



NATIONAL ENERGY TECHNOLOGY LABORATORY



Co-Simulation for Advanced Process Design and Optimization

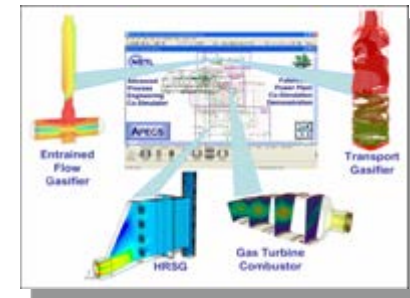
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Outline of Presentation

- **APECS Overview**
 - Workflow and Collaboration
 - Software Features and Capabilities
- **New Features**
 - Reduced Order Models (ROMs)
 - Design Optimization
- **APECS Co-Simulation Application**
 - Polygeneration Plant
- **Virtual Plant Co-Simulation**
 - APECS/VE-Suite Integration
- **Concluding Remarks**



APECS Co-Simulation



APECS/VE Collaboration

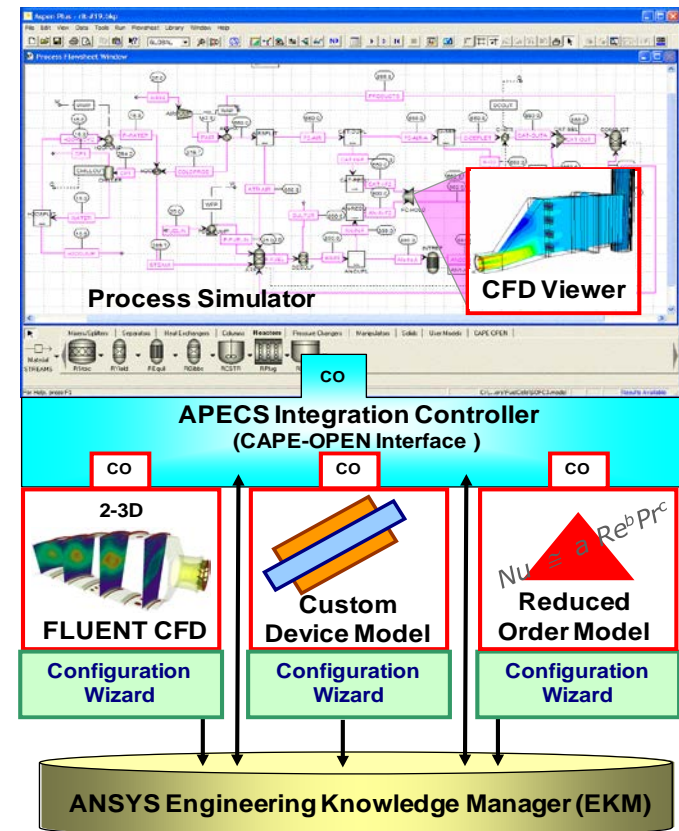


IGCC Power Plant

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



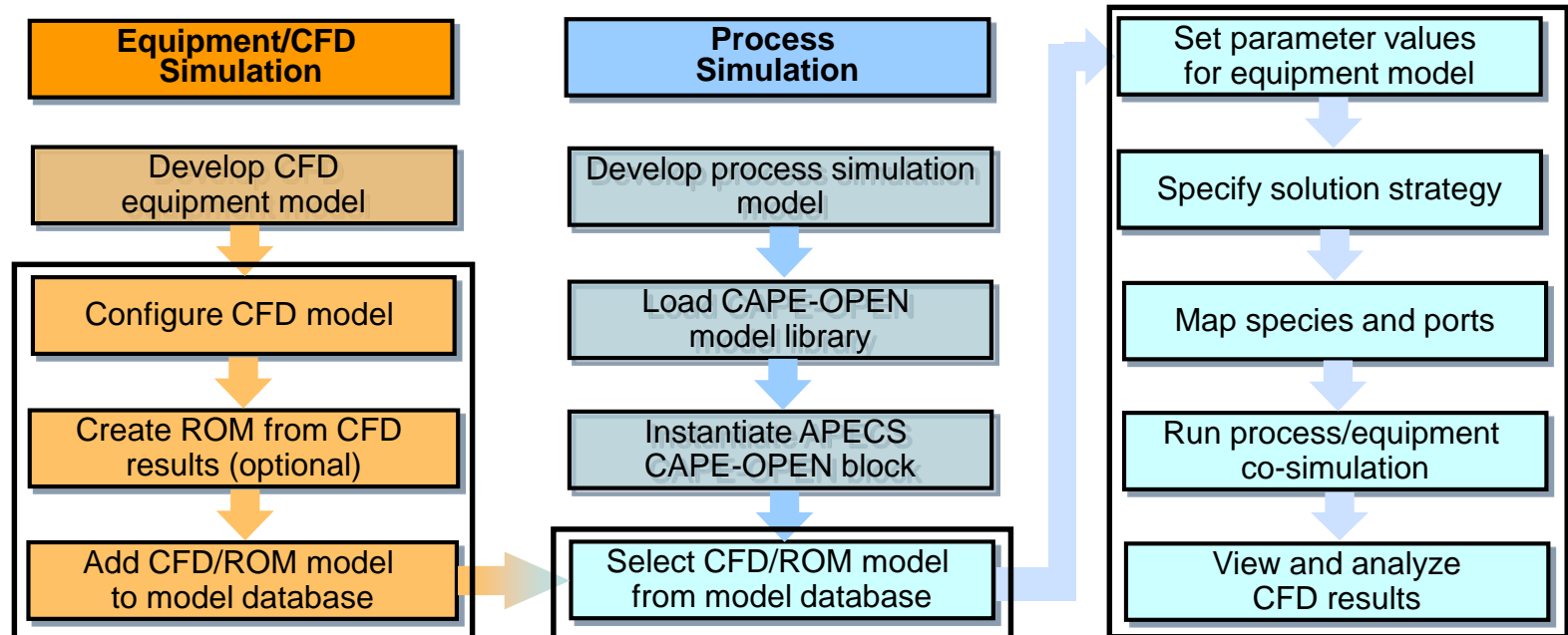
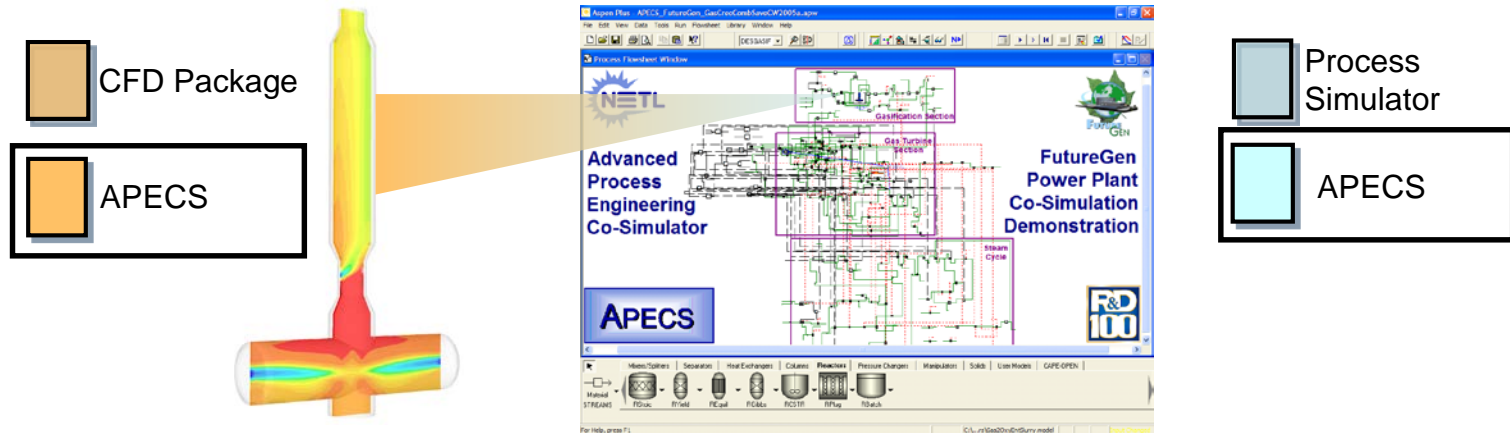
- 2004 R&D 100 Award (APECS)
- 2006, 2007 Federal Laboratory Consortium (FLC) Excellence in Technology Transfer Awards (APECS)
- 2008 R&D 100 Award (APECS with EKM)



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APECS Co-Simulation Workflow

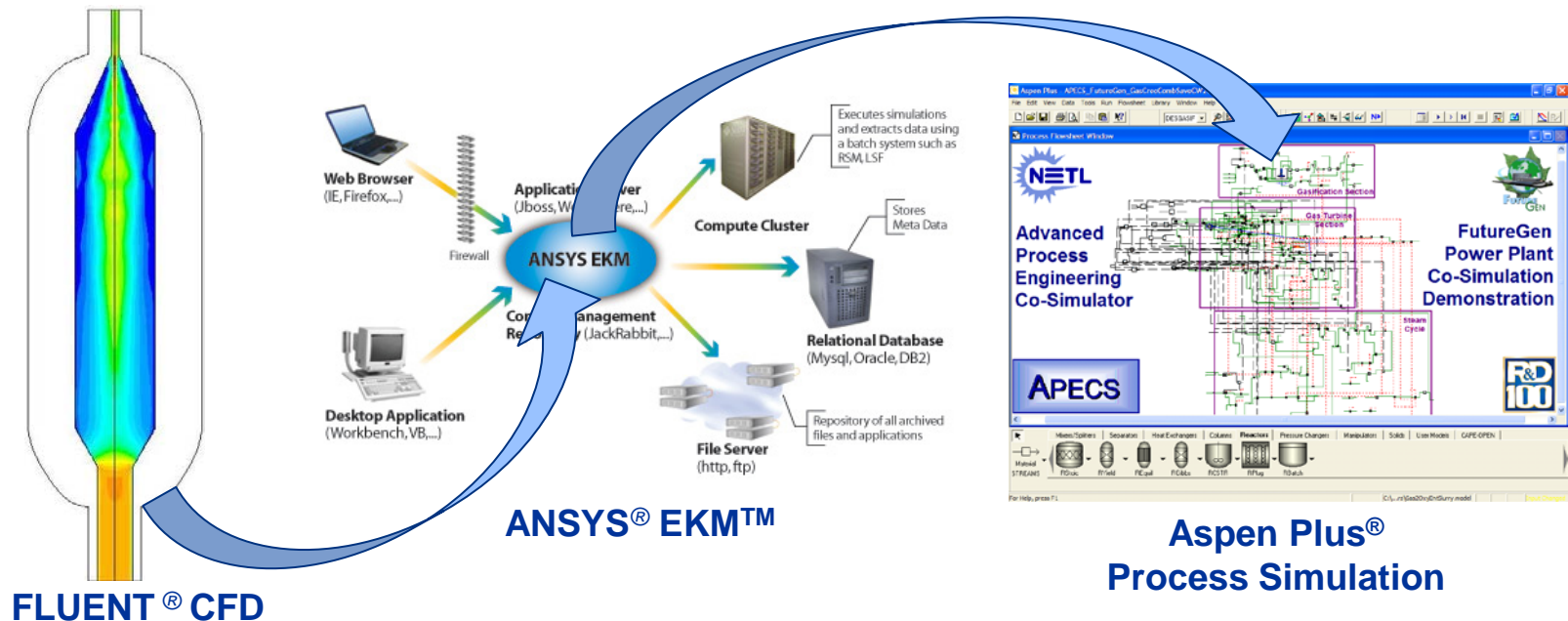
Separation of CFD and Process Simulation Tasks



APECS Co-Simulation Workflow

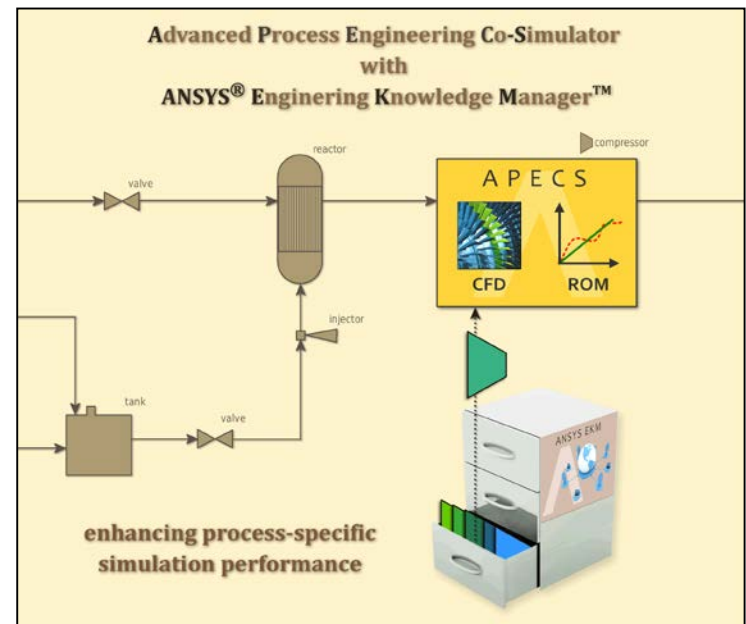
Seamless Integration of CFD/Process Simulation Tasks

- Fluid flow analyst creates CFD/CEMs/ROMs and uploads them to the model database
- Process engineer selects CFD/CEMs/ROMs from model database and seamlessly uses them in process simulation
- Process modeler does not need to be a CFD expert (and vice versa)



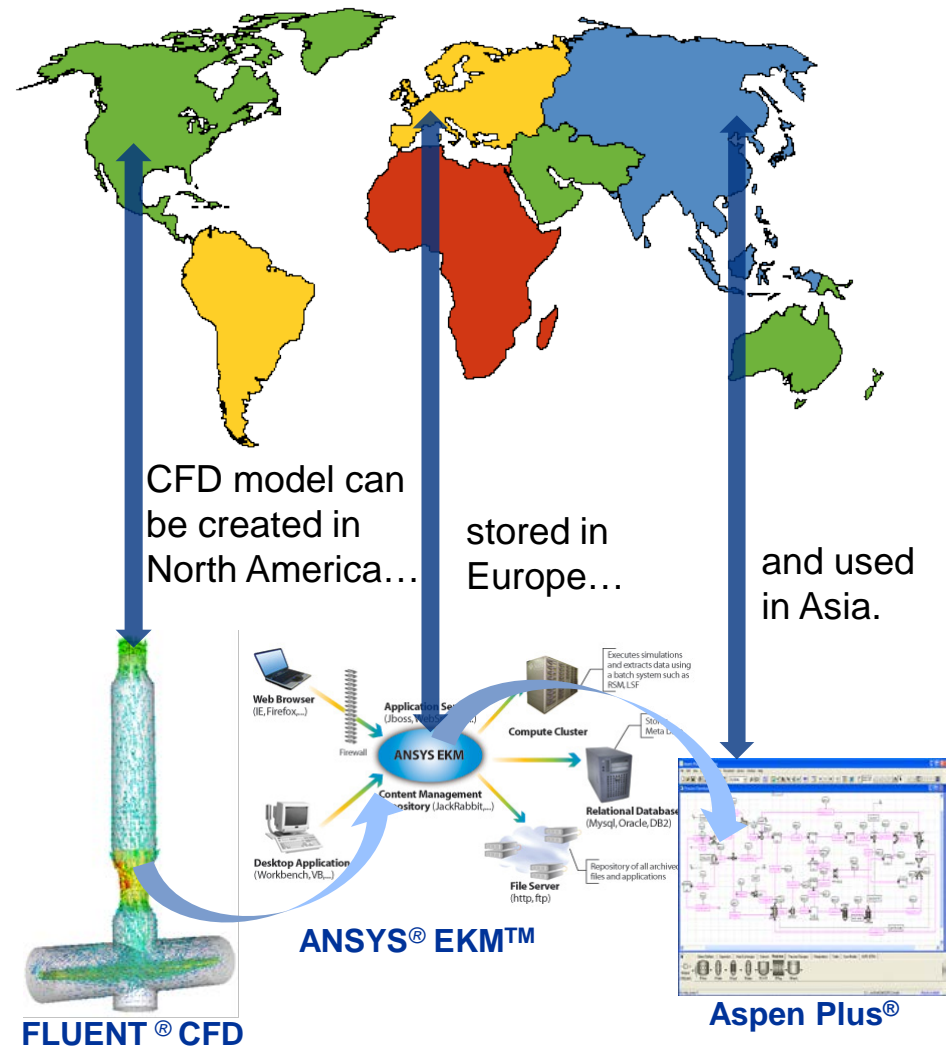
APECS with ANSYS® Engineering Knowledge Manager™ (EKM™)

- Manages equipment co-simulation data/model archiving and retrieval processes through the use of a single server-based, enterprise-wide repository
- Uses CAPE-OPEN software standard for plug-and-play model interoperability
- Benefits
 - Addresses challenge of managing the data, models, and engineering knowledge arising from advanced co-simulation applications
 - Improves workflow and asset utilization from plant innovation to design



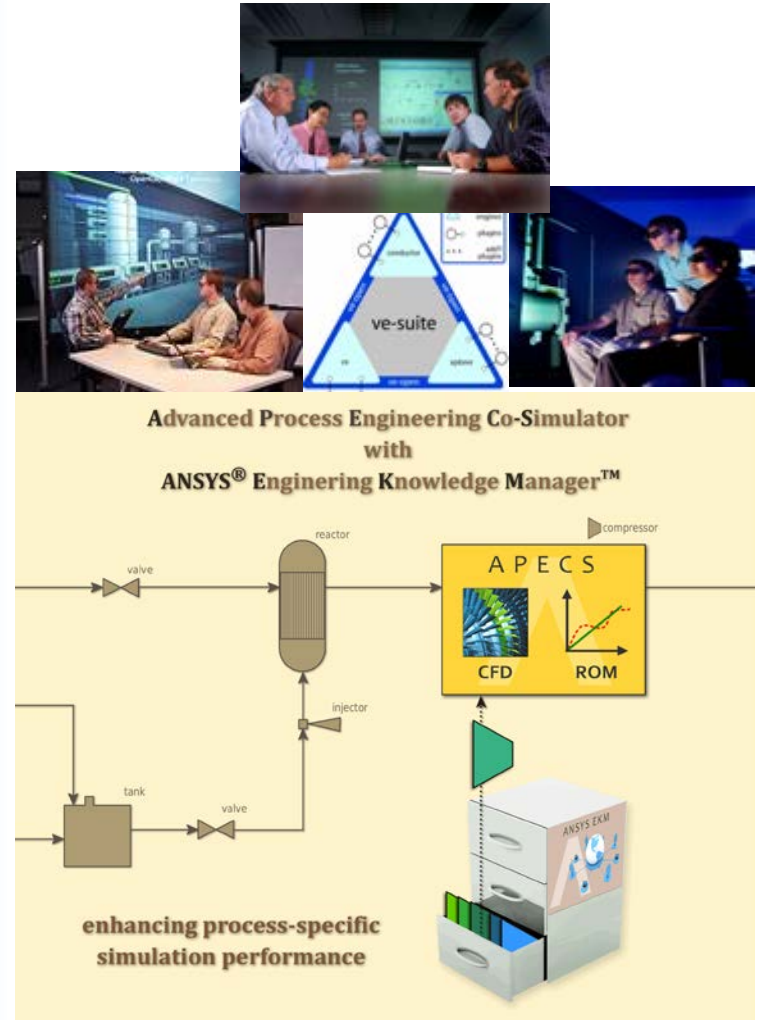
APECS with EKM™ Collaborative Co-Simulation

- Global companies can achieve new levels of simulation excellence and more rapid return on modeling investment through:
 - Better use of detailed equipment models to guide effective process systems engineering decisions
 - Collaborative detailed and process engineering solutions to enable global project execution



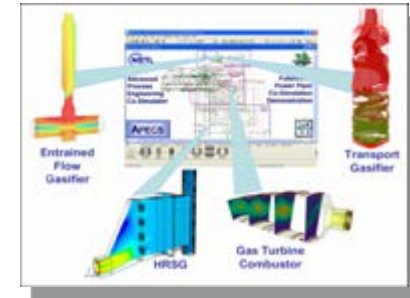
APECS Software Components and Features

- **Process Simulators**
 - CAPE-OPEN compliant
 - e.g., Aspen Plus®, HYSYS
- **Equipment Models and Database**
 - CAPE-OPEN compliant
 - ANSYS® EKM™
 - CFD: FLUENT®
 - CEMs: 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, Multi-objective Optimization
 - Geometry Parameterization
 - IGCC Cost Estimation
- **Distributed Execution**
 - CAPE-OPEN COM/Corba Bridge
 - Windows/Linux, Serial/Parallel
- **Virtual Engineering**
 - CFD Viewer (2D), Paraview (3D)
 - VE-Suite



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APECS Co-Simulation



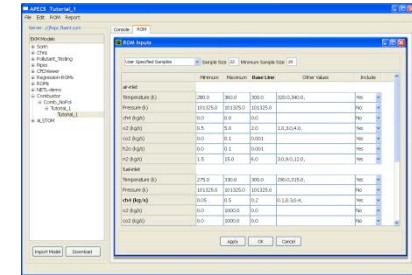
APECS/VE Collaboration



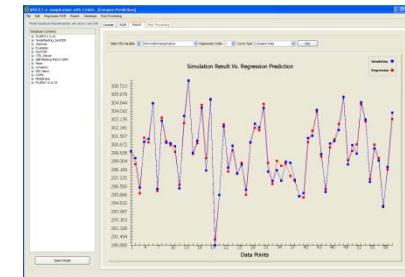
IGCC Power Plant

APECS Reduced Order Models (ROMs)

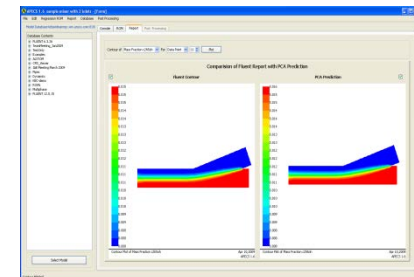
- APECS ROM Builder for automatic ROM generation from CFD simulations
- Design of experiments (DoE) using Latin Hypercube sampling
- CFD simulations can be run in advance and in serial/parallel on a remote cluster
- ROM methods include Regression and NN
- Principal Component Analysis (PCA) used to regenerate 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



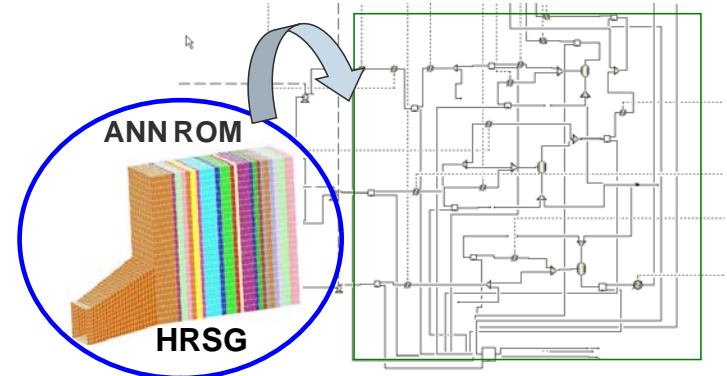
PCA-based ROM Contours

Industrial Applications of APECS ROMs

ALSTOM Power

- **IGCC with ANN ROM for HRSG**

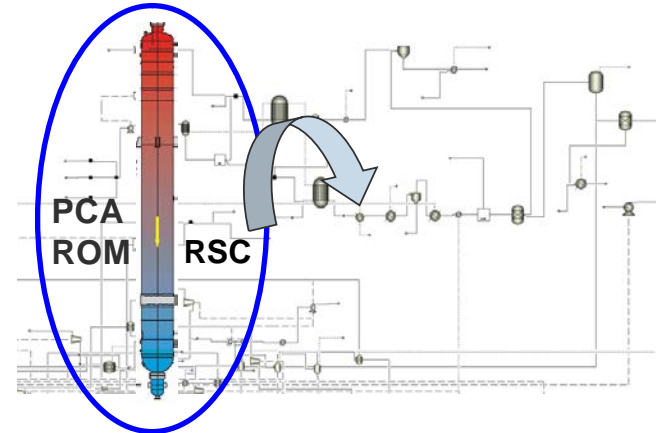
- Objective
 - Optimize heat integration
- CPU Time
 - FLUENT CFD: >1 CPU hour
 - ANN ROM: ~2 CPU seconds
- Convergence
 - Final ANN ROM flow rates for all streams are within 0.5% of FLUENT® CFD flow rates
- Reference
 - Osawe et al., AIChE Annual Meeting (2006)



250 MWe IGCC Co-Simulation with Artificial Neural Net (ANN) ROM for Heat Recovery Steam Generator (HRSG)

- **IGCC with PCA ROM for RSC**

- Objective
 - Analyze integration with gasifier via passing of multi-dimensional boundary conditions
 - Optimize heat integration with overall plant
 - Work in progress at ALSTOM Power

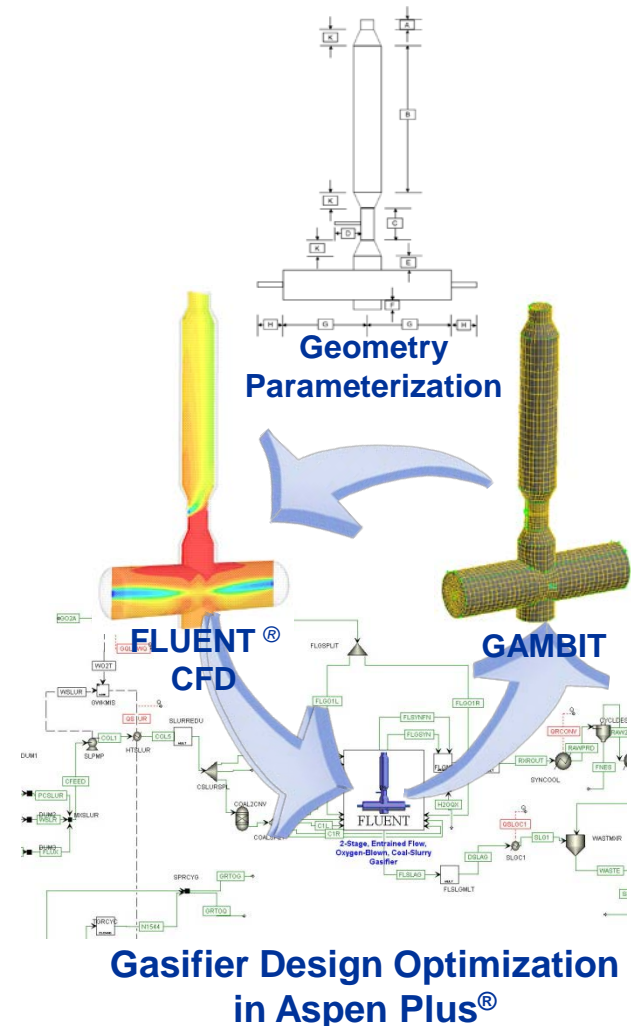
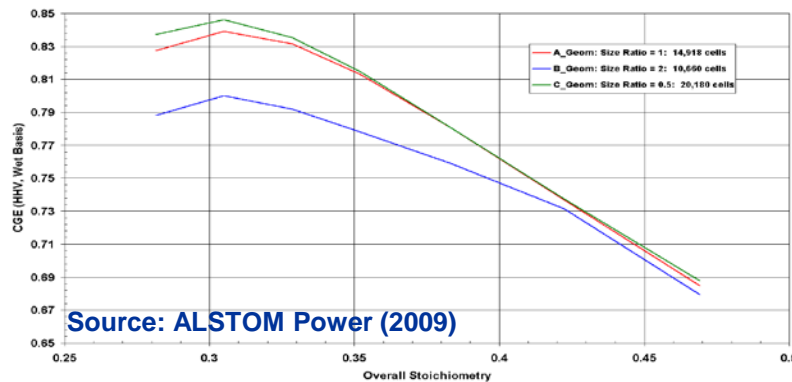


556 MWe IGCC Co-Simulation with ROM for Radiant Syngas Cooler (RSC)

APECS Geometry Parameterization

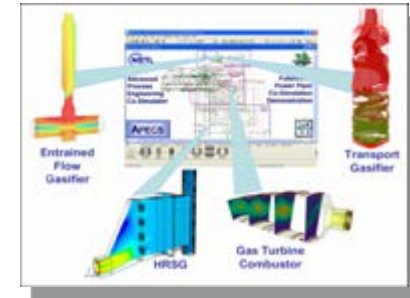
Design Optimization

- Conduct geometry parameterization studies within process simulation
- Automated regeneration of CFD geometry and mesh via CAPE-OPEN parameters
 - 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



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APECS Co-Simulation



APECS/VE Collaboration

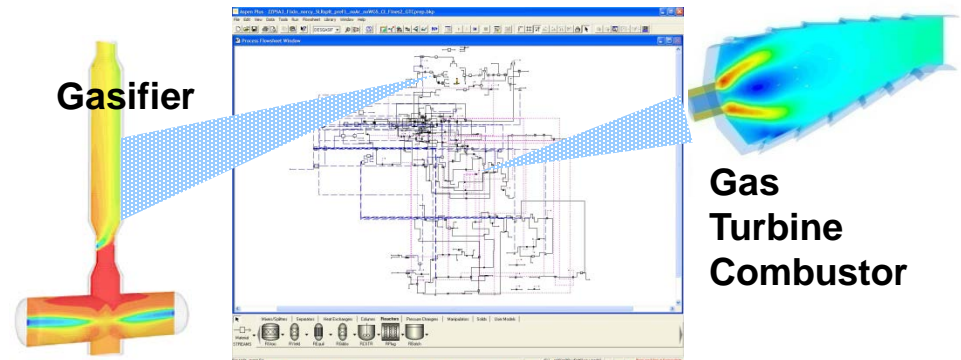


IGCC Power Plant

APECS Application – Polygeneration Plant *Power and Hydrogen Production with CO₂ Capture*

- **Process Simulation**

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

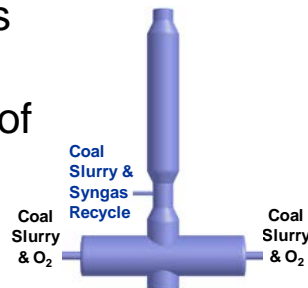


APECS Co-Simulation of Polygeneration Plant

- **CFD Simulations**

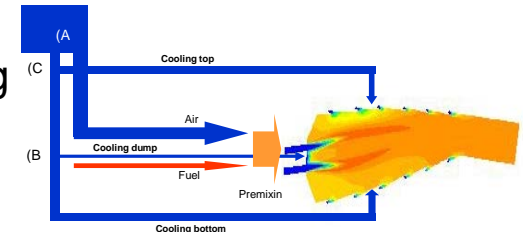
- Entrained-Flow Gasifier

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



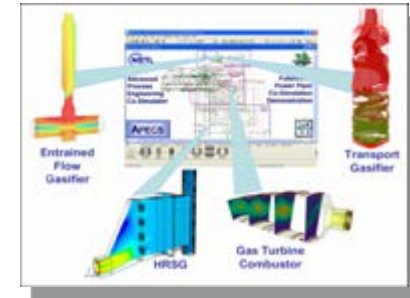
- Gas Turbine Combustor

- FLUENT® 3D/ROM
- Partially pre-mixed combustion
- Embedded in design spec loop to determine power/H₂ production
- Accurate calculation of GT inlet temperature
- Optimized cooling strategy to minimize NO_x



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APECS Co-Simulation



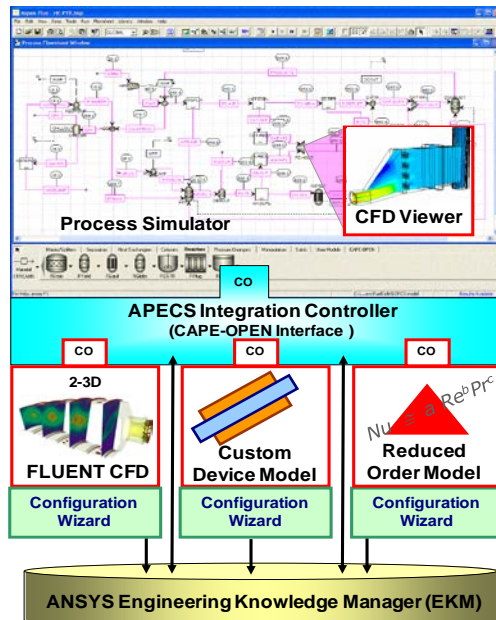
APECS/VE Collaboration



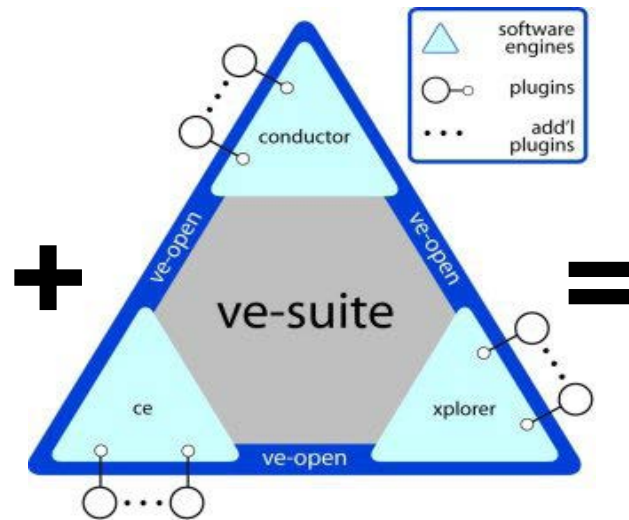
IGCC Power Plant

Virtual Power Plant Co-Simulation

APECS/VE-Suite Integration



APECS

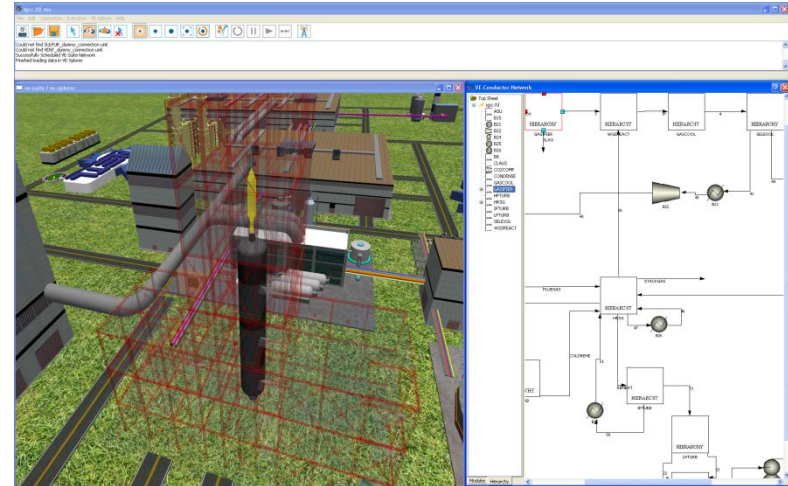


**Virtual Plant
Co-Simulation**

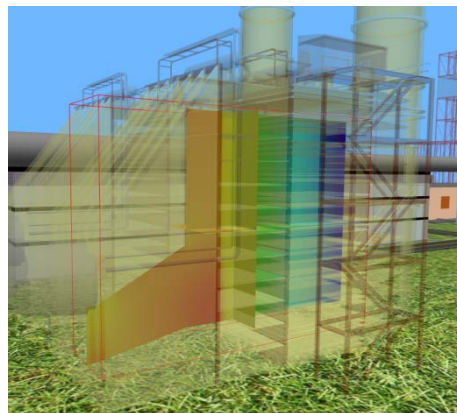
Virtual Power Plant Co-Simulation

APECS/VE-Suite Integration

- VE-Suite is a 3D immersive, interactive plant walkthrough environment for deployment of APECS process/CFD co-simulation results
- Provides graphic display of process simulation, CFD, and CAD data
- Supports hardware from the desktop to multi-wall caves
- Enables collaborative design and optimization for wide range of project stakeholders



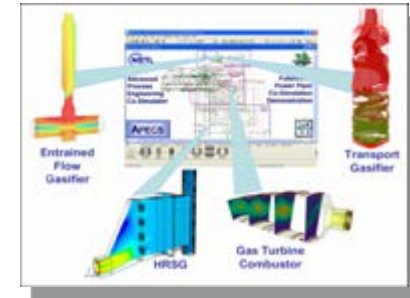
Using VE-Suite to analyze gasifier CFD data from APECS co-simulation of IGCC plant



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

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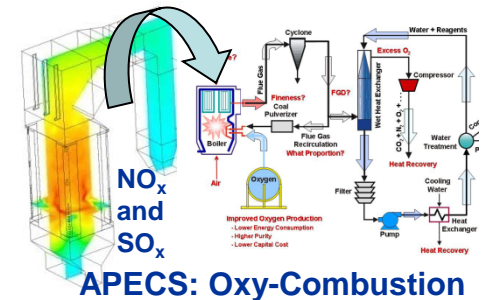
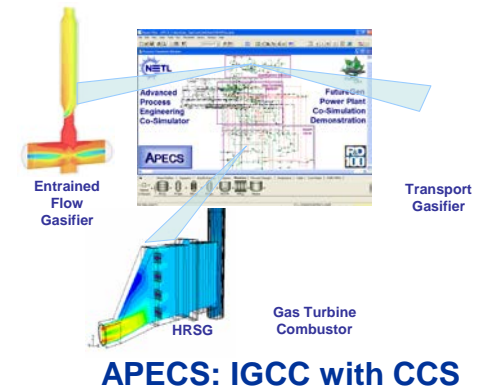
APECS/VE Collaboration



IGCC Power Plant

Concluding Remarks

- APECS is enabling software to facilitate effective integration, solution, and analysis of process/CFD co-simulations
- APECS helps to optimize fluid flow and related phenomena that impact overall plant performance
- APECS is built on the integrated access, workflow, and data services of EKM™
- APECS offers many advanced capabilities including ROMs, design optimization, stochastic analysis, parallel execution, and virtual plant co-simulations
- 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