasifier Model Connectivity and Temperature Contours

The FutureGen plant configuration considered here is modeled using the steady-state process simulator, Aspen Plus (Version 12.1), and based on several recent NETL reference cases for Integrated Gasification Combined Cycle (IGCC) systems with CO_2 capture (Parsons *et al.*, 2002; Shelton and White, 2004). As shown in Figure 6, the highly-integrated process flowsheet contains over 250 unit operation models comprising all of the major plant sections including gasification, air separation unit (ASU), cold gas cleanup (CGCU), gas turbine, and steam cycle.

The high-pressure, cryogenic ASU is heat integrated with the gas turbine section and supplies oxidant to the gasification section at a rate of 45.8 kg/s (oxidant = 94.4% O2, 1.5% N2, 4.1% Ar). The gasification section employs two oxygen-blown, entrained-flow gasifiers, each operating at 28 atm and firing (nominally) 27.5 kg/s Illinois #6 coal assumed to be 49.72% fixed carbon, 39.37% volatiles, and 1.91% ash by weight (dry basis). The slurry feed is assumed to be 67.7% solids by weight (dry basis).

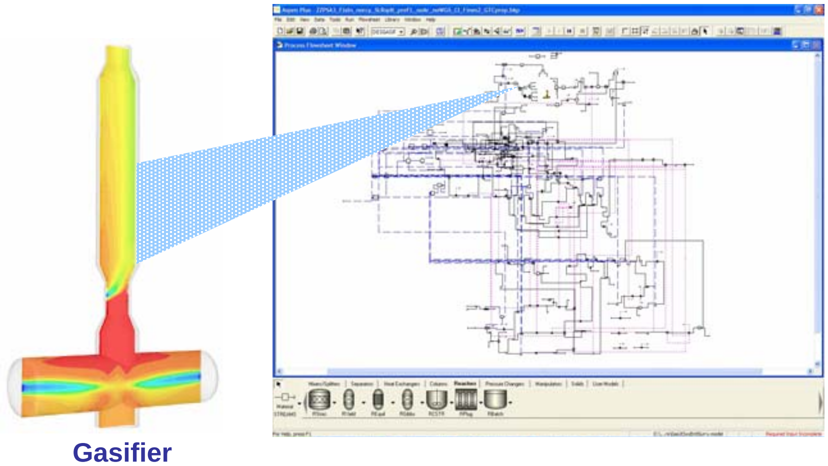


Figure 6. APECS FutureGen Simulation with CFD Model of an Entrained-Flow Gasifier

Following the gasification section is a syngas cooler for generating high-pressure superheated steam and a cyclone for capturing particulates for recycle to the gasifiers. The syngas is further cooled and scrubbed and then sent to a gas cooling/heat recovery section before entering the shift-reaction section. The water-gas shift reaction and carbonyl sulfide (COS) hydrolysis reaction generate hydrogen and hydrogen sulfide (H_2S), respectively, along with additional CO_2. In the cold gas cleanup (CGCU) section, a Selexol solvent process is used to selectively remove the H_2S in a product stream that is sent to a Claus unit for elemental sulfur recovery and to recover the CO_2 in a product stream that is sent to a compression unit for sequestration. The CO_2 is compressed in a multistage (5 stages), intercooled compressor, cooled to 310.9 K (liquid), and pumped to 204 atm for storage.

The cleaned syngas aimed at power production is reheated and sent to the gas turbine combustor, while the remainder is sent to a pressure swing adsorption (PSA) unit for generating hydrogen with a residual fuel stream available for use in power generation. Using a design specification, the syngas split between the PSA unit and the gas turbine is adjusted to maintain the turbine inlet temperature at 1619.3 K. Since combustor performance determines the turbine inlet temperature, the gas turbine combustor is simulated using a high-fidelity CFD model (Figure 3) described in more detail in the next section. The gas turbine exhaust enters a heat recovery steam generator (HRSG) that produces steam for a three pressure level, subcritical reheat steam cycle (122.5 atm / 838.7 K / 26.5 atm / 838.7 K / 2.4 atm).

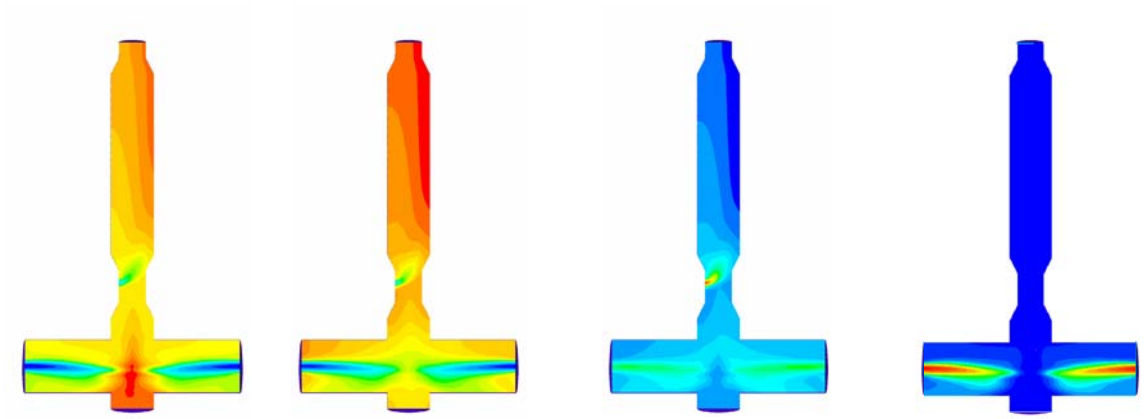
APECS Co-Simulation and Entrained-Flow Gasifier Results

When the FutureGen plant specifications are complete, the APECS co-simulation is ready to run. Using an iterative sequential-modular solution process, Aspen Plus controls the integrated simulation and automatically executes the FLUENT gasifier and combustor CFD models as needed to converge the tail gas recycle loop and the design specification on the gas turbine inlet temperature. The FLUENT results are saved at each flowsheet iteration so that subsequent CFD simulations converge more quickly.

Depending on the initial solution estimates in Aspen Plus and FLUENT, the co-simulation typically required several hours of CPU time to converge the "turbine inlet temperature" design specification case on a single-CPU workstation PC running Windows XP. The turnaround time for the co-simulation was improved by running the computationally-intensive CFD models in parallel on 2-8 CPUs of the Linux clusters at NETL and/or Pittsburgh Supercomputing Center (Zitney, 2004a). The number of CPUs, message-passing communication protocol, and name of the hosts file containing the list of computers on which to run the parallel job were specified on the solver tab of the APECS Model Edit GUI for the equipment model.

For the FutureGen design case, the APECS results show that the "turbine inlet temperature" target of 1619.3 K is met when 43% of the syngas is sent to the gas turbine combustor and the remainder goes to the PSA unit for hydrogen production. The corresponding net equivalent power output from the plant is 243.8 MW, corresponding to an HHV thermal efficiency of 53%.

The temperature contours for the gasifier are provided in Figure 6. The hot gas generated from combustion of the volatiles in the first stage provides the necessary energy for the second-stage coal gasification. The char conversion is 100% for the first stage and 86% for the second stage. The mole fraction contours of some major chemical species are shown in Figures 7a-d. Note here that the dark red represents the highest level while the dark blue represents the lowest level. Figure 7d shows that all of the oxygen is depleted by combustion in the first stage.



(a) CO **(b) H_2** **(c) H_2O** **(d) O_2**

Figure 7. Species mole fraction contours at the center plane of the entrained-flow gasifier

The species mole fractions at the outlet of the entrained-flow gasifier are shown in Table 1. The benefit of using the CFD gasifier model is that it predicts the syngas composition based on fluid flow (Figure 8), heat and mass transfer, and chemical reactions in the specified geometry and at the specified boundary/operating conditions. On the other hand, the Aspen Plus syngas composition must be tuned by specifying temperature approaches in the restricted equilibrium reactor models representing the two stages of the gasifier.

Table 1. Syngas Composition

Chemical Species	Mole Fractions	
	Aspen Plus	FLUENT
CO	0.339	0.359
H_2	0.212	0.229
CO_2	0.105	0.122
CH_4	0.021	0.017
H_2S	0.006	0.006
Ar	0.007	0.008
N_2	0.020	0.020
H_2O	0.290	0.239

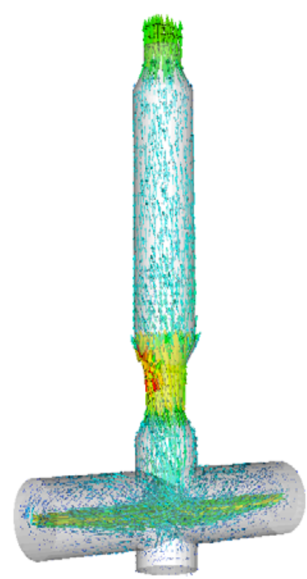


Figure 8. Velocity vectors for 3D gasifier

TRANSPORT GASIFIER

The Power Systems Development Facility (PSDF), located in Wilsonville, Alabama is a joint project between the U.S. DOE, Southern Company Services (SCS), Kellogg Brown & Root (KBR), and other industrial partners to demonstrate an advanced coal-fueled power system (Smith *et al.*, 1999). The major component of this power system is a transport gasifier which operates at higher circulation rates, velocities, and riser densities than conventional circulating fluidized bed technology, thereby resulting in higher throughput, better mixing, and increased mass and heat transfer.

At NETL, scientists and engineers are using the two-fluid model MFIX (Multiphase Flow with Interphase eXchanges) to model the hydrodynamic behavior inside the transport gasifier and account for chemical reactions and heat transfer (Guenther *et al.*, 2002, 2003). Two-fluid hydrodynamic models, also referred to as Eulerian-Eulerian models, treat the fluid and solid as two continuous and fully miscible phases. This approach results in mass, momentum, and energy balance equations for both the gas and solids phases. The MFIX model has been in use at the NETL for over fifteen years and has been become internationally recognized as one of the premier two-fluid models available to researchers (www.mfix.org). Fully optimized to run on high performance computers, its open source format and FORTRAN coding of subroutines and versatile post-processing tools makes MFIX an ideal platform to develop, validate and test sub-models (e.g., coal combustion and gasification) within a two-fluid framework.

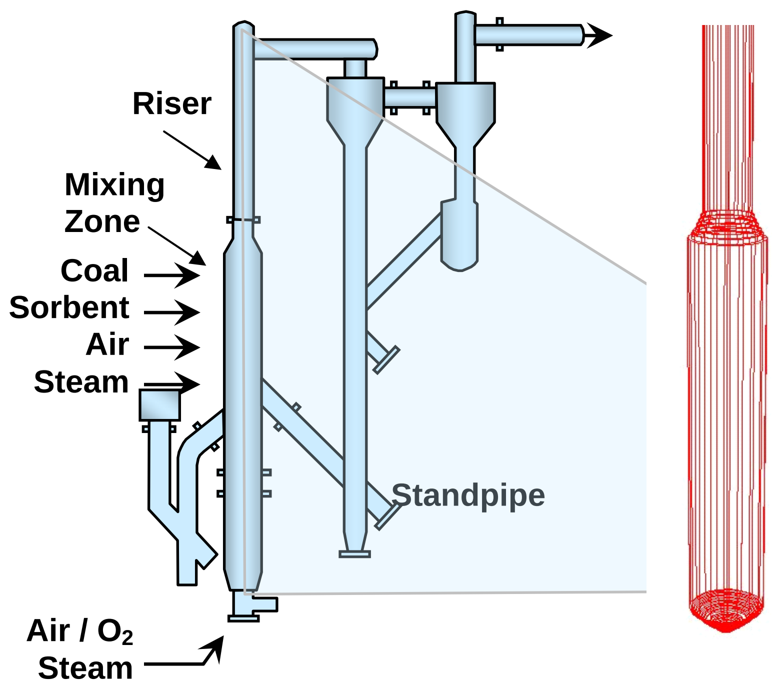


Figure 9. Schematic of transport gasifier and computational model

The MFIX model provides PSDF engineers with transient hydrodynamic, chemistry, and energy information inside the mixing zone and riser (Figure 9). The computational model uses a cylindrical coordinate system with over 250K computational cells. The chemistry sub-model considers combustion, gasification, devolatilization, tar cracking and water-gas-shift reactions and tracks eight gas species and four solids species. To validate the model simulations were completed considering both bituminous (Hiawatha) and sub-bituminous (PRB) coals under air and oxygen blown conditions. Mole fractions of the syngas, exit temperature, carbon conversion, and syngas rates are given in Table 2.

Table 2. MFIX predictions and experimental results

MFIX/Experiment	PRB Oxygen Blown	PRB Air Blown	Hiawatha Oxygen Blown	Hiawatha Air Blown
CO	12.7/11.7	14/11	8.5/6.4	3.4/3.5
CO2	11.2/14.1	5.1/7.4	13.8/12.6	11/9.3
CH4	2.2/2.8	1.9/1	3.5/2.3	2.6/1.3
H2	18/14.7	3/6.2	11/9.4	4.3/4.8
H2O	28/22.9	7/8.3	37/33.8	17/23
CO/CO2	.72/.8	.3/1.5	.62/.5	.3/.4
Exit Temp (F)	1668/1674	1749/1757	1783/1714	1763/1779
Percentage of Carbon Conversion	66%/87%	98%/98%	100%/97%	99%/97%
Syngas Rate in lbs/hr	13400/16000	19800/21000	13200/14600	19400/21000

Under the U.S. Department of Energy's Clean Coal Power Initiative, SCS, KBR, and Orlando Utilities Commission will team up to construct a commercial scale 285 MW coal-based gasification plant in Orlando, Florida. This plant will scale-up a transport gasifier in an air-blown mode. However, actual gasifier design is problematic because there is no well established method for scale-up. To help address some of these questions, NETL scientists working with SCS and KBR engineers have performed several MFIX simulations based on a conceptual design. The MFIX simulations provide transient three-dimensional detailed information inside the transport gasifier which would otherwise be unobtainable through experiments due to the high operating pressures and temperatures. For example, the red and blue isosurfaces in Figure 10 denote decreasing oxygen mass fraction when going from the lower to middle sections of the mixing zone. The green isosurface at the top of the mixing zone denotes a high concentration of carbon in the solids phase. Figure 10 also shows particle path lines in gray.

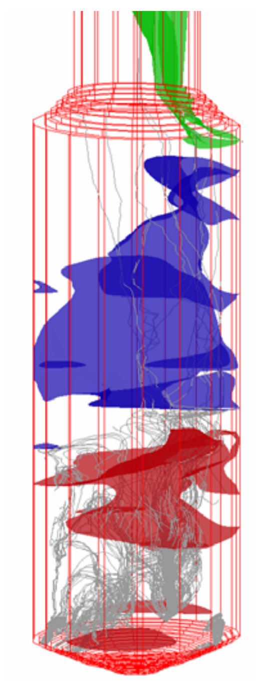


Figure 10. Oxygen and carbon mass fractions with particle trajectories inside the mixing zone

Table 3 presents the species mole fractions in the exit syngas for the MFIX simulations, along with theoretical predictions, for both air and oxygen blown conditions for a sub-bituminous coal. It should be noted that the large discrepancy between the MFIX and PSDF-model carbon monoxide (CO) mole fraction is due to a difference in input conditions into the respective models. The PSDF-model used less steam in the mixing zone than the MFIX model. With less steam available for gasification carbon combustion plays a more dominate role and results in increased production of CO.

Table 3. MFIX and PSDF predictions of syngas mole fractions

MFIX/PSDF-Model	Air Blown	Oxygen Blown
CO	21%/22.5%	24.0%/34%
CO_2	7.0%/6.7%	16.0%/13.5%
CH_4	2.3%/2.1%	3.8%/2.5%
H_2	12.7%/11.4%	27.0%/29.2%
H_2O	2.0%/5.5%	17.8%/18.9%

The MFIX simulations require 1.2 million computational cells to adequately resolve the commercial-scale transport gasifier. To run these large-scale simulations, NETL scientists rely heavily on high performance computers at NETL and the Pittsburgh Supercomputing Center (PSC). At NETL's Morgantown, WV and Pittsburgh, PA campuses, two clusters are readily available to NETL researchers working in the area of CFD and computational chemistry, respectively. Comparable in performance to computers currently listed in the top 500 in the world, the 256-processor cluster in Morgantown has been optimized for CFD calculations with 256 Xeon 3.0-GHz processors with gigabit ethernet interconnection and the 232-processor cluster in Pittsburgh has been optimized for computational chemistry calculations with 232 Opteron 2.0-GHz processors with gigabit ethernet interconnection. Furthermore, there exists 3.5 terabytes of mirrored raid level 5 data storage available at both the Morgantown and Pittsburgh campuses. High-performance computing at NETL is further enhanced through a regional Super Computing Science Consortium $(SC)^2$. This consortium is a partnership between NETL, PSC, West Virginia University, Carnegie Mellon University, University of Pittsburgh, West Virginia Governor's Office of Technology, Institute for Scientific Research, Duquesne University, Waynesburg College, and the NASA Independent Verification and Validation Facility. Through this consortium researchers have remote access to a variety of cluster and supercomputing platforms located at PSC.

The high-end computers at NETL and the PSC provide the MFIX performance required to generate a CFD results database over a wide range of operating conditions for use in developing reduced-order models (ROMs). Coupling these fast CFD-based ROMs together with plant-wide simulations using NETL's APECS system offers an opportunity to investigate the effect of transport gasifier fluid dynamics on overall power plant performance and efficiency.

SUMMARY AND FUTURE WORK

In this paper we have described recent progress on developing CFD models for two commercial-scale gasifiers, including a two-stage, coal slurry-fed, oxygen-blown, pressurized, entrained-flow gasifier and a scaled-up design of the PSDF transport gasifier. Also highlighted was NETL's Advanced Process Engineering Co-Simulator for coupling high-fidelity equipment models with process simulation for the design, analysis, and optimization of advanced power plants. Using APECS, we have coupled the entrained-flow gasifier CFD model into a coal-fired, gasification-based FutureGen power and hydrogen production plant. The results for the FutureGen co-simulation illustrate how the APECS technology can help engineers better understand and optimize gasifier fluid dynamics and related phenomena that impact overall power plant performance.

Development and validation of the MFIX transport gasifier model is continuing. Additional experimental data, axial gas and solids samples from both the mixing zone and riser are being generated for validation. The effects of mass transfer coefficients and gas/solids dispersion coefficients are currently being evaluated and their sensitivity within the MFIX model are being analyzed. In addition to these activities, the MFIX model is currently being used to study the effects of pressure and evaluate the effect of particle size.

Future work will include the development of additional gasifier CFD models and ROMs for use in advanced power plant simulations. For example, we are developing a FLUENT Eulerian-Eulerian multiphase model of the commercial-scale transport gasifier for use in generating a ROM based on the time-averaged transient CFD results (Shi *et al.*, 2005a). We are also considering the integration of a FLUENT CFD model of the Boeing/RocketDyne gasifier (Hartung, 2005) into an Aspen Plus simulation of a potential FutureGen plant configuration.

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