

## CAPE-OPEN Integration for Advanced Process Engineering Co-Simulation

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### ABSTRACT

This paper highlights the use of the CAPE-OPEN (CO) standard interfaces in the Advanced Process Engineering Co-Simulator (APECS) developed at the National Energy Technology Laboratory (NETL). The APECS system uses the CO unit operation, thermodynamic, and reaction interfaces to provide its plug-and-play co-simulation capabilities, including the integration of process simulation with computational fluid dynamics (CFD) simulation. APECS also relies heavily on the use of a CO COM/CORBA bridge for running process/CFD co-simulations on multiple operating systems. For process optimization in the face of multiple and some time conflicting objectives, APECS offers stochastic modeling and multi-objective optimization capabilities developed to comply with the CO software standard. At NETL, system analysts are applying APECS to a wide variety of advanced power generation systems, ranging from small fuel cell systems to commercial-scale power plants including the coal-fired, gasification-based FutureGen power and hydrogen production plant.

### INTRODUCTION

The Department of Energy's (DOE's) National Energy Technology Laboratory (NETL) is collaborating with its R&D technology partners to develop the Advanced Process Engineering Co-Simulator (APECS). APECS is as an integrated software suite that combines process simulation, high-fidelity computational fluid dynamics (CFD), immersive and interactive 3D plant walk-through virtual engineering, and advanced analysis capabilities for the improved design, operation, and optimization of process engineering systems (Zitney *et al.*, 2006).

For users in the process and energy industries, APECS offers process/CFD co-simulations that provide the necessary level of detail and accuracy required for engineers to analyze and optimize the coupled fluid flow, heat and mass transfer, and chemical reactions that drive overall plant performance and efficiency. At NETL, APECS facilitates for the first time the efficient and systematic integration of process simulation with CFD models of key power plant equipment items, such as combustors, gasifiers, syngas coolers, steam and gas turbines, heat recovery steam generators, and fuel cells. By coupling process/CFD co-simulations with advanced visualization and high-performance computing, APECS also offers opportunities for exploiting virtual plant simulation to reduce the time, cost, and technical risk of developing high-efficiency, zero-emission power plants such as the DOE's FutureGen plant (Zitney, 2005a).

In the APECS system, plug-and-play model interoperability is achieved by using the process industry-standard CAPE-OPEN (CO) interfaces (Osawe, 2005; Zitney, 2005b; Syamlal *et al.*, 2004). The CO standard for process simulation was developed as an international collaborative among leading process industry companies, academic institutions, and software vendors (Braunschweig and Gani, 2002). The standard provides interfaces for process unit operations, physical properties, reaction kinetics, and numerical solvers. The interfaces are open, multi-platform, available free of charge, and supported by

many of the leading commercial process simulators. Today the CAPE-OPEN Laboratories Network (CO-LaN, [www.colan.org](http://www.colan.org)) is the internationally recognized, user-driven organization for the management, exploitation, and promotion of the CO standard. A recent review of industrial applications of the CO standard, including a brief discussion of the process/equipment co-simulation solution described here, can be found in Pons (2003).

This paper describes the APECS integration framework for combining process simulation and CFD software using the CO interfaces. The application of APECS to process and fossil energy systems is also highlighted.

## APECS FEATURES AND CAPABILITIES

The APECS integration framework uses the CAPE-OPEN (CO) software interfaces for unit operations, physical properties, and reaction kinetics. The methods of the CO unit operation interfaces enable the seamless use (e.g., Initialize, Edit, Calculate, Load, Save) of equipment models in the process flowsheet. The interfaces also facilitate the bi-directional exchange of stream information (flow rate, temperature, pressure, and compositions) between the process simulator and the equipment model. For CFD models, the multi-dimensional boundary conditions are mapped automatically to process streams and vice versa. The CO physical property interface is used to transfer constant or temperature-dependent physical properties (e.g., density, viscosity, heat capacity, thermal conductivity, molecular weight) from the process simulator to the equipment models. Similarly, the CO reaction kinetics interface facilitates the automatic transfer of reaction stoichiometry and power-law parameters from the process simulator to the equipment models.

As shown in Figure 1, the hierarchy of unit operation/equipment models used by APECS ranges from high-fidelity CFD models to custom engineering models (CEMs) to fast reduced-order models (ROMs). The CFD models provide a detailed and accurate representation of a wide variety of process equipment items, while CEMs are typically engineering models that calculate mass and energy balances, phase and chemical equilibrium, and reaction kinetics. ROMs are a class of equipment models that are based on pre-computed CFD solutions over a range of parameter values, but are much faster than CFD models. For example, the APECS system currently provides for automatically generating and using a ROM based on multiple linear regression to demonstrate the concept (Syamlal and Osawe, 2004). Future ROM solvers will include non-linear regression, neural networks (Osawe et al., 2006), and proper orthogonal decomposition.

The APECS system drastically reduces the time and effort required to couple CFD-based equipment models into plant-wide simulations. Today, design engineers can use APECS to integrate CFD models into a process simulation in a matter of an hour or two using the CO software interfaces and easy-to-use configuration wizards. The wizards are used

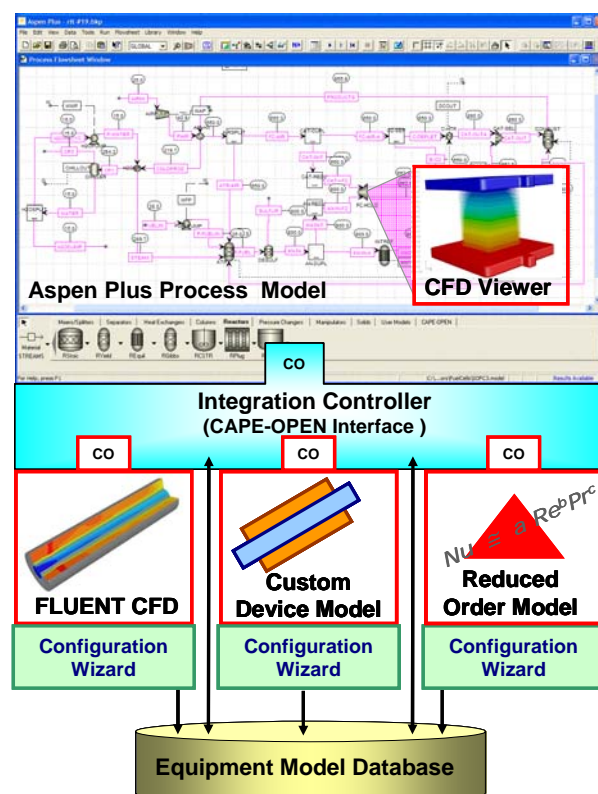


Figure 1. APECS Software Integration Framework

primarily to specify which equipment model parameters and stream ports to make available in the process simulator. Examples of common equipment parameters include the current and voltage for a fuel cell, or the impeller speed for a stirred tank reactor.

Use of the CAPE-OPEN standard ensures that any equipment model can be linked to the CO-compliant APECS framework. An easy-to-use template is provided for wrapping equipment models as CO-compliant models that can be executed in the APECS environment. The configured equipment models are stored in an equipment model database. After placing the detailed equipment model on the process flowsheet, a model selection GUI can be used to browse and select a suitable equipment model from the model database. Upon selection, the corresponding ports and parameters are automatically associated with the equipment model instantiated on the flowsheet. This then allows the process engineer to connect the appropriate number of input and output streams to the equipment model ports. The model edit GUI enables the process engineer to modify equipment parameters. The initial parameter values correspond to those set in the configuration wizard.

The model edit GUI is also used to define a solution strategy consisting of a combination of one or more models/solvers ranging from fast ROMs to CEMs to rigorous CFD models. For example, one common solution strategy is to have the initial flowsheet iterations use a fast ROM and the final iterations use a high-fidelity CFD model. In this way, a process engineer can customize solution strategies from a hierarchy of models/solvers, thereby achieving the desired trade-off between speed and accuracy.

If a parallel solver is available for a given equipment model, improved performance can be achieved by using multiple processors that may be executing on the same computer, or on different computers in a network. In the model edit GUI, an APECS user can specify the number of processors to be used, message passing protocol, and hosts file containing the list of computers on which to run the parallel job. The CAPE-OPEN COM/CORBA bridge implementation in APECS allows process simulations running under the Windows operating system to use equipment models running locally/remotely and serially/in parallel on Linux clusters and/or supercomputers (Zitney, 2004).

The APECS system also provides a wide variety of powerful analysis tools for optimizing overall plant performance (Zitney *et al.*, 2006). Design specifications are used to calculate operating conditions or equipment parameters to meet specified performance targets. Case studies are used to run multiple simulations with varying input. Sensitivity analysis shows how process performance varies with changes to selected equipment specifications and operating conditions. Optimization is used for maximizing plant efficiency, energy production, and process economics. For process optimization in the face of uncertain variables — such as feed flow rates, or fluctuating prices of raw materials — and multiple and some time conflicting objectives, APECS offers stochastic modeling and multi-objective optimization capabilities (Figure 2) developed to comply with the CO software standard (Subramanyan and Diwekar, 2006).

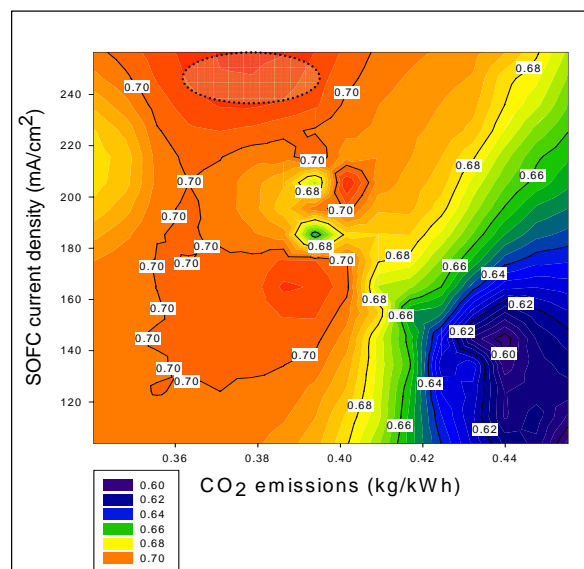


Figure 2. Multi-objective optimization trade-off surface between CO<sub>2</sub> emissions, fuel cell current density and efficiency for next-generation power plant





Research engineers at NETL are also developing APECS co-simulations to analyze potential FutureGen plant configurations (Zitney et al., 2006). In a recent demonstration case, the FutureGen co-simulation combined a plantwide Aspen Plus simulation with two FLUENT CFD-based equipment models, one for the entrained flow gasifier where fluid dynamics strongly affect synthesis gas quality and carbon conversion, and another for the gas turbine combustor where the blending of air and fuel is vital to gas turbine combustor performance and efficiency. Using APECS, Aspen Plus controls the co-simulation and automatically executes the gasifier and combustor CFD models as needed to converge the tail gas recycle loop and a design specification on the gas turbine inlet temperature. The design specification is met by manipulating the synthesis gas split between power production and hydrogen production. This co-simulation typically requires several hours of CPU time to converge on a single-CPU workstation. The turnaround time for the co-simulation is improved by running the computationally intensive CFD models in parallel on 2–8 CPUs of the Linux clusters at NETL and/or Pittsburgh Supercomputing Center.

The co-simulation applications described above illustrate how APECS is helping NETL engineers optimize the coupled fluid flow, heat and mass transfer, and related phenomena that drive overall system performance. By combining process simulation and CFD software, together with advanced visualization and high-performance computing, APECS provides the high-fidelity solution and analysis capabilities required to achieve the aggressive integration, environmental, and performance goals for advanced power generation systems such as the DOE's FutureGen plant.

## APECS R&D COLLABORATIONS

NETL initiated APECS development in 2000 with a four-year cooperative R&D project with Fluent and its collaboration partners, AspenTech, Alstom Power, and West Virginia University. In March 2005, U.S. Secretary of Energy, Samuel Bodman, announced that Fluent and Reaction Engineering International were awarded \$1.9M and \$0.5M APECS projects, respectively, as part of a portfolio of \$62.4 million for 32 clean coal research projects. The ongoing projects are focused on achieving the following APECS R&D objectives:

- Enhancement of APECS *ease-of-use* for configuring, managing, integrating, solving, and visualizing CFD-based equipment models within a CO-compliant process simulation environment.
- Demonstration of fast *reduced-order models* (ROMs) based on 2-3D CFD results.
- Integration of APECS power plant co-simulations to user-centered, interactive, hierarchical *visualization* environments at the immersive, 3D plant walkthrough level.
- Demonstration of a prototype *dynamic* APECS co-simulation capability for use in designing *control* strategies for advanced power plants.
- Development of a prototype *parallel-modular* solution approach in APECS for improving turnaround time for large-scale co-simulations involving the use of multiple high-fidelity, CFD-based equipment models.

Under the auspices of a U.S.-U.K. Memorandum of Understanding and Implementing Agreement (<http://us-uk.fossil.energy.gov/>) signed in November 2000, NETL is collaborating with the U.K.'s Virtual Plant Demonstration Model (VPDM) team, including Alstom Power U.K., Engineous Software, Fluent U.K., KS-Tech, ME Engineering, Mitsui Babcock, Process Systems Enterprise (PSE) Limited, RWE Innogy, and the University of Ulster. The main objective of the collaboration is to develop compatible, CAPE-OPEN standards-based software platforms for virtual power plant simulation for advanced fossil energy systems. The VPDM team is leveraging NETL's APECS technology to integrate high-fidelity FLUENT CFD equipment models into overall power plant models developed with PSE's gPROMS simulator (Williams, 2006). The APECS co-simulation tool will help the U.K. power generation and

associated industries to develop competitive power plant solutions and ultimately zero-emission technologies with significantly reduced development costs and technical risk.

In the research community, NETL is working in close cooperation with Carnegie Mellon University on the development of CO-compliant reduced-order models based on CFD results; Iowa State University and Ames National Laboratory on coupling process/CFD co-simulation to immersive 3D virtual engineering software (Rubin, et al., 2006); Vishwamitra Research Institute on CO-compliant stochastic analysis and multi-objective optimization capabilities for process/CFD co-simulation (Subramanyan and Diwekar, 2006); and Reaction Engineering International on the development of CO-compliant power plant equipment models including a CAPE-OPEN interface to the GateCycle software, which is widely used in the power generation industry for process modeling (Swensen, 2006).

## SUMMARY

This paper has highlighted NETL's Advanced Process Engineering Co-Simulator (APECS) for coupling high-fidelity equipment models with process simulation for the design, analysis, and optimization of process engineering systems. The APECS integration framework and its capabilities have been described, including the use of the process-industry CAPE-OPEN (CO) software interfaces. Also highlighted was the application of the co-simulation technology to fossil-energy power generation systems including the coal-fired, gasification-based FutureGen power and hydrogen production plant. At NETL, the CO-compliant APECS process/CFD co-simulation technology is helping engineers to better understand and optimize the fluid dynamics and related phenomena that impact overall power plant performance.

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**3rd Annual U.S. CAPE-OPEN Conference**  
**AICHE 2006 Annual Meeting**  
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***November 12-17, 2006***

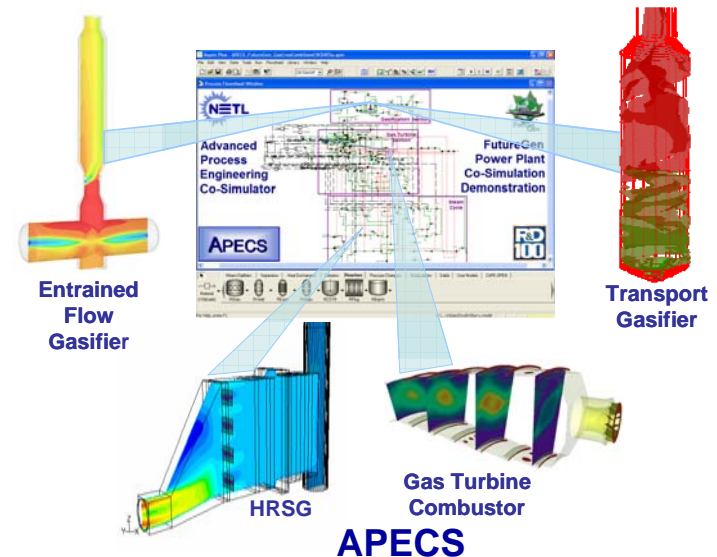
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# Outline of Presentation

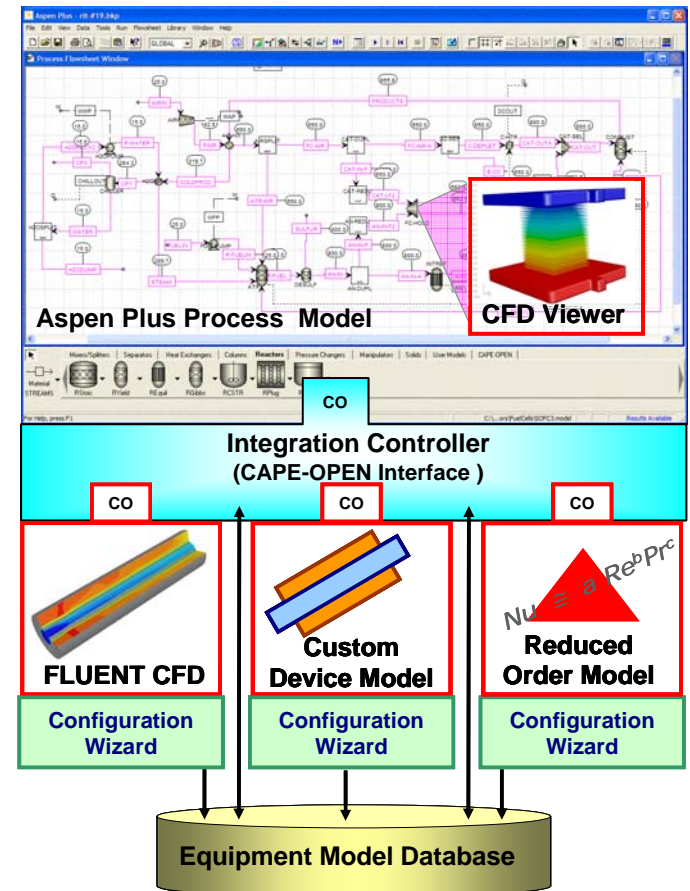
- **Advanced Process Engineering Co-Simulator (APECS)**
  - Introduction
  - Software Components and Features
  - Co-Simulation Workflow
  - Use of CAPE-OPEN
- **APECS Power Generation Applications at NETL**
- **Concluding Remarks**





# Advanced Process Engineering Co-Simulator (APECS)

- Co-simulation software framework for CAPE-OPEN 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

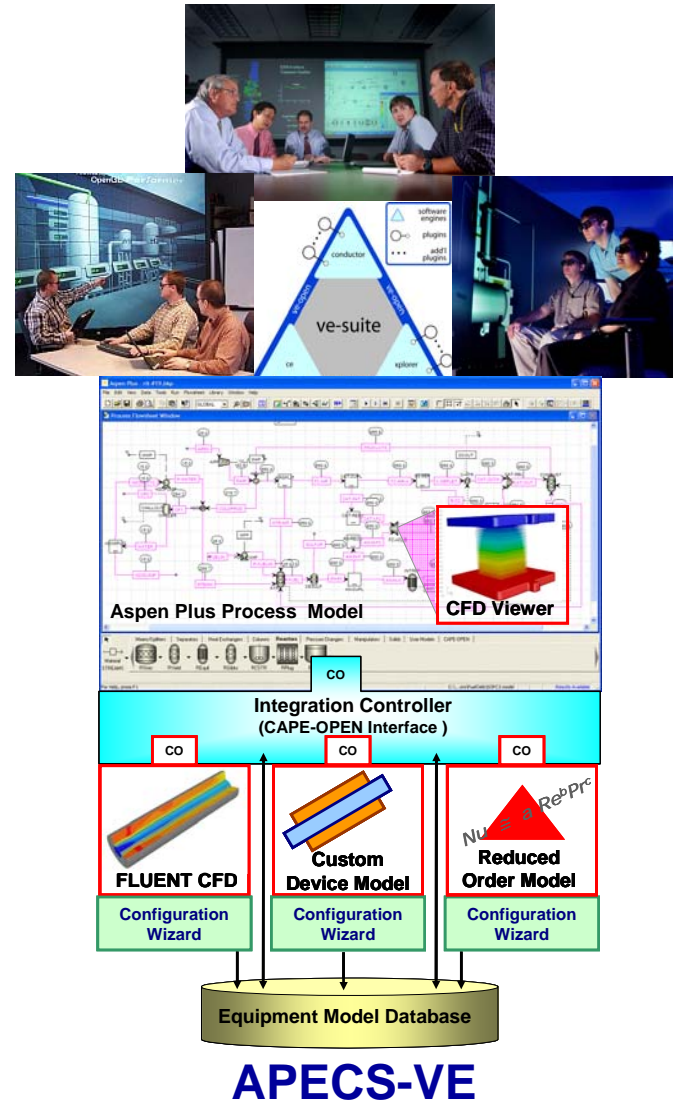
## *Brief History*

- 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)
- 2<sup>nd</sup> 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 Award (2006) 

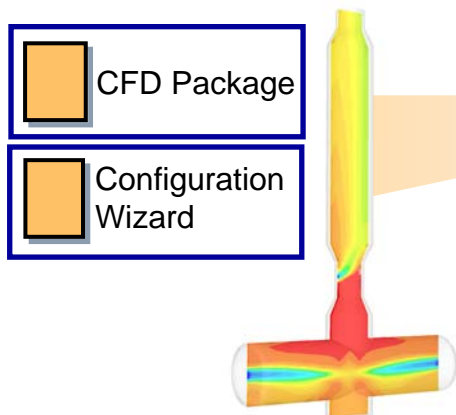




# APECS Software Components and Features

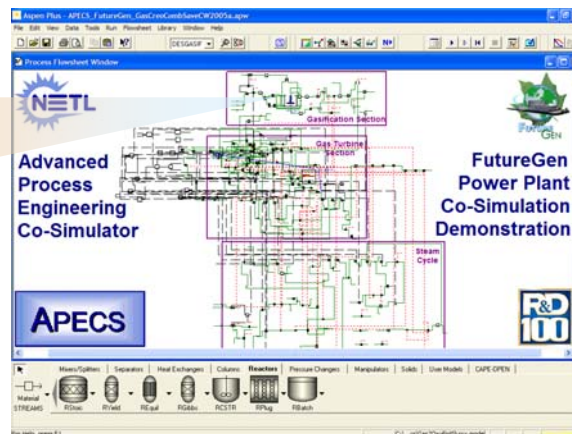
- **Process Simulators**
  - CAPE-OPEN compliant
  - Aspen Plus®, HYSYS®, gPROMS®
- **Equipment Models and Database**
  - CAPE-OPEN compliant
  - CFD: FLUENT®
  - Custom Models: e.g., INDVU
  - ROMs: LR, NN
- **Integration Controller**
  - CAPE-OPEN v1.0 Interfaces
  - Unit Ops, Phys Props, Reactions
- **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







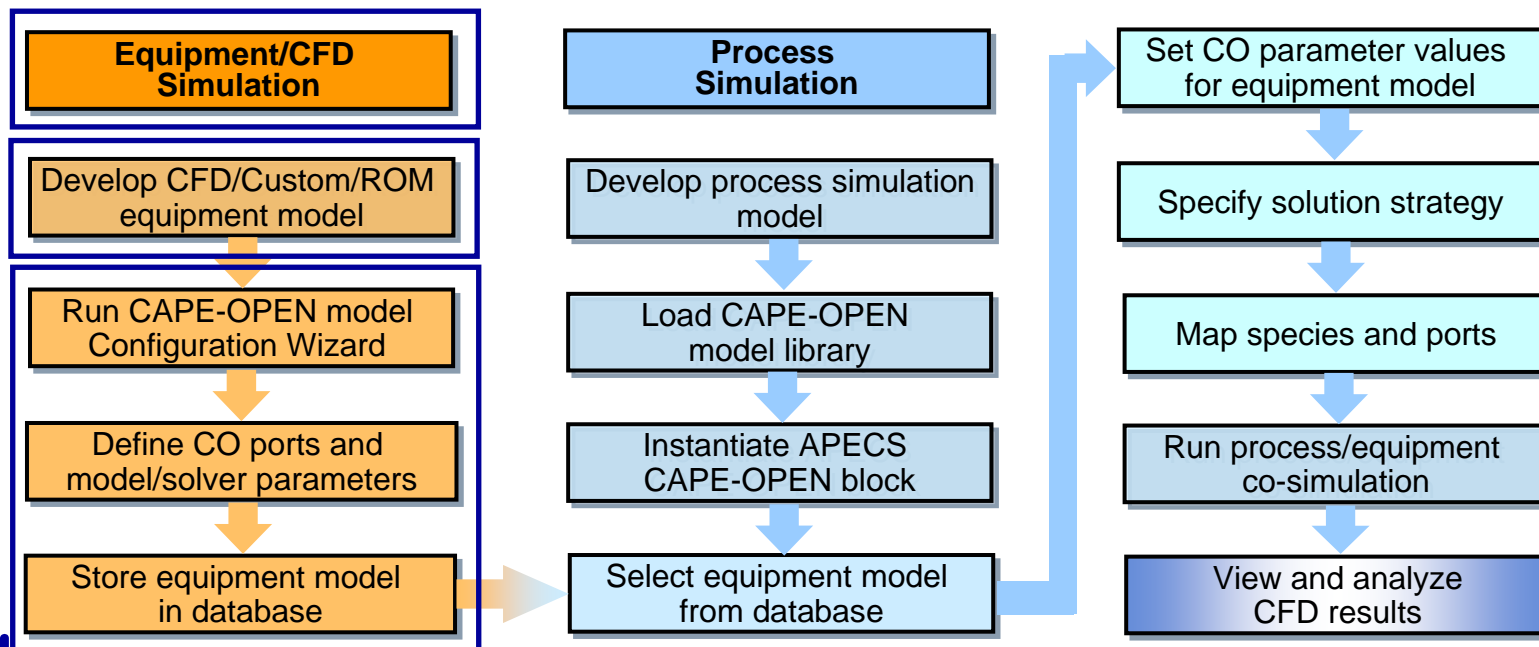
# APECS CFD/Process Co-Simulation Workflow



-  CFD Package
-  Configuration Wizard



-  Process Simulator
-  Model Selection GUI
-  Model Edit GUI
-  CFD Viewer/Paraview

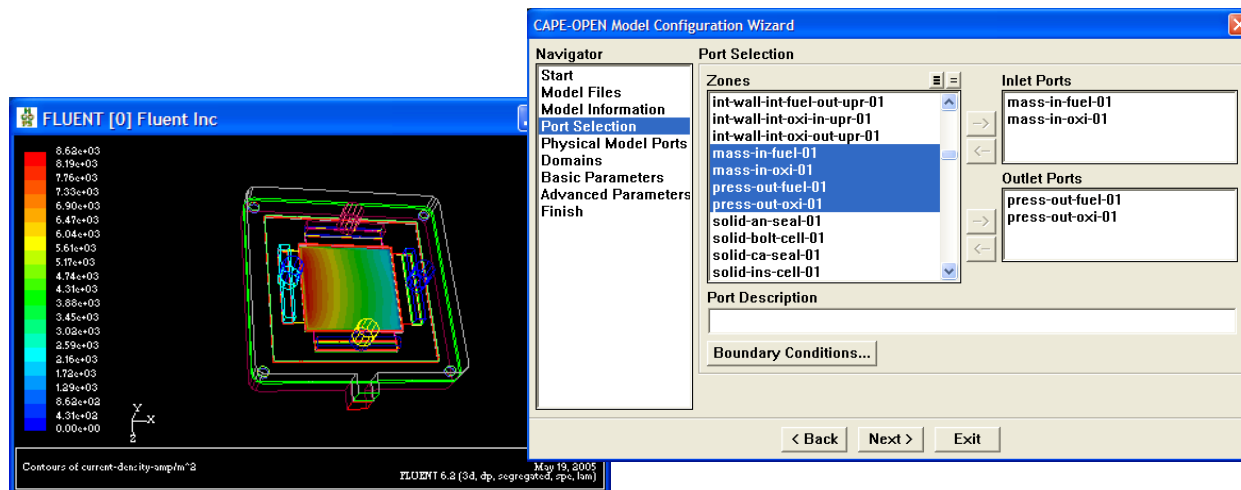




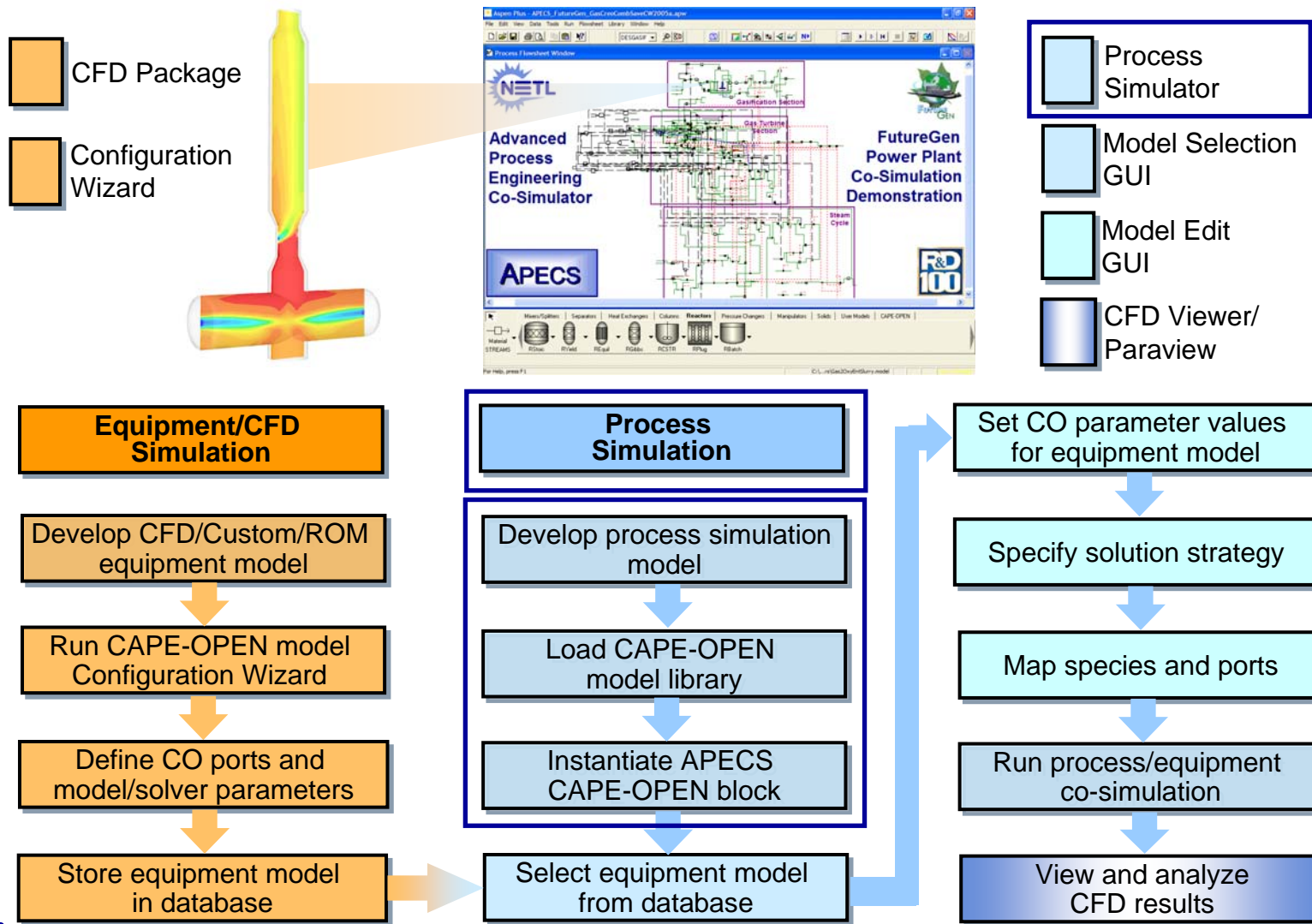
# Use of CAPE-OPEN in APECS

## *Unit Operation: Configuration Wizards*

- Prepare equipment/CFD models as CAPE-OPEN (CO) models for use in CO-compliant simulators
- Invoke as standalone tool or from within FLUENT
- Define CO ports (e.g., BCs, physical model ports)
- Define CO model parameters (e.g., fuel cell current)
- Define CO solver parameters (e.g., max. CFD iterations)
- Store CO-compliant model in the Model Database



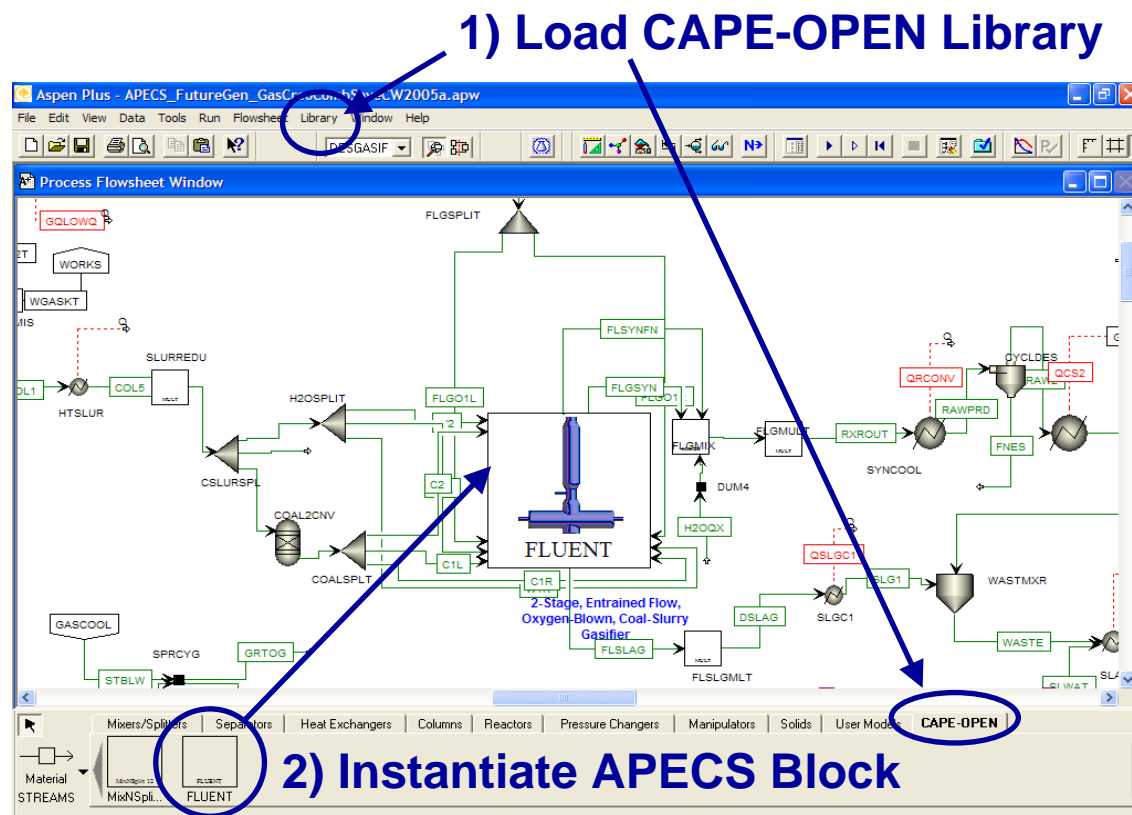
# APECS CFD/Process Co-Simulation Workflow



# Use of CAPE-OPEN in APECS

## *Unit Operation: Instantiation*

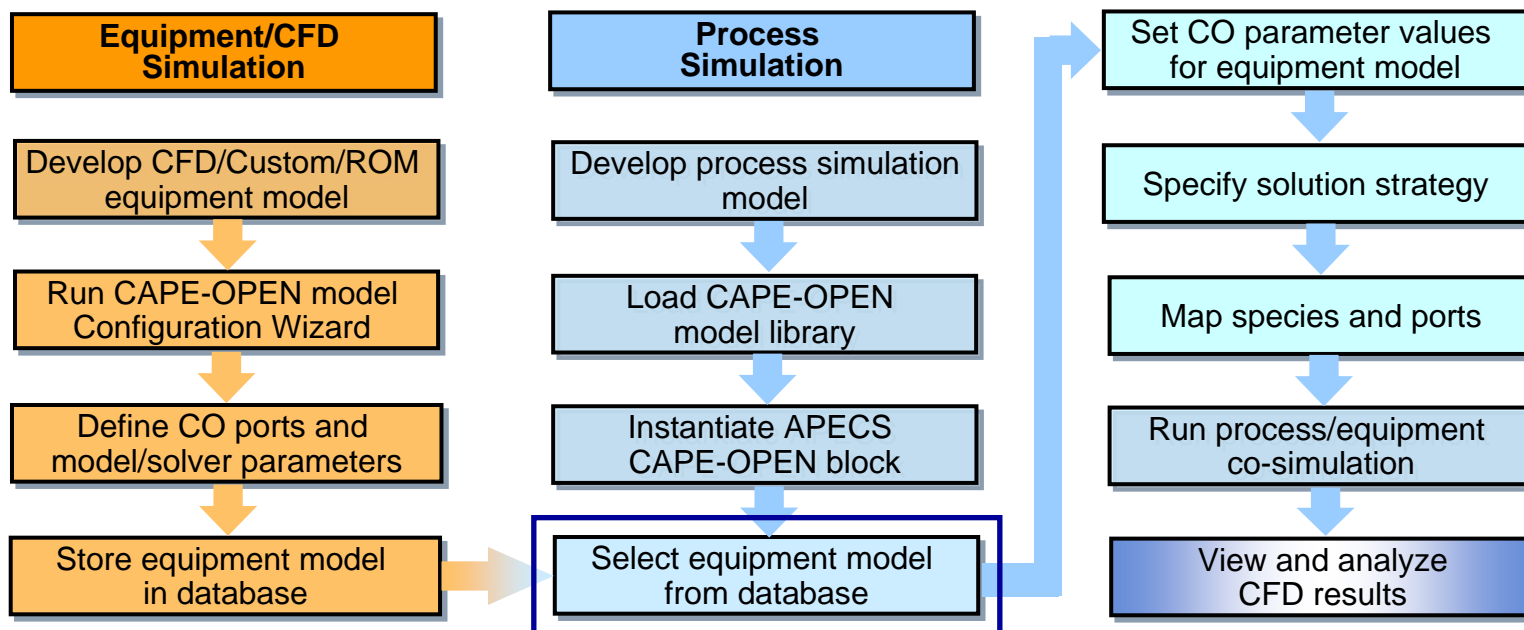
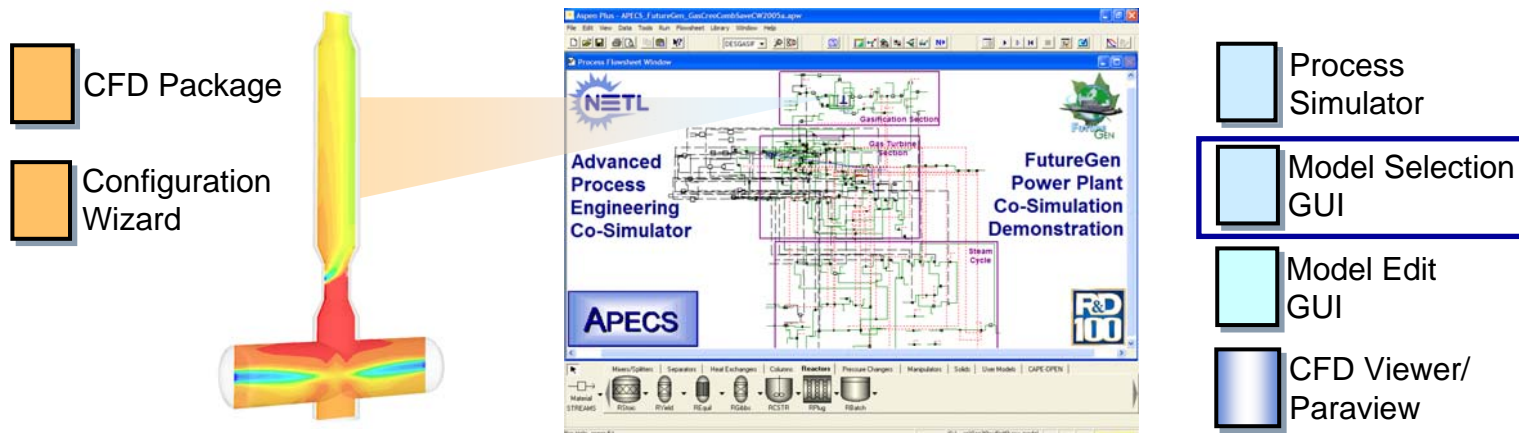
- APECS unit operation
  - Available via CAPE-OPEN Model Library
  - Drag-and-drop block on to process flowsheet



Process Simulator GUI



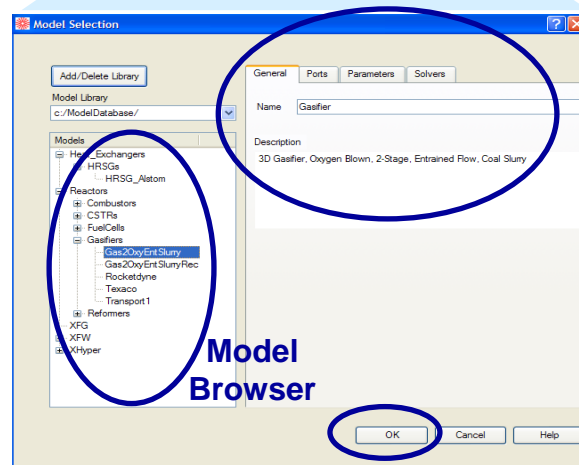
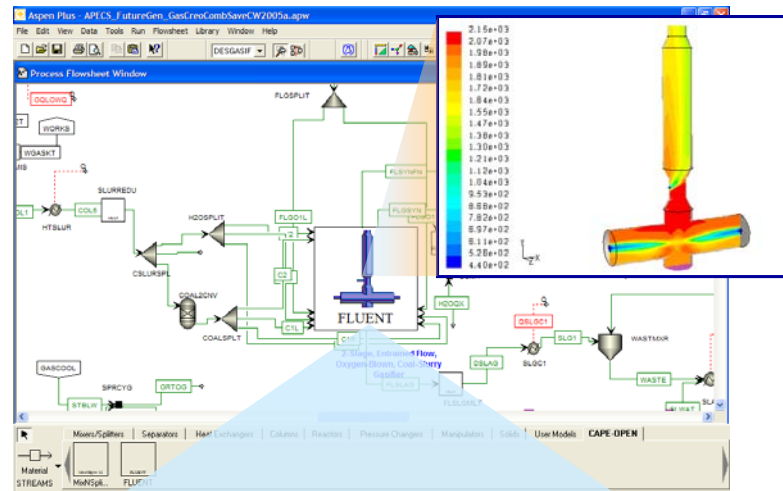
# APECS CFD/Process Co-Simulation Workflow



# Use of CAPE-OPEN in APECS

## *Unit Operation: Model Selection*

- Model Selection GUI
  - Browse CO-compliant CFD, Custom, and ROM models
  - View general, port, parameter, and solver info for each model
  - Select equipment model to associate with instantiated APECS block
  - CO parameters and ports defined upon model selection

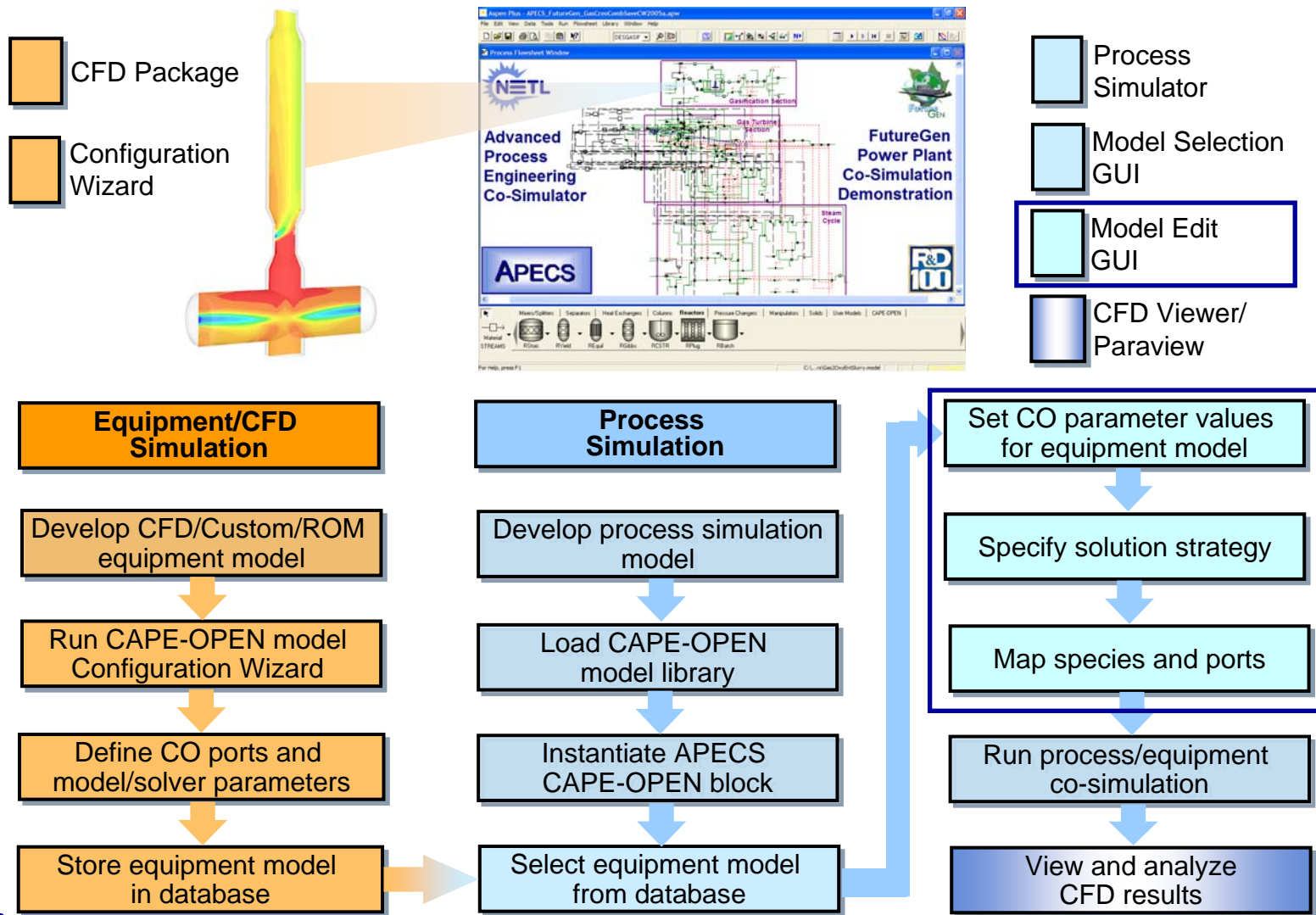


## Model Selection GUI



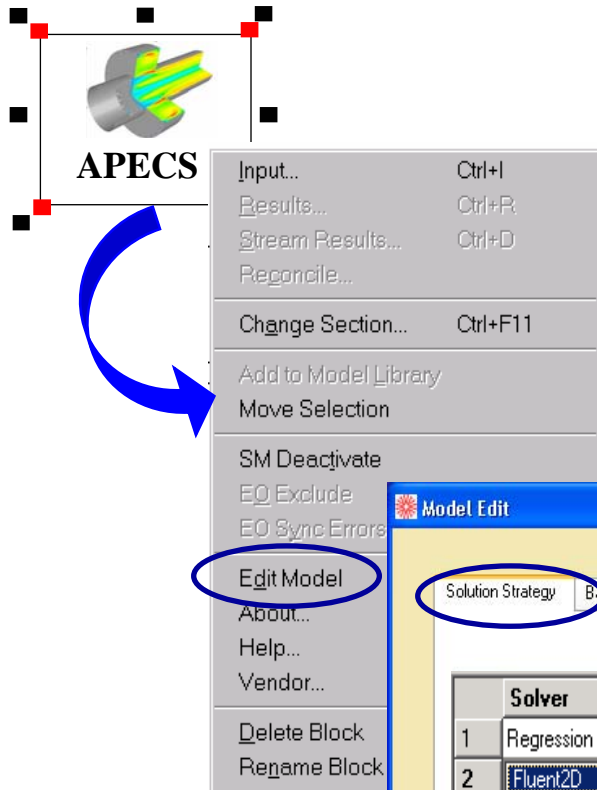


# APECS CFD/Process Co-Simulation Workflow



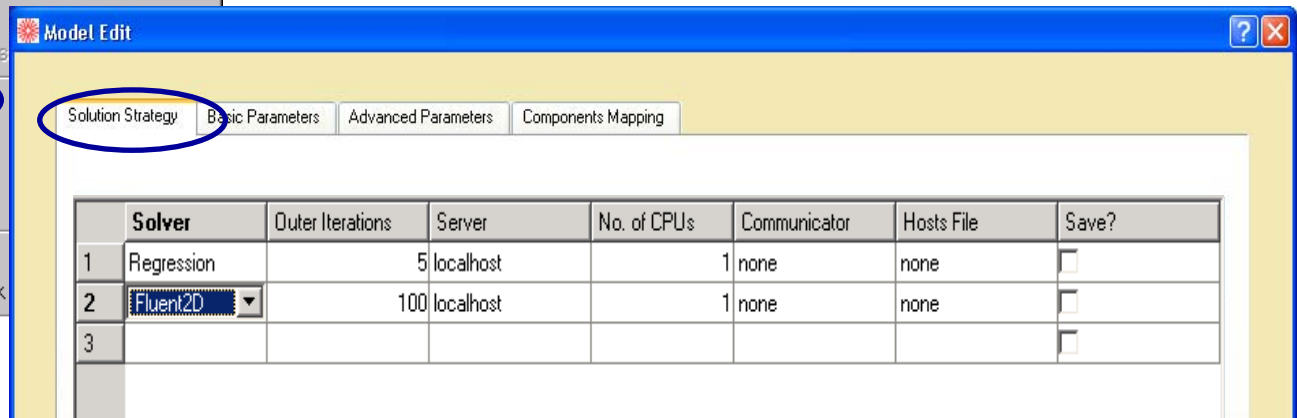
# Use of CAPE-OPEN in APECS

## *Unit Operation – Model Edit*



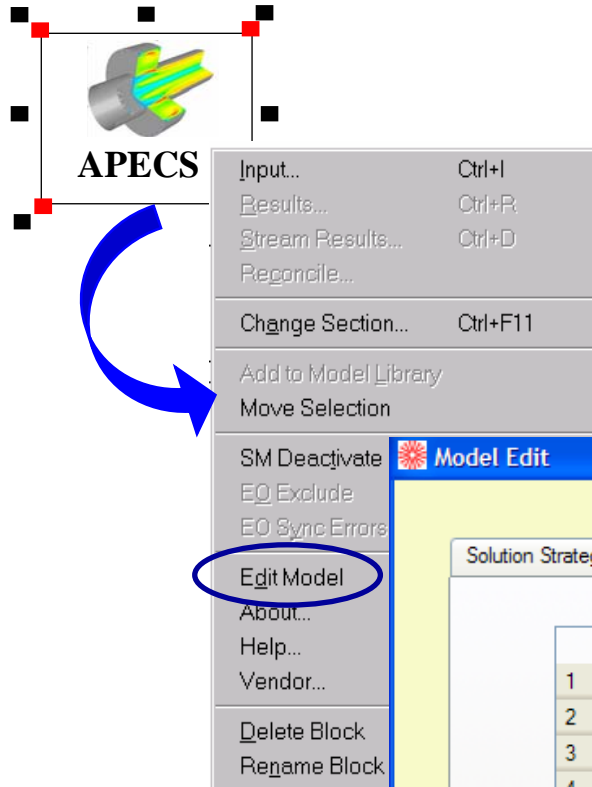
- **Solution Strategy**

- Combination of ROM, Custom, and CFD models/solvers
- Server (Local vs. Distributed)
- Parallel execution
- Save results



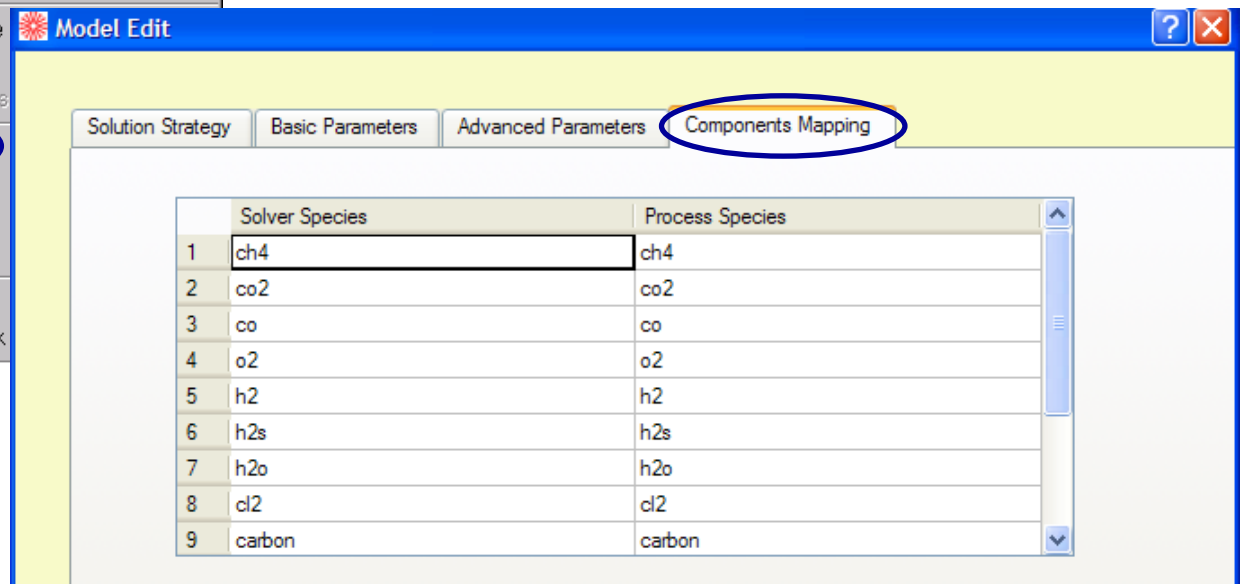
# Use of CAPE-OPEN in APECS

## *Unit Operation – Model Edit*



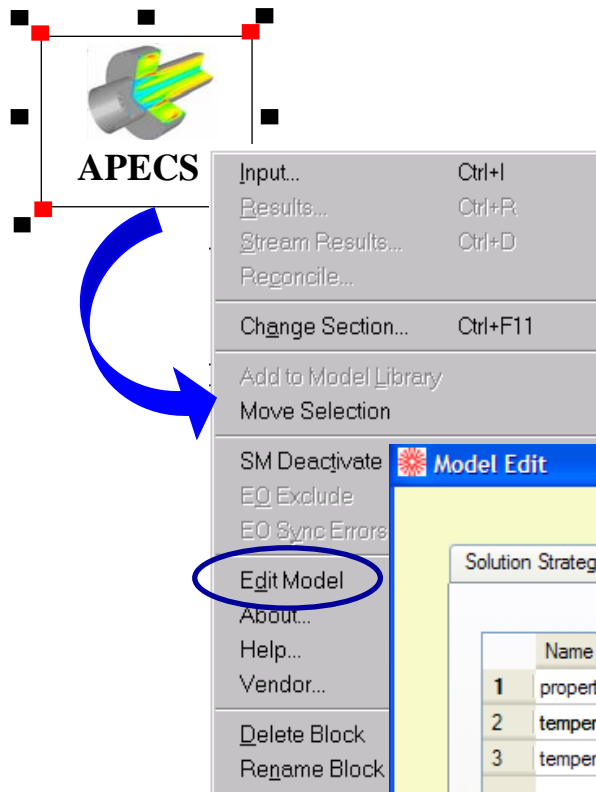
- **Species Mapping**

- Map chemical species between equipment model (Solver) and process model



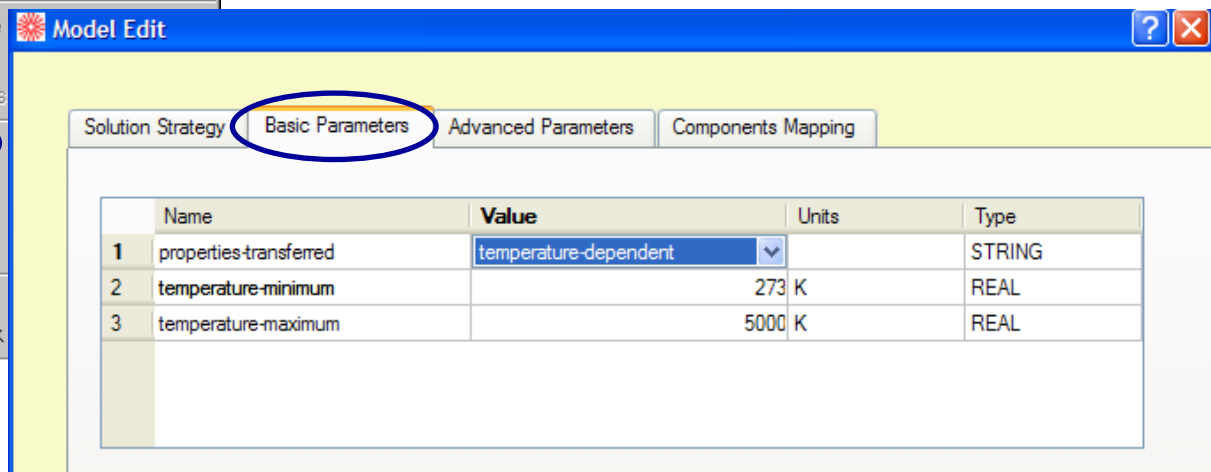
# Use of CAPE-OPEN in APECS

## *Unit Operation – Model Edit*



### • CAPE-OPEN Parameters

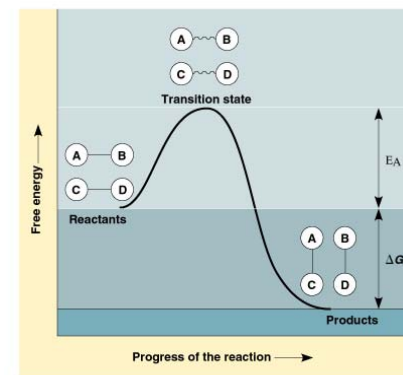
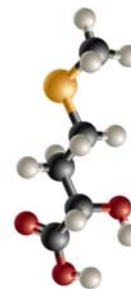
- Basic: Model, Thermo parameters
- Advanced: Solver parameters



# Use of CAPE-OPEN in APECS

## *Physical Properties and Reactions*

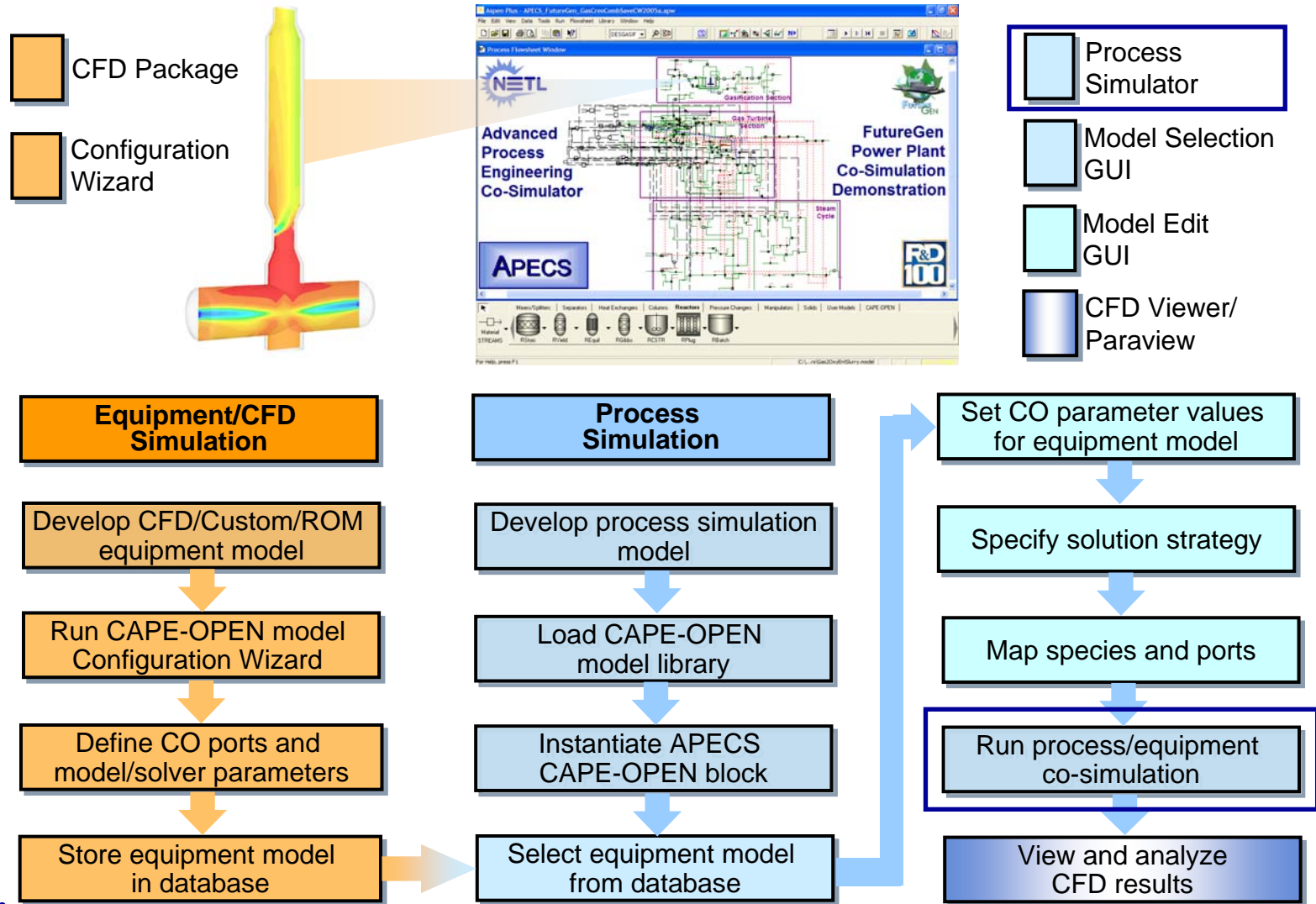
- Automatic data transfer from process simulator to CFD equipment model
- Physical properties
  - Temperature-dependent (i.e.,  $C_p$ ,  $\mu$ ,  $\rho$ ,  $k$ )
  - Constant (i.e.,  $h_0$ ,  $s_0$ , MW)
- Reactions
  - Stoichiometry (i.e., species, coefficient, rate exponent)
  - Power-law parameters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



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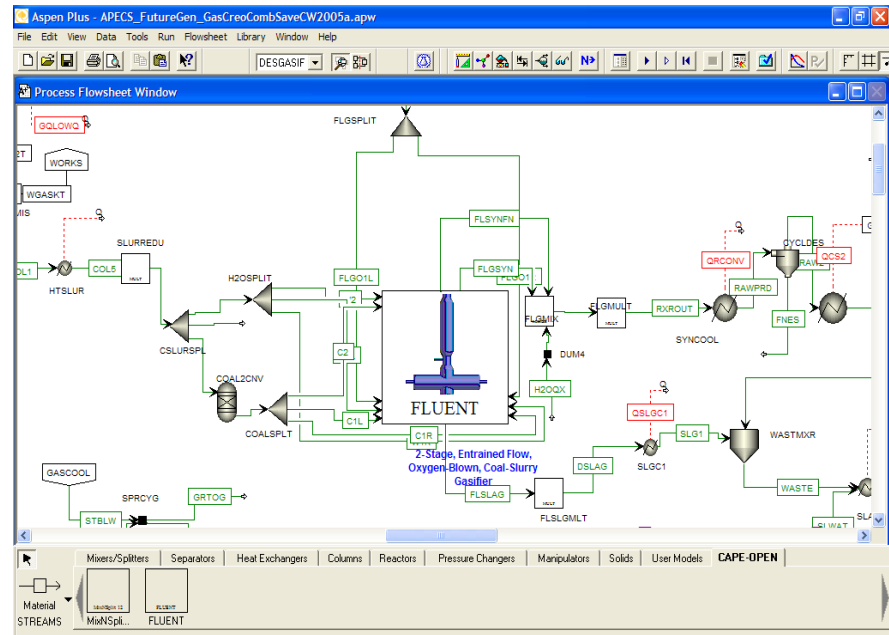
# APECS CFD/Process Co-Simulation Workflow



# Use of CAPE-OPEN in APECS

## *Process/CFD Co-Simulation*

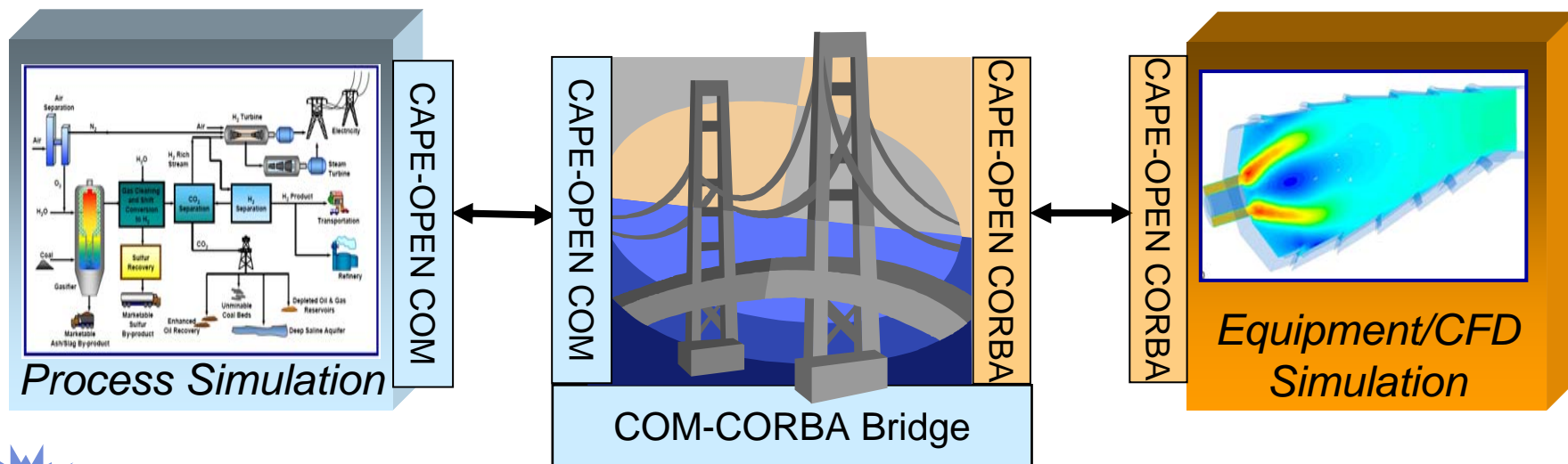
- Process material streams connected to CAPE-OPEN ports of CFD block
- Bi-directional exchange of process stream data ( $F$ ,  $x_i$ ,  $T$ ,  $P$ ) at flow boundaries
- Integrated averages at CFD outlet boundaries
- CFD block executed multiple times during flowsheet convergence if embedded in a recycle loop
- CFD results saved at each process iteration so that subsequent CFD simulations start at better starting points



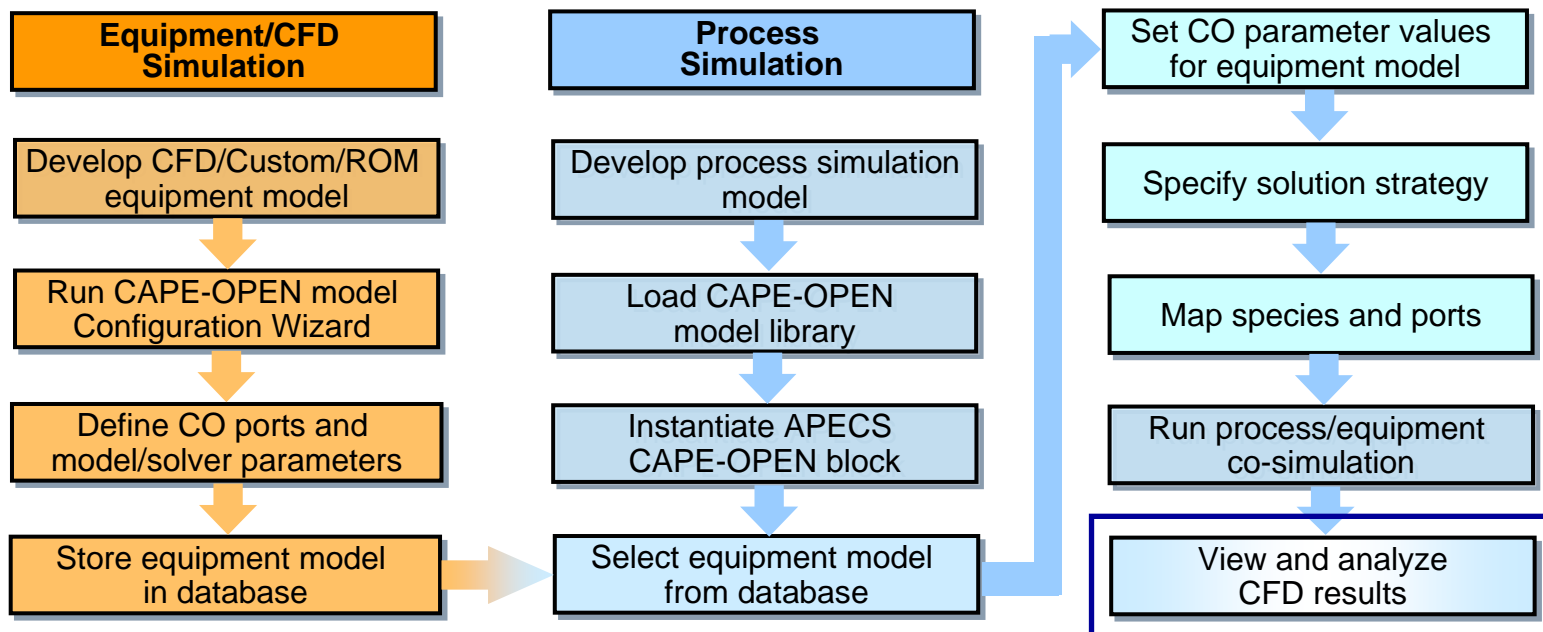
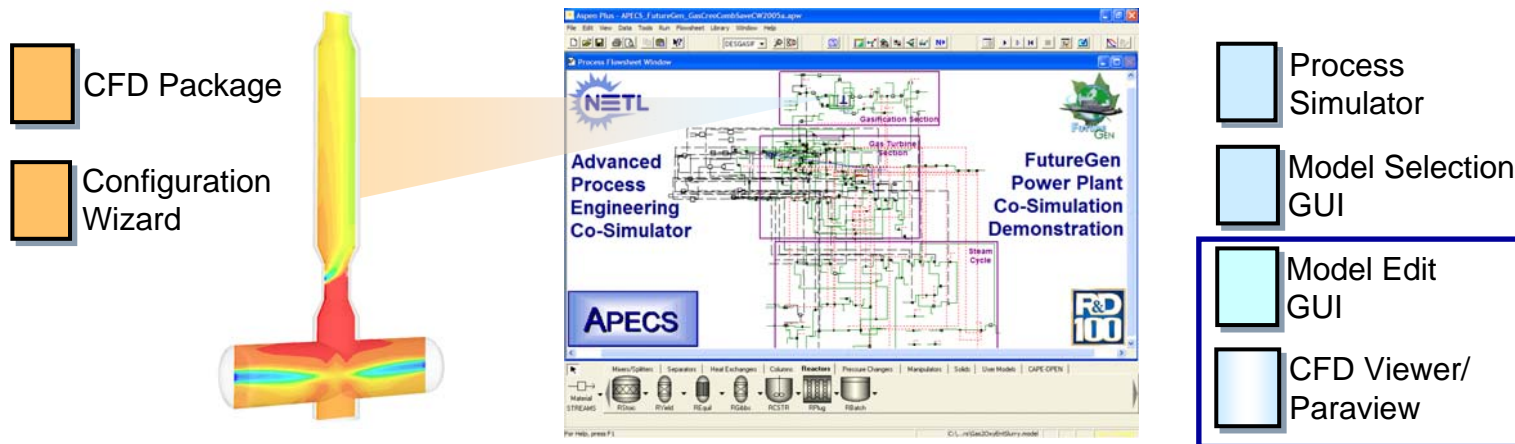
# Use of CAPE-OPEN in APECS

## *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

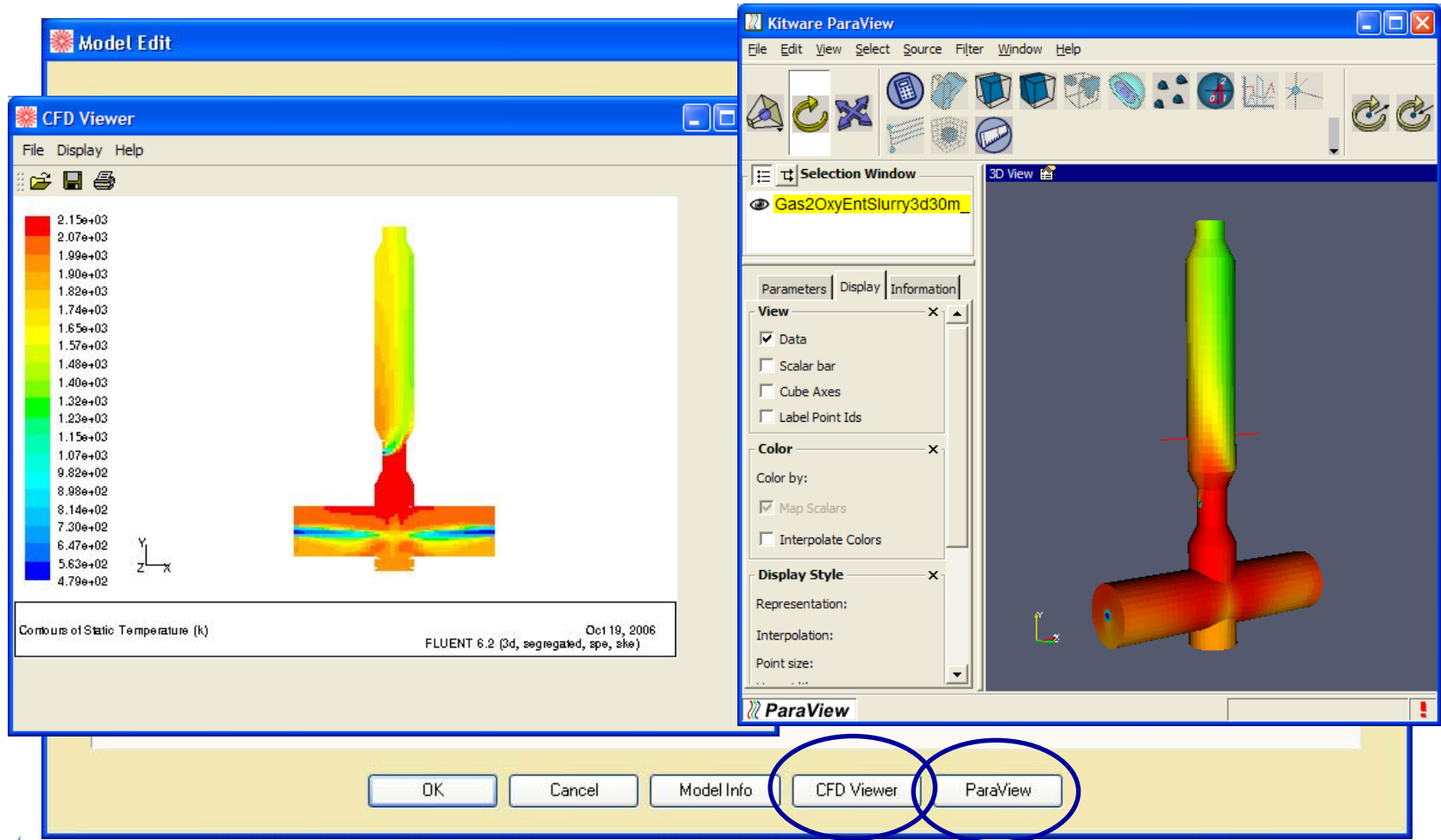


# APECS CFD/Process Co-Simulation Workflow



# Use of CAPE-OPEN in APECS

## *Unit Operation – Model Edit/Viewing CFD Results*

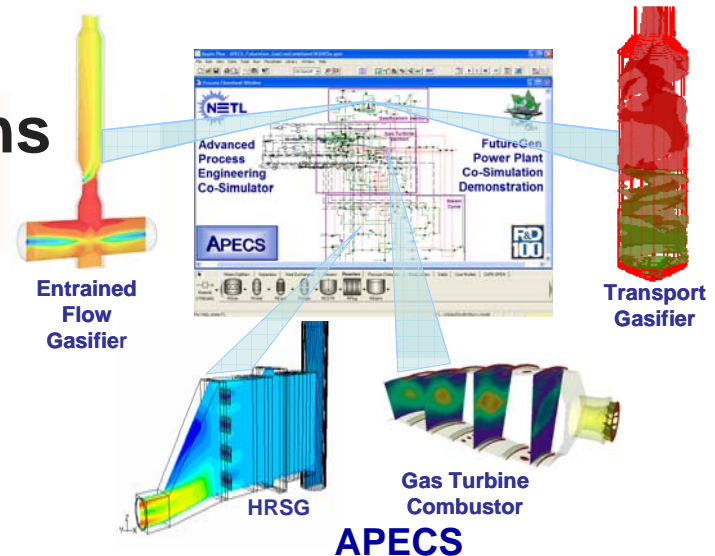


**Model Edit GUI**



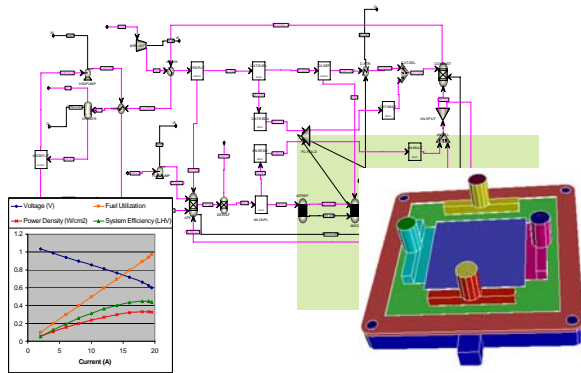
# Outline of Presentation

- **Advanced Process Engineering Co-Simulator (APECS)**
  - Introduction
  - Software Components, Features, and Workflow
  - Use of CAPE-OPEN
- **Power Generation Applications at NETL**
- **Concluding Remarks**

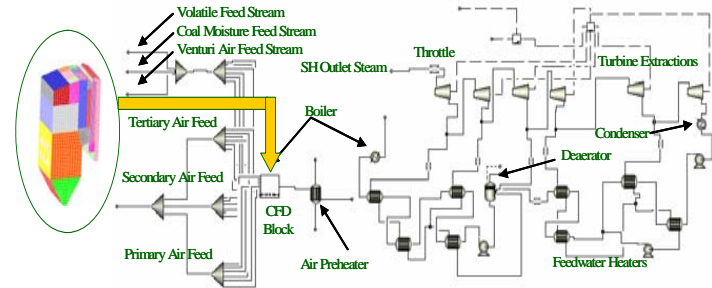


# APECS Power Generation Applications

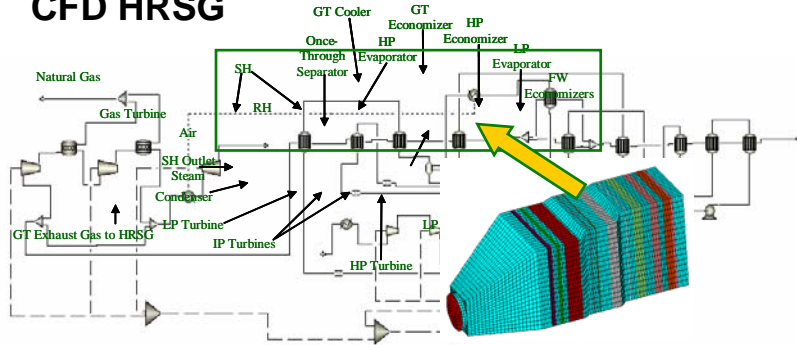
- **Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC**



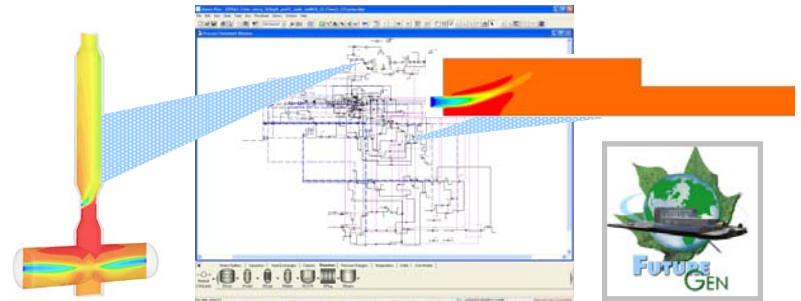
- **ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler**



- ALSTOM NGCC (250MWe ) with 3D CFD HRSG
  - GT Cooler
  - GT
  - Exhaust
  - HP

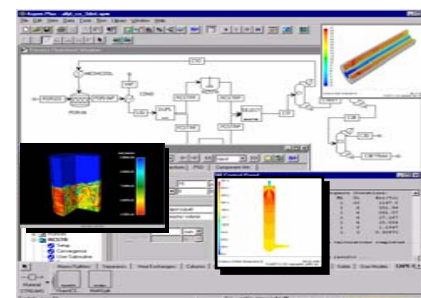


- **FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor**



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



# CAPE-OPEN Integration for Advanced Process Engineering Co-Simulation

Thank You!

Questions?

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