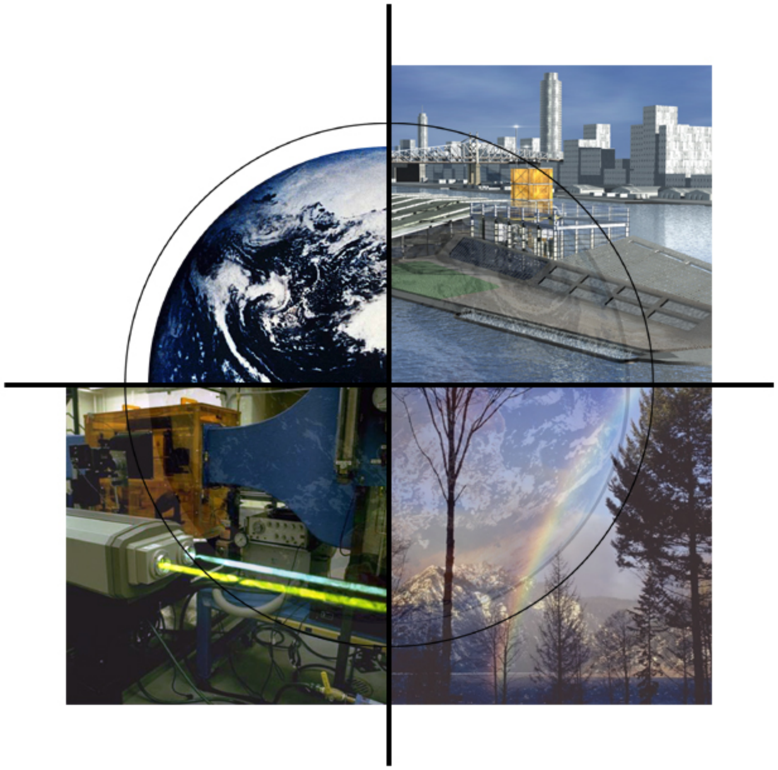
Using Process/CFD Co-Simulation for the Design and Analysis of Advanced Energy Systems



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presented at

2007 Aspen Engineering Suite (AES) User Group Meeting

Houston, TX
April 10-11, 2007

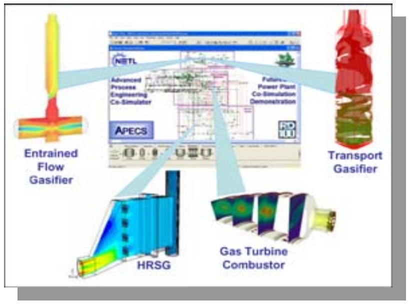
National Energy Technology Laboratory

Office of Fossil Energy

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
- **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

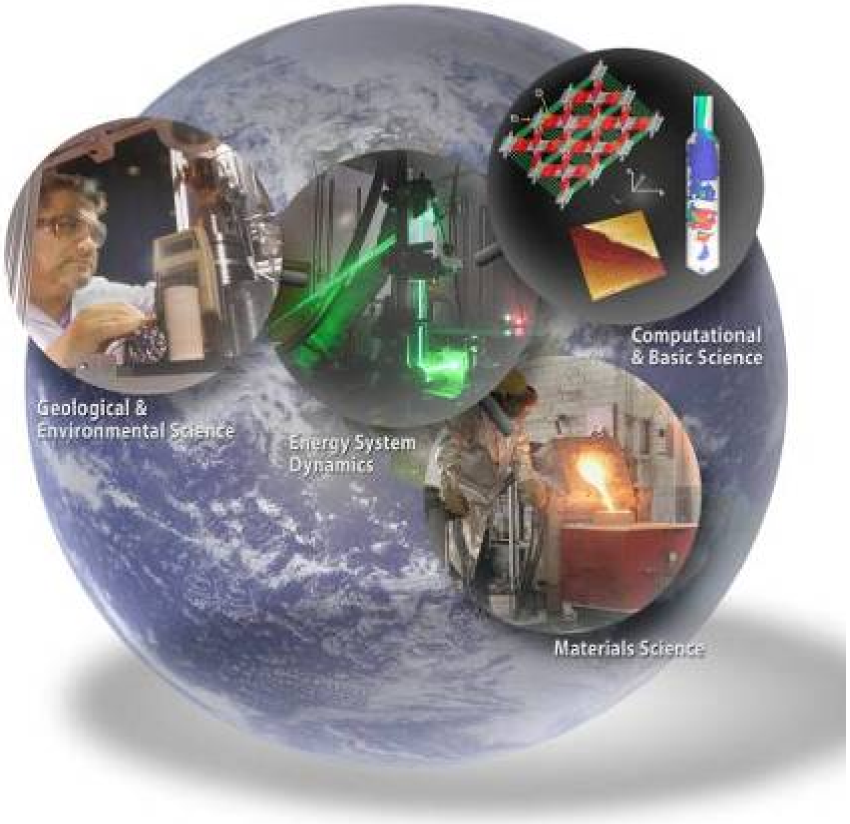
Accomplishing Our Mission

- **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

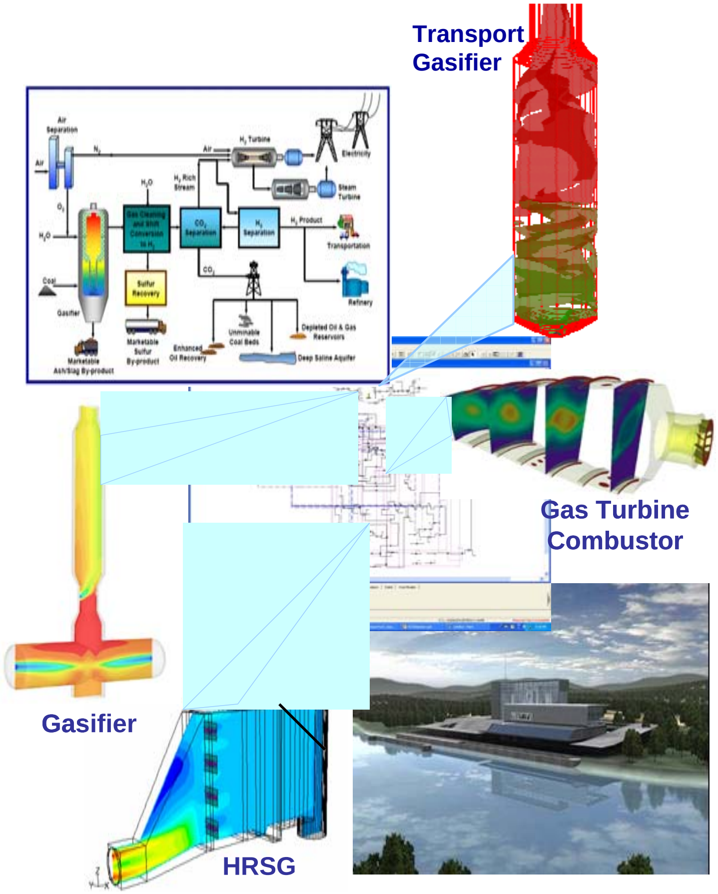
Focus Areas

- **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
R&D 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-based *FutureGen* Plant Simulation

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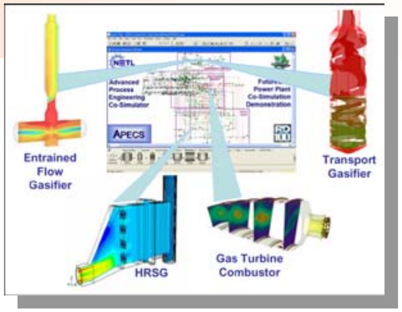
NETL Onsite R&D

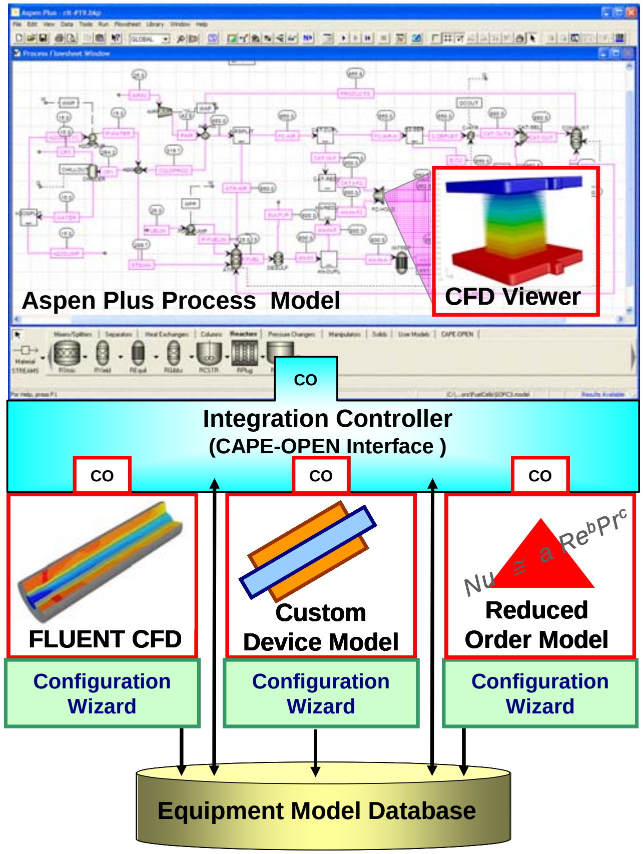


APECS Co-Simulation

FutureGen Plant

Advanced Process Engineering Co-Simulator (APECS)

- Co-simulation software framework for integration of process simulation with high-fidelity equipment simulations, including computational fluid dynamics (CFD)
- Enables analysis and optimization of overall plant performance with respect to complex thermal and fluid flow phenomena



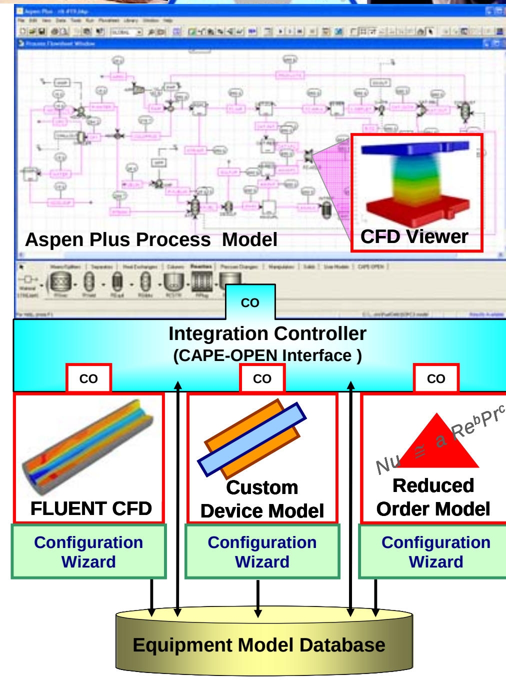
APECS Software Integration Framework

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)

APECS Software Components and Features

- **Process Simulators**
  - CAPE-OPEN compliant
  - Aspen Plus®, HYSYS
- **Equipment Models and Database**
  - CAPE-OPEN compliant
  - CFD: FLUENT®
  - Custom Models: e.g., INDVU
  - ROMs: LR, NN
- **Integration Controller**
  - CAPE-OPEN v1.0 Interfaces
  - Unit Ops, Phys Props, Reactions
- **Configuration Wizards**
  - FLUENT®, Custom Model, and ROM
- **Solution/Analysis Tools**
  - CAPE-OPEN compliant
  - 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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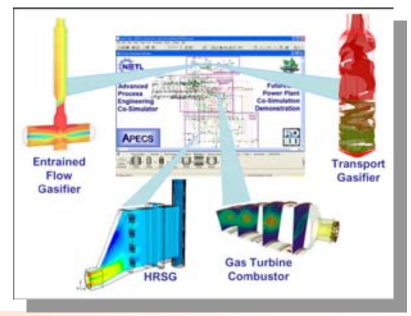
NETL Onsite R&D



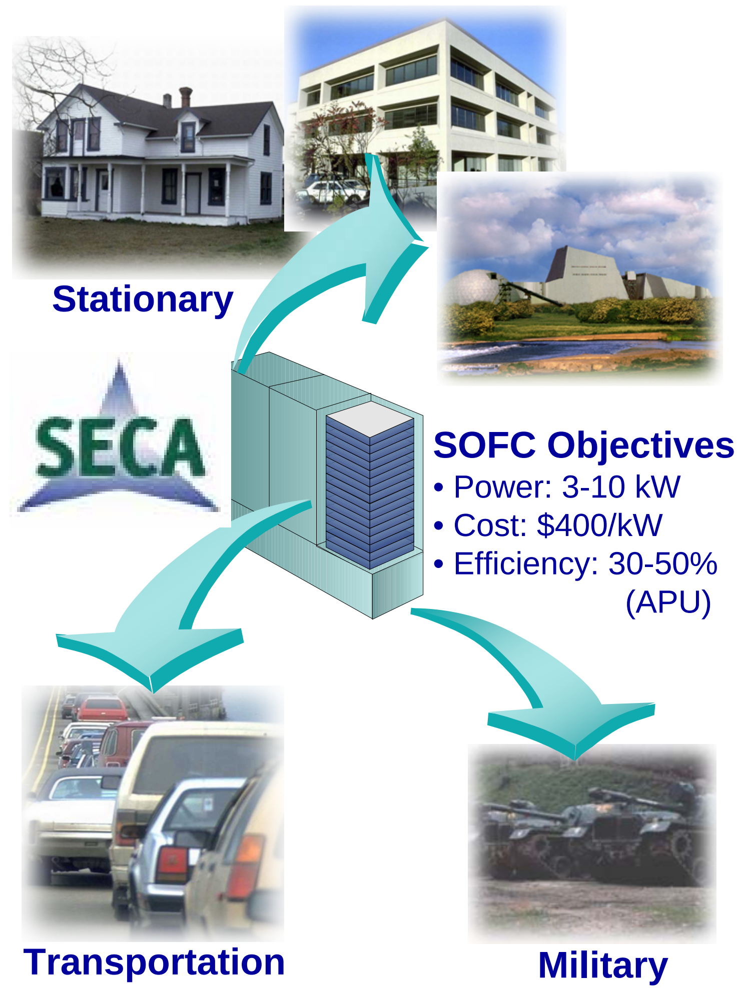
APECS Co-Simulation

***FutureGen* Plant**

APECS Application - Fuel Cell APU Systems

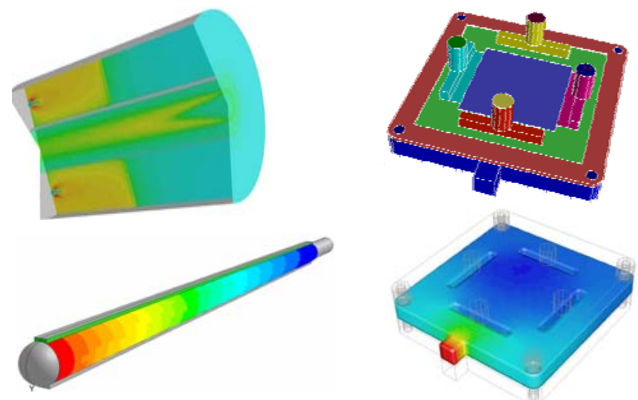
- **Fuel cell systems are emerging as versatile energy solutions**
- **DOE-sponsored Solid state Energy Conversion Alliance**
- **Solid oxide fuel cells (SOFC)**
- **Auxiliary power units (APU) for transportation can reduce:**
  - Diesel fuel consumption
  - Cost
  - Pollutant emissions

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

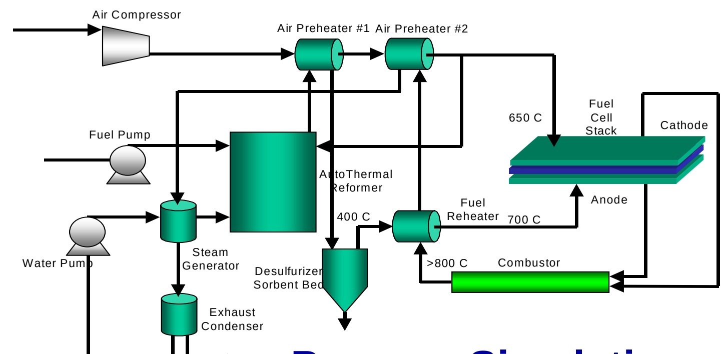


Modeling and Analysis Requirements

- **Device-scale Modeling**
  - Wide variety of key devices
    - Reformer, desulfurizer, fuel cell stack, combustor
  - Complex 2-3D geometries
  - Coupled multiphysics
    - Fluid flow, heat/mass transfer
    - Chemical reactions
- **System Analysis**
  - Many interlinked devices
  - Tight process integration
    - Stack exhaust recycle
    - Heat/water management
  - Couple in high-fidelity device models for improved design, analysis, and optimization



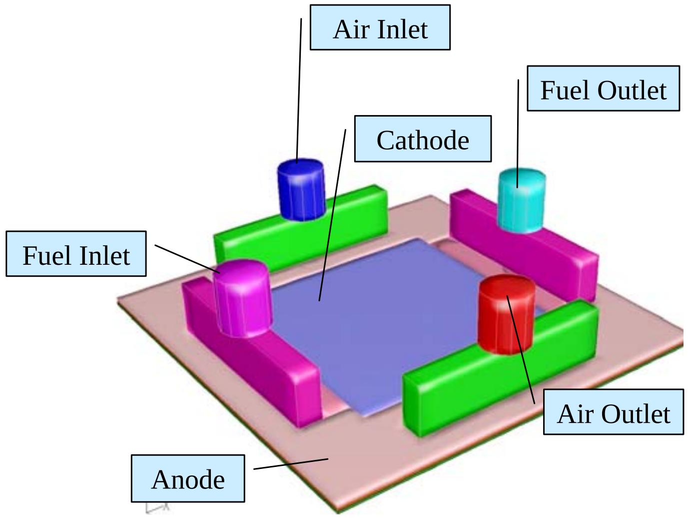
Computational Fluid Dynamics (CFD)

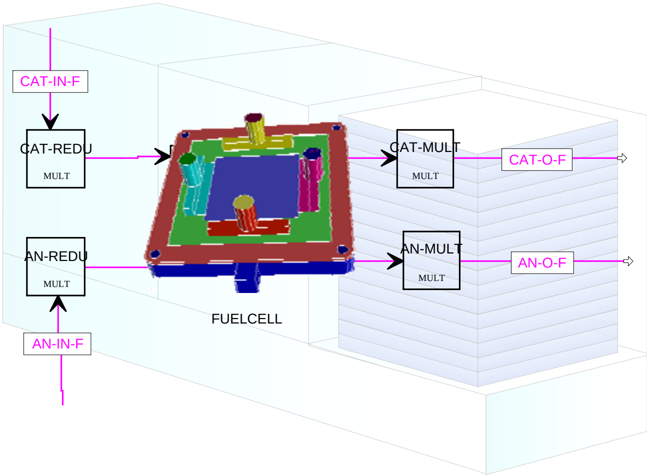


Process Simulation

CFD Model of SOFC in Aspen Plus

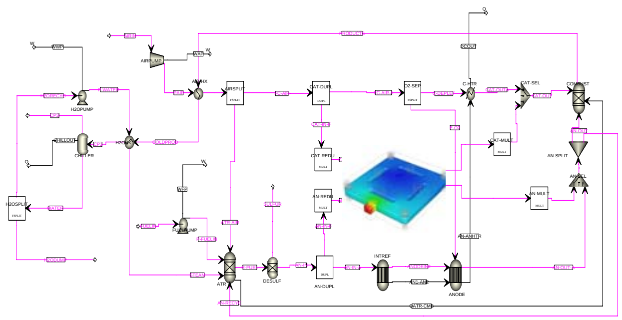
- **Single cross-flow planar cell**
  - FLUENT 3D CFD (steady-state)
  - H_2 and CO chemistry
  - Cell area: 36 cm^2
  - Grid: 58k cells
  - Specify I, calculate V and fuel use
- **Stack Model**
  - Total number of cells: 360
  - Use single cell FLUENT model
  - Assume no cell-to-cell variations
  - Connected to Aspen Plus by four material streams
  - CO parameters: current and voltage

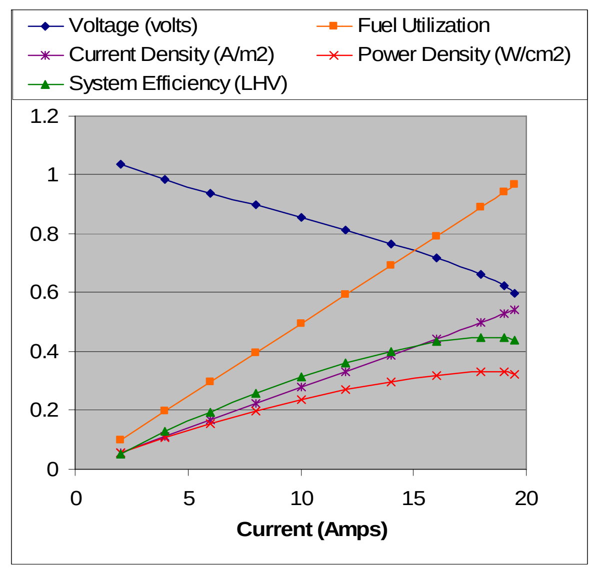


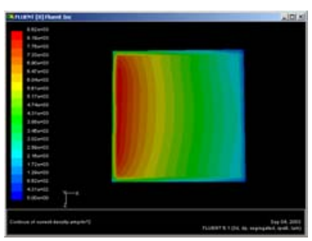


APECS Application - SECA Fuel Cell APU System

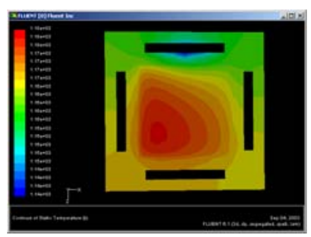
- Aspen Plus process model of Auxiliary Power Unit (APU)
- FLUENT 3D CFD model of SECA solid oxide fuel cell
- Optimize process efficiency by varying CFD parameter (fuel cell current)
- Maximum system efficiency (LHV) of 45% at 18 amps
- Max. system power of 4.3 kW







Current density for cathode

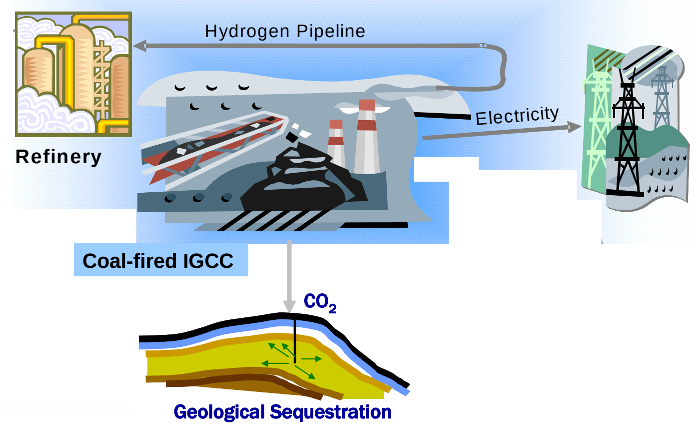


Temperature for anode

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.

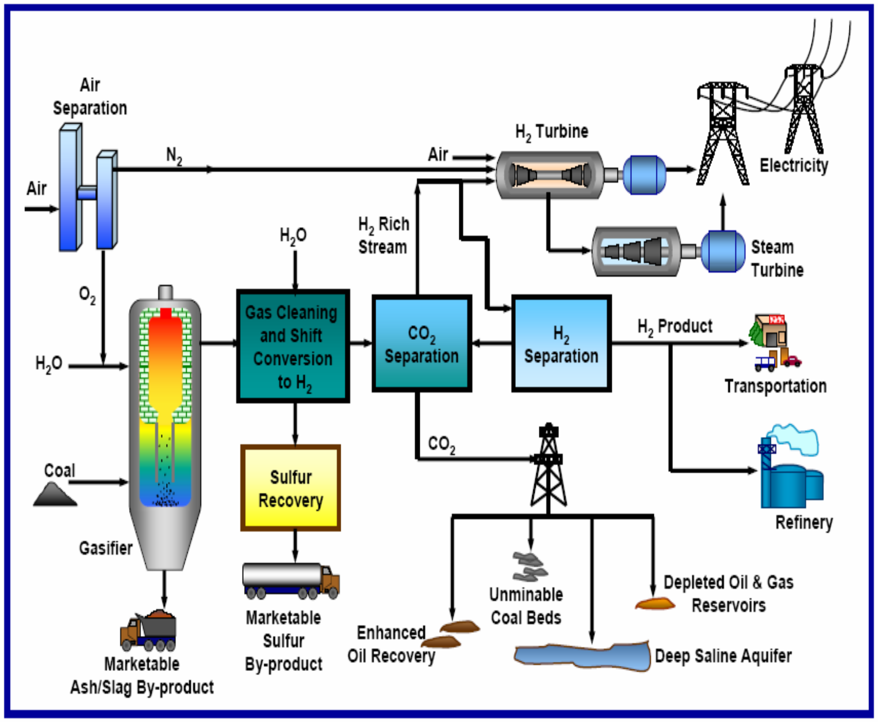
U.S. DOE *FutureGen* Initiative
Pathway to Zero Emissions

- 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

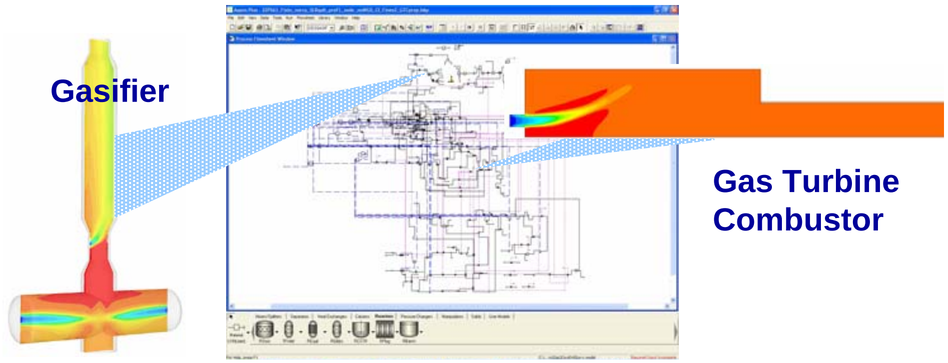


***FutureGen* Process Diagram**

- **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

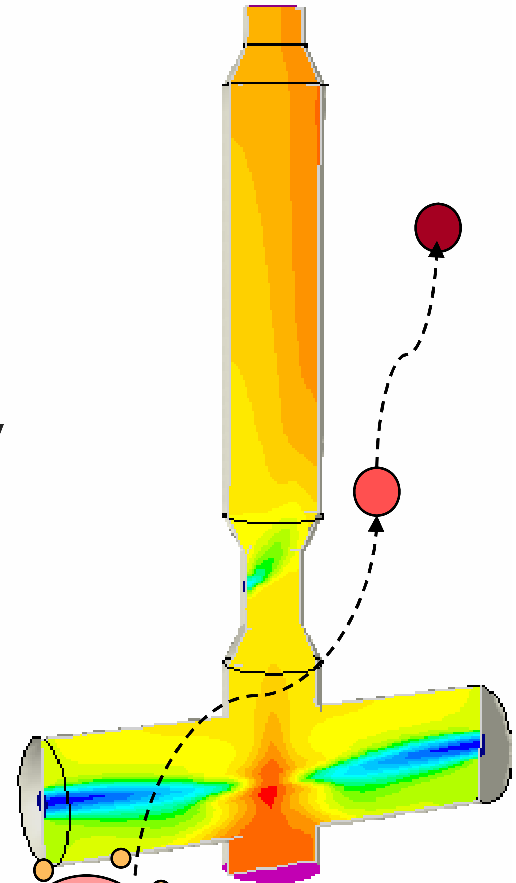


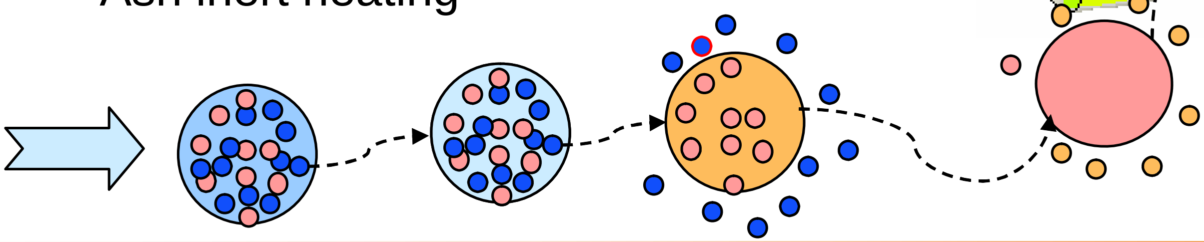
APECS Co-Simulation of FutureGen Power Plant

- **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

Gasification CFD Model

- **Two-stage, entrained-flow, oxygen-blown, coal-slurry gasifier**
- **Fluid flow, heat and mass transfer, and chemical kinetics**
- **Eulerian-Lagrangian multiphase method**
  - Continuous gas phase with reactions
  - Discrete Phase Model (DPM) for coal slurry
- **Coal particle processes**
  - Particle injections
  - Inert heating
  - Moisture release
  - Devolatilization
  - Char combustion and gasification
  - Ash inert heating

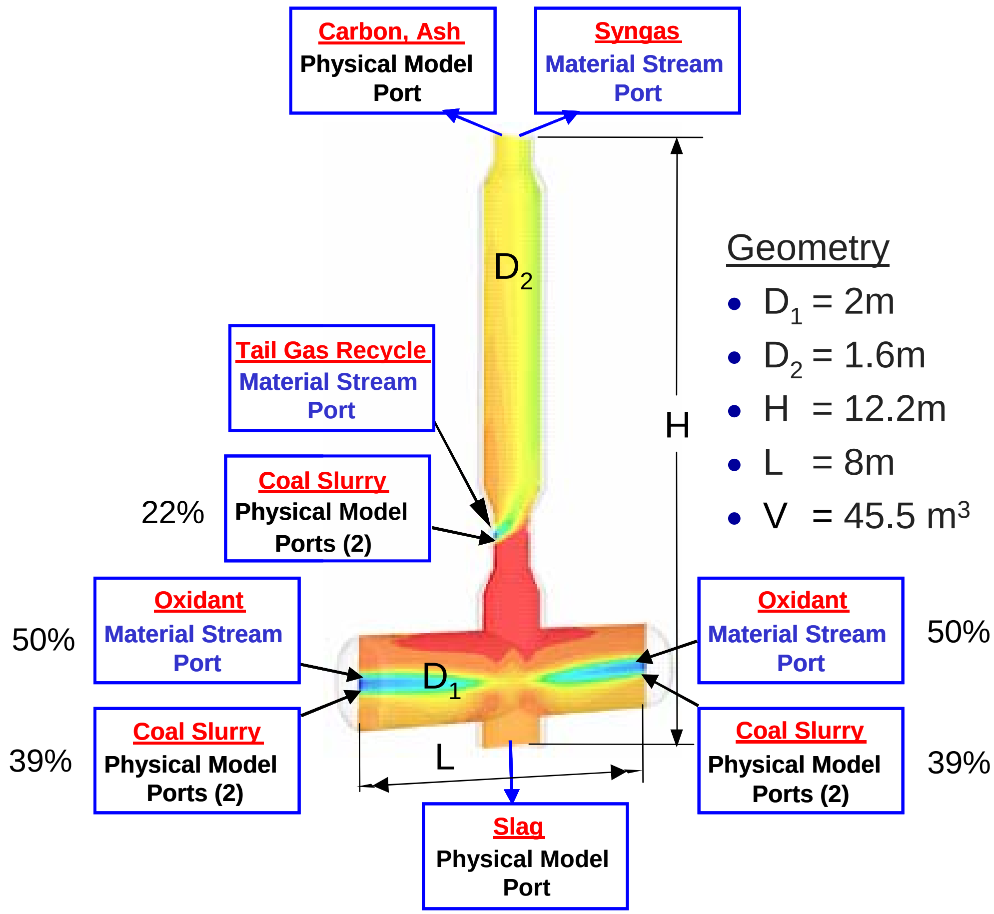




Two-Stage Entrained Flow Gasifier

- Illinois #6 coal
- Rosin-Rammler distribution for particle size
  - 10-50 microns
  - Average of 30 microns
- Coal slurry: 39.7 kg/s, 450K
- Oxidant: 22.9 kg/s, 411K

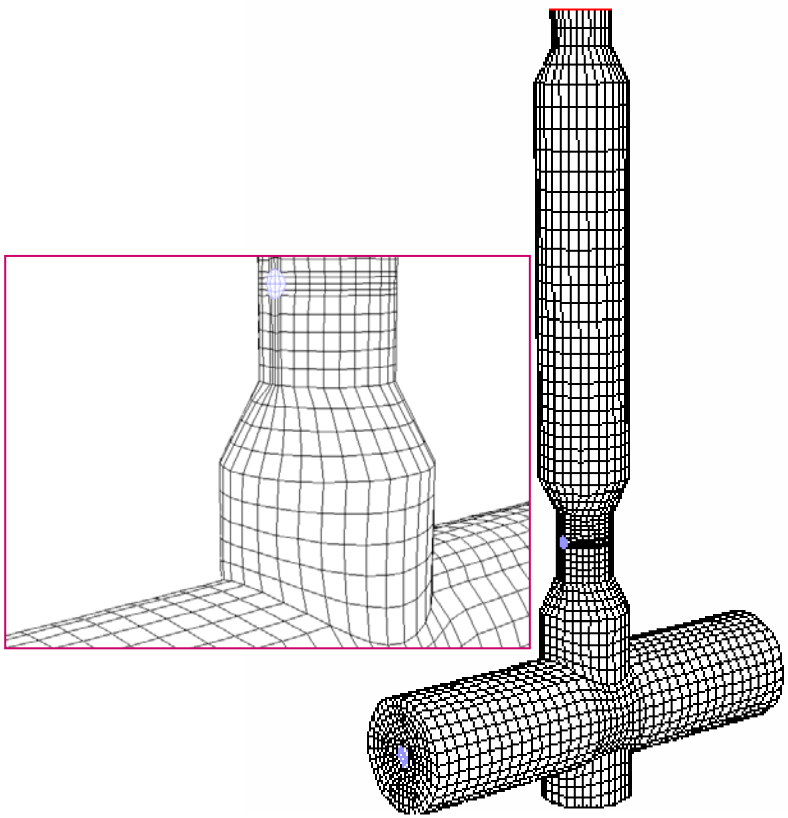
  95%O_2, 1.7N_2, 3.3%Ar
- Particle volume fraction: 4%
- Operating pressure: 28 atm
- Chemical species: CO, H_2, CO_2, H_2O, CH_4, H_2S, Ar, N_2



Geometry
- D_1 = 2m
- D_2 = 1.6m
- H = 12.2m
- L = 8m
- V = 45.5 m^3

FLUENT CFD Model Preparation

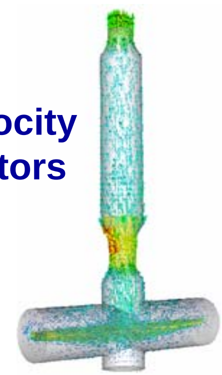
- 12,256 hexahedral computatonal cells
- Converged using approximately 50,000 gas phase iterations
- Temperature of 2500K was patched in gasifier to initialize combustion reaction
- DPM calculations were performed at every 50th iteration of the fluid phase calculation



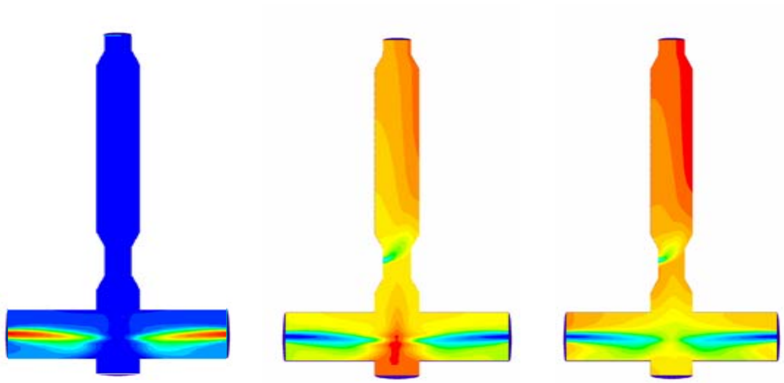
FutureGen Process/CFD Co-Simulation Results

- **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%

Velocity vectors



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



Species mole fraction contours at the center plane

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

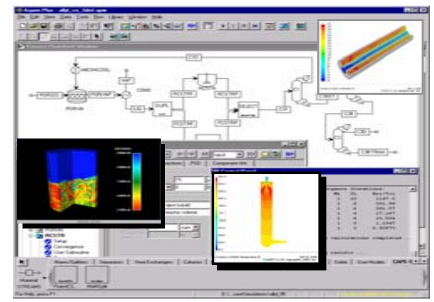
Synthesis Gas Composition

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).

Concluding Remarks

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

- APECS helps to optimize fluid flow and related phenomena that impact overall plant performance



- NETL is using APECS to reduce the time, cost, and technical risk of developing high-efficiency, zero-emission power plants

Thank You

Questions?

- **For additional information on APECS, please contact:**
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    - EML: stephen.zitney@netl.doe.gov
    - TEL: 304-285-1379