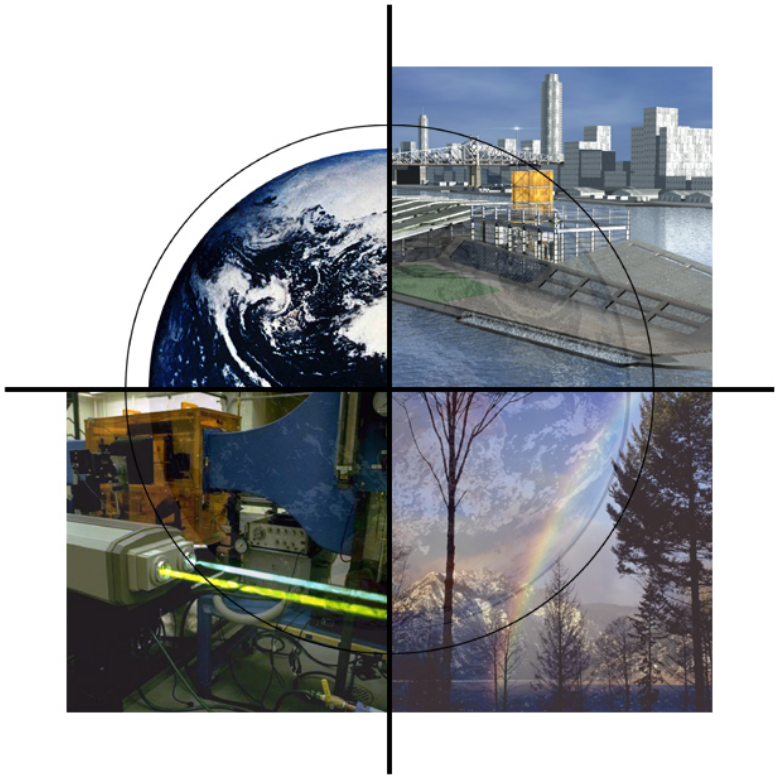
CAPE-OPEN Integration for Advanced Process Engineering Co-Simulation



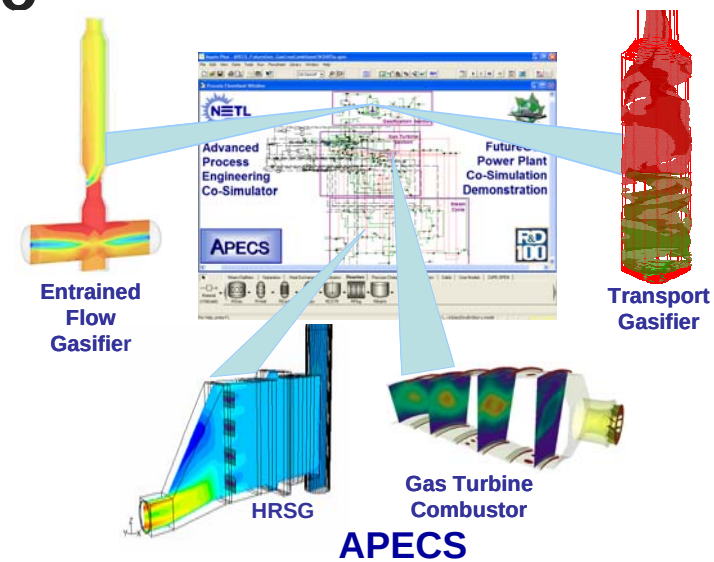
2nd Annual U.S. CAPE-OPEN Meeting
May 25-26, 2005
Morgantown, WV

Stephen E. Zitney
Research Group Leader
Device-Scale & Systems Modeling

National Energy Technology Laboratory
Morgantown, WV

Outline of Presentation

- Motivation
- Advanced Process Engineering Co-Simulator (APECS)
- Use of CAPE-OPEN in APECS
- APECS FutureGen Plant Demo
- Concluding Remarks
- Additional CAPE-OPEN Requirements for APECS



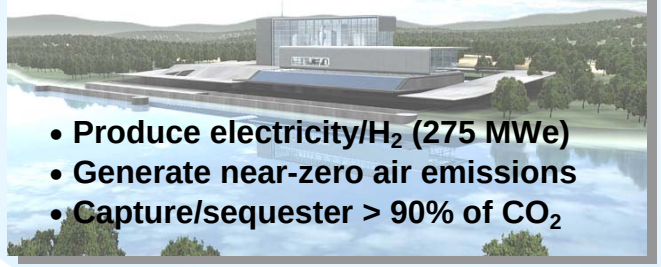
Motivation

Fuel Cells

Carbon Sequestration

FutureGen

- $1B, 10-year demonstration project
- Coal-fired, gasification-based plant

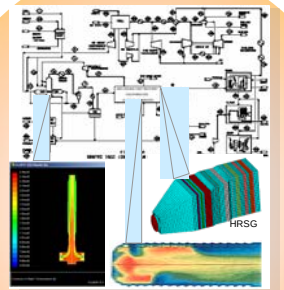


- Produce electricity/H_2 (275 MWe)
- Generate near-zero air emissions
- Capture/sequester > 90% of CO_2

Gasification with Cleanup & Separation

H_2 Production

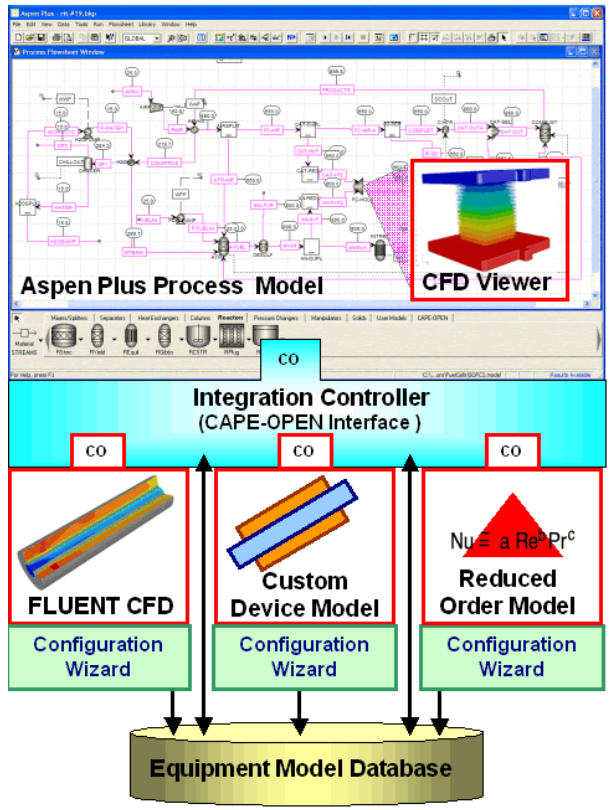
Optimized Turbines



Systems Analysis & Integration

Advanced Process Engineering Co-Simulator (APECS)

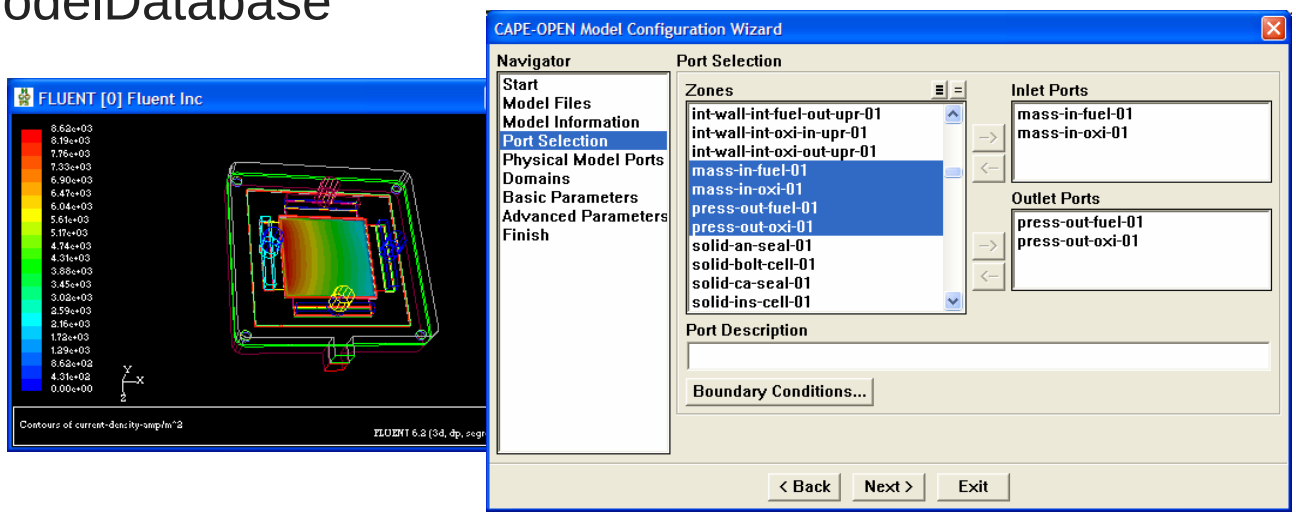
- **Equipment/Process Co-Simulation**
  - Computational fluid dynamics (CFD)
  - Custom equipment models
  - Reduced order models (ROMs)
- **High-Performance Options**
  - Computationally inexpensive ROMs
  - Parallel/distributed simulation
- **Advanced Visualization**
  - Post-processing of CFD results
  - 3D Immersive plant walk-through
- **CAPE-OPEN Software Standard**
  - Unit operations
  - Thermodynamics/Physical properties
  - Reaction kinetics



APECS Software Integration Framework

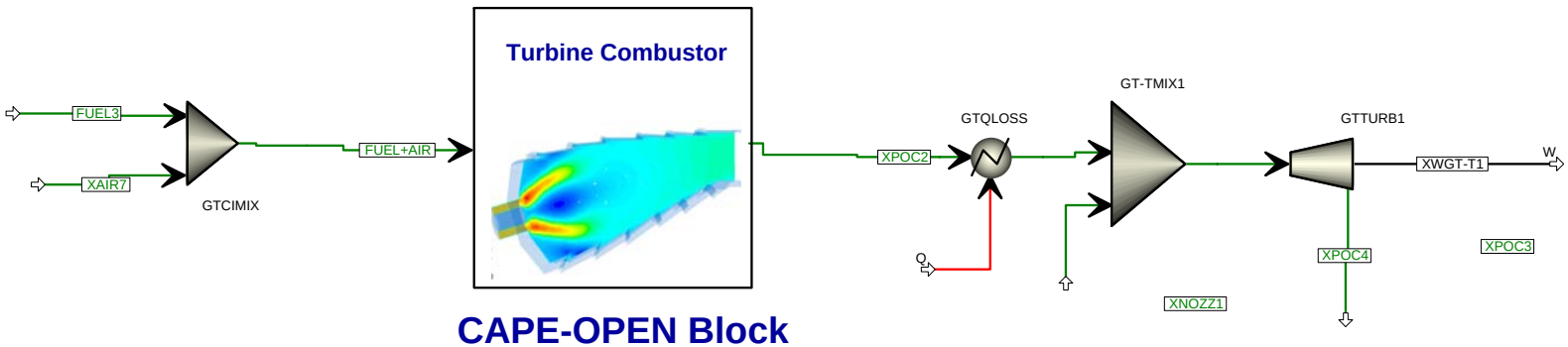
Use of CAPE-OPEN in APECS
Configuration Wizards

- **Custom/CFD Configuration Wizards**
  - Prepare equipment/CFD models as CAPE-OPEN (CO) models for use in CO-compliant simulators
  - Define CO ports (e.g., BCs, physical model ports)
  - Define CO model and solver parameters (e.g., current and voltage for fuel cell, maximum CFD iterations)
  - Generate model and solver XML files for use by the ModelDatabase



Use of CAPE-OPEN in APECS
Unit Operation

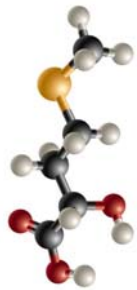
- CAPE-OPEN unit operation block for accessing equipment/CFD models from Model Database using Model Selection GUI
- Model Edit GUI for specifying CO parameter values and solution strategy
- Process streams connected to CO ports
- Bi-directional exchange of process stream data (F, x_i, T, P) at flow boundaries
- Integrated averages at CFD outlet boundaries

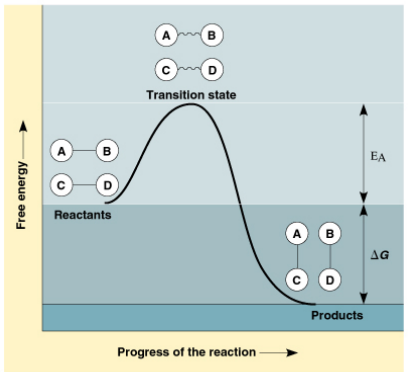


CAPE-OPEN Block

Use of CAPE-OPEN in APECS
Physical Properties and Reactions

- Automatic data transfer from process simulator to CFD equipment model
- Physical properties
  - Temperature-dependent (i.e., C_p, μ, ρ, k)
  - Constant (i.e., h_0 , s_0, MW)
- Reactions
  - Stoichiometry (i.e., species, coefficient, rate exponent)
  - Power-law parameters (i.e., pre-exponential factor, activation energy, temperature exponent)





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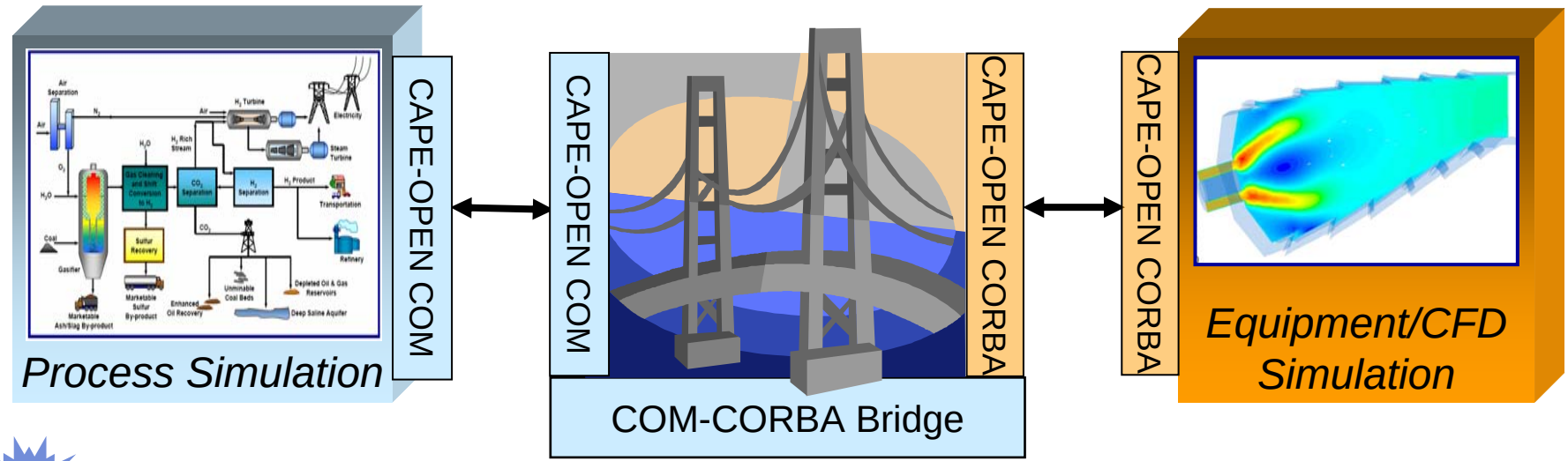
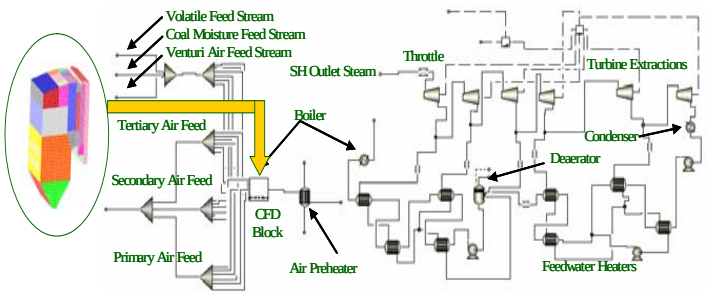
Use of CAPE-OPEN in APECS
COM-CORBA Bridge

- **CO-Compliant COM-CORBA Bridge Architecture**
  - Process simulation on local Windows system
  - Equipment simulation on remote Windows/Linux system in serial/parallel

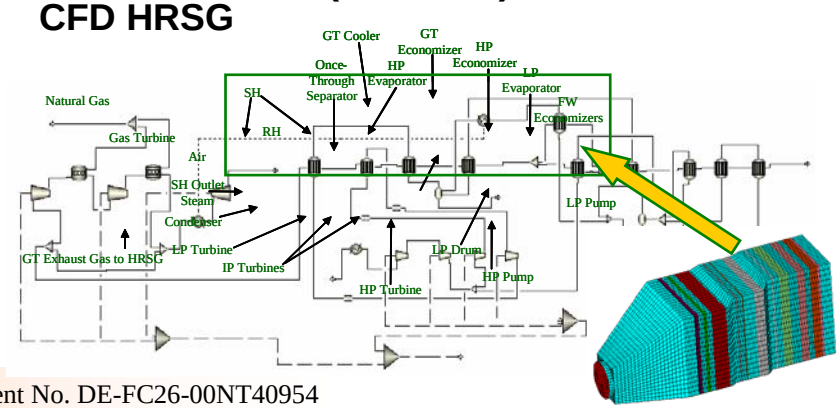


APECS Power Generation Applications

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

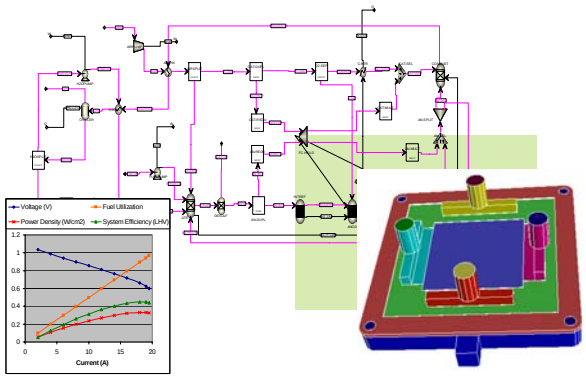


- **ALSTOM NGCC (250MWe) with 3D CFD HRSG**

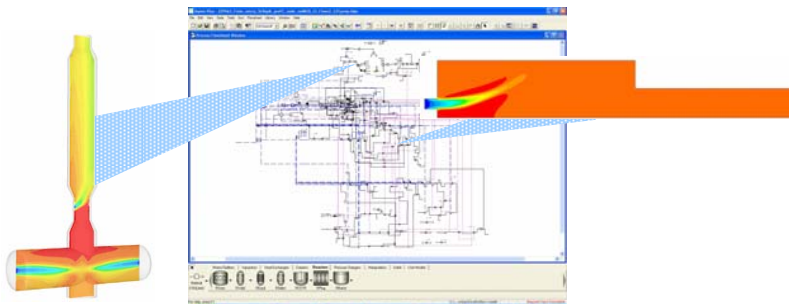


NETL-Fluent Inc Cooperative Agreement No. DE-FC26-00NT40954

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

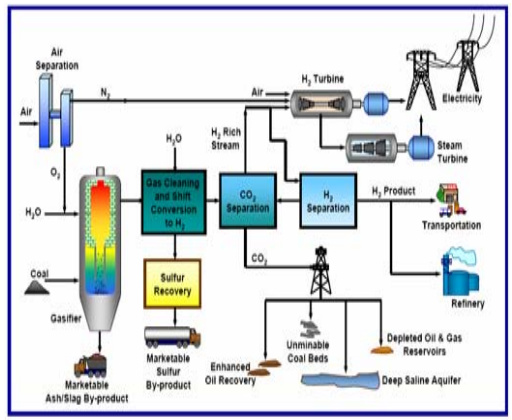


- **FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor**

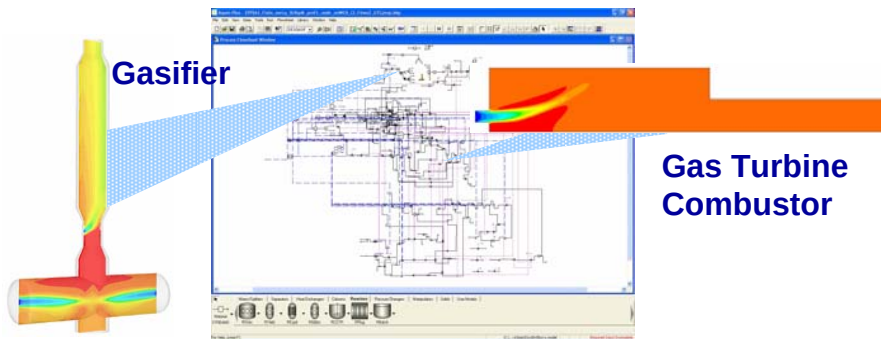


APECS Demonstration of FutureGen Plant

- **FutureGen Power Plant**
  - IGCC with CO_2 capture and H_2 production (~250 MWe)
  - Two-stage, oxygen-blown, entrained flow gasifier
  - GE 7FB gas turbine (GT)
  - Pressure-swing adsorption for generating H_2 stream
- **APECS Co-Simulation**
  - Process Simulation
    - Aspen Plus® steady-state
    - All major plant sections, over 250 unit operations
    - Design specification on GT inlet temperature
  - CFD Simulations
    - FLUENT® 3D Gasifier
    - FLUENT® 2D GT Combustor



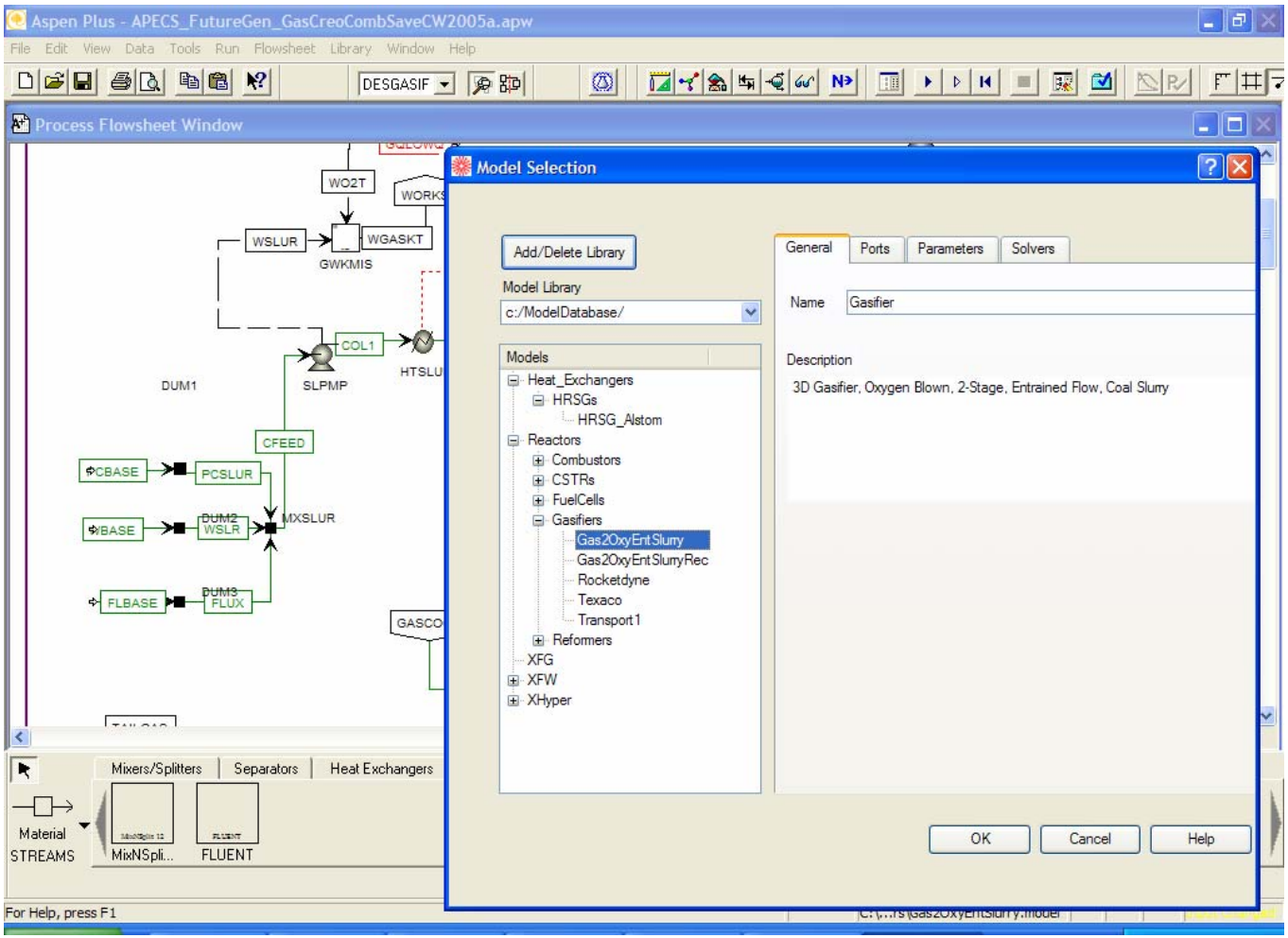
FutureGen Process Diagram



APECS Co-Simulation of FutureGen Power Plant

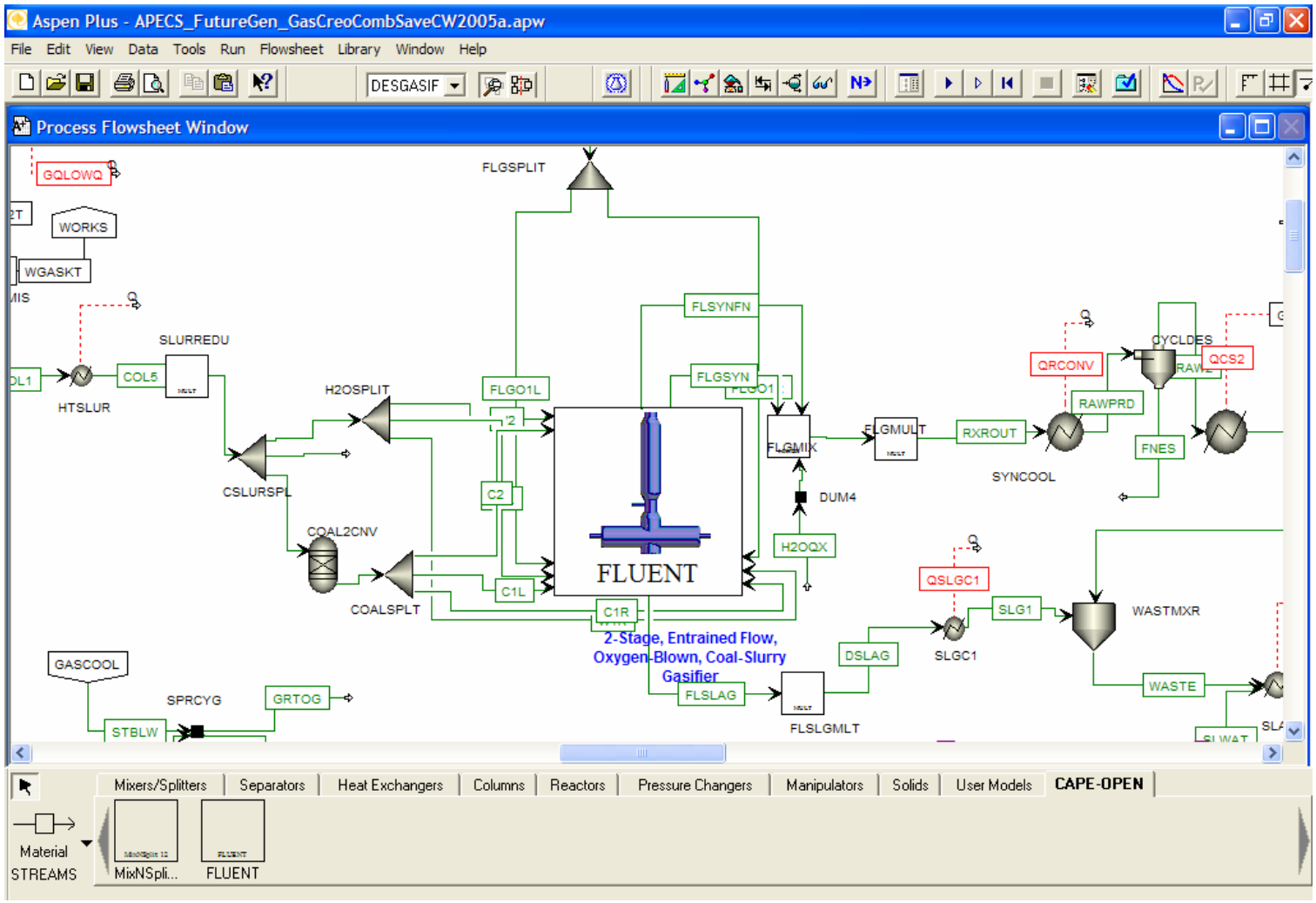
APECS Demonstration of FutureGen Plant

Model Selection GUI for CFD/Equipment Model Database



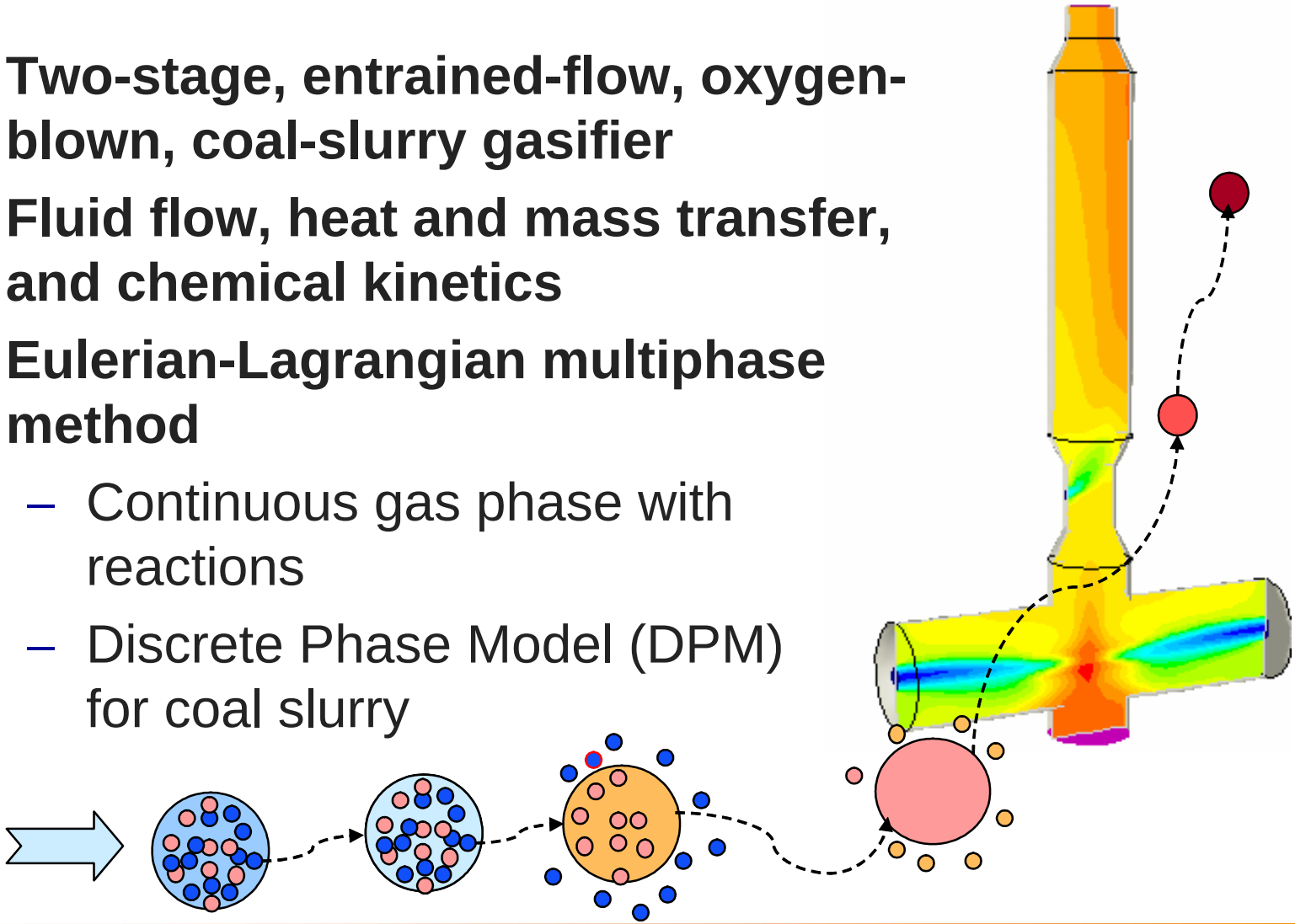
APECS Demonstration of FutureGen Plant

Instantiation of CAPE-OPEN Gasifier CFD Model



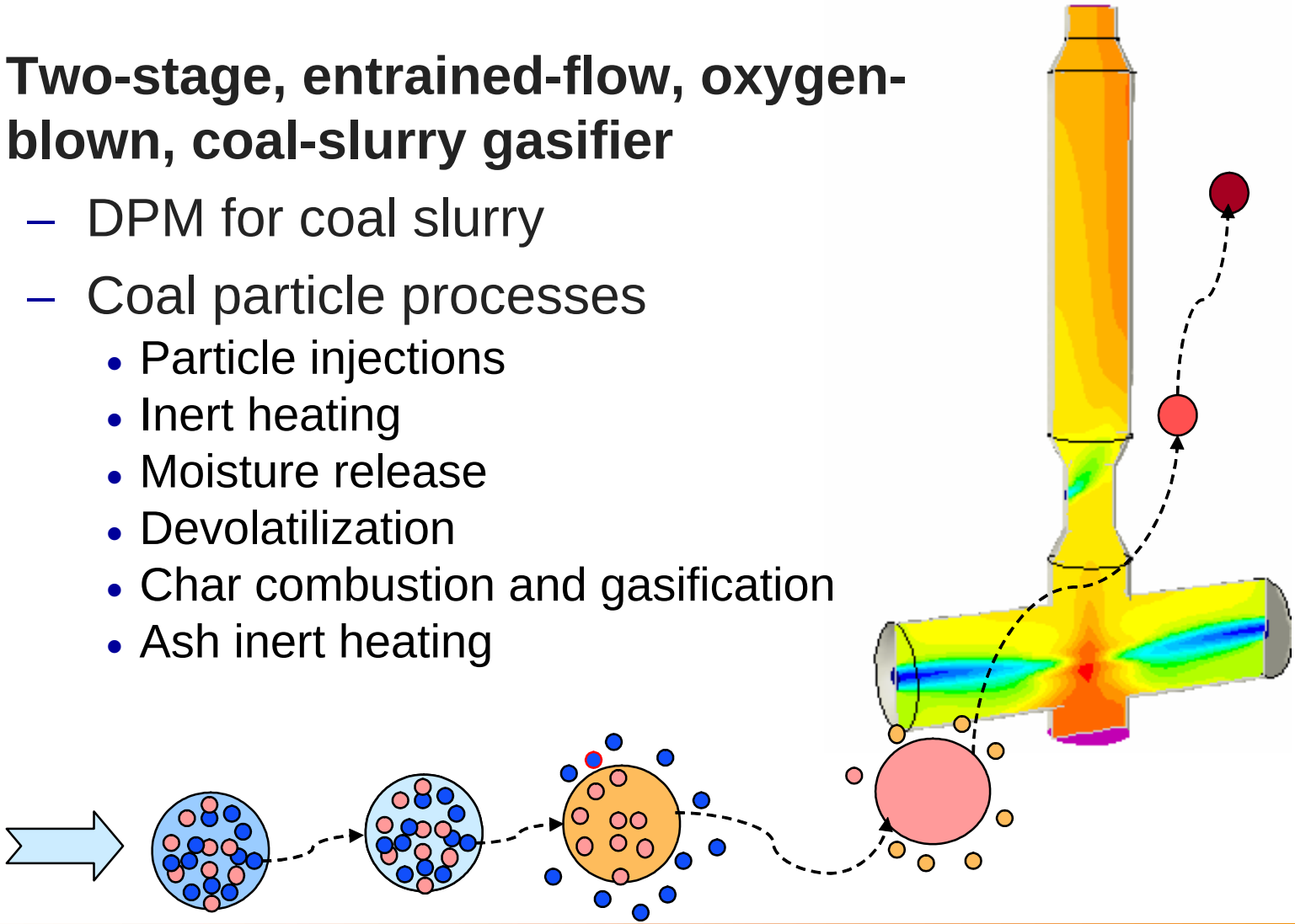
Gasification CFD Model

- **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



Gasification CFD Model

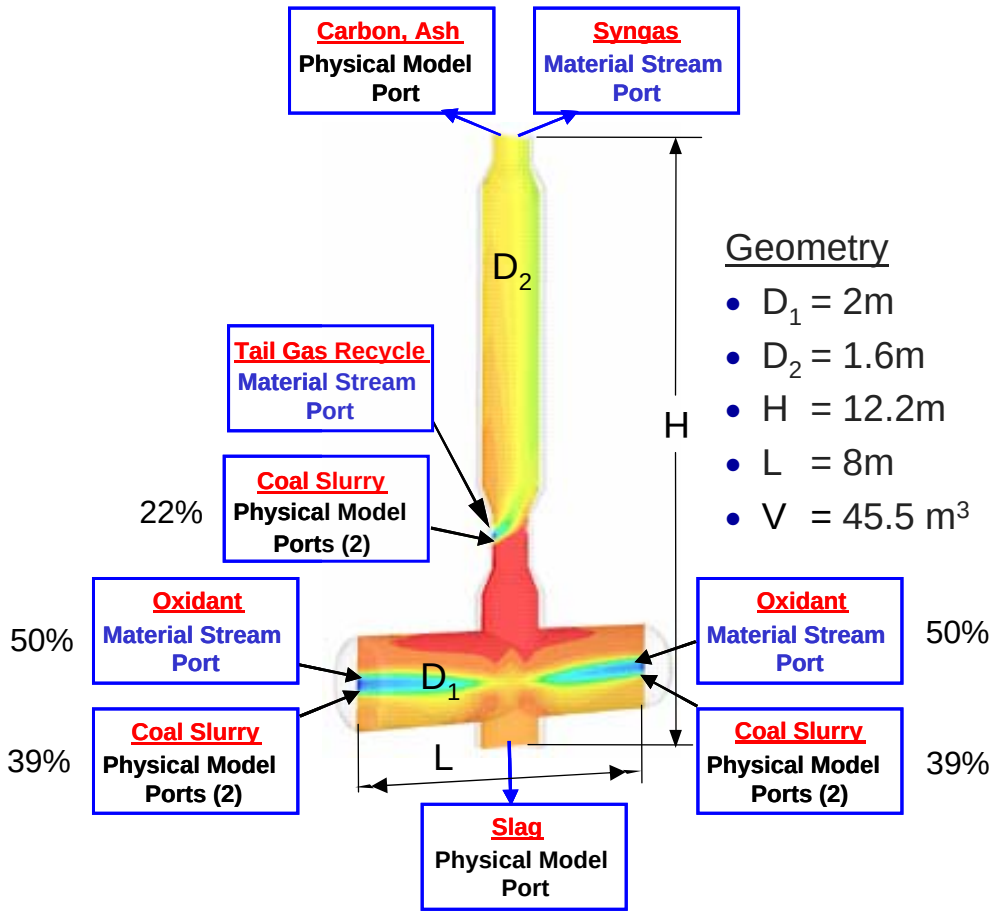
- **Two-stage, entrained-flow, oxygen-blown, coal-slurry gasifier**
  - DPM for coal slurry
  - Coal particle processes
    - Particle injections
    - Inert heating
    - Moisture release
    - Devolatilization
    - Char combustion and gasification
    - Ash inert heating



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

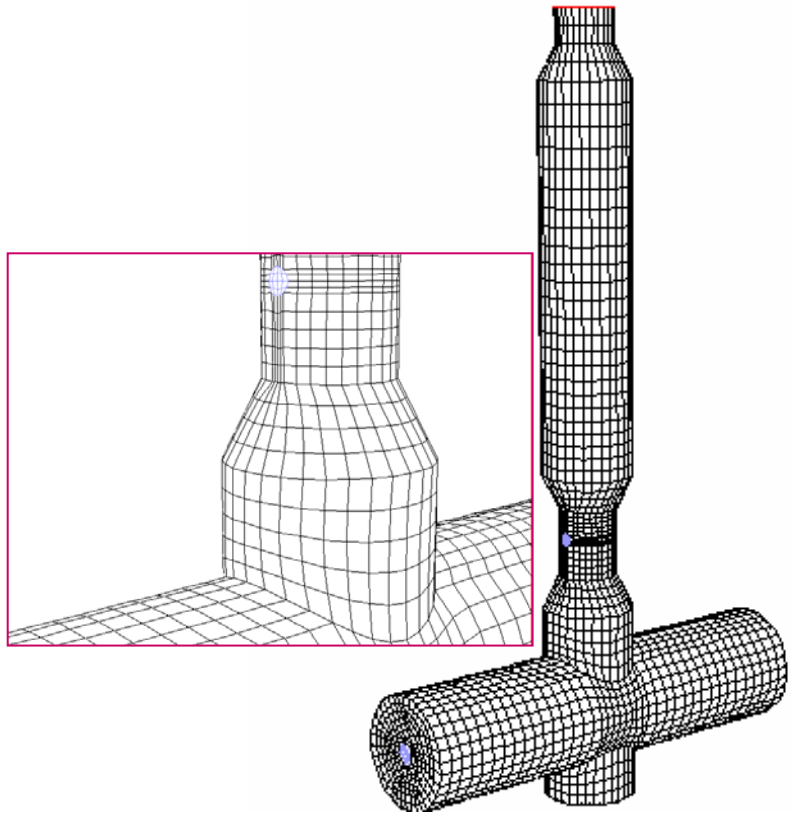


Geometry

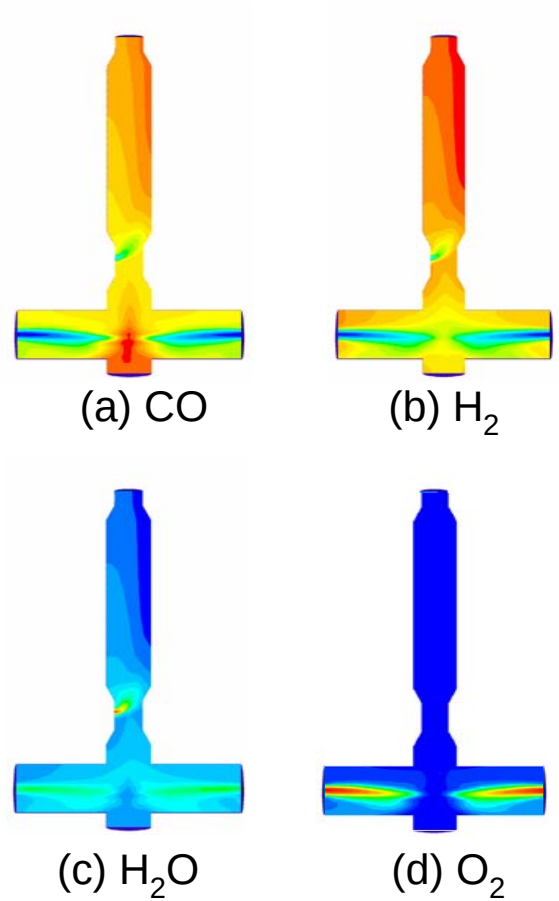
- D_1 = 2m
- D_2 = 1.6m
- H = 12.2m
- L = 8m
- V = 45.5 m^3

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

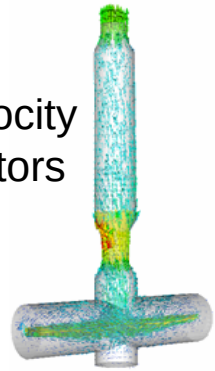


APECS Results: Entrained Flow Gasifier



Species mole fraction contours at the center plane

Velocity vectors



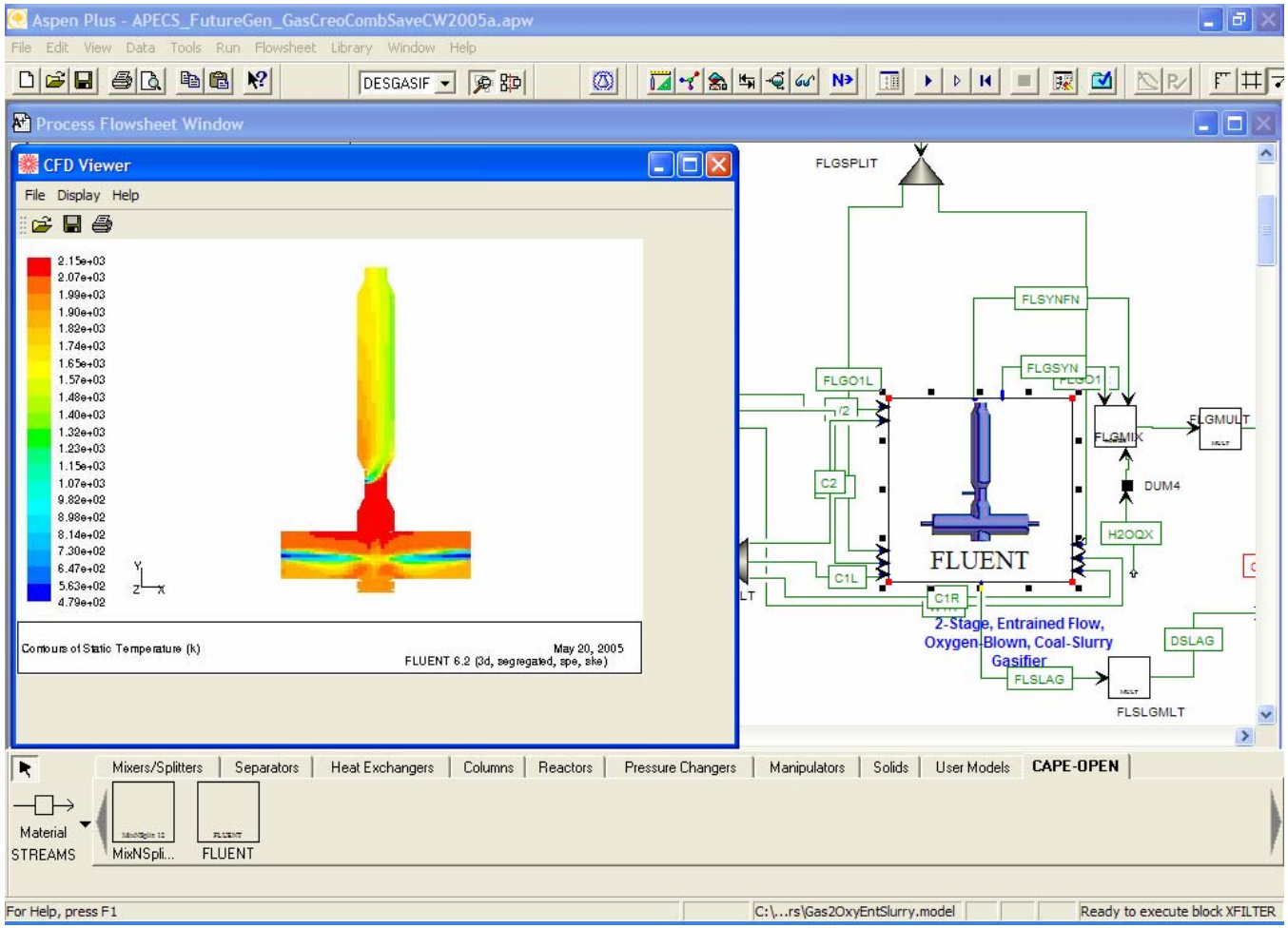
Char Conversion
- 1st Stage
  - 100%
- 2nd Stage
  - 86%

Synthesis Gas 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

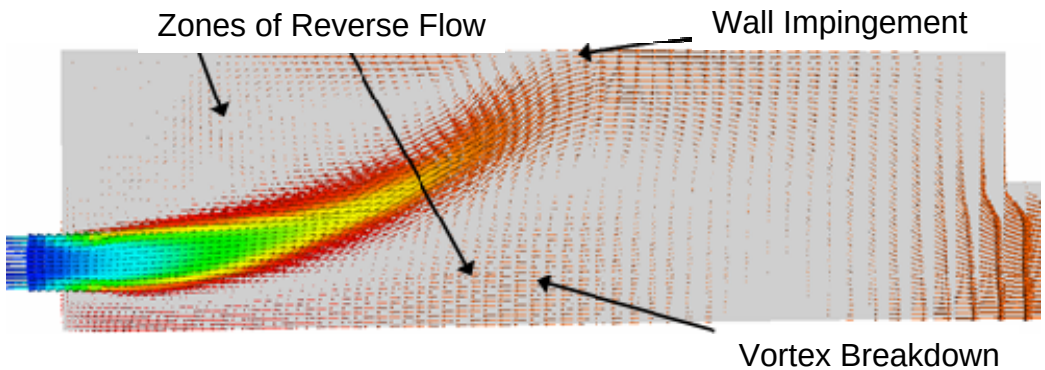
APECS Demonstration of FutureGen Plant

CFD Viewer – Gasifier Temperature Contours



APECS Results: Turbine Combustor

Velocity vectors colored by temperature for the main chamber



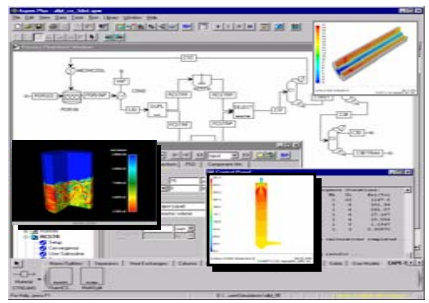
Inlet and outlet stream compositions

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	---	---

Concluding Remarks

- CAPE-OPEN standard facilitates the seamless integration of CFD and process simulation in APECS

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



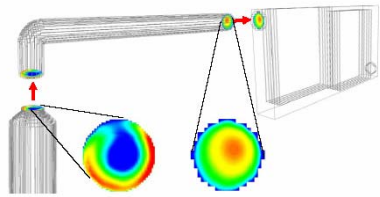
- NETL is using APECS to reduce the time, cost, and technical risk of developing high-efficiency, zero-emission power plants

Use of CAPE-OPEN in APECS

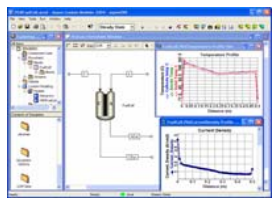
Additional Requirements

- **Solids Handling**
  - CISOLID/NC substreams
  - Particle size distributions (PSD)
  - Coal analysis data
- **Multi-Dimensional BCs**
  - Transfer 1-2D boundary conditions
  - For use in coupling multiple CFD models
- **Dynamics**
  - CAPE-OPEN specification for modular and equation-oriented simulators
  - Vendor support in commercial simulators
- **Flowsheet Interconnectivity**
  - Get list of blocks and streams, as well as their interconnectivity
  - Handle flowsheet section and hierarchy block concepts

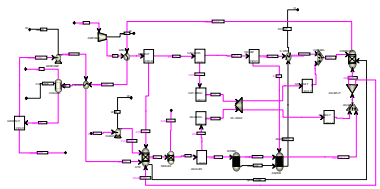
Coal



CFD Models in Series (REI)



Dynamic Simulation



Flowsheet Interconnectivity