Advanced Process Engineering Co-Simulation of the FutureGen Power and Hydrogen Production Plant

Stephen E. Zitney
National Energy Technology Laboratory
Morgantown, WV 26507-0880
stephen.zitney@netl.doe.gov
http://www.netl.doe.gov

Paper 375c, Session: TE003 Sustainable Energy II
AIChE 2005 Annual Meeting, October 30-November 4, Cincinnati, OH

ABSTRACT

In this paper we describe progress toward developing an Advanced Process Engineering Co-Simulator (APECS) for the design and optimization of future energy plants to achieve a sustainable balance between efficiency, economics, and environmental performance. The APECS integration framework combines process simulation and computational fluid dynamics (CFD) software, together with advanced visualization and high-performance computing. We apply APECS here to the U.S. Department of Energy's coal-fired FutureGen power plant that will produce both hydrogen and electricity without emissions. Two high-fidelity CFD simulations, one for an entrained-flow gasifier and one for a gas turbine combustor, are coupled into an overall process simulation of a potential FutureGen plant configuration. The co-simulation results illustrate how APECS can help engineers understand and optimize the fluid mechanics, heat and mass transfer, and chemical reactions that drive overall power plant performance and sustainability.

INTRODUCTION

The U.S. Department of Energy (DOE) is investing heavily in Fossil Energy R&D programs to promote the development of advanced power generation systems that meet the Nation's energy needs while achieving a sustainable balance between economic, environmental, and social performance. One prime example is the DOE's $1 billion, 10-year, FutureGen Research Initiative aimed at creating the world's first coal-based, near-zero emissions electricity and hydrogen production power plant (DOE, 2004). The 275-megawatt 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). It 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. In order to achieve the aggressive integration, environmental, performance, and economic goals for the FutureGen plant, it will be necessary to extend the DOE's systems analysis capabilities to include rigorous modeling and simulation coupled with advanced visualization and high-performance computing. Such capabilities represent a necessary step in the deployment of virtual plant models that should speed technology development by reducing pilot/demo-scale facility design time and operating campaigns, thereby lowering the

cost and technical risk in realizing high efficiency, near-zero emission power plants (NETL, 2001; DOE, 2003).

At the DOE's National Energy Technology Laboratory (NETL), computational scientists and engineers, building on collaborations with NETL R&D technology partners (e.g., Syamlal *et al.*, 2001; Sloan *et al.*, 2002; Bockelie *et al.*, 2005; McCorkle *et al*., 2003) are developing the Advanced Process Engineering Co-Simulator (APECS) to address the need for high-fidelity, high-performance, virtual power plant models (Zitney, 2004a). One APECS concept receiving considerable attention is the ability to integrate process simulation with detailed 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; Zitney *et al*., 2004). Other examples of recent research efforts in the area of process and CFD co-simulation include Bezzo *et al.* (2000) who coupled the gPROMS® process simulator with the FLUENT CFD package for studying a batch reactor system; Aumiller *et al*. (2002) who combined the RELAP5-3D© thermo-hydraulics systems code with CFD models based on the CFX package for analysis of water-cooled nuclear power plants; and Mota *et al*. (2004) who coupled the FLUENT CFD code with their AngTank dynamic process simulator to accurately model the performance of a new adsorption storage tank design for methane-fueled vehicles.

In NETL's APECS system, plug-and-play interoperability is achieved by using the process industry-standard CAPE-OPEN (CO) interfaces for unit operations, physical properties, and reaction kinetics (Osawe *et al.*, 2002; Syamlal *et al.*, 2004; Zitney, 2004b). The CO standard for process simulation was developed as an international collaborative involving more than thirty leading process-industry companies, academic institutions, and software vendors (Braunschweig and Gani, 2002). The standard provides interfaces for process unit operations, physical properties, reaction kinetics, and numerical solvers. The interfaces are open, multi-platform, available free of charge, and supported by many of the leading commercial process simulators. Today the CAPE-OPEN Laboratories Network (CO-LaN, www.colan.org) is the internationally recognized, user-driven organization for the management, exploitation, and promotion of the CO standard. A recent review of industrial applications of the CO standard, including a brief discussion of the integrated Aspen Plus and FLUENT solution described here, 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.

This paper describes the APECS integration framework for combining process simulation and CFD software, together with advanced visualization and high-performance computing. The application of the APECS system to a potential FutureGen plant configuration is also highlighted.

APECS INTEGRATION FRAMEWORK

As shown in Figure 1, the APECS framework integrates process simulators (e.g., Aspen Plus) with various equipment models including CFD models (e.g., FLUENT), custom equipment models, and reduced-order models (ROMs). CFD models provide a detailed and accurate representation of a wide variety of process equipment items such as combustors, gasifiers, synthesis gas coolers, gas and steam turbines, and fuel cells. Custom equipment models are typically engineering models that calculate mass and energy balances, phase and chemical equilibrium, and reaction kinetics. Custom models can also be legacy computer programs based on empirical information obtained from many years of experience in designing and operating certain equipment items. Such models are typically very fast and accurate within a certain parameter range. ROMs are a class of equipment models that are based on previously-computed CFD solutions over a range of parameter values, but are much faster than CFD models. For example, the APECS system currently provides for automatically generating and using a ROM based on (piecewise) multiple linear regression to demonstrate the concept. Future ROMs may include non-linear regression, neural networks, proper orthogonal decomposition, and network-of-zones (e.g., Bezzo *et al.*, 2004).

The APECS integration framework drastically reduces the time and effort required to integrate CFD models into plant-wide simulations. Previously, such integration was not practicable, requiring months of effort by expert programmers. Using APECS, a CFD model can now be coupled systematically into a process simulation in a matter of an hour or two. The ease of integration and solution was achieved by using the CAPE-OPEN standard and by providing a number of timesaving features including easy-to-use Configuration Wizards, Equipment Model Database, Model Selection/Edit Graphical User Interfaces (GUIs), and CFD Viewer.

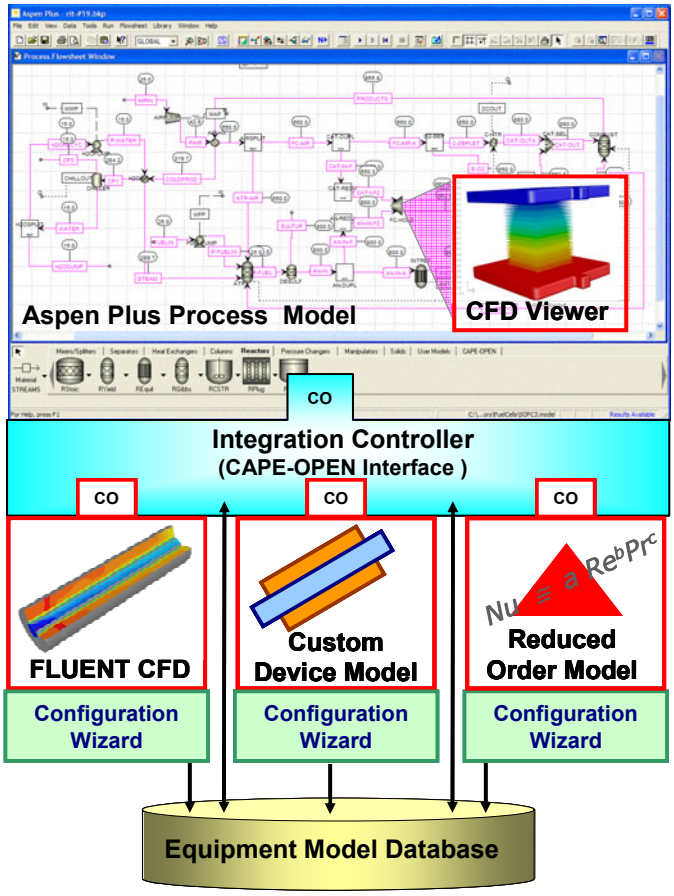


Figure 1. APECS Integration Framework

The APECS system exploits three major classes of CAPE-OPEN (CO) interfaces—unit operations, physical properties, and reaction kinetics. The methods of the CO unit operation interfaces enable the seamless use (e.g., Initialize, Edit, Calculate, Load, Save) of equipment models in the process flowsheet. The interfaces also facilitate the bi-directional exchange of stream information (flow rate, temperature, pressure, and compositions) between the process simulator and the equipment model. For CFD models, the multi-dimensional boundary conditions are mapped automatically to process streams and vice versa. The CO physical property interface is used to transfer constant or temperature-dependent physical properties (e.g., density, viscosity, heat capacity, thermal conductivity, molecular weight) from the process simulator to the equipment models. Similarly, the CO reaction kinetics interface facilitates the automatic transfer of reaction stoichiometry and power-law parameters from the process simulator to the equipment models.

The CAPE-OPEN COM/CORBA bridge implementation (Osawe *et al.*, 2002) in APECS allows process models running under the Windows operating system to exchange stream, physical property, and reaction kinetic information with equipment models running locally/remotely and serially/in parallel under a different operating system such as Linux. By using the CO standard we also ensure that any CFD model, custom equipment model, or ROM that uses CO interfaces can be linked to the APECS framework. We provide an easy-to-use template for wrapping equipment models as CO-compliant models that can be executed in the APECS environment.

To further facilitate the efficient preparation of equipment models as CAPE-OPEN models for use in APECS, two configuration wizards are provided, one for FLUENT and one for custom equipment models, ROMs, and other CFD codes. The wizards are used primarily to specify which equipment model parameters and stream ports to make available in the process simulator. Examples of common equipment parameters include the current and voltage for a fuel cell, or the impeller speed for a stirred tank reactor. The configured equipment models are then stored in an equipment model database.

After placing the detailed equipment model on the process flowsheet, a model selection GUI can be used to browse and select a suitable equipment model from the model database. Upon selection, the corresponding ports and parameters are automatically associated with the equipment model instantiated on the flowsheet. This then allows the process engineer to connect the appropriate number of input and output streams to the equipment model ports. The model edit GUI enables the process engineer to modify equipment parameters. The initial parameter values correspond to those set in the configuration wizard.

The model edit GUI is also used to define a solution strategy consisting of a combination of one or more models/solvers ranging from fast ROMs to 0-1D custom equipment models to rigorous 2-3D CFD models. For example, one common solution strategy is to have the initial flowsheet iterations use a fast ROM and the final iterations use a high-fidelity CFD model. In this way, a process engineer can customize solution strategies from a hierarchy of models/solvers, thereby achieving the desired trade-off between speed and accuracy. If a parallel solver is available for a given equipment model (e.g., FLUENT), improved performance can be achieved by using multiple processes that may be executing on the same computer, or on different computers in a network. In the model edit GUI, an APECS user can specify the number of processors to be used, message passing protocol, and hosts file containing the list of computers on which to run the parallel job.

In Aspen Plus, the process engineer interactively runs and monitors the combined simulation, which involves an iterative sequential-modular solution process. Aspen Plus controls the integrated simulation and automatically executes the detailed equipment model (e.g., FLUENT) at each flowsheet iteration. The CFD results are saved at each Aspen Plus iteration so that subsequent FLUENT simulations converge more quickly. Stream information, physical properties, and reaction kinetic data are transferred automatically from Aspen Plus to FLUENT by the APECS integration framework. Using the CFD parameter values specified in Aspen Plus, FLUENT computes the flow pattern and chemical species distribution. The mass-weighted average of the stream variables at the equipment outlets are sent back to Aspen Plus. This direct coupling of FLUENT and Aspen Plus avoids the time-consuming, error-prone, manual back-and-forth calculations required when a CFD model is embedded in a process recycle loop or heat integration loop.

Upon completion of the integrated simulation, the process engineer reviews the results for streams, blocks, and overall convergence in Aspen Plus. The CFD viewer then allows the process engineer to display, within the process simulator, the results of a CFD simulation conducted as a part of an integrated simulation. Typical CFD results include 2D contours of velocity, temperature, pressure, and species mass fractions for a specified surface in the equipment item. The ParaView scientific visualization tool (www.paraview.org) is available in APECS for viewing 3D CFD results.

FUTUREGEN PROCESS MODEL

To highlight the capabilities of the APECS system, we focus on a FutureGen plant with a nominal 250 MW net equivalent output from producing both electricity and hydrogen. Figure 2 provides a simplified flow diagram of the prototype 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.

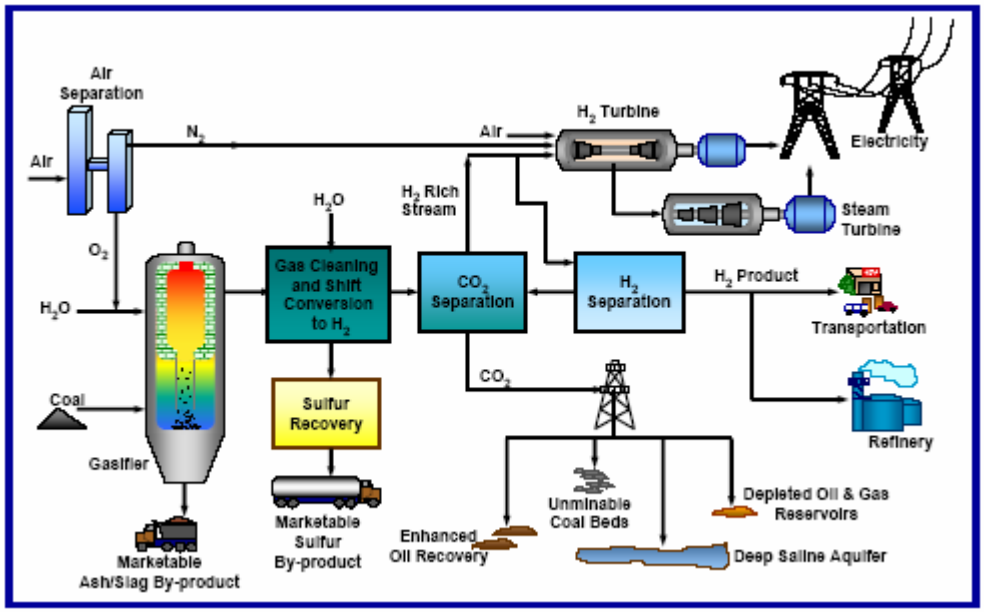


Figure 2. FutureGen Plant Configuration

The FutureGen plant configuration considered here is modeled using the steady-state process simulator, Aspen Plus (Aspen Technology, 2003) 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 3, 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).

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.

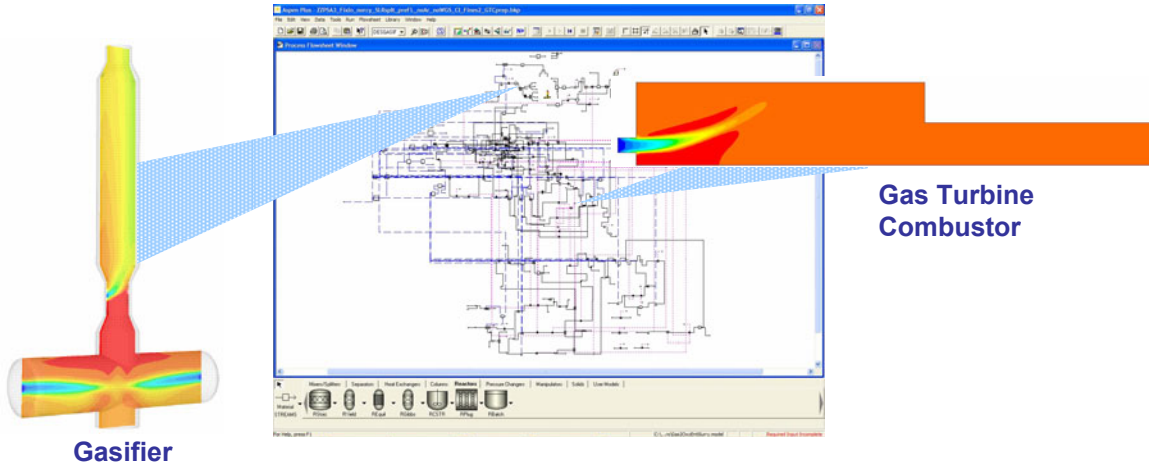


Figure 3. APECS FutureGen Simulation with CFD Models of Gasifier and Combustor

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).

CFD MODELS

To build a comprehensive simulation of the FutureGen power plant described above, we are developing high-fidelity CFD models for process units in which fluid flow, heat and mass transfer, and chemical reactions impact performance of the unit as well as the overall plant. In this paper, we start with CFD models of the gasifier and gas turbine combustor. Gasifier fluid dynamics strongly affect syngas quality and carbon conversion. Similarly, the blending of air and fuel is at the heart of gas turbine combustor performance and efficiency. Details of the CFD models used here to simulate the gasifier and turbine combustor are provided in the next section.

Entrained-Flow Gasifier

The entrained-flow, coal-slurry gasifier in the FutureGen plant is simulated using the steady-state, three-dimensional FLUENT CFD model described by Shi *et al.* (2004, 2005). 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 impact of the coal particles on the gas phase are computed by adding an appropriate source term to the conservation equations. The discrete phase model (DPM) is used to simulate the coal slurry flow. Using DPM, the particle trajectories, along with mass and energy transfer to/from the particles, are computed with a Lagrangian formulation. The coupling between the continuous phase (gas) and the discrete phase (particle) is solved by tracking the exchange of mass, momentum, and energy. 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 two-stage, up-flow gasifier consists 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.

In preparation for coupling with the FutureGen process simulation, the gasifier CFD model with 12,256 hexahedral computational cells was converged using approximately 50,000 gas phase iterations. 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 50^{th} iteration of the fluid phase calculation.

Gas Turbine Combustor

NETL researchers are using CFD analysis to assess new combustor concepts for future power plants that may operate on hydrogen-rich fuels, such as coal-derived syngas, or pure hydrogen derived from shifting the syngas. In this paper, we consider a turbulent, lean-premixed, swirl-stabilized combustor based on the NETL research combustor described by Sidwell *et al.* (2005). A FLUENT CFD model of the NETL combustor was scaled up to represent a single combustor can in a 250MW gas turbine with 16 combustor cans. Using flow rates from the FutureGen plant, the combustor size was increased to match the nozzle velocity

(42.1 m/s) of the NETL research combustor to maintain flame stability. The 2D axisymmetric combustor geometry with nearly 6000 computational cells is shown in Figure 4.

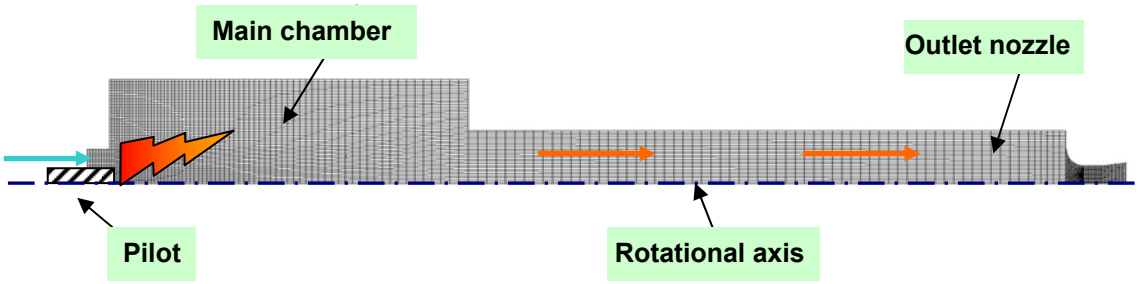


Figure 4. Gas turbine combustor geometry

The FLUENT combustor model uses the finite rate/eddy dissipation model in which the reaction rate is defined by taking the minimum of the chemical reaction rate and the turbulent mixing rate. This reaction model prevents immediate combustion at the combustor inlet by providing a *kinetic switch*. Once the flame is ignited, the eddy-dissipation rates are generally smallest; that is, the reactions are mixing-limited. The global reactions are given in Table 1.

$2CO + O_2 \rightarrow 2CO_2$
$2H_2 + O_2 \rightarrow 2H_2O$
$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Table 1. Gas-phase reactions

In preparation for coupling with the FutureGen process simulation, the baseline case was simulated at the following conditions: equivalence ratio = 0.51, mass flow rate = 20.5 kg/s, inlet temperature = 658.9 K, and operating pressure = 18.3 atm. A fixed mass flow with completely premixed reactants was assumed at the inlet.

FUTUREGEN PLANT SIMULATION

Using the APECS framework, FLUENT (Version 6.1.22) CFD models for the entrained-flow gasifier and gas turbine combustor are integrated with the Aspen Plus (Version 12.1) process simulation of the entire FutureGen plant (Figure 3). The CFD models are instantiated on the process flowsheet via the Fluent block in the CAPE-OPEN Model Library. The two-stage CFD gasifier model replaces two restricted equilibrium reactor models (REquil) from the Aspen Plus Model Library. The combustor CFD model replaces a stoichiometric reactor model that assumes 100% conversion for the combustion reactions.

Flowsheet Connectivity for CFD Models

The FLUENT gasifier 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 FLUENT 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 Fluent block via "physical model ports" representing FLUENT DPM injections for coal particles and water droplets. The solid particles exiting the top and bottom of the FLUENT gasifier are calculated in the UDF and passed back to Aspen Plus using "physical model ports".

As shown in Figure 4, the FLUENT combustor model has a single inlet boundary (mass-flow-inlet) and a single outlet boundary (pressure-outlet). These boundaries are connected to Aspen Plus "material streams" via standard "material stream ports".

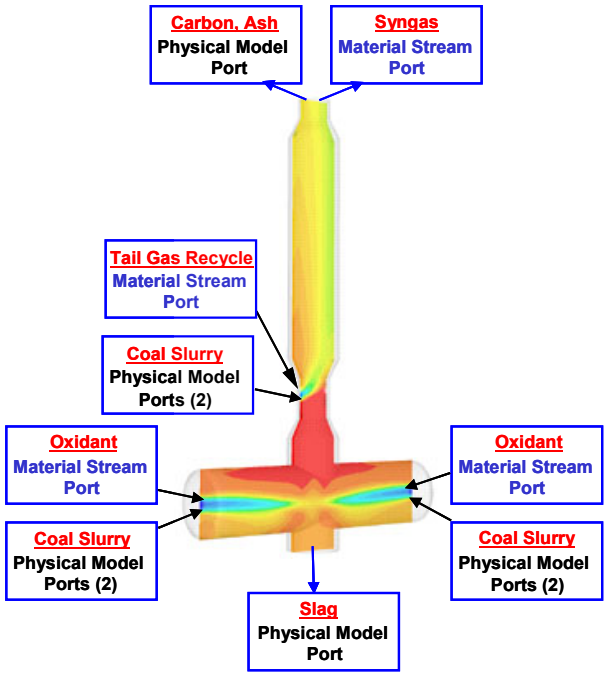


Figure 5. Gasifier Model Connectivity and Temperature Contours

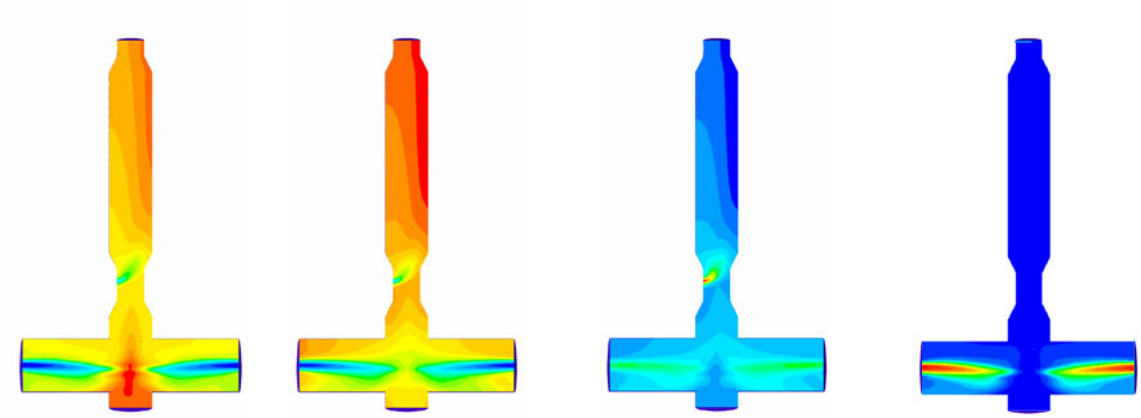
APECS Co-Simulation and Results

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 2000. 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 5. 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 6a-d. Note here that the dark red represents the highest level while the dark blue represents the lowest level. Figure 6d 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 6. Species mole fraction contours at center plane of entrained-flow gasifier

The species mole fractions at the outlet of the entrained-flow gasifier are shown in Table 2. The benefit of using the CFD gasifier model is that it predicts the syngas composition based on fluid flow (Figure 7), 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 2. 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

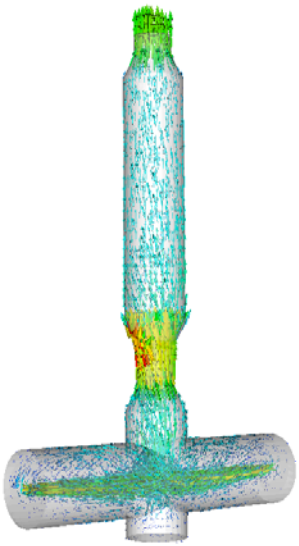


Figure 7. Velocity vectors for 3D gasifier

The temperature contours for the gas turbine combustor are shown in Figures 3. The predicted average outlet temperature is 1813 K which when mixed with the 10% bypassed air at 656.5 K yields a turbine inlet temperature of 1697 K. By comparison, Aspen Plus predicts an outlet temperature of 1710.2 K when using a stoichiometric reactor for the combustor. Figure 8 shows the velocity vectors for the main chamber of the gas turbine combustor. The recirculation zone at the rotational axis of symmetry promotes mixing of the hot combustion products with incoming air and fuel.

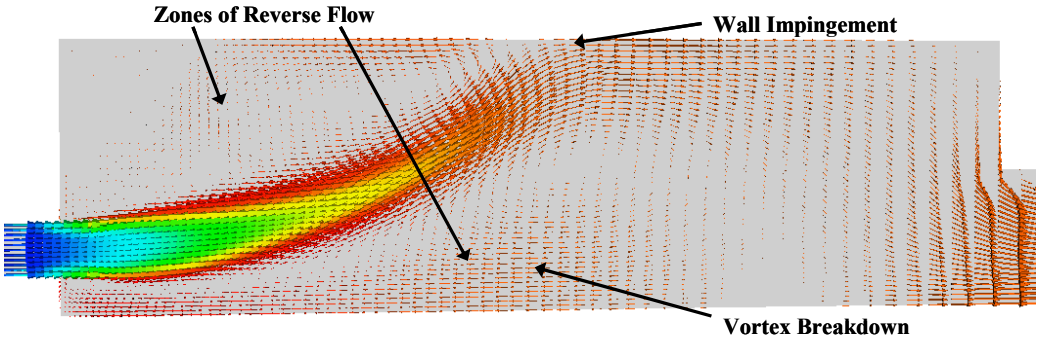


Figure 8. Velocity vectors colored by temperature for main chamber of combustor

Table 3 presents the fuel and oxidant inlet stream compositions, as well as a comparison of the product outlet stream compositions as calculated by the stoichiometric reactor model in Aspen Plus and the CFD model in FLUENT. In this case, the CFD results match the Aspen Plus results which assume complete conversion of the combusting species. In addition to ensuring complete burnout for a given syngas fuel and combustor length, the CFD model provides a more accurate prediction of the combustor outlet temperature and NO_x formation.

Table 3. Inlet and outlet stream compositions for the turbine combustor

Stream→ Species	Fuel Inlet Mole Fractions	Oxidant Inlet Mole Fractions	Aspen Plus Outlet Mole Fractions	FLUENT CFD Outlet Mole Fractions
O2	0.001	0.207	0.095	0.094
N2	0.145	0.774	0.681	0.680
Ar	0.015	0.009	0.011	0.011
H2	0.530	0.000	0.000	0.000
CO	0.035	0.000	0.000	0.000
CO2	0.026	0.000	0.022	0.022
H2O	0.211	0.010	0.191	0.193
CH4	0.037	0.000	0.000	0.000
Total	0.210	0.790	---	---

SUMMARY AND FUTURE WORK

In this paper we have highlighted NETL's Advanced Process Engineering Co-Simulator (APECS) for coupling high-fidelity equipment models with process simulation for the design, analysis, and optimization of power generation systems. The APECS integration framework and its capabilities have been described, including the use of the process-industry CAPE-OPEN software standards. Also highlighted was the application of the co-simulation technology to a coal-fired, gasification-based FutureGen power and hydrogen production plant. Using APECS, we have coupled CFD equipment models for an entrained-flow gasifier and gas turbine combustor into a FutureGen power plant simulation. The results for the FutureGen co-simulation illustrate how the APECS technology can help engineers better understand and optimize the fluid dynamics and related phenomena that impact overall power plant performance.

Future work will include the integration of higher-fidelity and/or additional CFD equipment models into the FutureGen co-simulation. For example, we are developing an industrial-scale 3D FLUENT gas turbine combustor model to replace the 2D model used in this work. We will also consider a commercial-scale transport gasifier simulated using a ROM based on time-averaged transient CFD results from FLUENT and MFIX Eulerian-Eulerian multiphase models (Guenther *et al*., 2002, 2003). In addition, we will make use of the FLUENT 3D CFD model of a heat recovery steam generator (HRSG) discussed by Sloan *et al*. (2005) and consider adding a FLUENT 3D solid oxide fuel cell (SOFC) stack model (Rogers *et al*., 2003; Zitney *et al*., 2004) to make use of the hydrogen generated from the syngas via pressure swing adsorption in the FutureGen plant.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support of the U.S. Department of Energy, Fossil Energy Advanced Research Program. We also gratefully acknowledge Walter Shelton of EG&G for providing the Aspen Plus simulation of the FutureGen plant.

REFERENCES

Aspen Technology, Aspen Plus 12.1 User Guide, Cambridge, MA (2003).

Aumiller, D.L., E.T. Tomlinson, and W.L. Weaver, "An integrated RELAP5-3D and multiphase CFD code system utilizing a semi-implicit coupling technique," *Nuclear Engineering and Design*, 216, 77-87 (2002).

Bezzo, F., S. Macchietto and C.C. Pantelides, "A General Framework for the Integration of Computational Fluid Dynamics and Process Simulation," *Computers and Chemical Engineering*, 24, 653-658 (2000).

Bezzo, F., S. Macchietto and C.C. Pantelides, "A general methodology for hybrid multizonal/CFD models Part I. Theoretical framework," *Computers and Chemical Engineering*, 28, 501-511 (2004).

Bockelie, M.J., D.A. Swensen, C. Yang, M.K Denison, C.L. Senior, and A.F. Sarofim, "A Software Framework for Modeling Advanced Power Generation Systems," In *Proc. of the 30th International Technical Conference on Coal Utilization & Fuel Systems*, April 16-21, Clearwater, Florida (2005).

Braunschweig, B.L. and R. Gani, *Software Architectures and Tools for Computer Aided Process Engineering*, 1st ed., Elsevier Science, Amsterdam (2002).

Department of Energy (DOE), "Revolutionary Advanced Energy System Modeling," *Clean Coal Today*, Issue No. 55, Fall/Winter, DOE/FE-0462, Office of Fossil Energy, Germantown, MD, pp. 13-14 (2003).

Department of Energy (DOE), "FutureGen Report to Congress, FutureGen: Integrated Hydrogen Electric Power Production and Carbon Sequestration Research Initiative," March (2004).

Fluent Incorporated, FLUENT User's Guide, Lebanon, NH (2004).

Guenther, C., M. Shahnam, M. Syamlal, J. Longanbach, D. Cicero, and P. Smith, "CFD Modeling of a Transport Gasifier," *Proc. of the 19th Annual Pittsburgh Coal Conference*, September 23-27, Pittsburgh, PA (2002).

Guenther, C., M. Syamlal, P.V. Smith, J. Longanbach, "Two-fluid model of an industrial scale transport gasifier," Presented at the *AIChE 2003 Annual Meeting*, November 16-21, San Francisco, CA (2003).

McCorkle, D.S., K.M. Bryden, and S.J. Kirstukas, "Building a Foundation for Power Plant Virtual Engineering," In *Proc. of the 28th International Technical Conference on Coal Utilization & Fuel Systems*, Clearwater, FL, pp. 118-127 (2003).

Mota, J.P.B., I.A.A.C. Esteves, and M. Rostam-Abadi, "Dynamic modeling of an adsorption storage tank using a hybrid approach combining computational fluid dynamics and process simulation," *Computers and Chemical Engineering*, 28, pp. 2421–2431 (2004).

National Energy Technology Laboratory (NETL), U.S. Department of Energy, Vision 21 Technology Roadmap, Morgantown, WV (2001).

Osawe, M.O, P. Felix, M. Syamlal, I. Lapshin, K.J. Cleetus, and S.E. Zitney, "An Integrated Process Simulation and CFD Environment Using the CAPE-OPEN Interface Specifications," Presented at the *AIChE 2002 Annual Meeting*, November 3-8, Paper No. 250c, Indianapolis, IN (2002).

Parsons, E.L., W.W. Shelton, and J.L. Lyons, "Advanced Fossil Power Systems Comparison Study, Final Report", EG&G, December (2002).

Pons, M., "Industrial implementations of the CAPE-OPEN standard," Presented at the *Sixth Italian Conference on Chemical and Process Engineering (IcheaP-6)*, June 8-11, Pisa, Italy (2003).

Rogers, W.A., Gemmen, R.S., Johnson, C., Prinkey, M.T., Shahnam, M., Validation and Application of a CFD-based Model for Solid Oxide Fuel Cells and Stacks, *Proc. of First International Conference on Fuel Cell Science, Engineering and Technology*, April 21-23, Rochester, NY, pp. 517-520 (2003).

Shahnam, M., M. Syamlal, and D. Cicero, "Numerical Modeling of Combustion and Gasification Processes using the Discrete Particle Method," ASME Fuels & Combustion Technologies Division, *2000 International Joint Power Generation Conference*, Miami, FL (2000).

Shelton, W.W. and C.W. White, "The Application of an In Situ Oxygen Membrane for an IGCC Process with CO2 Capture, Final Report," EG&G, August (2004).

Shi, S., M. Shahnam, M. Syamlal, S.E. Zitney, and W.A. Rogers, "Coal Gasification for Future Power Generation," *Fluent News*, p. S11, Fall (2004).

Shi, S., S.E. Zitney, M. Shahnam, M. Syamlal, W.A. Rogers, "Modeling Coal Gasification with CFD and the Discrete Phase Method," Accepted for publication in *Proc. of the 4th International Conference on Computational Heat and Mass Transfer*, May 17-20, Paris-Cachan, France (2005).

Sidwell, T., K. Casleton, D. Straub, D. Maloney, G. Richards, P. Strakey, D. Ferguson, S. Beer, “Development and Operation of a Pressurized Optically-Accessible Research Combustor for Simulation Validation and Fuel Variability Studies,” ASME GT2005-68752. To appear ASME TurboExpo, June 6-9, 2005, Reno-Tahoe, NV, USA (2005).

Sloan, D.G., W.A. Fiveland, S.E. Zitney, and M. Syamlal, "Software Integration for Power Plant Simulations," In *Proc. of the 27th International Technical Conference on Coal Utilization & Fuel Systems*, March 4-7, Clearwater, FL (2002).

Sloan, D.G., W.A. Fiveland, S.E. Zitney, and M. Syamlal, "Power Plant Simulations Using Process Analysis Software Linked to Advanced Modules," In *Proc. of the 29th International Technical Conference on Coal Utilization & Fuel Systems*, April 18-22, Clearwater, FL (2004).

Sloan, D.G., W.A. Fiveland, M.O. Osawe, S.E. Zitney, and M. Syamlal, " Demonstrations of Coupled Cycle Analyses and CFD Simulations over a LAN," In *Proc. of the 30th International Technical Conference on Coal Utilization & Fuel Systems*, April 17-21, Clearwater, FL (2005).

Syamlal, M., and L.A. Bissett, "METC Gasifier Advanced Simulation (MGAS) Model," Technical Note, NTIS report No. DOE/METC-92/4108, DE92001111 (1992).

Syamlal, M, P.E. Felix, M.O. Osawe, W.A. Fiveland, D.G. Sloan, S.E. Zitney, F. Joop, J. Cleetus, and I.B. Lapshin, “Virtual Simulation of Vision 21 Energy Plants,” Presented at the U.S. DOE NETL Vision 21 Program Review Meeting, November 6-7, Morgantown, WV (2001).

Syamlal, M., J.I. Madsen, W.A. Rogers, and S.E. Zitney, “Application of an Integrated Process Simulation and CFD Environment to Model Fuel Cell Systems,” Presented at the *AIChE 2003 Spring Meeting*, March 30 - April 3, New Orleans, LA (2003).

Syamlal, M. and M.O. Osawe, “Reduced Order Models for CFD Models Integrated with Process Simulation,” Presented at the *AIChE 2004 Annual Meeting*, November 7-12, Austin, TX (2004).

Syamlal, M., S. Venkatesan, S.M. Cho, “Modeling of Coal Conversion in a Carbonizer,” *Proc. of Thirteenth Annual International Pittsburgh Coal Conference*, Vol. 2, Ed. S.-H. Ciang, University of Pittsburgh, pp. 1309-1314, September 3-7, Pittsburgh, PA (1996).

Syamlal, M. and S.E. Zitney, “Virtual Demonstration to Model Future Power Plants,” Presented at the *2001 International Joint Power Generation Conference*, June 4-7, New Orleans, LA (2001).

Syamlal, M., S.E. Zitney, and M.O. Osawe, “Using CAPE-OPEN Interfaces to Integrate Process Simulation and CFD,” *CAPE-OPEN Update Newsletter*, Volume 7, January (2004).

Zitney, S.E., “High-Performance Process Simulation of Advanced Power Generation Systems,” Presented at *SMART TechTrends 2004*, August 3-6, Pittsburgh, PA (2004a).

Zitney, S.E., “CAPE-OPEN Integration of CFD and Process Simulation for Advanced Power Generation Applications,” Presented at *CAPE-OPEN Meetings*, August 25-26, Cincinnati, OH (2004b).

Zitney, S.E., M.T. Prinkey, M. Shahnam, and W.A. Rogers, “Coupled CFD and Process Simulation of a Fuel Cell Auxiliary Power Unit,” In *Proc. of the ASME Second International Conference on Fuel Cell Science, Engineering, and Technology*, Eds. R. Shah and S.G. Kandlikar, June 13-16, Rochester NY, Paper 2490, pp. 339-345 (2004).

Zitney, S. E. and M. Syamlal, “Integrated Process Simulation and CFD for Improved Process Engineering," *Proc. of the European Symposium on Computer Aided Process Engineering–12, ESCAPE-12*, May 26-29, The Hague, The Netherlands, eds. J. Grievink and J. van Schijndel, pp. 397-402 (2002).