Towards the Integration of APECS and VE-Suite for Virtual Power Plant Co-Simulation

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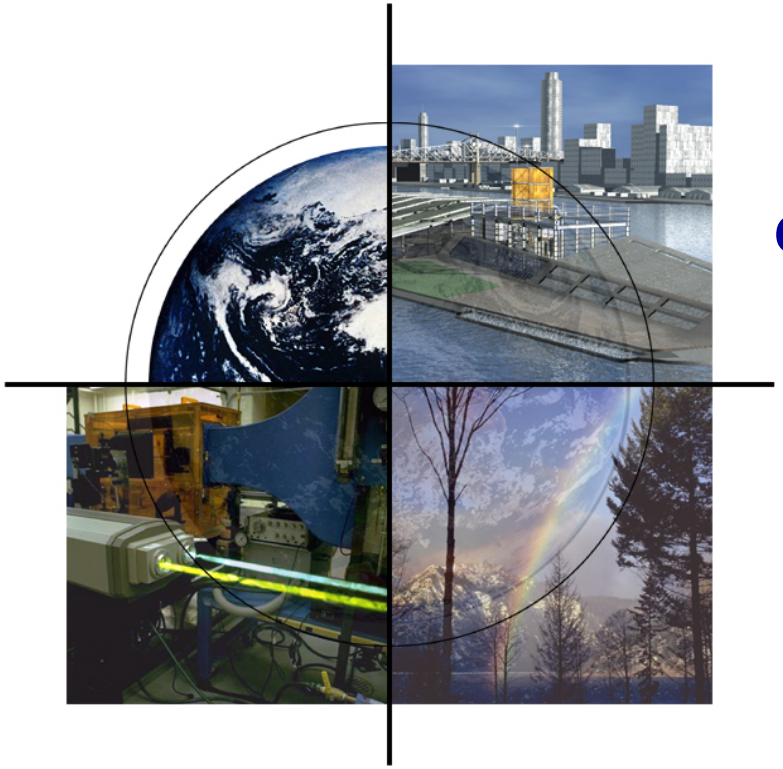
Process modeling and simulation tools are widely used for the design and operation of advanced power generation systems. These tools enable engineers to solve the critical process systems engineering problems that arise throughout the lifecycle of a power plant, such as designing a new process, troubleshooting a process unit or optimizing operations of the full process. To analyze the impact of complex thermal and fluid flow phenomena on overall power plant performance, the Department of Energy's (DOE) National Energy Technology Laboratory (NETL) has developed the Advanced Process Engineering Co-Simulator (APECS). The APECS system is an integrated software suite that combines process simulation (e.g., Aspen Plus) and high-fidelity equipment simulations such as those based on computational fluid dynamics (CFD), together with advanced analysis capabilities including case studies, sensitivity analysis, stochastic simulation for risk/uncertainty analysis, and multi-objective optimization.

In this paper we discuss the initial phases of the integration of the APECS system with the immersive and interactive virtual engineering software, VE-Suite, developed at Iowa State University and Ames Laboratory. VE-Suite uses the ActiveX (OLE Automation) controls in the Aspen Plus process simulator wrapped by the CASI library developed by Reaction Engineering International to run process/CFD co-simulations and query for results. This integration represents a necessary step in the development of virtual power plant co-simulations that will ultimately reduce the time, cost, and technical risk of developing advanced power generation systems.

Towards the Integration of APECS and VE-Suite for Virtual Power Plant Co-Simulation



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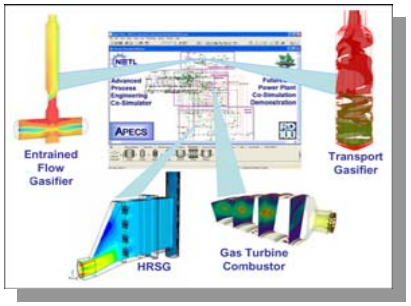
Outline of Presentation

- **Introduction**
  - NETL/Office of R&D/Process & Dynamic Systems Research
- **Advanced Process Engineering Co-Simulator (APECS)**
  - Brief Overview and History
  - Process/CFD Software Components and Features
- **APECS Energy Applications**
  - Fuel Cell Auxiliary Power Unit
  - *FutureGen* Power Plant
- **Virtual Power Plant Co-Simulation**
  - Goals/Objectives
- **Concluding Remarks**

NETL Onsite R&D



APECS Co-Simulation

***FutureGen* Plant**

National Energy Technology Laboratory

- **Only DOE national lab dedicated to fossil energy**
  - Fossil fuels provide 85% of U.S. energy supply
- **One lab, five locations, one management structure**
- **1,200 Federal and support-contractor employees**
- **NETL's Fossil Energy Mission**
  - Implement an R&D and demonstration program to resolve the environmental, supply, and reliability constraints of producing and using fossil energy

Morgantown, WV

Pittsburgh, PA

Tulsa, Oklahoma

Albany, Oregon

Fairbanks, Alaska

Accomplishing Our Mission

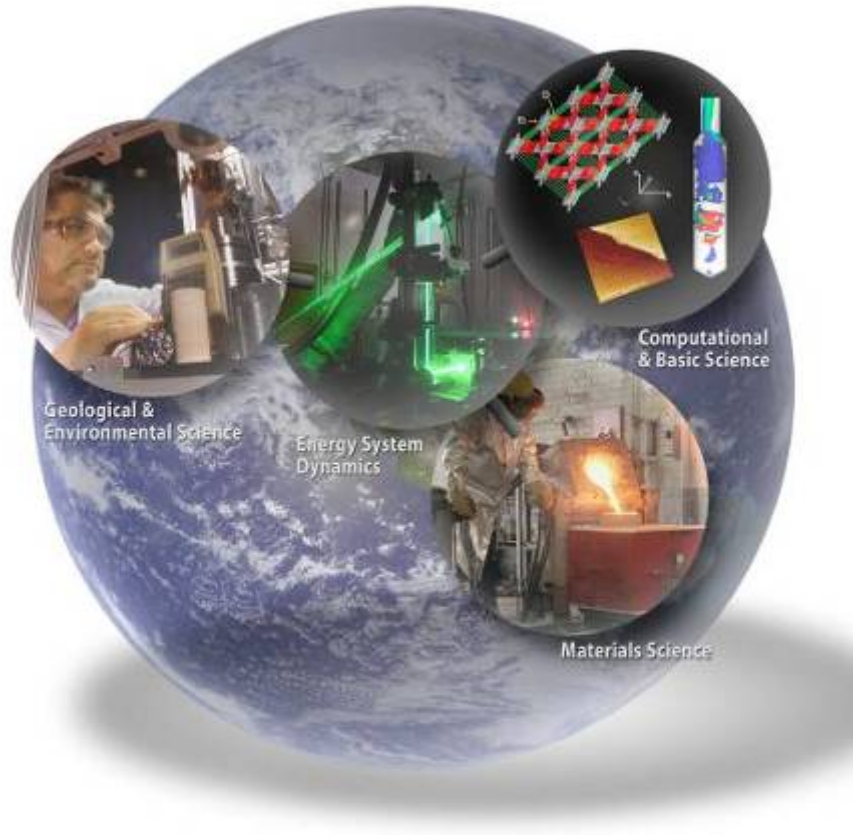
- **Support energy policy development**
  - Clean Coal Power (IGCC), Hydrogen
  - Clear Skies, Climate Change
  - *FutureGen*
- **Implement and manage extramural RD&D**
  - Over 1,800 research activities in U.S. and more than 40 foreign countries
  - Total award value over $9 billion
  - Private sector cost-sharing over $5 billion
- **Conduct onsite research**
  - Approximately 550 engineers and scientists
  - Over 150 PhDs
  - Office of Research and Development

Office of Research and Development

Creates and Transfers Innovative Fossil Energy Technologies

Focus Areas

- **Energy System Dynamics**
- **Geological & Environmental Science**
- **Materials Science**
- **Computational & Basic Science**
  - Computational Chemistry
  - Multiphase Flow
  - Model Validation
  - Device-Scale Simulation
  - Process & Dynamic Systems



Process & Dynamic Systems Research
Goals and Objectives

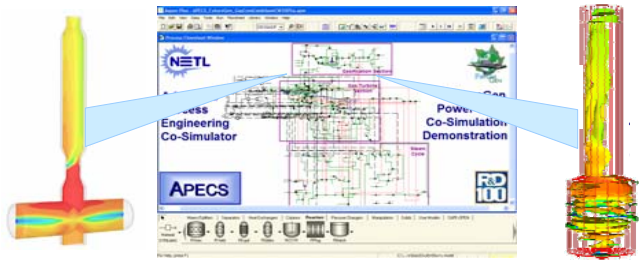
- Research and develop innovative computational models, methods, and tools
- Apply to advanced fossil energy (FE) systems
  - IGCC, *FutureGen*
  - Polygeneration
- Establish strong R&D collaborations
- Transfer technology to process and energy industries

NETL
Carnegie Mellon
University of Pittsburgh
West Virginia University

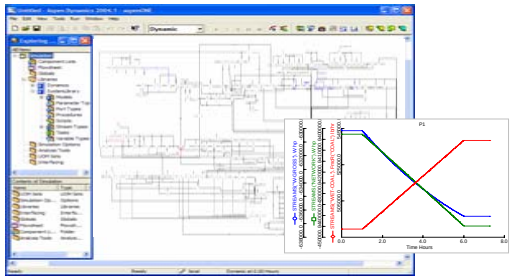
NETL Collaboratory for Process & Dynamic Systems Research

Process & Dynamic Systems Research
Focus Areas

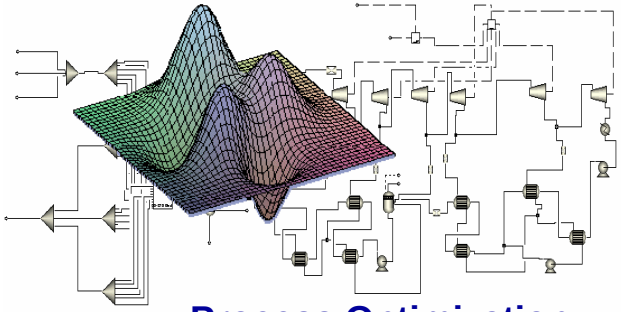
- **High-Fidelity Systems**
  - Advanced process engineering co-simulation (APECS)
  - Virtual power plant simulation
- **Dynamic Systems**
  - Dynamic simulation
  - Process control
  - Real-time applications
- **Systems Optimization**
  - Plant-wide optimization
  - Stochastic simulation for uncertainty/risk analysis
  - Cost estimation



APECS FutureGen



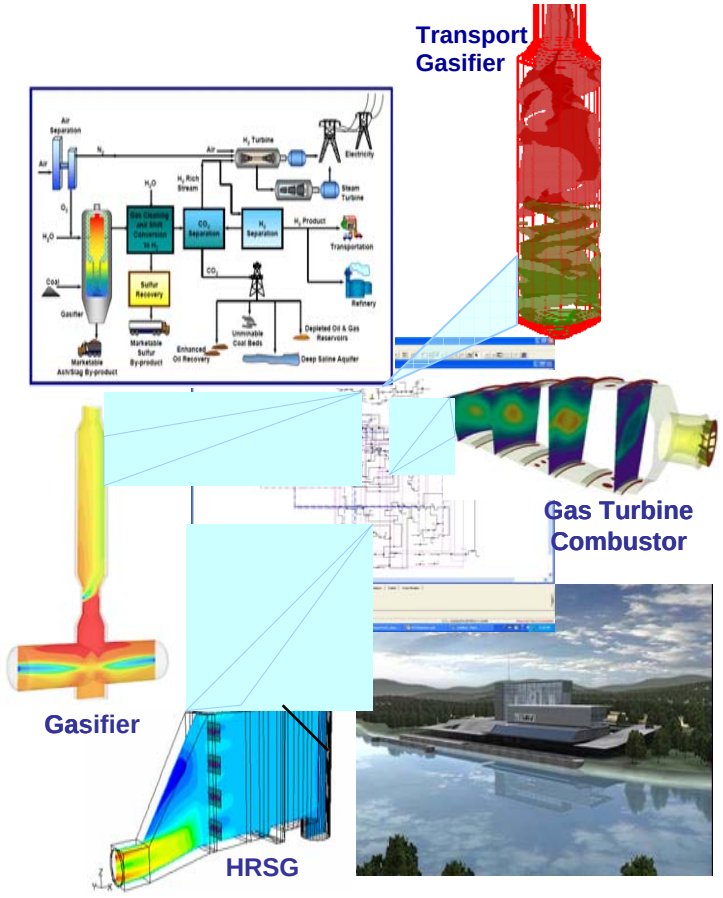
IGCC Dynamic Simulation



Process Optimization

Advanced Process Engineering Co-Simulator (APECS)

- Combines process simulation with computational fluid dynamics (CFD)
- Provides engineers with a better understanding of the fluid dynamics impacting overall plant performance
- Provides high-fidelity process co-simulation essential for advanced power plant design and optimization



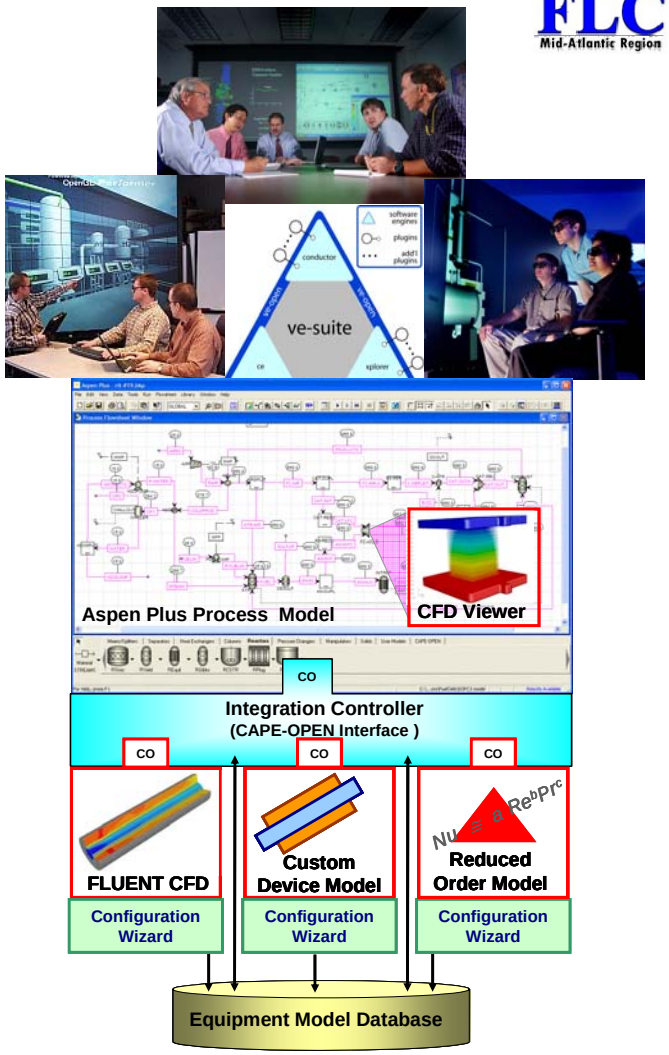
APECS-based *FutureGen* Plant Simulation

Advanced Process Engineering Co-Simulator
Brief History

- Phase-1 APECS R&D Project Start (2000)
- Steady-State Co-Simulation Prototype (2001)
- Commercial Release by Ansys/Fluent (2003)
- First Commercial Success (2004)
- R&D 100 Award (2004)
- APECS *FutureGen* Demo at Supercomputing (2004)
- 2nd Annual CAPE-OPEN Meeting at NETL (2005)
- Phase-2 APECS R&D Project Start (2005)
- US/APECS – UK/VPDM Collaboration (2005)
- APECS/VE-Suite Integration Prototype (2006)
- US Federal Technology Transfer Awards (2006/7)

Advanced Process Engineering Co-Simulator (APECS)

- **Process Simulators**
  - CAPE-OPEN compliant
  - Aspen Plus®, HYSYS®, gPROMS®
- **Equipment Models and Database**
  - CAPE-OPEN compliant
  - CFD: FLUENT®
  - Custom Models: e.g., INDVU
  - ROMs: LR, NN, PCA
- **Integration Controller**
  - CAPE-OPEN v1.0 Interfaces
  - Unit Ops, Phys Props, Reactions
- **Configuration Wizards**
  - FLUENT®, Custom Model, and ROM
- **Solution/Analysis Tools**
  - Hybrid: Speed (ROM), Accuracy (CFD)
  - Stochastic, Optimization
- **Distributed Execution**
  - CAPE-OPEN COM/Corba Bridge
  - Windows/Linux, Serial/Parallel
- **Virtual Engineering**
  - CFD Viewer (2D), Paraview (3D)
  - **VE-Suite**



APECS/VE-Suite

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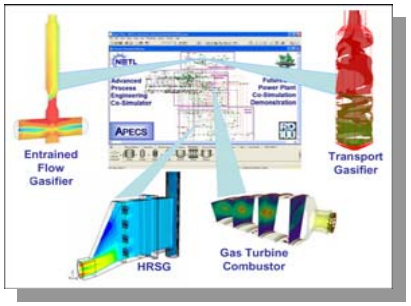
  - Fuel Cell Auxiliary Power Unit
  - *FutureGen* Power Plant
- **Virtual Power Plant Co-Simulation**
  - Goals/Objectives
- **Concluding Remarks**

NETL Onsite R&D

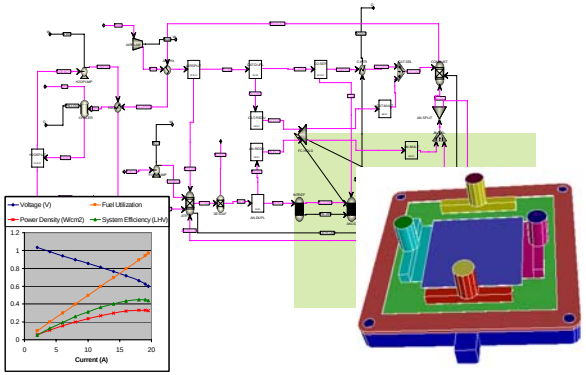


APECS Co-Simulation

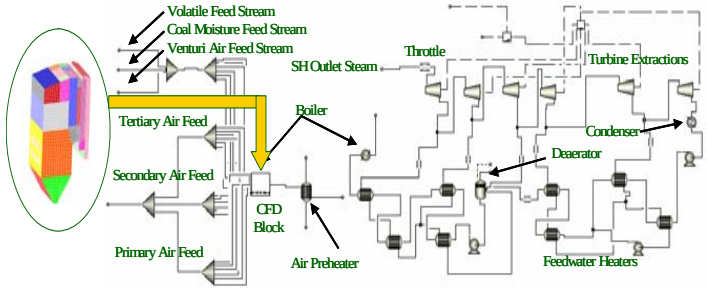
***FutureGen* Plant**

APECS Power Generation Applications

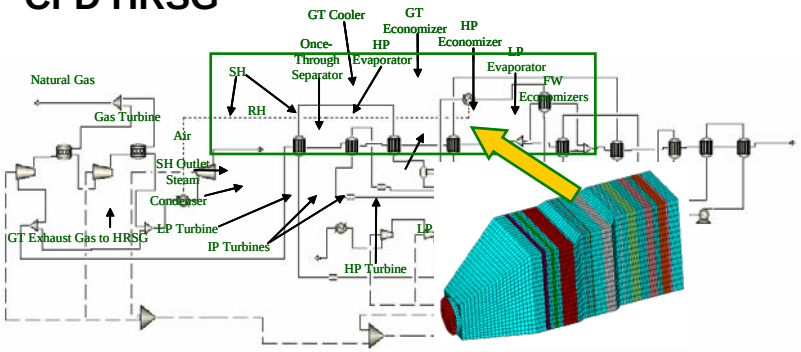
- **Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC**



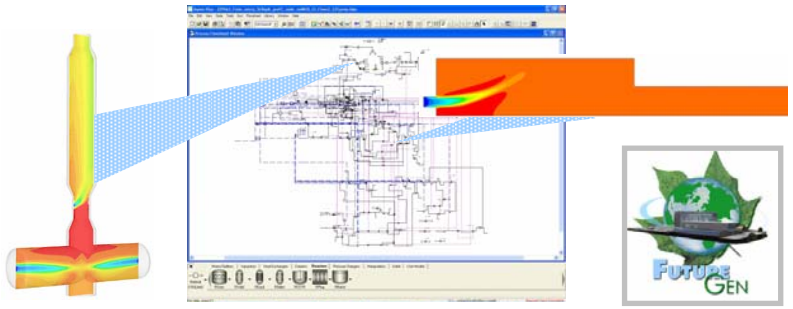
- **ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler**



- **ALSTOM NGCC (250MWe) with 3D CFD HRSG**



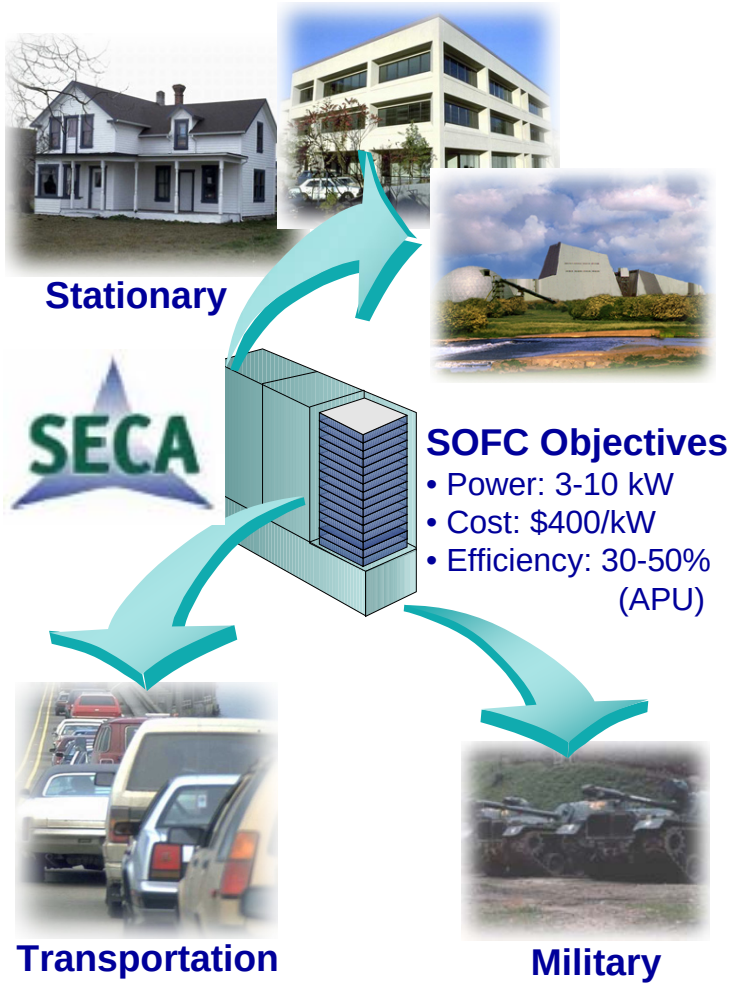
- **FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor**



APECS Application - Fuel Cell APU Systems

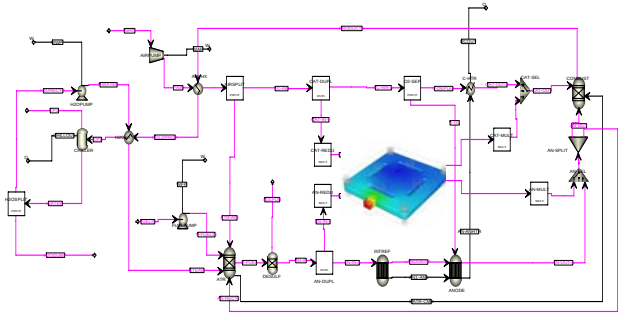
- **Fuel cell systems are emerging as versatile energy solutions**
- **DOE-sponsored Solid state Energy Conversion Alliance**
- **Solid oxide fuel cells (SOFC)**
- **Auxiliary power units (APU) for transportation can reduce:**
  - Diesel fuel consumption
  - Cost
  - Pollutant emissions

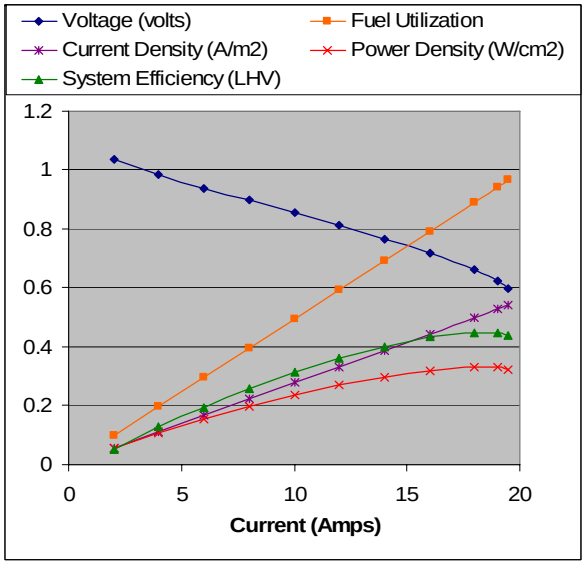
- **Need to analyze fuel cell APU systems for low cost, high efficiency, and maximum integration**

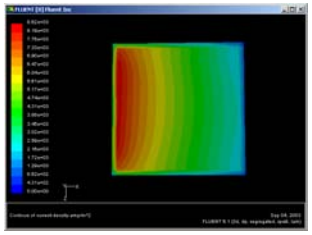


APECS Application - SECA Fuel Cell APU System

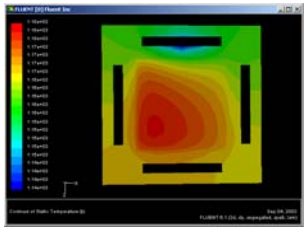
- Aspen Plus process model of Auxiliary Power Unit (APU)
- FLUENT 3D CFD model of SECA solid oxide fuel cell
- Optimize process efficiency by varying CFD parameter (fuel cell current)
- Maximum system efficiency (LHV) of 45% at 18 amps
- Max. system power of 4.3 kW







Current density for cathode

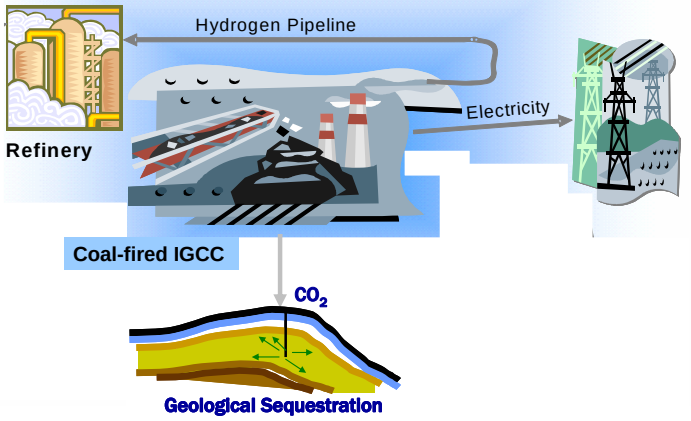


Temperature for anode

Zitney, S.E., Prinkey, M.T., Shahnam, M., and Rogers, W.A. (2004), "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, Rochester NY, June 13-16, 2004, Paper 2490, pp. 339-345.

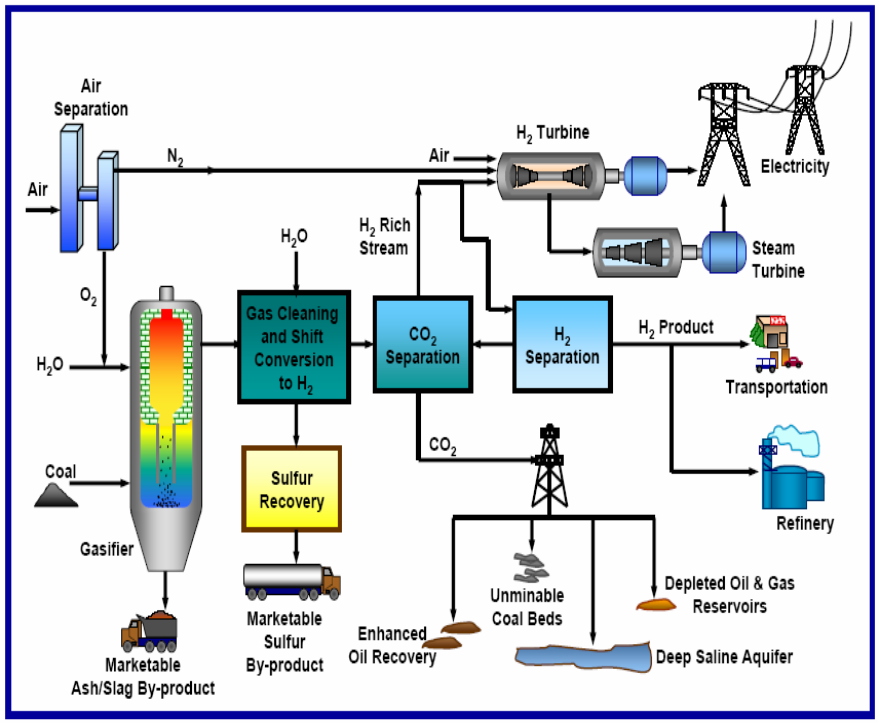
U.S. DOE *FutureGen* Initiative
Pathway to Zero Emissions

- 10-year, $1B DOE project
- Commercial-scale, coal-fired, gasification-based plant
- Co-production of H_2 and electricity (275 MWe)
- Sequester >90% CO_2 with potential for ~100%
- Minimum 1-million tons/year CO_2 captured and sequestered
- “Living R&D laboratory” for cutting-edge technologies
- FutureGen Alliance
- On-line 2012



FutureGen Power/Hydrogen Production Plant

- **IGCC with CO_2 capture and H_2 generation**
  - Air separation unit (ASU) integrated with gas turbine
  - Entrained-flow, coal-slurry, oxygen-blown gasifier
  - Water gas shift
  - Gas cleanup for particulates, Cl_2, and S_2
  - Selexol for CO_2 capture with compression to liquid
  - Pressure-swing adsorption (PSA) for generating H_2
  - GE 7FB gas turbine
  - Steam cycle with three pressure levels and HRSG

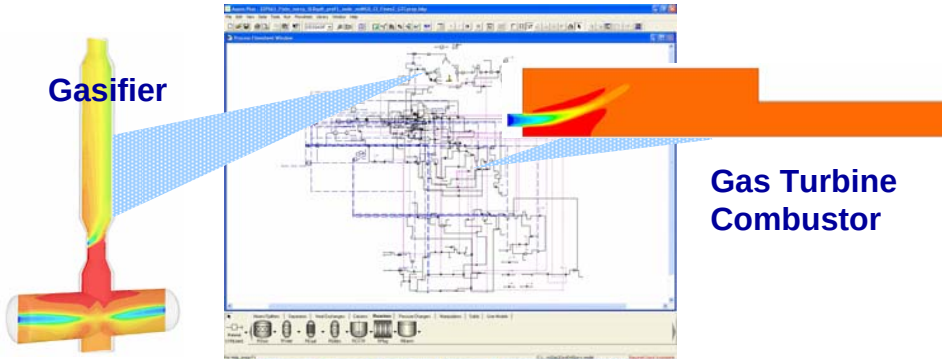


***FutureGen* Process Diagram**

- **IGCC plant with advanced technology modules and aggressive integration, performance, and environment goals**

APECS Application - *FutureGen* Plant

- **Process Simulation**
  - Aspen Plus® steady-state
  - All major plant sections
  - Over 250 unit ops

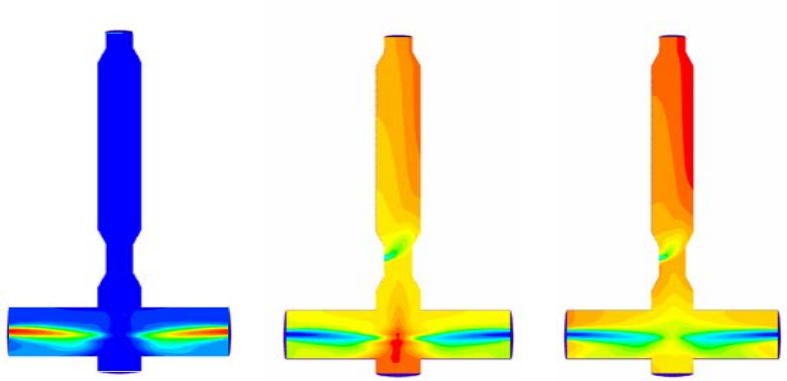


APECS Co-Simulation of FutureGen Power Plant

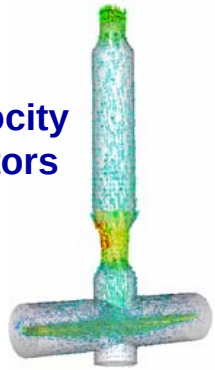
- **CFD Simulations**
  - Entrained-Flow Gasifier
    - FLUENT® 3D/ROM
    - Accurate calculation of synthesis gas composition
    - Embedded in syngas recycle loop
  - Gas Turbine Combustor
    - FLUENT® 2D/3D/ROM
    - Accurate calculation of GT inlet temperature
    - Embedded in design spec loop to determine power/H2 production

FutureGen Process/CFD Co-Simulation Results

- **Gas turbine inlet temperature specification of 1619.3 K is met when:**
  - 43% of syngas is sent to GT combustor and remainder goes to PSA unit for H2 production
  - Net equivalent power output from plant is 243.8 MW, corresponding to HHV thermal efficiency of 53%



Species mole fraction contours at the center plane



Velocity vectors

Char Conversion
- 1st Stage
  - ➢ 100%
- 2nd Stage
  - ➢ 86%

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

Synthesis Gas Composition

Zitney, S.E., M.O. Osawe, L. Collins, E. Ferguson, D.G. Sloan, W.A. Fiveland, and J.M. Madsen, "Advanced Process Co-Simulation of the FutureGen Power Plant," *Proc. of the 31st International Technical Conference on Coal Utilization & Fuel Systems*, May 21-25, Clearwater, FL (2006).

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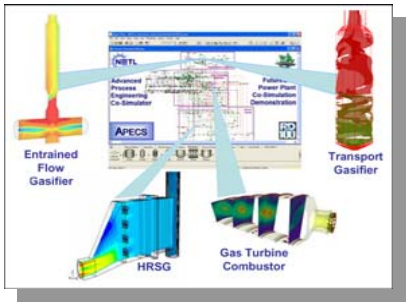
NETL Onsite R&D



APECS Co-Simulation

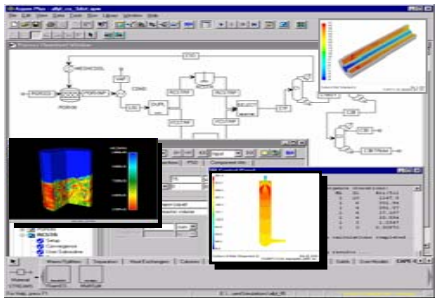
***FutureGen* Plant**

Virtual Power Plant Co-Simulation
Integration of APECS and VE-Suite

- **Goals**
  - Reduce the time, cost, and technical risk to develop high-efficiency, near zero-emission power generation systems, such as *FutureGen*
  - Promote collaborative engineering and design, as well as communication of advanced power plant concepts to other key stakeholders
- **Objectives**
  - Deploy process/equipment co-simulations in a 3D, immersive and interactive, virtual plant walkthrough environment
  - Automate complex virtual engineering workflow across the plant lifecycle, from design to operations

Concluding Remarks

- APECS facilitates the effective integration, solution, and analysis of process/CFD co-simulations

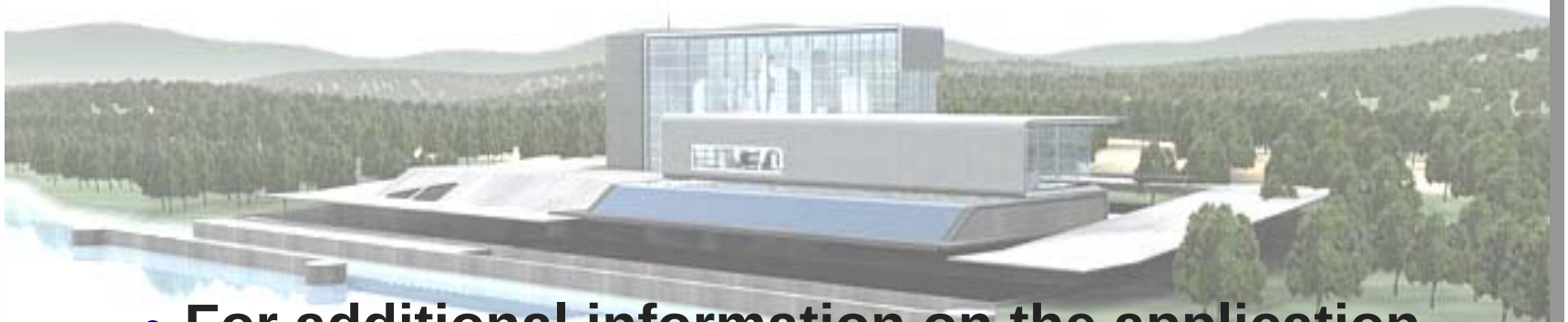


- NETL is using APECS to optimize a wide variety of advanced power generation systems

- Virtual power plant simulation with APECS/VE-Suite offers opportunities for accelerating the development of future zero-emission power plants

Thank You

Questions?



- **For additional information on the application of APECS to power generation applications, please contact:**
  - Stephen E. Zitney, NETL
    - EML: stephen.zitney@netl.doe.gov
    - TEL: 304-285-1379