NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL 2009 Workshop on Advanced Process Engineering Co-Simulation (APECS)

Pittsburgh, PA
October 20-21, 2009

Co-Simulation for Design and Optimization of Advanced Energy Systems with Carbon Capture

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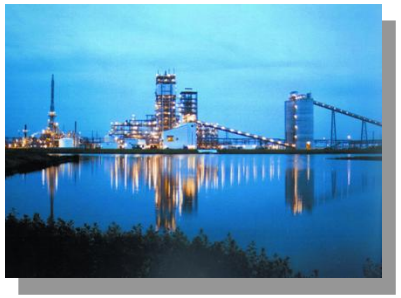
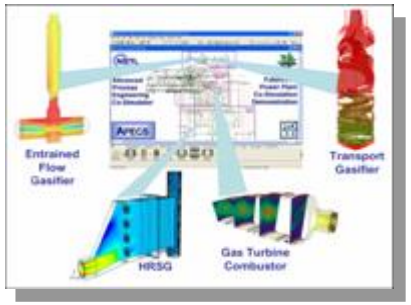
U.S. DEPARTMENT OF ENERGY

Outline of Presentation

- **Introduction**
  - U.S. Energy Challenges
  - Design and Optimization of Advanced Energy Systems
    - Simulation Tools and Challenges
- **Advanced Process Engineering Co-Simulation (APECS)**
  - Basic Features
    - Process/CFD Workflow/Integration
    - Engineering Knowledge Manager™
    - Reduced Order Models (ROMs)
  - Power Generation Applications
  - Advanced Features
    - Design Optimization
    - Virtual Power Plant Co-Simulation
  - Future Work
    - Extension to Carbon Management
- **Concluding Remarks**



IGCC Power Plant



APECS Co-Simulation

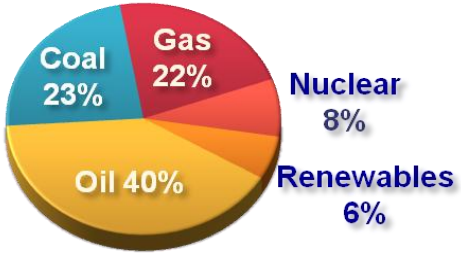
APECS/VE Collaboration

U.S. Energy Challenges

- **Meet increasing demand**

Today

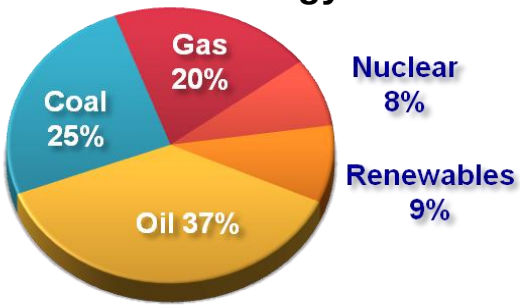
101 QBtu / Year
85% Fossil Energy



+ 16%
United States

2030

118 QBtu / Year
82% Fossil Energy



- **Provide secure, affordable, and clean energy**
- **Address energy-water nexus**

U.S. data from EIA, Annual Energy Outlook 2008

U.S. Energy Challenges
DOE 2020 Goals

- Clean energy
  - Near-zero levels of NO_x, SO_x, PM, and Hg
  - 90% CO_2 capture and 99%+ storage permanence
- Affordable energy
  - <35% increase in COE for post- and oxy-combustion capture
  - <10% increase in COE for pre-combustion capture (e.g., IGCC)
- Energy-water nexus
  - Reduce freshwater withdrawal and consumption by 70% or greater

IGCC Power Plant

References:
1. *Existing Plants—Emissions and Capture Program Goals, U.S. DOE/National Energy Technology Laboratory, Draft Final Report, February 2009*
2. *Impact of Cost Escalation on Power Systems R&D Goals—Re-baselining APS, CS & FC GPRA R&D Goals, July 2008*

U.S. Energy Challenges
Fossil Energy Industry

- Optimize/retrofit existing fleet of combustion power plants
  - Ultra-supercritical (USC)
  - Oxy-combustion
  - Chemical looping combustion (CLC)
- Design next-generation plants
  - Integrated gasification combined cycle (IGCC)
  - Polygeneration
    - Chemicals, Liquid fuels, SNG, H_2
  - Chemical looping gasification (CLG)
  - Gas turbine/fuel cell hybrids
- Use carbon capture and storage (CCS)
- Minimize air emissions and water use

Combustion Power Plant

IGCC Power Plant with CCS

References:

1. *Existing Plants—Emissions and Capture Program Goals, U.S. DOE/National Energy Technology Laboratory, Draft Final Report, February 2009*
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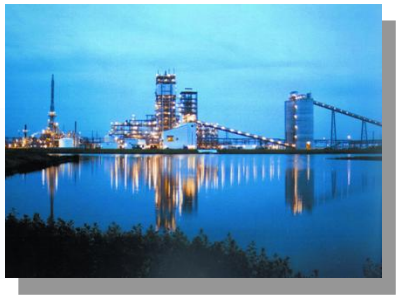
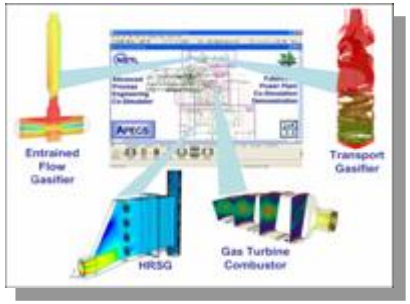


IGCC Power Plant

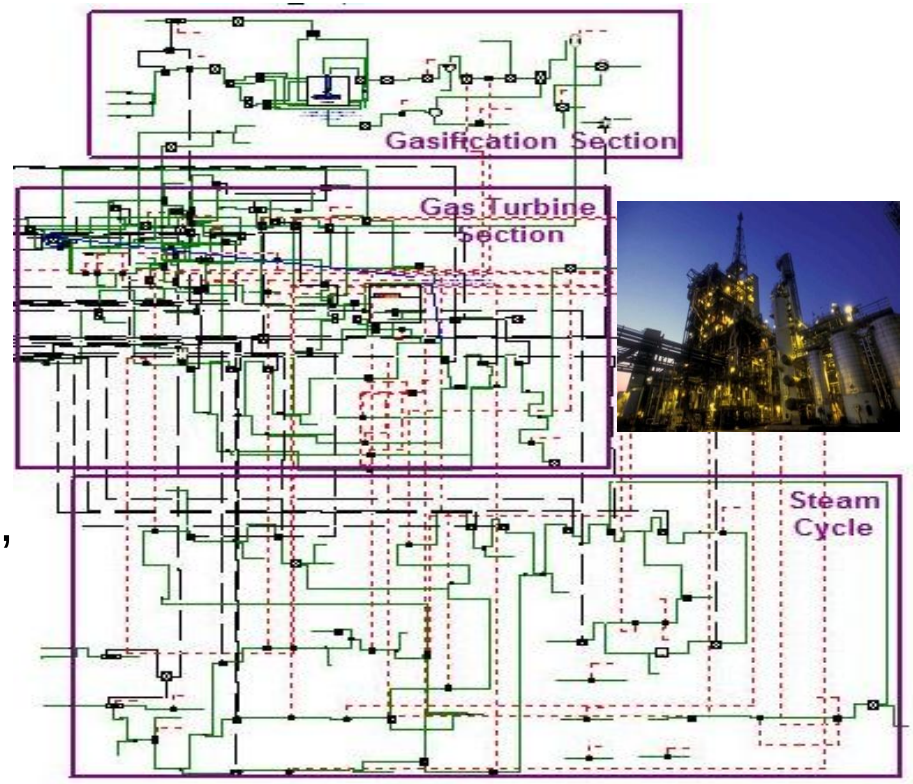


APECS Co-Simulation

APECS/VE Collaboration

Design and Optimization of Advanced Energy Systems
Process Simulation

- Power output, overall efficiency, environmental performance
- Hundreds of process units and streams
- Mass and energy balances
- Lumped-parameter models
- Extensive physical properties, including solids (coal)
- Recycles, heat and water integration
- Analysis tools include design specifications, case studies, sensitivity analysis, and optimization

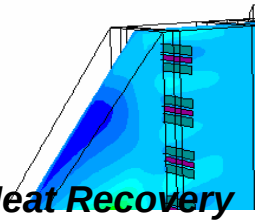


Aspen Plus® steady-state process simulation of an IGCC plant

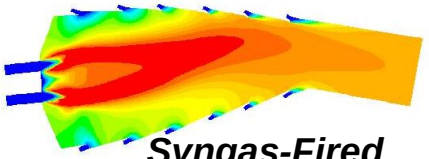
"Cost and Performance Baseline for Fossil Energy Power Plants Study, Volume 1: Bituminous Coal and Natural Gas to Electricity," NETL, www.netl.doe.gov, August 2007.

Design and Optimization of Advanced Energy Systems
Equipment Simulation

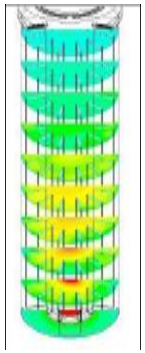
- Equipment design, analysis, and optimization
- Detailed engineering
- Complex geometries
- 2D/3D distributed-parameter models (PDEs)
- Coupled multiphysics: fluid flow, heat/mass transfer, and reactions
- Physical sub-models: mixing, turbulence, combustion
- Multiphase, e.g. gas-solids
- Flow field visualization
- High-performance computing



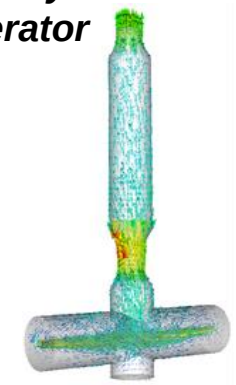
Heat Recovery Steam Generator



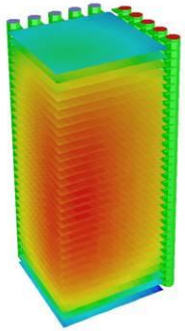
Syngas-Fired Turbine Combustor



Syngas Cooler



Entrained-Flow Gasifier

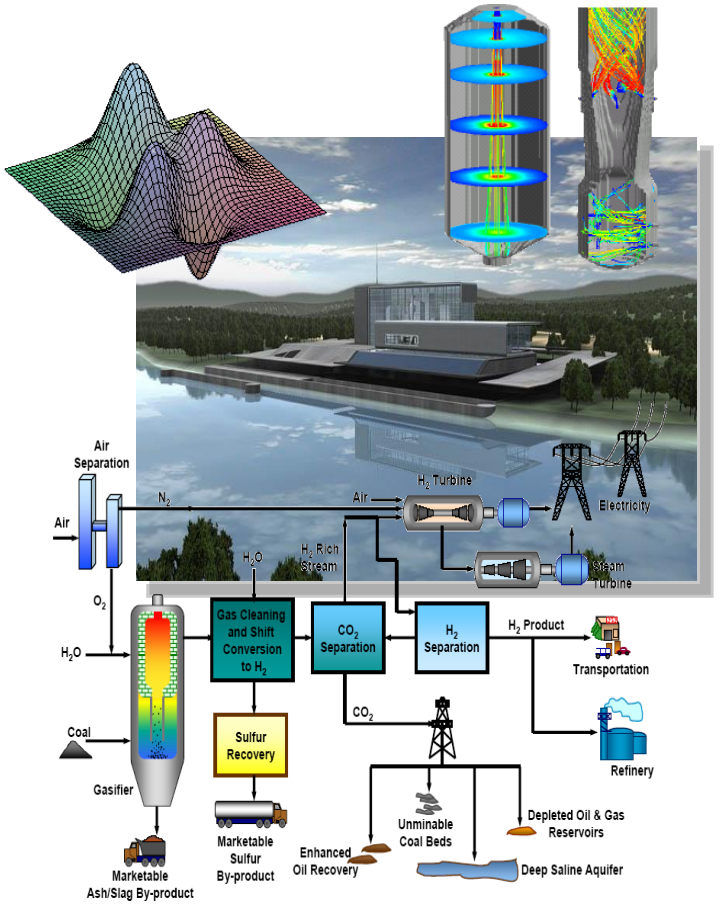


Solid Oxide Fuel Cell Stack

- Computational Fluid Dynamics (CFD)
- FLUENT® (ANSYS), MFIX (NETL)

Design and Optimization of Advanced Energy Systems *Challenges*

- Large, highly-integrated, and multipurpose systems with heat and water network management
- Wide variety of advanced equipment items with complex geometries and multiphysics
- Limited number of demo plants
- High-fidelity simulations required to:
  - Predict, analyze, and optimize plant performance
  - Meet aggressive design goals
    - Near-zero emissions and CCS
    - Unprecedented efficiency
  - Reduce design time, cost, and risk



IGCC Power Plant with CCS

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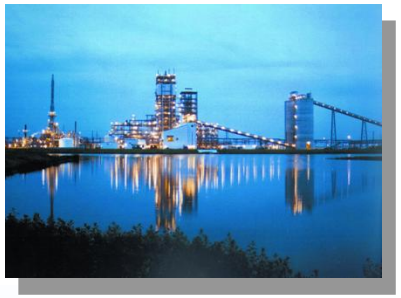
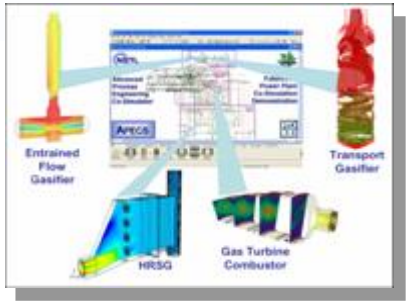


IGCC Power Plant



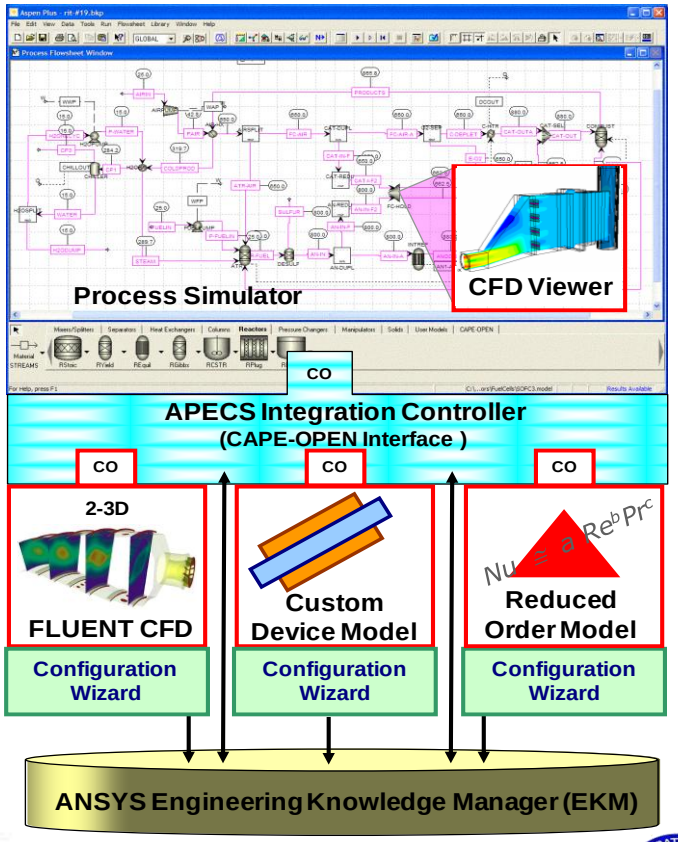
APECS Co-Simulation

APECS/VE Collaboration

Advanced Process Engineering Co-Simulator (APECS)

High-Fidelity Process/Equipment Design and Optimization

- Collaborative co-simulation software framework for seamless and efficient integration of:
  - Process simulation
  - Detailed equipment simulations
    - Computational fluid dynamics (CFD) models
    - PDE-based custom equipment models (CEMs)
    - Reduced-order models (ROMs)
- Analysis and optimization of overall plant performance with respect to complex thermal and fluid flow phenomena



- *2004 R&D 100 Award (APECS)*
- *2006,2007 Federal Laboratory Consortium (FLC) Excellence in Technology Transfer Awards (APECS)*
- *2008 R&D 100 Award (APECS with EKM)*
- *2009 R&D 100 Award (VE-PSI: APECS with VE-Suite)*

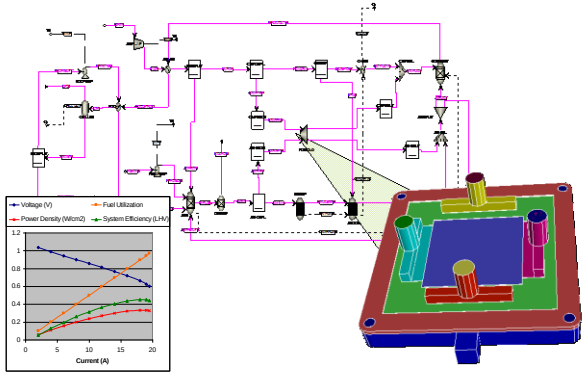
Advanced Process Engineering Co-Simulator (APECS)
Brief History

- 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&D100 Award - APECS (2004)
- Phase-2 APECS R&D Project Start (2005)
- US Federal Technology Transfer Awards (2006/7)
- US/APECS – UK/VPDM Collaboration (2005-8)
- R&D100 Award – APECS with ANSYS® EKM™ (2008)
- R&D100 Award – APECS with VE-Suite (2009)
- Phase-2 APECS R&D Project Extension (2009)

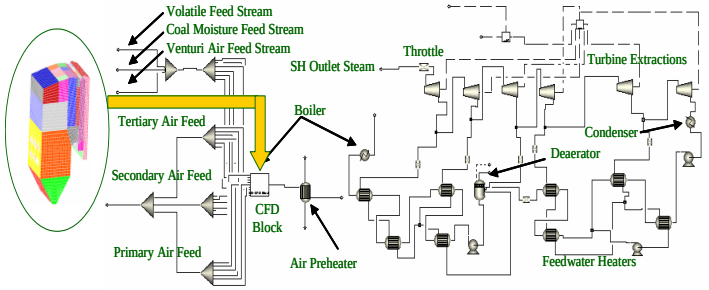
APECS Process Simulation/CFD Integration

Power Generation Applications

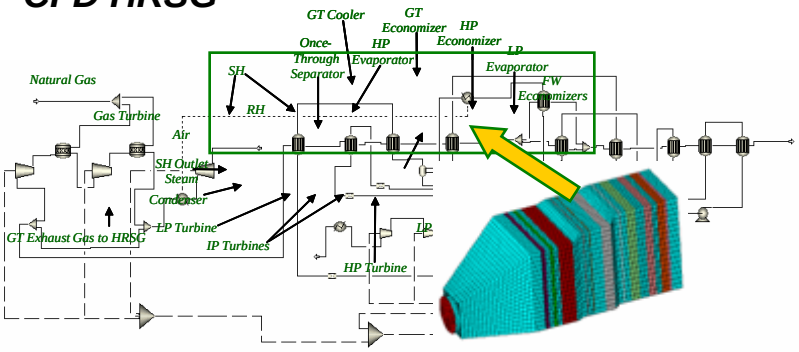
- ***Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC***



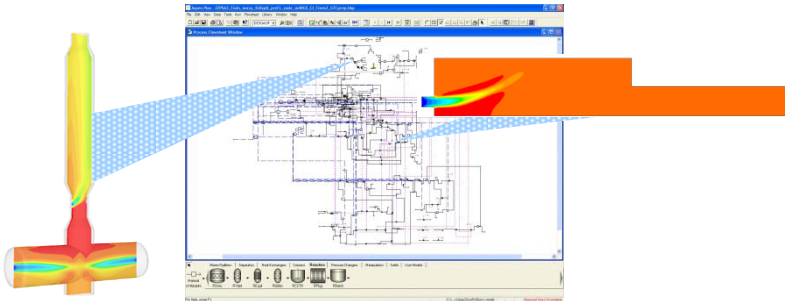
- ***ALSTOM Conventional Steam Plant (30MWe) with 3D CFD Boiler***



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



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



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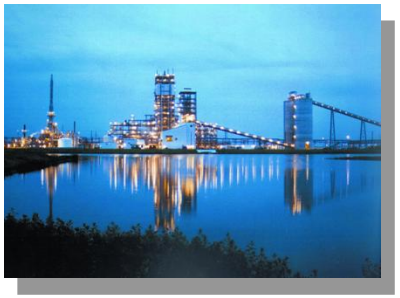
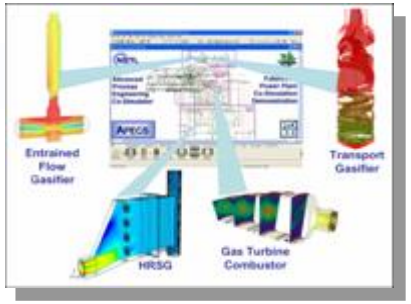


IGCC Power Plant



APECS Co-Simulation

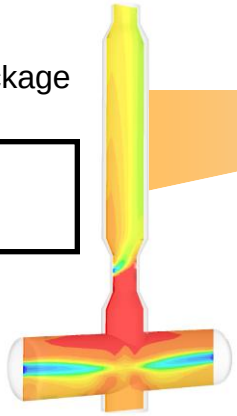
APECS/VE Collaboration

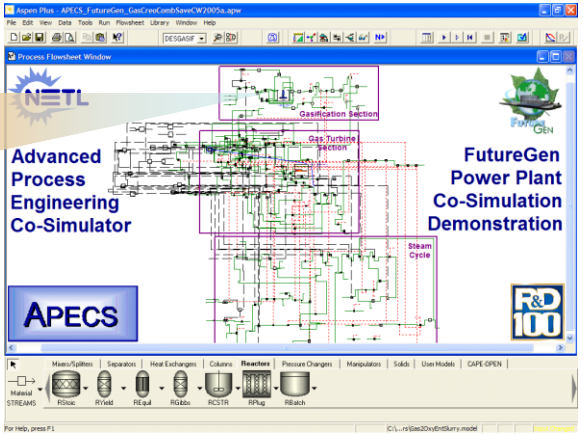
APECS Co-Simulation Workflow

Seamless Integration of CFD and Process Simulation Tasks

CFD Package

APECS





Process Simulator

APECS

Equipment/CFD Simulation

Develop CFD equipment model

Configure CFD model

Create ROM from CFD results (optional)

Add CFD/ROM model to model database

Process Simulation

Develop process simulation model

Load CAPE-OPEN model library

Instantiate APECS CAPE-OPEN block

Select CFD/ROM model from model database

Set parameter values for equipment model

Specify solution strategy

Map species and ports

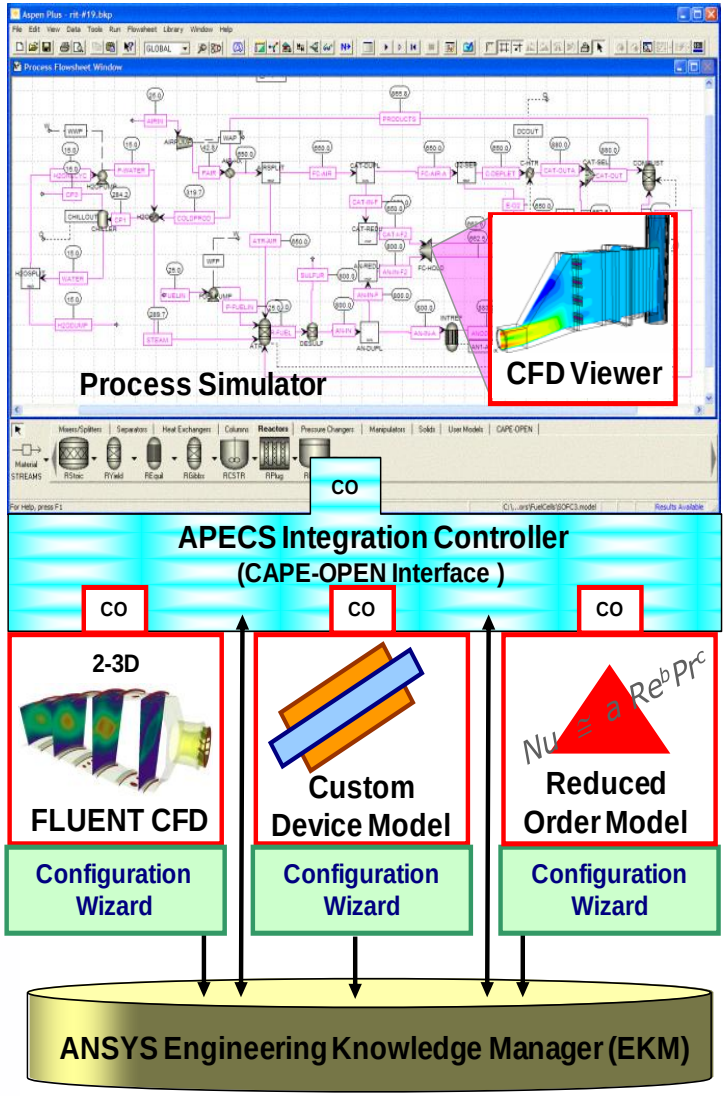
Run process/equipment co-simulation

View and analyze CFD results

APECS Process/Equipment Co-Simulation Workflow (with Demo) – *Erik Ferguson, ANSYS Inc.*

APECS Software Components and Features

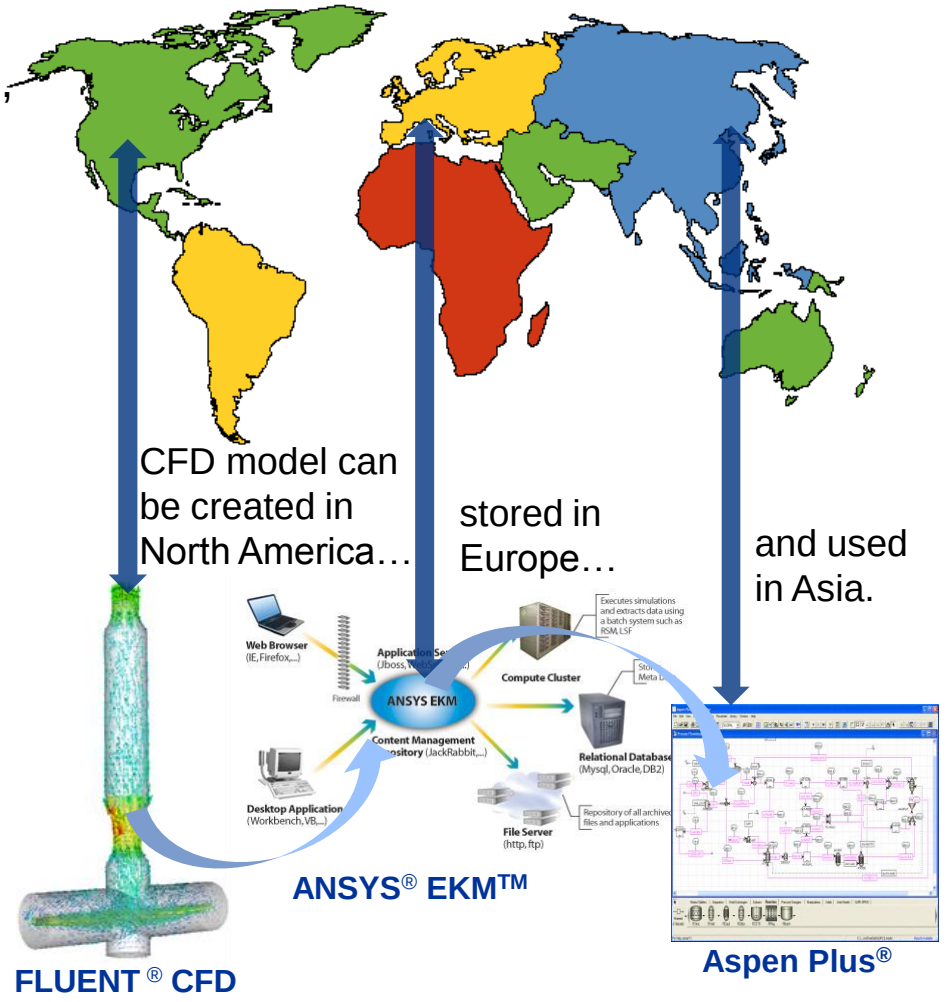
- **Process Simulators**
  - CAPE-OPEN compliant
  - Aspen Plus®, HYSYS®, gPROMS®, PRO/II®, COCO
- **Equipment Models and Database**
  - CAPE-OPEN compliant
  - ANSYS® EKM™
  - CFD: FLUENT®
  - CEMs: e.g., ALSTOM's INDVU
  - ROMs: LR, ANN, PCA
- **Integration Controller**
  - CAPE-OPEN v1.0 Interfaces
  - Unit Ops, Phys Props, Reactions
- **Configuration Wizards**
  - FLUENT®, Custom Model, and ROM
- **Solution/Analysis Tools**
  - ROM Builder
  - Hybrid: Speed (ROM), Accuracy (CFD)
  - Stochastic, Multi-objective Optimization
  - Design Optimization
  - PC/IGCC Cost Estimation
- **Distributed Execution**
  - CAPE-OPEN COM/Corba Bridge
  - Windows/Linux, Serial/Parallel
- **Virtual Engineering**
  - CFD Viewer (2D), Paraview (3D)
  - VE-Suite



APECS Collaborative Co-Simulation Workflow

ANSYS® Engineering Knowledge Manager™ (EKM™)

- APECS with EKM™ addresses challenge of managing data, models, and engineering knowledge arising from advanced co-simulation applications
  - CAPE-OPEN software standard for plug-and-play model interoperability
  - Archiving/retrieval processes
  - Server-based, enterprise-wide repositories
- Better use of detailed equipment models to guide effective process systems engineering decisions
- Collaborative detailed and process engineering solutions to enable global project execution

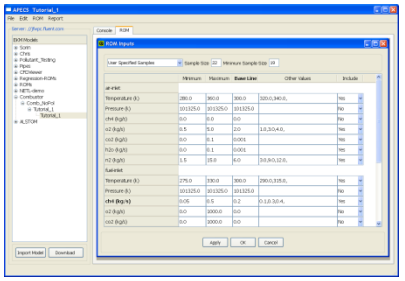


APECS with ANSYS® Engineering Knowledge Manager™ (with Demo) – *Sorin Munteanu, ANSYS Inc.*

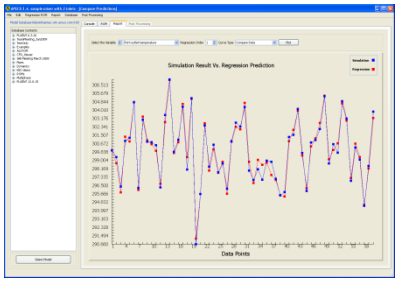
APECS Reduced Order Models (ROMs)

Fast CFD-Based ROMs for Process Design and Optimization

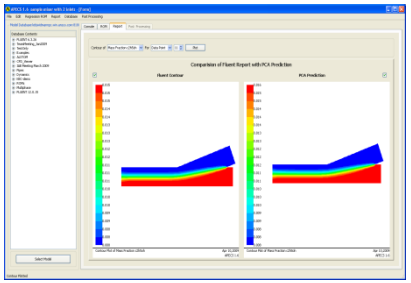
- APECS ROM Builder for automatic ROM generation from CFD simulations
- Design of experiments (DoE) using Latin Hypercube sampling
- CFD simulations can be run in advance and in serial/parallel on a remote cluster
- ROM methods include Regression and ANN
- Principal Component Analysis (PCA) used to regenerate flow field and other contours
- Accuracy of ROMs can be compared to CFD results
- ROMs stored in EKM™ model database
- ROMs run very fast for use in process simulation and optimization
- CFD Viewer available for displaying ROM results in process simulator



ROM Builder GUI



CFD/ROM Comparisons

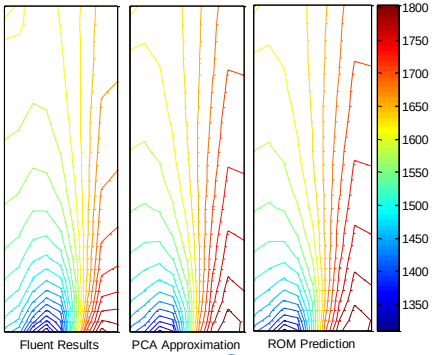


PCA-based ROM Contours

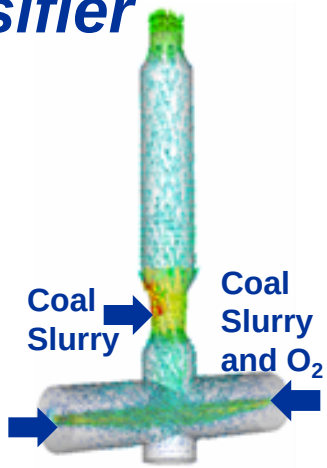
APECS ROM Application

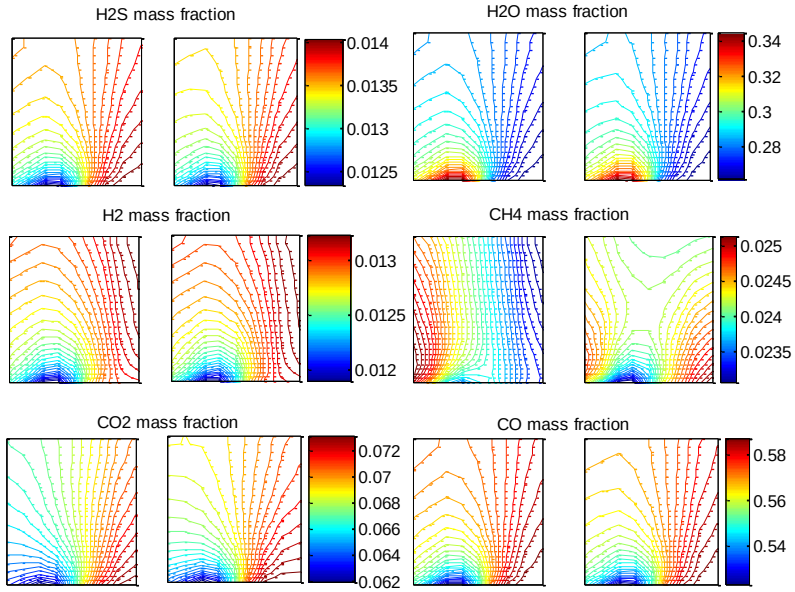
Optimal Design of Entrained-Flow Gasifier

- **2-stage, coal slurry, O_2-blown, entrained-flow gasifier**
- **FLUENT® CFD model *(Shi et al., 2006)***
  - Eulerian-Lagrangian multiphase
    - Continuous gas phase with reactions
    - Discrete Phase Model (DPM) for coal slurry
- **3 independent inputs selected for variation over restricted input range**
  - Coal feed split to stage 1 (75-85%)
  - O_2/coal ratio (.75-.85)
  - Water % in slurry (25-35%)
- **CFD executed 30 times according to Latin Hypercube sampling**
- **ANN-based ROM created from data**
- **PCA-based method *(Lang et al., 2009)***
  - 8 principal components
  - Ratio of energies = 0.99995
  - Used with ANN-ROM to provide output contours for arbitrary input (over the input range)



Temperature Contours



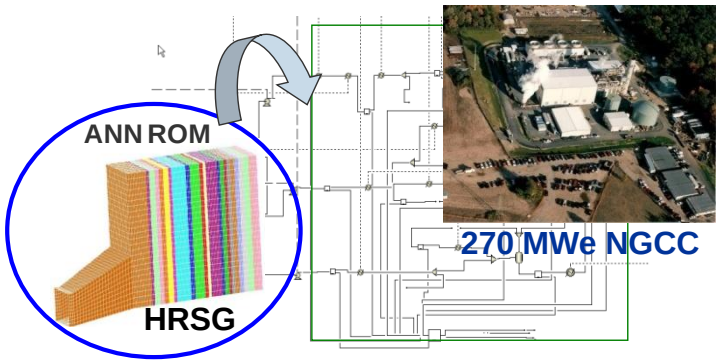


Contours of Species Mass Fractions (FLUENT/ROM)

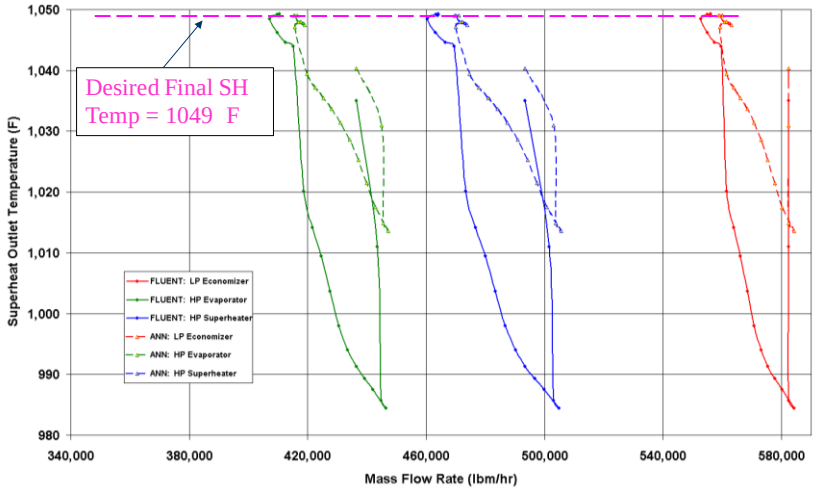
APECS ROM Applications at ALSTOM Power

HRSG ANN-ROMs for NGCC and IGCC Co-Simulations

- **Applications**
  - 270 MWe Natural Gas Combined Cycle (NGCC)
  - 250 MWe IGCC with Carbon Capture
- **Objective**
  - Use APECS to optimize HRSG heat integration in context of Aspen Plus® process simulations
- **FLUENT® HRSG CFD Model**
  - 18 Tube banks, HP/LP/Reheat
  - 40,000 computational cells; >1 CPU hr
- **Artificial Neural Network (ANN) ROM**
  - Logistic activation function and hybrid of SA/CG training algorithms
  - Trained on 76 CFD simulations
  - ~2 CPU seconds
- **Co-Simulations**
  - 2 material stream connections (gas-side)
  - 12 physical model port (inlet/outlet) connections
  - ANN-ROM flow rates for all streams are within 0.5% of CFD flow rates
  - Sensitivity analysis using APECS co-simulations for different initial economizer flow rate conditions



Co-Simulation with ANN-ROM for a Heat Recovery Steam Generator (HRSG)

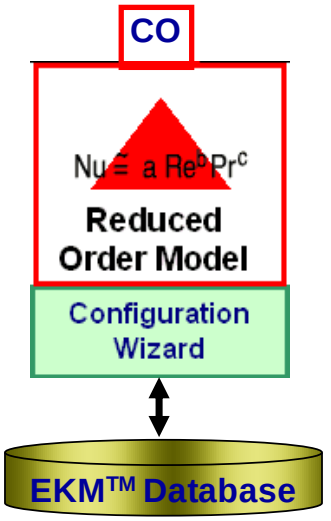


ANN / FLUENT® Results for NGCC Run: +20,000 lb_m/hr Perturbation

APECS Reduced-Order Models (ROMs)

Wednesday, October 21, 2009 (8:00-11:00am)

- **Principal Component Analysis (PCA)-based ROMs**
  Larry Biegler, Carnegie Mellon University
- **APECS ROM Builder (with Demo)**
  John Widmann, ANSYS Inc.
- **APECS ROM Applications at ALSTOM Power**
  David Sloan, ALSTOM Power



- **Development of CAPE-OPEN ROMs for APECS Power Generation Applications**
  Mike Bockelie, Reaction Engineering International
- **Recent Advances in Reduced-Order Modeling for Transport Phenomena**
  Paul Cizmas, Texas A&M University
- **Multizonal Reactor Network ROMs**
  Scott Drennan, Reaction Design

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  - Design and Optimization of Advanced Energy Systems
    - Simulation Tools and Challenges
- **Advanced Process Engineering Co-Simulation (APECS)**
  - Basic Features
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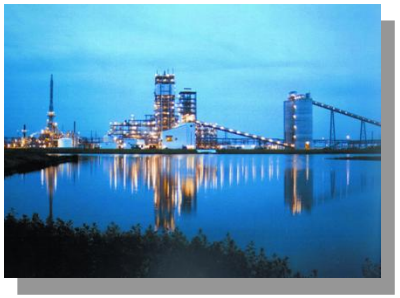
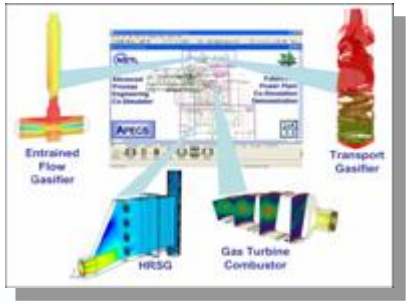
  - Power Generation Applications
  - Advanced Features
    - Design Optimization
    - Virtual Power Plant Co-Simulation
  - Future Work
    - Extension to Carbon Management
- **Concluding Remarks**



IGCC Power Plant



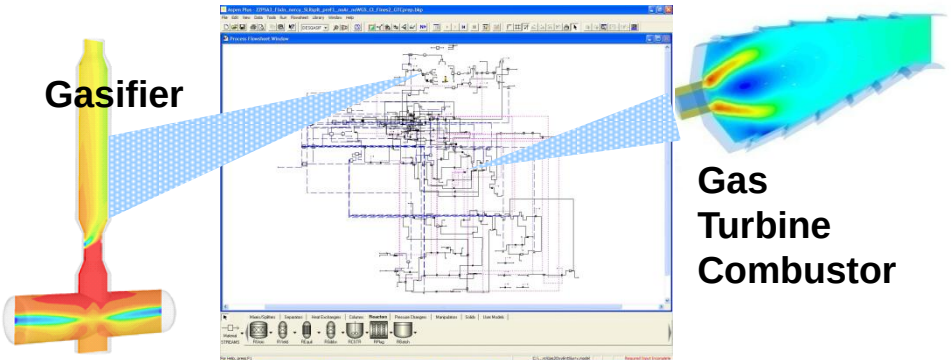
APECS Co-Simulation

APECS/VE Collaboration

APECS Application – Polygeneration Plant

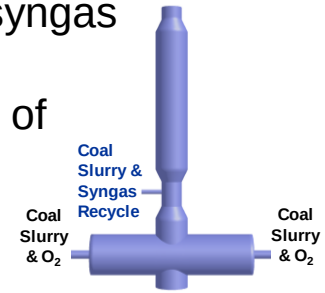
Power and Hydrogen Production with CO_2 Capture

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

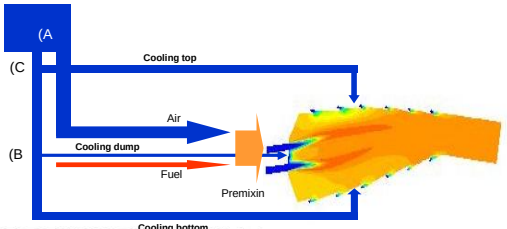


APECS Co-Simulation of Polygeneration Plant

- **CFD Simulations**
  - Entrained-Flow Gasifier
    - FLUENT® 3D/ROM
    - Accurate calculation of synthesis gas composition
    - Embedded in syngas recycle loop
    - Optimized flow of coal slurry and syngas recycle to 2nd stage

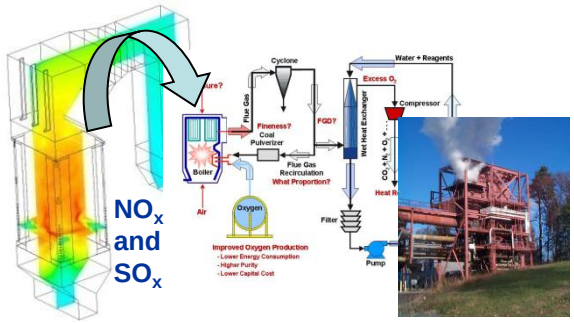


  - Gas Turbine Combustor
    - FLUENT® 3D/ROM with partially pre-mixed combustion
    - Accurate calculation of GT inlet temperature
    - Embedded in design spec loop to determine power/H_2 production
    - Optimized cooling strategy to minimize NO_x

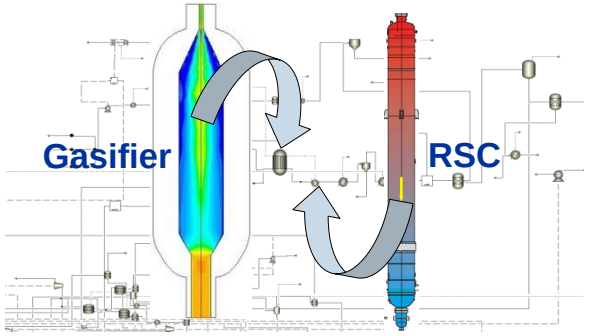


APECS Application Projects at ALSTOM Power

- **Oxy-Combustion**
  - 18 MW_{th} Boiler Simulation Facility (BSF)
  - BSF island (gas side only) with flue gas recycle (FGR)
  - FLUENT® 3D CFD boiler with pollutant species (NO_x, SO_x) exposed to Aspen Plus® via CAPE-OPEN parameters
  - Characterize impact of various FGR and cleanup scenarios on pollutant emissions for candidate BSF configurations
- **IGCC with CO_2 Capture**
  - 556 MW_e IGCC simulated in Aspen Plus®
  - FLUENT® CFD models
    - Single-stage, downward-fired, coal-fed, entrained-flow gasifier
    - Radiant syngas cooler (RSC)
  - Transfer multi-dimensional boundary conditions
  - Analyze integration of gasifier and RSC
  - Optimize heat integration with overall plant
- **Chemical Looping Combustion**
  - APECS co-simulation of 65 kW_{th} pilot-scale facility
  - FLUENT® 3D CFD/ROMs for solid fuel and air reactors
  - Dense, multiphase flow using E-E solution



ALSTOM: Oxy-Combustion

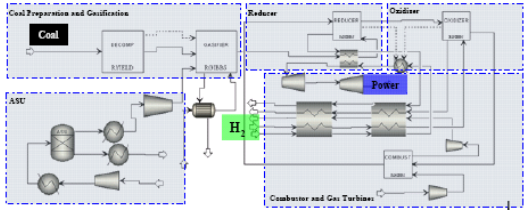


ALSTOM: IGCC with CO_2 Capture

ALSTOM: Chemical Looping Combustion

APECS Applications – Power Generation

- **Ohio State University: Syngas Chemical Looping (SCL)**
  - Aspen Plus® simulation of SCL process
  - Power generation and H_2 production
  - Patented Fe_2O_3-based composite oxygen carrier
  - FLUENT® CFD models/ROMs for air/fuel reactors
  - APECS co-simulation and validation using OSU's SCL test facility



Aspen Plus model of SCL Process

2.5 kW_{th} SCL Process at OSU

Process/Equipment Co-Simulation of a Syngas Chemical Looping Process - *L.S. Fan, Ohio State University*

- **West Virginia University: PC Power Plant with Cooling Tower**
  - Aspen Plus® simulation of pulverized coal (PC) power plant and water network
  - FLUENT® CFD models/ROMs for hyperbolic natural-draft cooling tower
  - Optimize energy/water system to minimize water consumption

Hyperbolic Cooling Tower

Cooling Tower Geometry

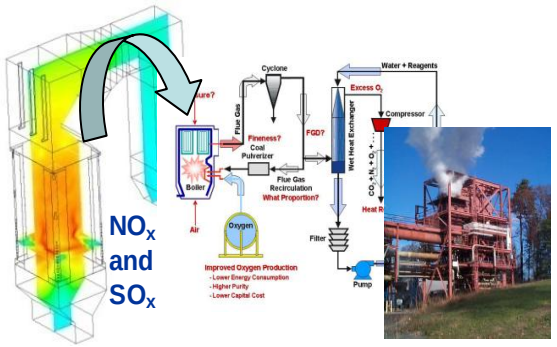
Process/Equipment Co-Simulation of a Pulverized Coal Plant with Cooling Tower – *W. Huebsch, WVU*

APECS Applications

Tuesday, October 20, 2009 (1:00-5:00pm)

APECS Applications at ALSTOM Power
David Sloan, ALSTOM Power

Co-Simulation of a Syngas Chemical Looping Process
L.S. Fan, Ohio State University



ALSTOM: Oxy-Combustion

Co-Simulation of a Pulverized Coal Plant with Cooling Tower
Wade Huebsch, West Virginia University

Co-Simulation for Gasification- and Combustion-based Energy Applications
Mike Bockelie, Reaction Engineering International

Co-Simulation: An Integrated Energy Company Perspective
Lanre Oshinowo, ConocoPhillips

Co-Simulation: A Chemical Process Industry Perspective
Kunle Ogunde, DuPont

Outline of Presentation

- **Introduction**
  - U.S. Energy Challenges
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    - Simulation Tools and Challenges
- **Advanced Process Engineering Co-Simulation (APECS)**
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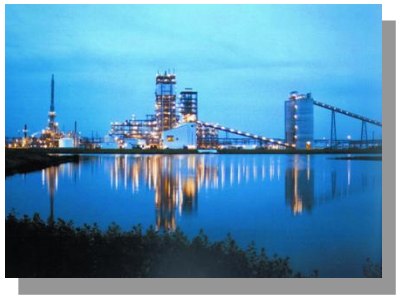
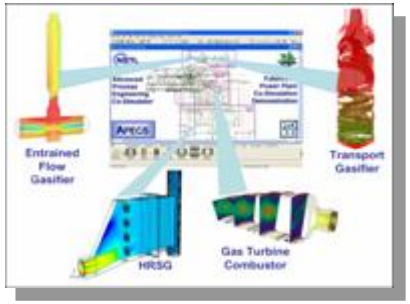
  - Future Work
    - Extension to Carbon Management
- **Concluding Remarks**



IGCC Power Plant



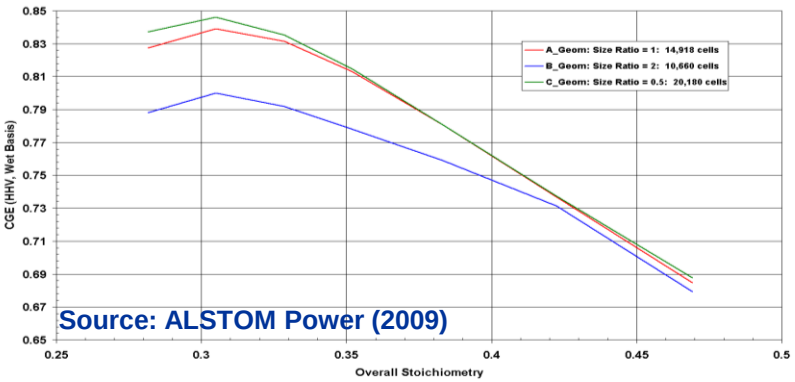
APECS Co-Simulation

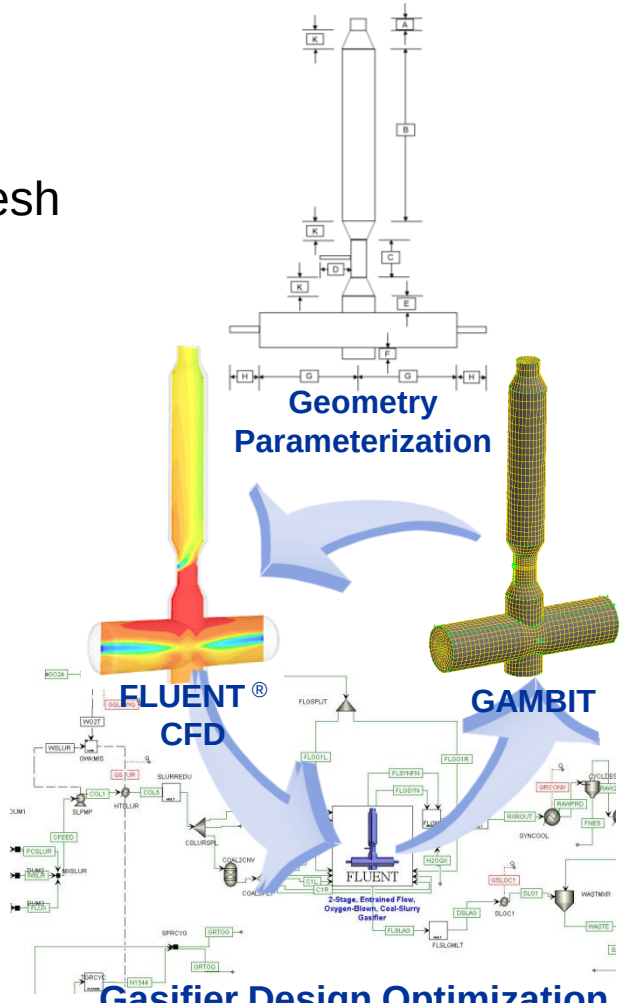
APECS/VE Collaboration

APECS Design Optimization

Case Study: Entrained-Flow Gasifier Design

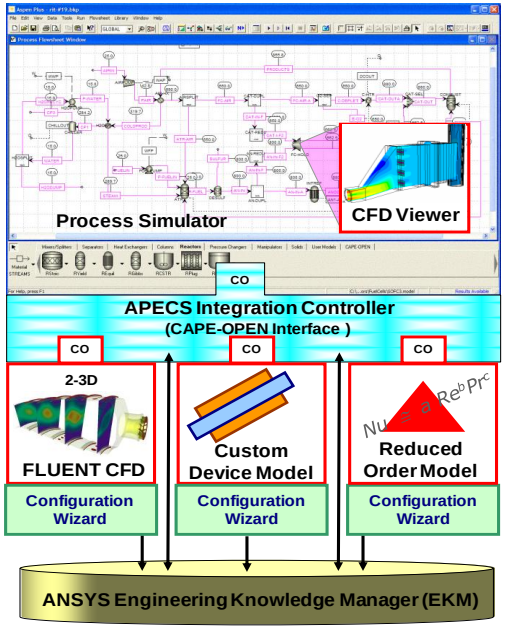
- Geometry parameterization within process simulation via CAPE-OPEN parameters
- Automated regeneration of CFD geometry/mesh
  - GAMBIT => FLUENT® => Aspen Plus®
- Case study: Gasifier design optimization
  - Geometry and inlet cross-sections scale with coal throughput in order to preserve cross-sectional velocities and residence times
  - Vary oxygen flow rate to maximize cold gas efficiency (CGE) for a given coal throughput





Virtual Power Plant Co-Simulation

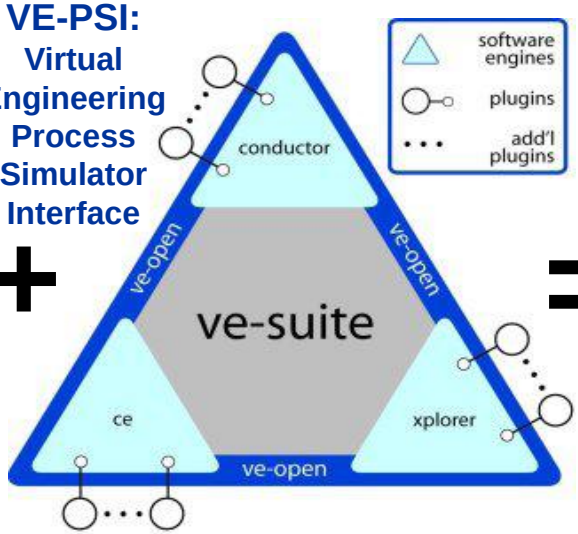
APECS/VE-Suite Integration



APECS

VE-PSI: Virtual Engineering Process Simulator Interface

+



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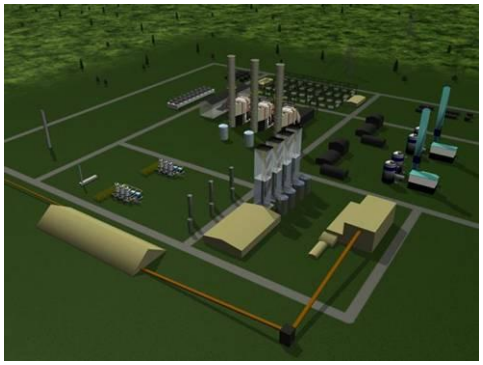


Virtual Plant Co-Simulation

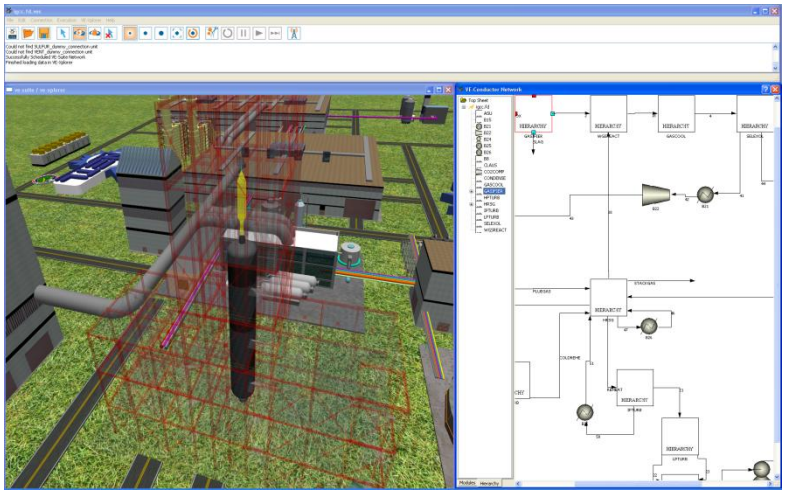
VE-Suite

IOWA STATE UNIVERSITY

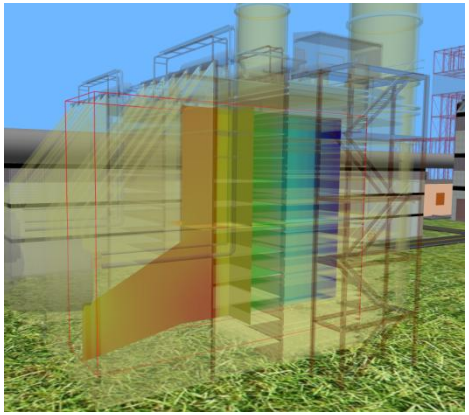
Virtual Power Plant Co-Simulation

APECS/VE-Suite Integration with VE-PSI

- Facilitates optimization of next-generation power plants within a virtual engineering software environment
- Integrates 3D immersive, interactive plant walkthrough environment in **VE-Suite** with **APECS** process/equipment co-simulations
- Provides graphic display of process simulation, CFD, and CAD data
- Supports hardware from the desktop to multi-wall caves
- Enables collaborative design for wide range of project stakeholders
- Collaboration Partners
  - DOE/NETL
  - Ames Laboratory/Iowa State Univ.
  - Reaction Engineering International
- Demonstrations
  - NETL: IGCC with carbon capture
  - ALSTOM Power: Power generation
  - INL: Biomass applications



Using VE-PSI with VE-Suite to analyze gasifier CFD data from APECS co-simulation of IGCC plant



Using VE-PSI in VE-Suite to overlay CFD results on 3D CAD for HRSG from APECS co-simulation of IGCC plant

Integration of APECS with VE-Suite for Virtual Plant Simulation – *Doug McCorkle, Iowa State University*

APECS Advanced Features

Wednesday, October 21, 2009 (11:00am-2:20pm)

- **APECS Design Optimization**

  David Sloan, ALSTOM Power

- **Stochastic Analysis and Multi-Objective Optimization**

  Urmila Diwekar, Vishwamitra Research Institute

- **Integration of APECS and Aspen Plus Dynamics**

  John Widmann, ANSYS Inc.

- **Integration of APECS with VE-Suite for Virtual Plant Simulation (with Demo)**

  Doug McCorkle, Iowa State University

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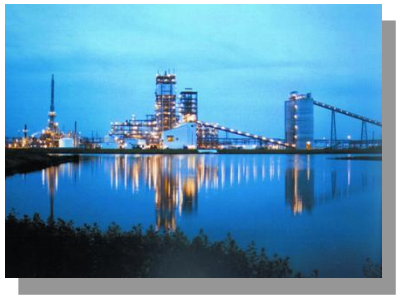
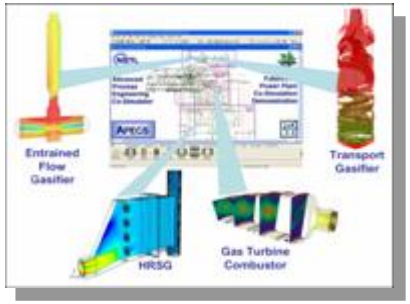


IGCC Power Plant



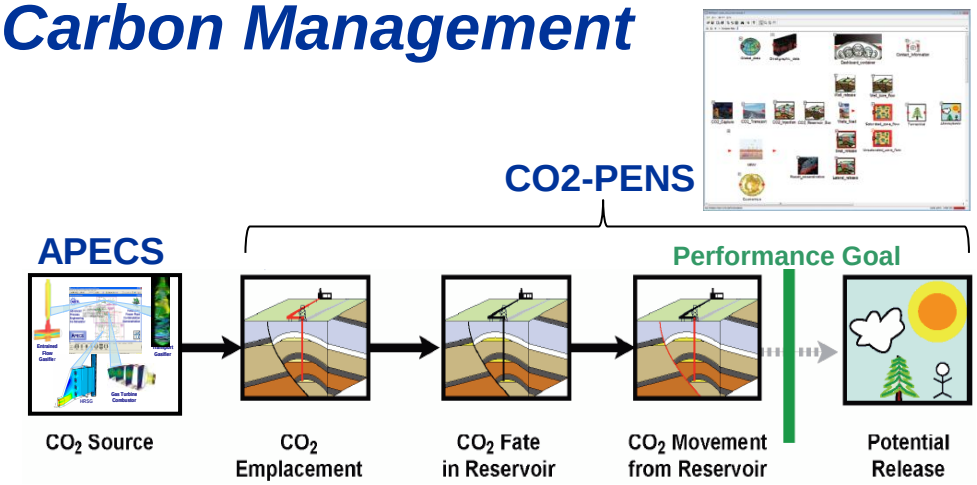
APECS Co-Simulation

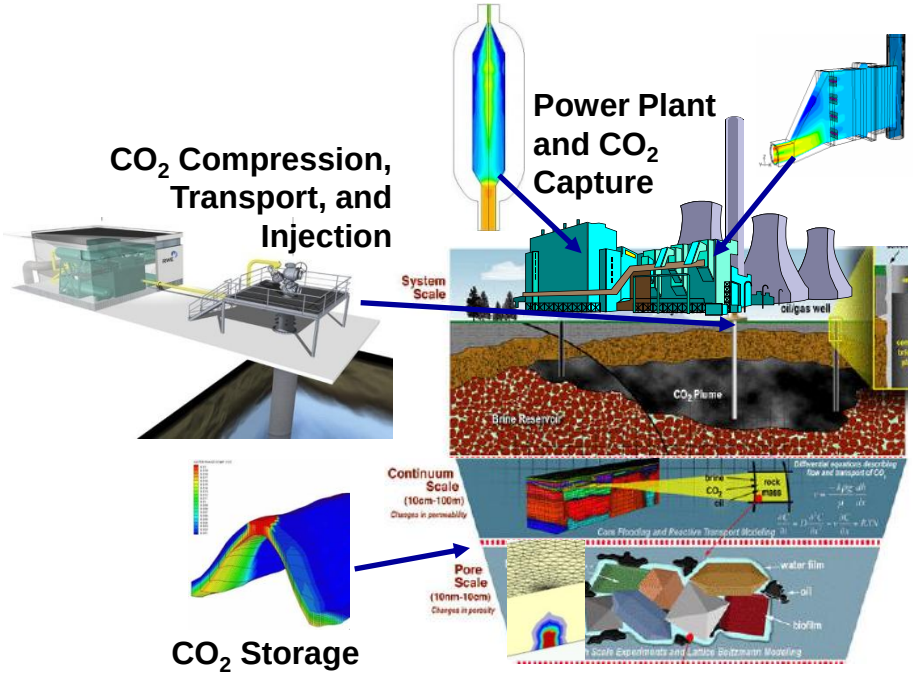
APECS/VE Collaboration

APECS Future Work

Extension to Carbon Management

- **Integrate APECS power plant co-simulations with high-fidelity simulations and ROMs for:**
  - CO_2 compression
  - CO_2 transport/pipelines
  - CO_2 injection
  - CO_2 storage sites (reservoirs)
- **Collaborate with LANL to couple APECS with CO_2-PENS***
  - Monte Carlo simulation software solution for evaluating environmental and economic impacts of geologic CO_2 sequestration
  - Los Alamos National Laboratory
- **Applications**
  - Site selection
  - CO_2 lifecycle management
  - Risk/performance assessment



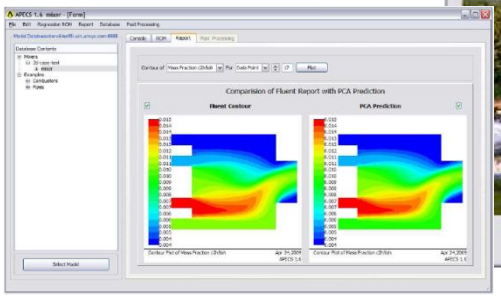


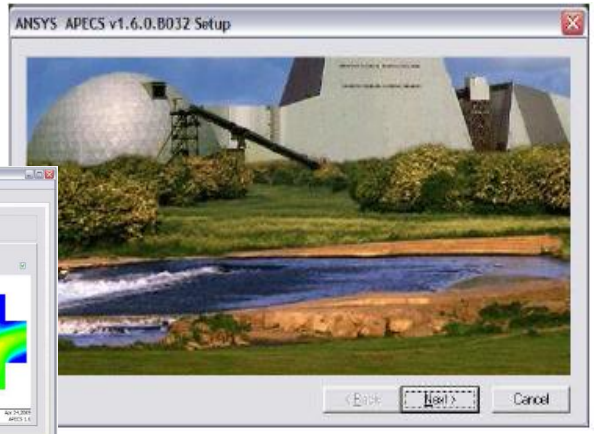
** Pawar, R. and D. Wildman, "A National Plan for Assessing the Risks of Engineered Geologic Storage of CO_2." LA-UR-08-2644, Los Alamos National Laboratory, National Energy Technology Laboratory (2008).*

APECS Future Work

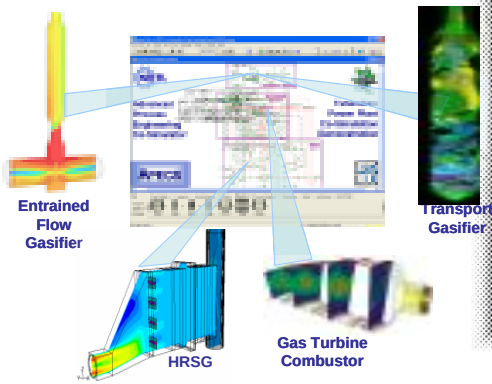
Wednesday, October 21, 2009 (2:30am-5:00pm)

- **APECS Development 2009/2010**
  John Widmann, ANSYS Inc.



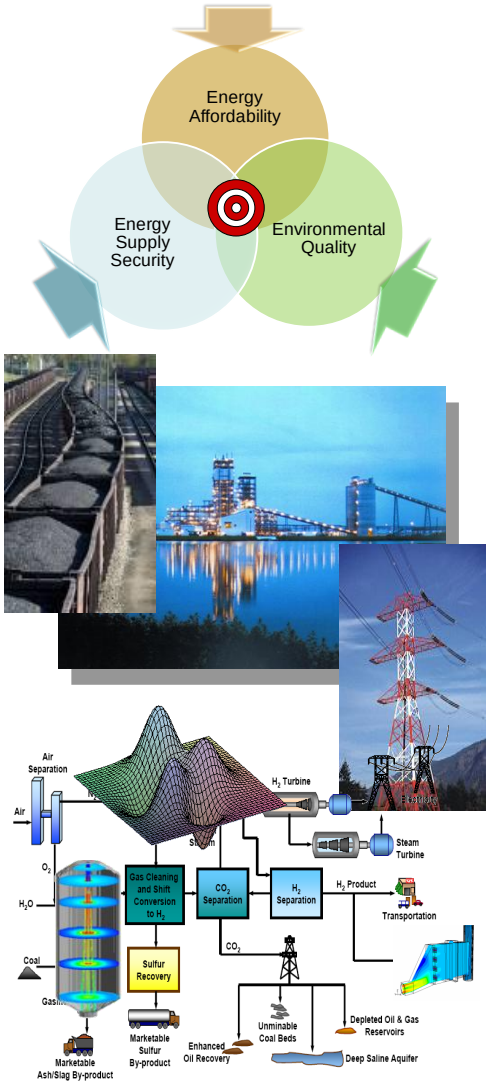


- **APECS Roadmapping Session**
  Ronald Breault, NETL
  Steve Zitney, NETL



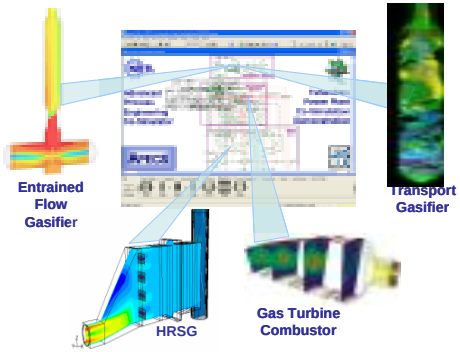
Concluding Remarks

- Meeting the increasing demand for clean, affordable, and secure energy is arguably the most important challenge facing the world today.
- Fossil fuels can play a central role in a portfolio of carbon-neutral energy options provided CO_2 emissions can be dramatically reduced by capturing CO_2 and storing it safely and effectively.
- Fossil energy industry faces the challenge of meeting aggressive design goals for next-generation power plants with CCS.
- Process designs will involve large, highly-integrated, and multipurpose systems with advanced equipment items with complex geometries and multiphysics.

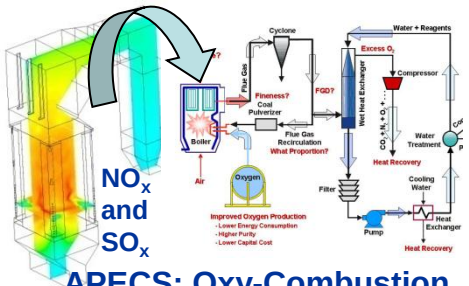


Concluding Remarks

- APECS is enabling software to facilitate effective integration, solution, and analysis of high-fidelity process/equipment (CFD) co-simulations.
- APECS helps to optimize fluid flow and related phenomena that impact overall power plant performance.
- APECS offers many advanced capabilities including ROMs, design optimization, parallel execution, stochastic analysis, and virtual plant co-simulations.
- NETL and its collaborative R&D partners are using APECS to reduce the time, cost, and technical risk of developing high-efficiency, zero-emission power plants with CCS.



APECS: IGCC with CCS

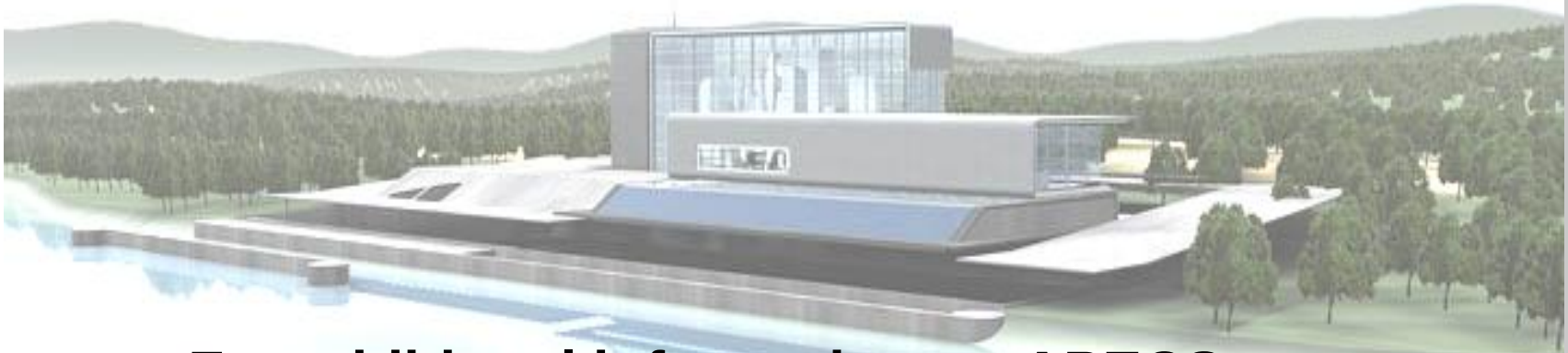


APECS: Oxy-Combustion

APECS/VE-Suite Collaboration

Thank You and Enjoy the Workshop

Questions?



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