The background features a central blue globe with the ANSYS logo overlaid. The globe is surrounded by a complex network of glowing blue and orange lines that radiate outwards, creating a sense of dynamic energy and connectivity. The overall aesthetic is high-tech and futuristic.

APECS Software and Architecture Overview

**NETL 2009 Workshop on
Advanced Process
Engineering Co-Simulation
October 20-21, 2009**

- **What is APECS?**
- **Overview of APECS Features**
- **Overview of APECS Architecture**

What is APECS?



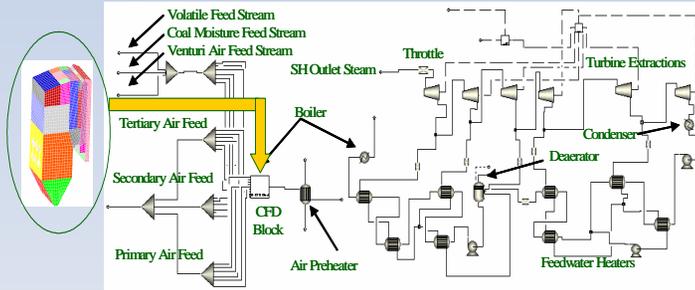
- **Enabling software that permits users to add high-fidelity CFD models (or ROMs) to process modeling environments**



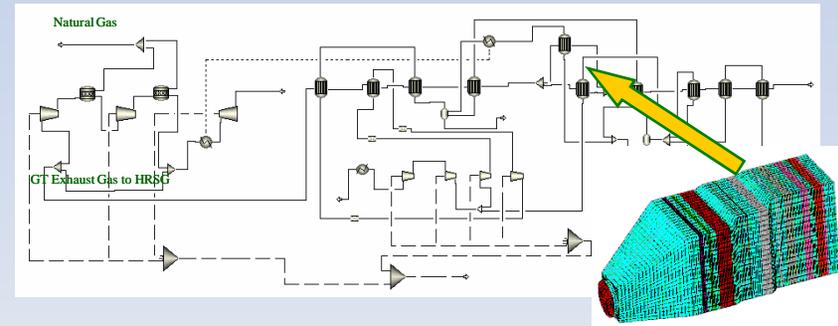
Examples



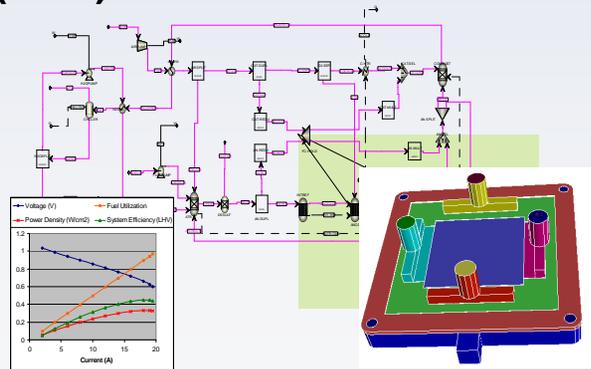
- ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler



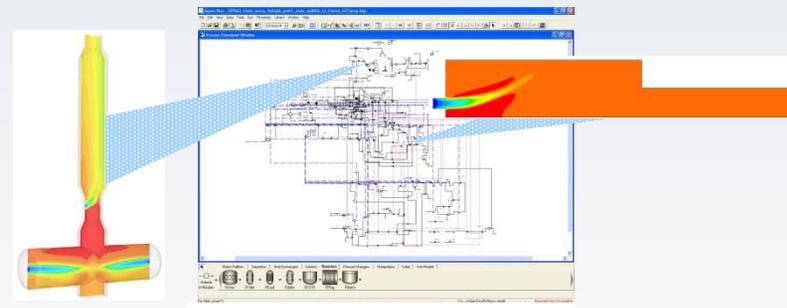
- ALSTOM NGCC (250MWe) with 3D CFD HRSG



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



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



Performed by collaborators at NETL and ALSTOM Power

User's Manual Available



**APECS: The Advanced Process Engineering
Co-Simulator**

User's Manual

Version 1.6.1

June 2009

APECS Features



- Easy to Use
- CAPE-OPEN (CO) Compliant
- Separation of Tasks between CFD and PME users
- Shared Model Database
- Physical Properties Transferred to FLUENT Model
- CFD Models can be Executed Remotely
- Geometric Parameterization Possible
- Reduced-Order Models can be Incorporated
- Sophisticated Solution Strategies Possible
- Results Easily Visualized in the PME
- Coupling with Virtual Reality Software

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What is CAPE-OPEN?



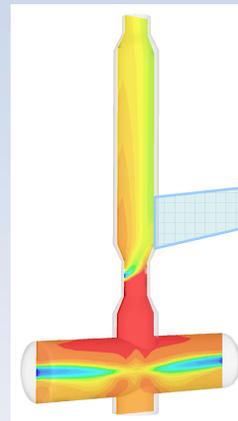
- **An Open Standard for Computer Aided Process Engineering**
- **Enables Software Interoperability**
 - 2-way exchange of stream information
 - Plug-and-play capabilities for compliant models
- **Standard maintained by CO-LaN**
 - The CAPE-OPEN Laboratories Network, www.colan.org
- **CO compliancy testing performed by AmsterCHEM**
 - Provider of COFE (CO Flowsheet Environment)
 - www.cocosimulator.org

CAPE-OPEN PMEs

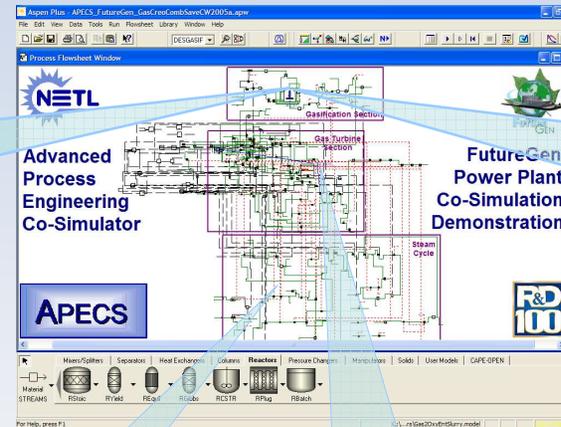


CAPE-OPEN Compliant Process Modeling Environments (PMEs)

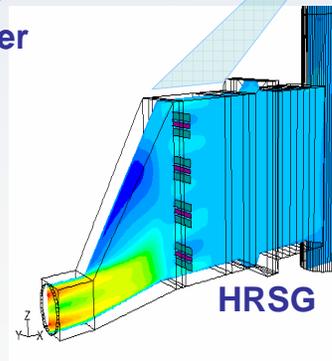
- Aspen Plus
- Aspen HYSYS
- UniSim Design
- gPROMS
- COCO
- ProSimPlus
- PRO/II
- Petro-SIM



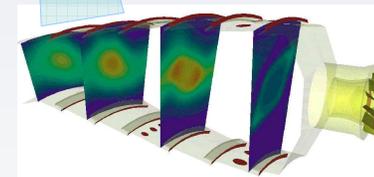
**Entrained
Flow
Gasifier**



**Transport
Gasifier**



HRSG



**Gas Turbine
Combustor**

APECS Features

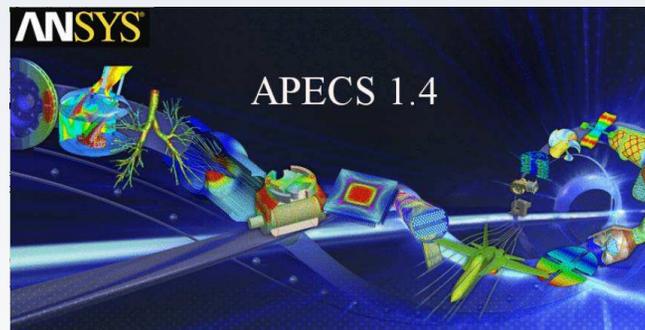
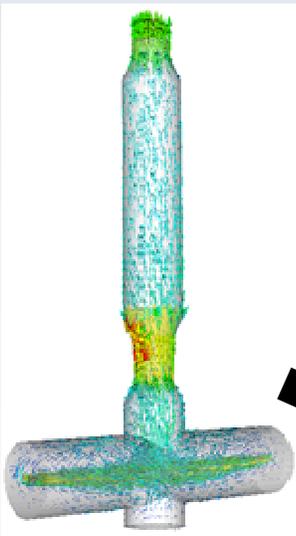


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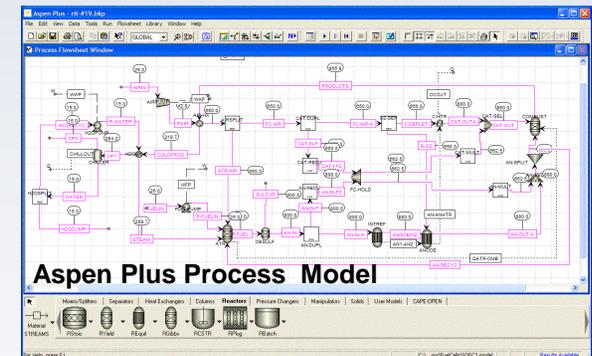
Separation of Tasks



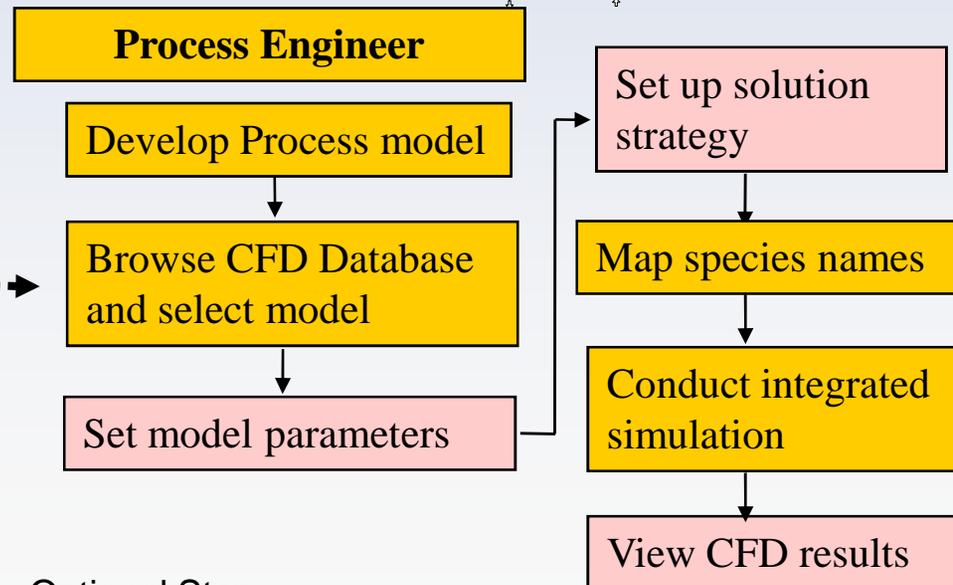
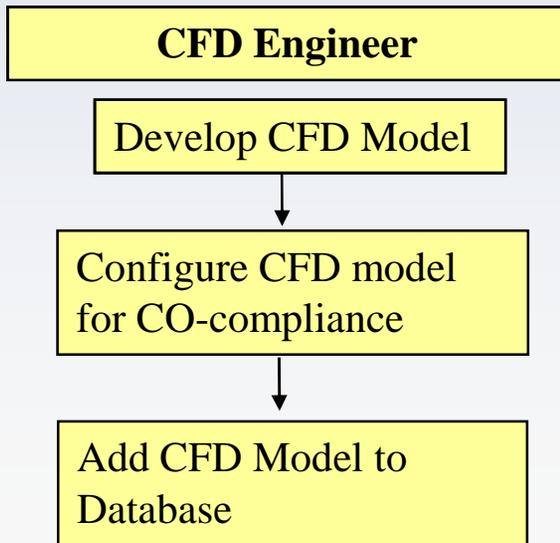
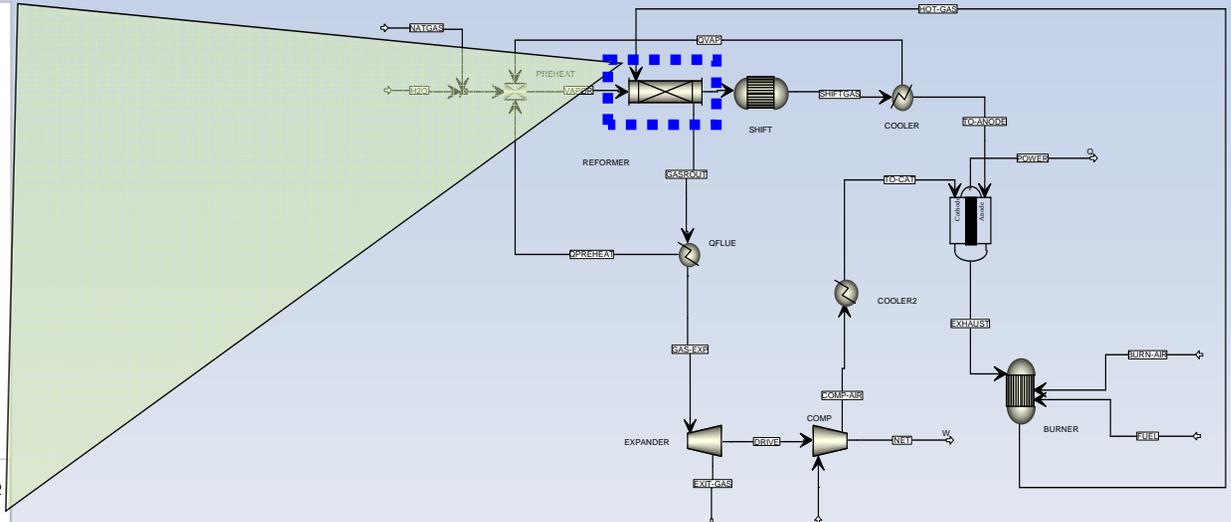
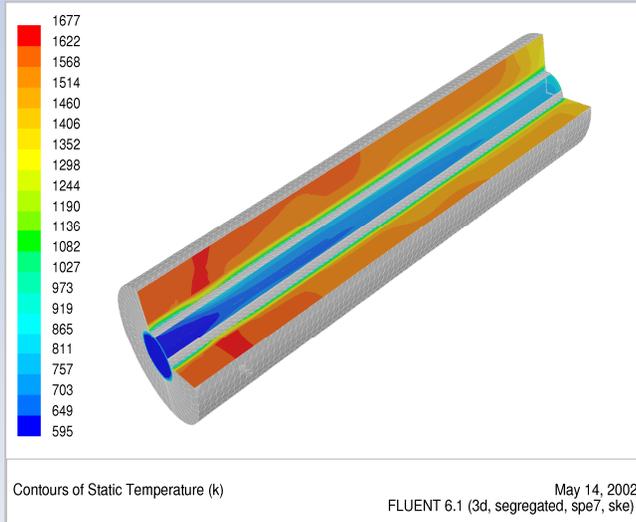
- It is not necessary for the process engineer to be a CFD expert (and vice versa)
- The CFD analyst creates models and uploads them to the Model Database
- The process engineer selects models from the database and uses them in process flowsheets



APECS Model Database



Typical Workflow

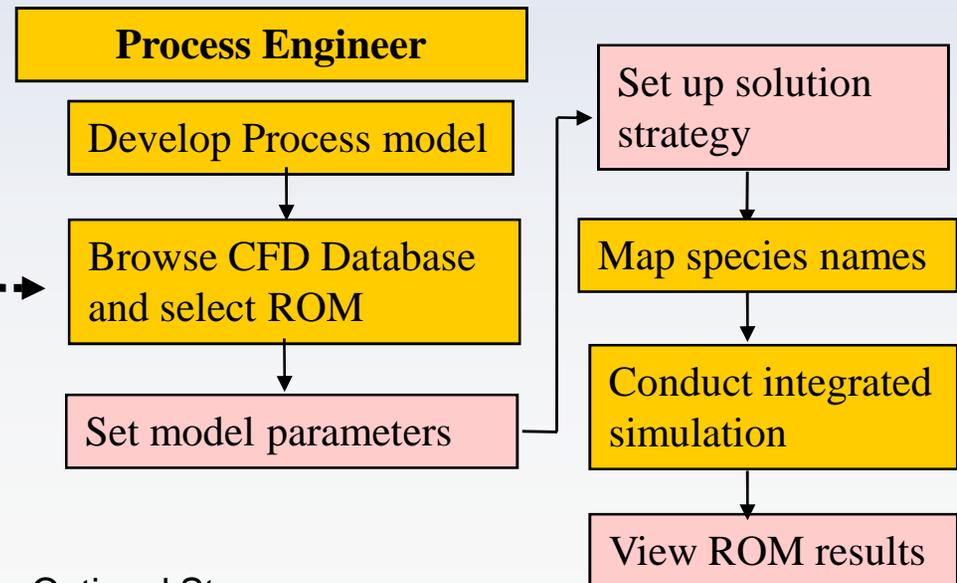
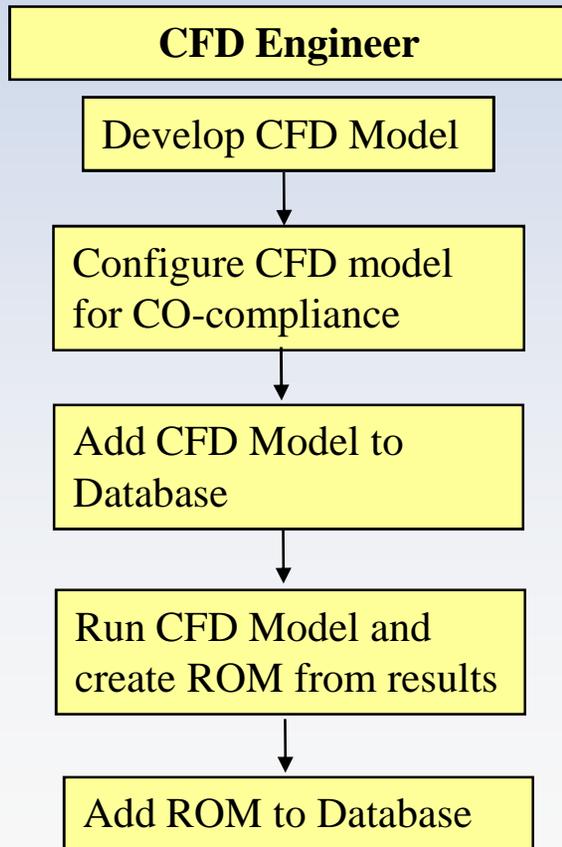
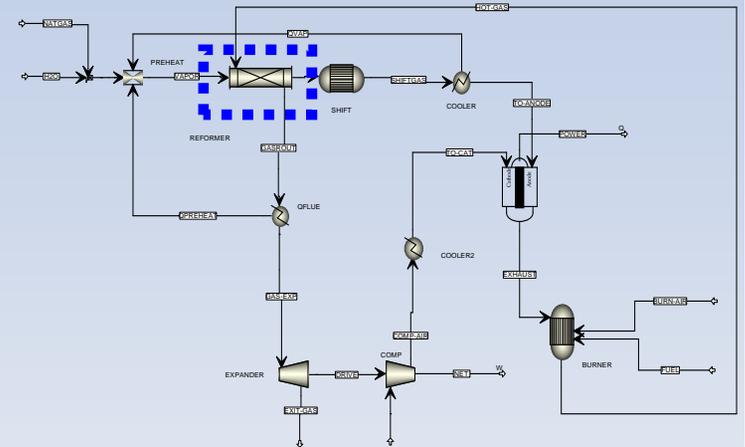


Indicates Optional Step

Alternative Workflow



- Replace FLUENT model with Reduced Order Model (ROM)



Indicates Optional Step

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Shared Model Database (EKM)



The screenshot displays the ANSYS User Interface window. The title bar reads "ANSYS User Interface". The menu bar includes "File", "Database", "ROM", "Display", and "Report". The status bar at the top indicates the "Model Database: lebjwidmannpc.win.ansys.com:8180". A red circle highlights this status bar. On the left, a tree view shows a hierarchical structure of model categories, including "APECS_Demos_Summer2009" (with sub-items like "Spray-Combustion", "Reacting-Spray Linear Regression Rom", "Reacting-Spray-Example", and "pipe model with 6 species"), "CFD_Viewer", "COM-based Models", "Cyclones", "Dynamics", "Examples", "FLUENT 12.0.16", "IAB Meeting March 2009", "Mixers", "Models-with-multiple-solvers", "Multiphase", "Pipes" (with sub-items like "Property-transfer", "Test pressure drop calculations", "Two public species", "no-properties-transferred", "pipe-model-ROM"), "ROMs", "Reactors", "Report Testing", "TeamMeeting_Jan2009", "Testing", and "VE Suite". At the bottom of the tree view is a button labeled "Select APECS Model". The main content area on the right contains a welcome message: "Welcome to ANSYS Advanced Process Engineering Co-Simulator 1.6", "Copyright 2008 ANSYS Inc. All Rights Reserved", and a paragraph of legal notice regarding data protection and government agreement No. DE-FC26-05NT42443.

APECS Features

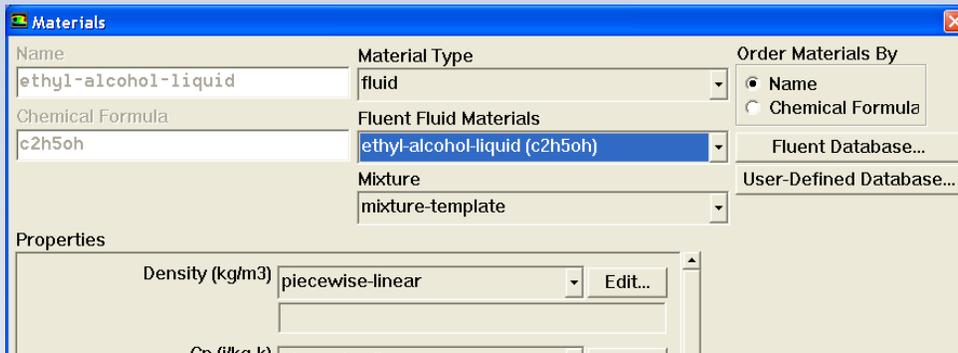


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Material Properties



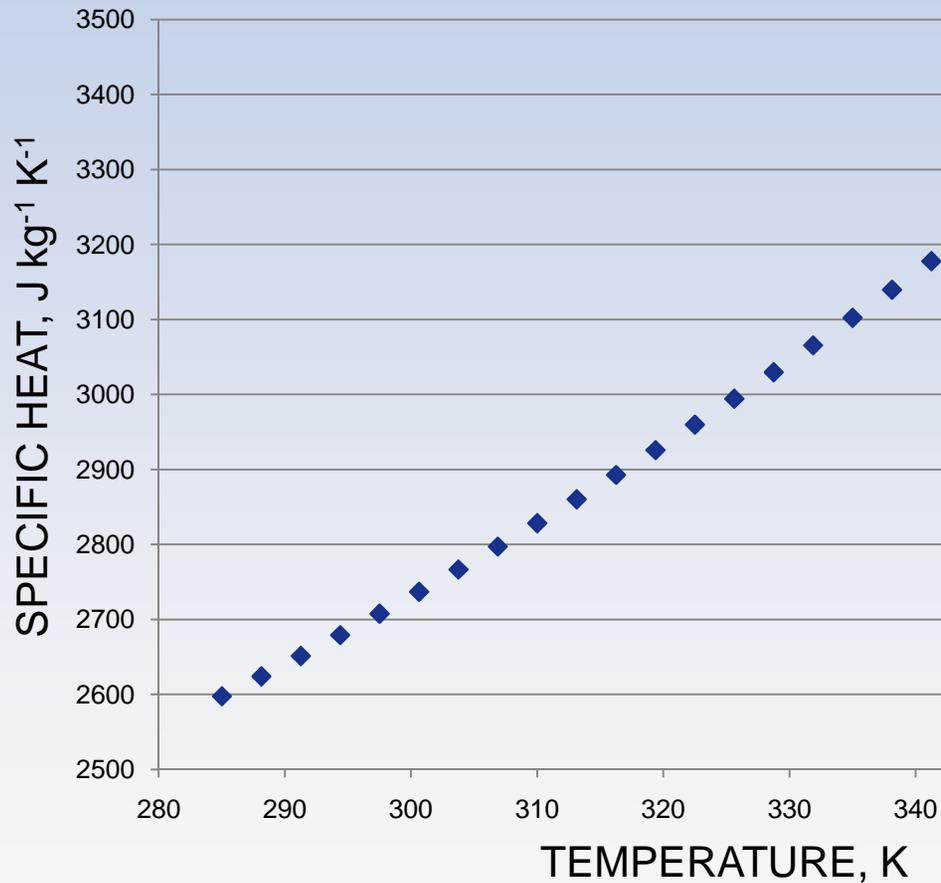
Can use the same material properties in the CFD model that are used in the PME flowsheet



Parameters available in flowsheet

	Name	Value	Units	Read Only	Description	Base Typ
Viscosity (kg/m-s)	viscosity-transferred	False		READ ONLY	Whether viscosity should be transferred to the solver.	BOOLEAN
	maximum-iterations	5	UNITLESS	READ-WRITE	Maximum number of FLUENT iterations	INTEGER
	molecular-weight-transferred	False	UNITLESS	READ ONLY	Whether molecular-weight should be transferred to the solver.	BOOLEAN
	density-transferred	False	UNITLESS	READ ONLY	Whether density should be transferred to the solver.	BOOLEAN
	converged	False	UNITLESS	READ ONLY	Whether FLUENT converged or not at the end of a given n	BOOLEAN
	temperature-maximum	400	UNITLESS	READ-WRITE	Maximum temperature for temperature dependent properti	DOUBLE
	geometry_parameter 2	3	UNITLESS	READ-WRITE	length of pipe	DOUBLE
	temperature-minimum	275	UNITLESS	READ-WRITE	Minimum temperature for temperature dependent propertie	DOUBLE
	specific-heat-transferred	False	UNITLESS	READ ONLY	Whether specific-heat should be transferred to the solver.	BOOLEAN
	geometry-parameterization	True	UNITLESS	READ-WRITE	indicates if parameterization is enabled	BOOLEAN
	thermal-conductivity-transferred	False	UNITLESS	READ ONLY	Whether thermal-conductivity should be transferred to the	BOOLEAN
	public-species	ch3oh	UNITLESS	READ ONLY	public species names	STRING
	geometry scale factor	1	UNITLESS	READ ONLY	meshing scale factor	DOUBLE
	geometry model name	pipe	UNITLESS	READ ONLY	base name of gambit journal file file	STRING
	geometry_parameter 1	0.1	UNITLESS	READ-WRITE	radius of pipe	DOUBLE
	file-system	pipe.jou	UNITLESS	READ ONLY	Files Required to run the case	STRING
	model-views	pipe	UNITLESS	READ ONLY	The equipment views for post-processing.	STRING
	archive-rom-data	False	UNITLESS	READ-WRITE	Whether to archive data for reduced order modeling.	BOOLEAN

C_p for Ethanol



Piecewise-Linear Profile

Define: Cp In Terms of: Temperature Points: 25

Data Points

Point	Temperature [k]	Value [j/kg-k]
8	306.875	2797.19

OK Cancel Help

Materials

Name	Material Type	Order Materials By
ethyl-alcohol-liquid	fluid	<input checked="" type="radio"/> Name
Chemical Formula	Fluent Fluid Materials	<input type="radio"/> Chemical Formula
c2h5oh	ethyl-alcohol-liquid (c2h5oh)	Fluent Database...
	Mixture	User-Defined Database...
	mixture-template	

Properties

Density (kg/m3)	piecewise-linear	Edit...
Cp (j/kg-k)	piecewise-linear	Edit...
Thermal Conductivity (w/m-k)	piecewise-linear	Edit...
Viscosity (kg/m-s)	piecewise-linear	Edit...

Change/Create Delete Close Help

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Remote FLUENT Execution



The screenshot displays the ANSYS APECS Unit Operation interface. The main window is titled "APECS Unit Operation" and has a blue header bar. On the left, the "Model Database" section shows a connection to "lebjwidmannpc.win.ansys.com:8180" and a tree view of "Database Contents" including "Pipes", "Property-transfer", and "pipe model". The main area is divided into tabs: "General", "Ports", "Parameters", "Solvers", and "APECS Log". The "General" tab is active, showing fields for "Name" (pipe model) and "Description" (FLUENT CFD Model). Below these are "Strategy" (StaticSolutionSteps) and "Solution Steps: pipe model" (1 pipe model). A "Solver" section is visible at the bottom of the main window. A "Server Configuration" dialog box is overlaid on top, with three red arrows pointing from the "Solver" section to its fields. The dialog box has a blue header bar and contains the following settings:

- Solution Step Details:**
 - Solver: pipe model (dropdown) Release solver license
 - Server: linux_1 (dropdown)
- FLUENT specific:**
 - Number of Processors: 4 (spin box) Communicator: smpi (dropdown)
 - FLUENT Host File or Compute Nodes: linux_1,linux_1,linux_2,linux_2| (text box)

Buttons for "OK" and "Cancel" are at the bottom right of the dialog box. The main window also has "Select Model", "Start Model", and "Close" buttons.

APECS Features

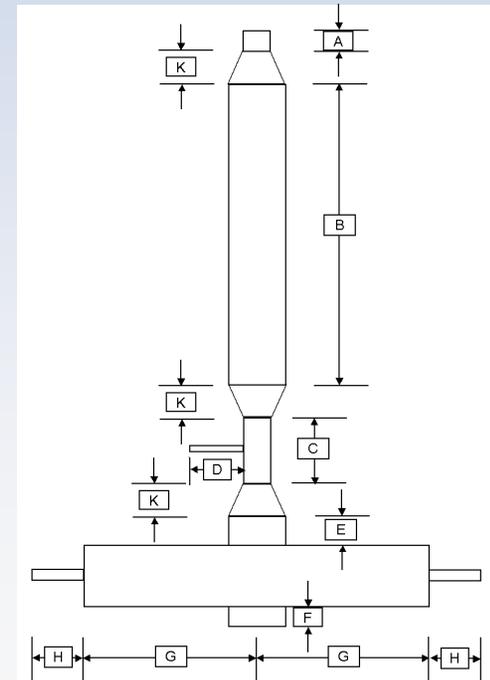
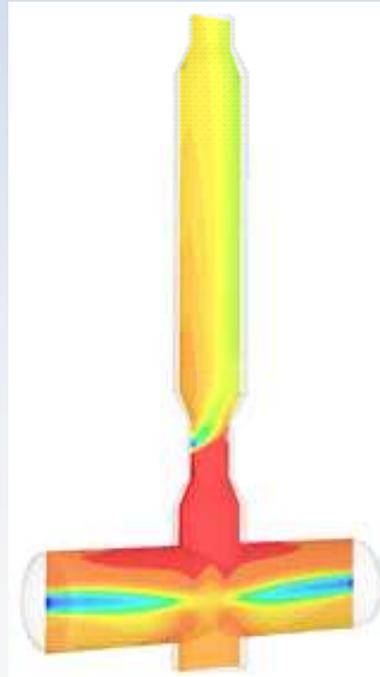
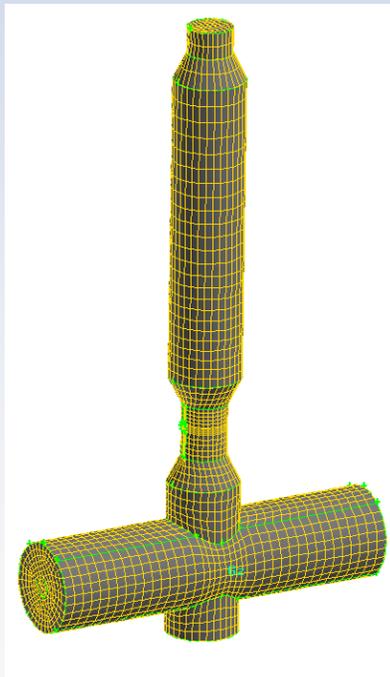


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Geometric Scaling / Parameterization



- Conduct geometry parameterization studies from within the process flowsheet



Geometry Scaling (2)



- Changing parameters in flowsheet reflected by automatic modifications of the CFD mesh
- Parameters passed from Aspen Plus to APECS as CAPE-OPEN parameters

Name	Value	Units	Read Only	Description	Base Type
viscosity-transferred	False		READ ONLY	Whether viscosity should be transferred to the solver.	BOOLEAN
maximum-iterations	5	UNITLESS	READ-WRITE	Maximum number of FLUENT iterations	INTEGER
molecular-weight-transferred	False	UNITLESS	READ ONLY	Whether molecular-weight should be transferred to the solver.	BOOLEAN
density-transferred	False	UNITLESS	READ ONLY	Whether density should be transferred to the solver.	BOOLEAN
converged	False	UNITLESS	READ ONLY	Whether FLUENT converged or not at the end of a given n	BOOLEAN
temperature-maximum	400	UNITLESS	READ-WRITE	Maximum temperature for temperature dependent properties	DOUBLE
geometry parameter 2	3	UNITLESS	READ-WRITE	length of pipe	DOUBLE
temperature-minimum	275	UNITLESS	READ-WRITE	Minimum temperature for temperature dependent properties	DOUBLE
specific-heat-transferred	False	UNITLESS	READ ONLY	Whether specific-heat should be transferred to the solver.	BOOLEAN
geometry-parameterization	True	UNITLESS	READ-WRITE	indicates if parameterization is enabled	BOOLEAN
thermal-conductivity-transferred	False	UNITLESS	READ ONLY	Whether thermal-conductivity should be transferred to the solver.	BOOLEAN
public-species	ch3oh	UNITLESS	READ ONLY	public species names	STRING
geometry scale factor	1	UNITLESS	READ ONLY	meshing scale factor	DOUBLE
geometry model name	pipe	UNITLESS	READ ONLY	base name of gambit journal file	STRING
geometry parameter 1	0.1	UNITLESS	READ-WRITE	radius of pipe	DOUBLE
file-system	pipe.jou	UNITLESS	READ ONLY	Files Required to run the case	STRING
model-views	pipe	UNITLESS	READ ONLY	The equipment views for post-processing.	STRING
archive-rom-data	False	UNITLESS	READ-WRITE	Whether to archive data for reduced order modeling.	BOOLEAN

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Reduced Order Models (ROMs)



- Build *inexpensive* ROMs from FLUENT results
- ROMs can be run within the PME

The screenshot displays the ANSYS APECS 1.6 interface. The main window shows a tree view on the left with categories like Reactors, Combustors, and CSTRs. The central pane displays a welcome message and copyright information. Overlaid on this is the 'ROM Inputs' dialog box, which contains a table of input parameters and simulation settings.

	Include	Lower Bound	Upper Bound	Base Values	Simulation #1	Simulation #2	Simulation #3	Simulation #4
air-inlet-4								
o2 (kg/s)	No	0.0	1000.0	0.0	0.0	0.0	0.0	0.0
c4h10 (kg/s)	Yes	0.0055	0.0075	0.0065	0.007389	0.006944	0.006722	0.00605
co2 (kg/s)	No	0.0	1000.0	0.0	0.0	0.0	0.0	0.0
h2o (kg/s)	No	0.0	1000.0	0.0	0.0	0.0	0.0	0.0
co (kg/s)	No	0.0	1000.0	0.0	0.0	0.0	0.0	0.0
Parameters								
temperature-maximum [Real]	No	0.0	5000.0	2500.0	2500.0	2500.0	2500.0	2500.0
temperature-minimum [Real]	No	0.0	1000.0	298.0	298.0	298.0	298.0	298.0

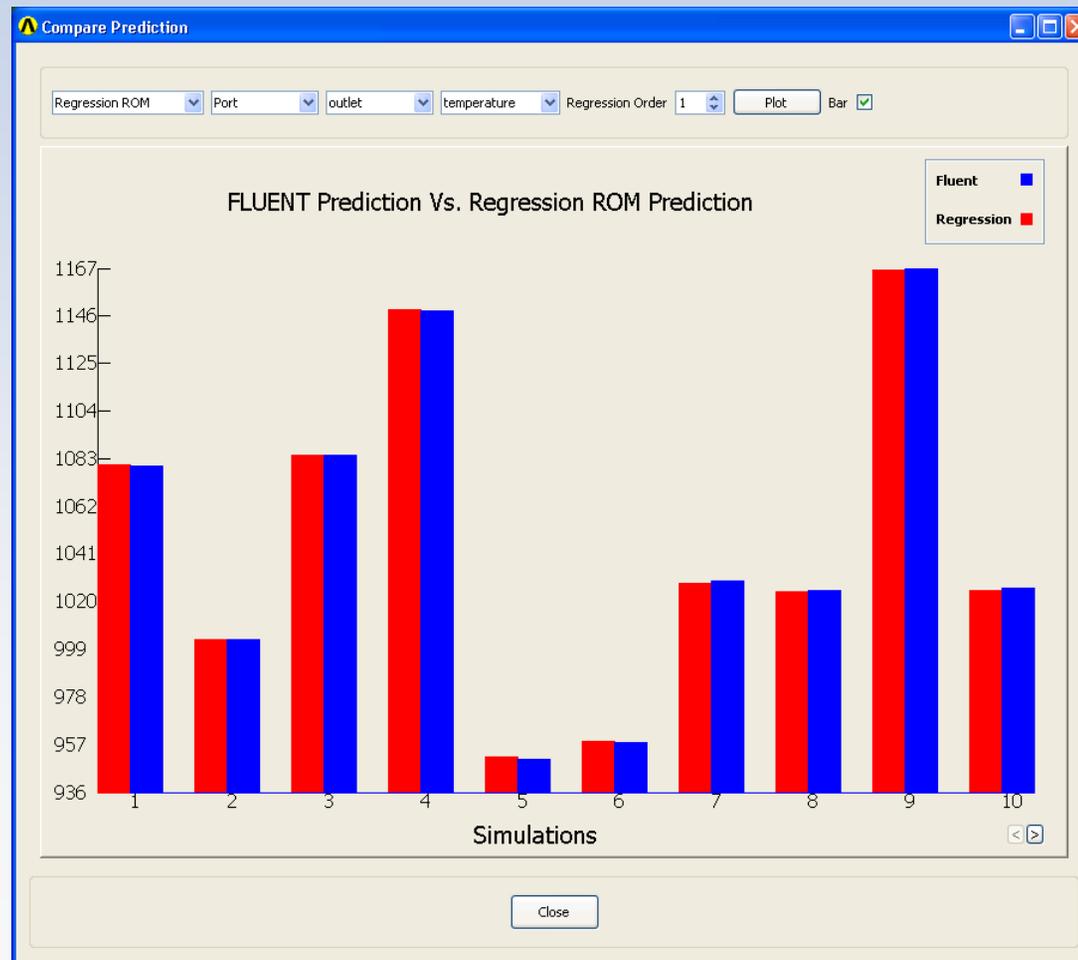
Below the table, the 'Specify Simulation Count' section shows: Total Simulations 10 = User Specified Simulations 9 + Simulation with Base Values 1 + Simulations with Min/Max Values 10 [Include?].

At the bottom of the dialog, there are buttons for 'Apply', 'OK', and 'Cancel'.

Reduced Order Models (2)



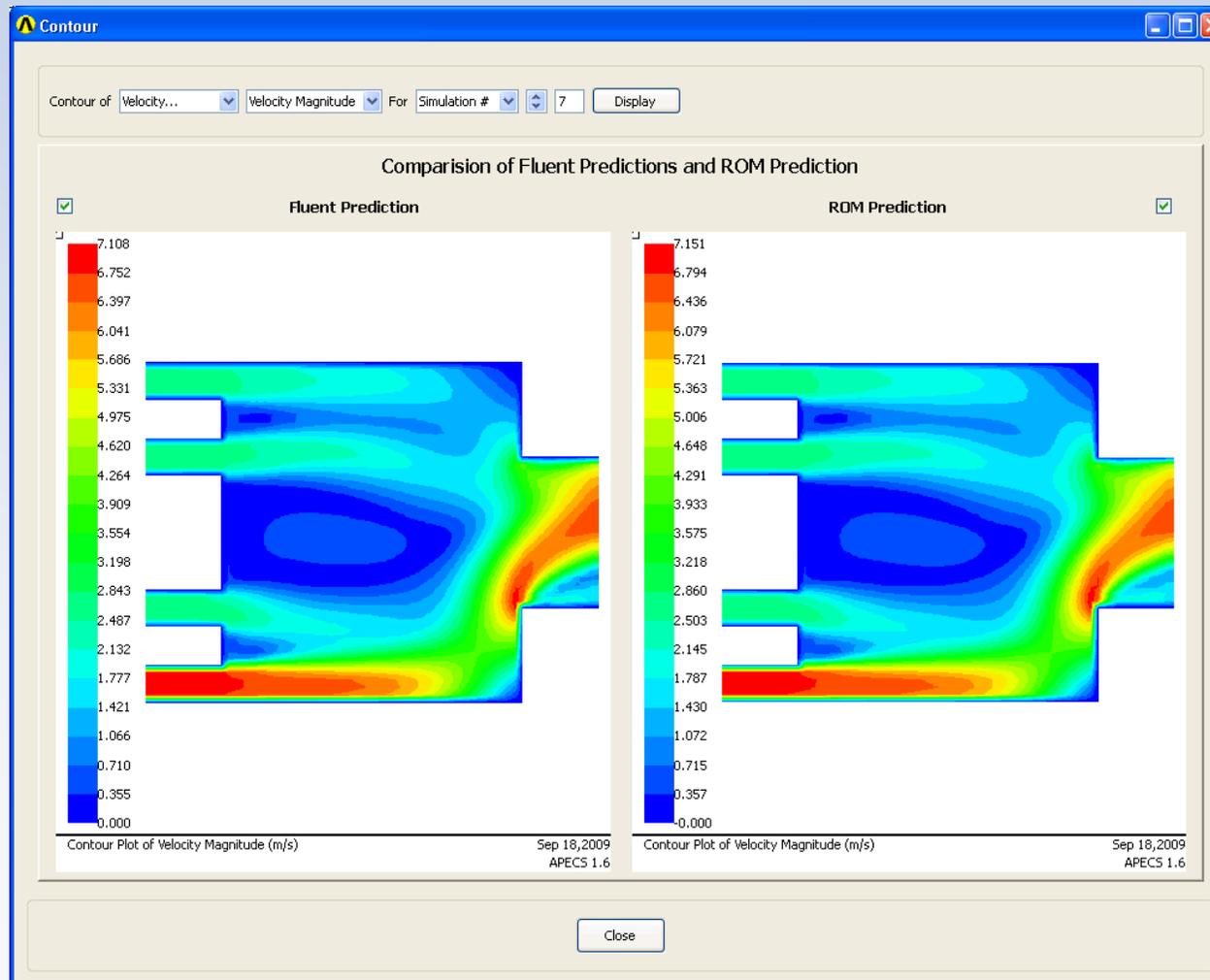
- APECS provides methods to evaluate the accuracy of the ROM



Reduced Order Models (3)



- ROMs with post-processing capabilities



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Solution Strategies



The screenshot shows the 'APECS Unit Operation' dialog box with the 'Solvers' tab selected. The 'Strategy' dropdown menu is open, showing options: 'Explicit solver', 'Static solution steps', 'Relative input change', and 'Explicit solver'. The 'Explicit solver' option is highlighted. Below the dropdown is a table with two columns: 'Max. Iterations' and 'Input change(%)'. The table contains two rows of data.

	Max. Iterations	Input change(%)
1 2d spray combustion	100	5.000000
2 Reacting Spray Example	100	5.000000

Buttons at the bottom of the dialog include 'Delete Solution Step', 'Reset Iterations', 'Add Solution Step', and 'Iteration Step 3'. A 'Close' button is located at the bottom right of the dialog.

APECS Features

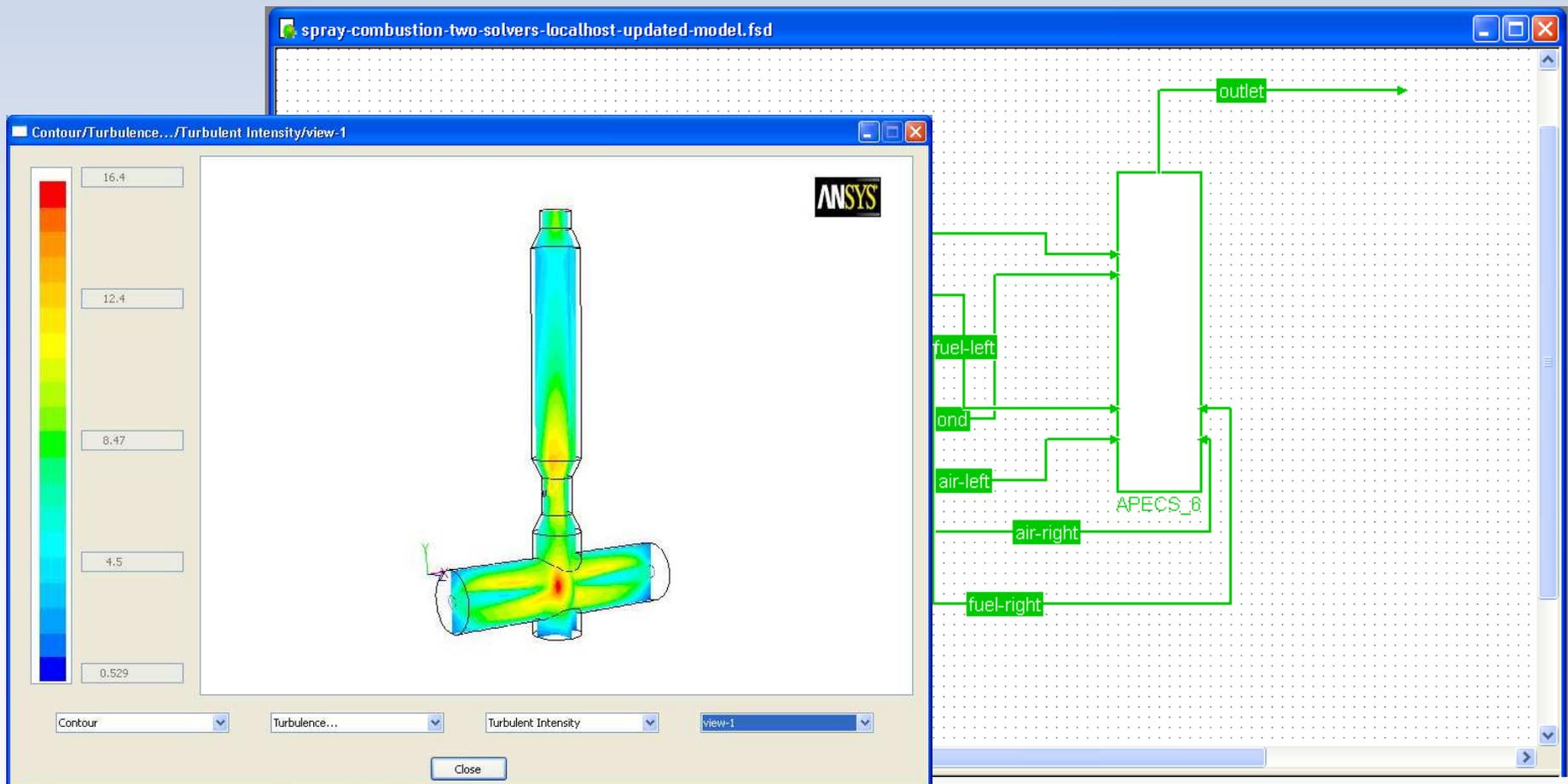


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CFD Viewer



- Permits the process modeler to view CFD or PCA ROM results from within the PME



APECS Features

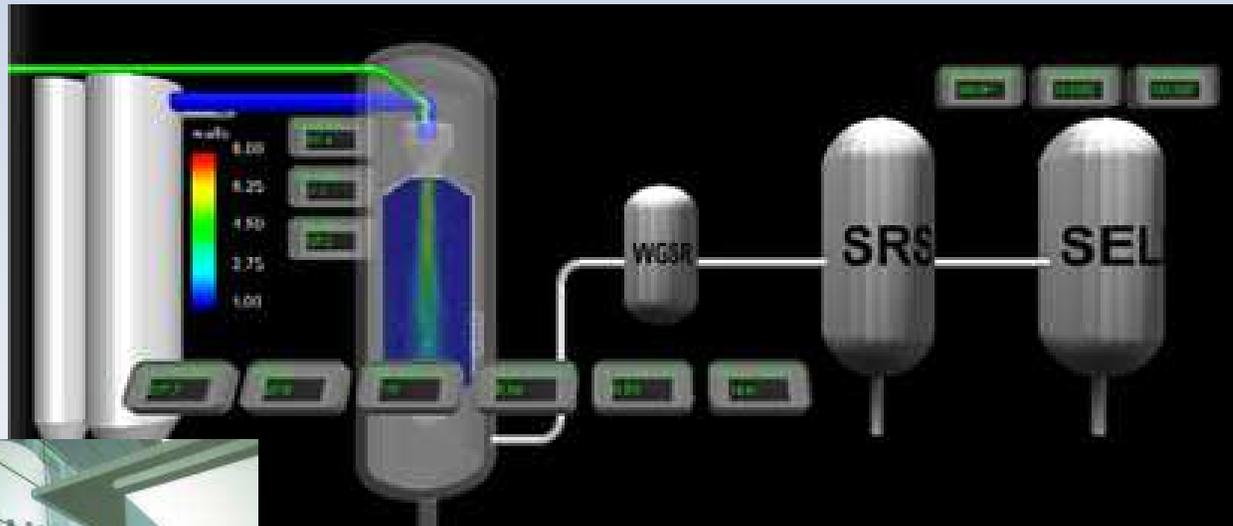


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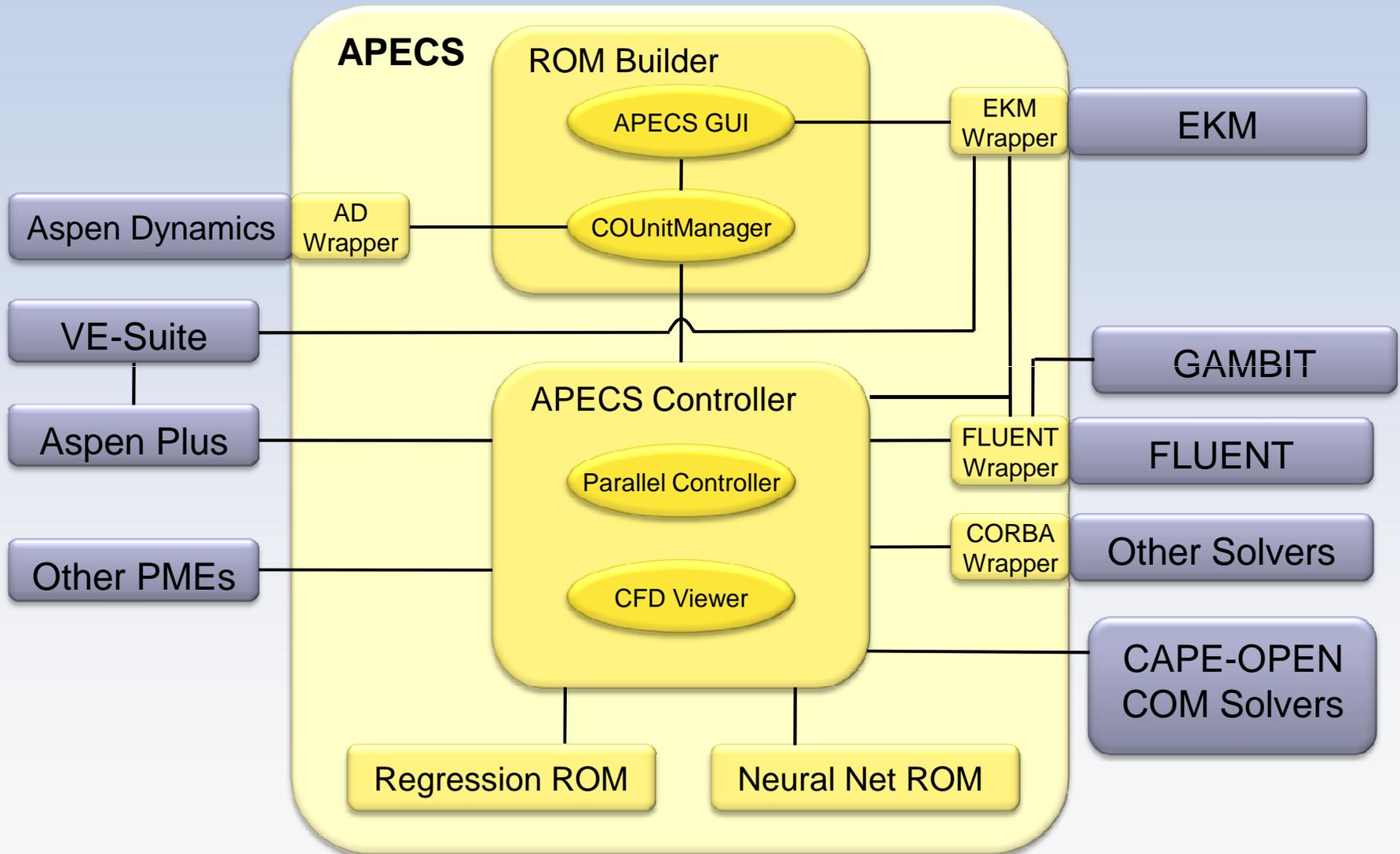
VE-Suite Coupling



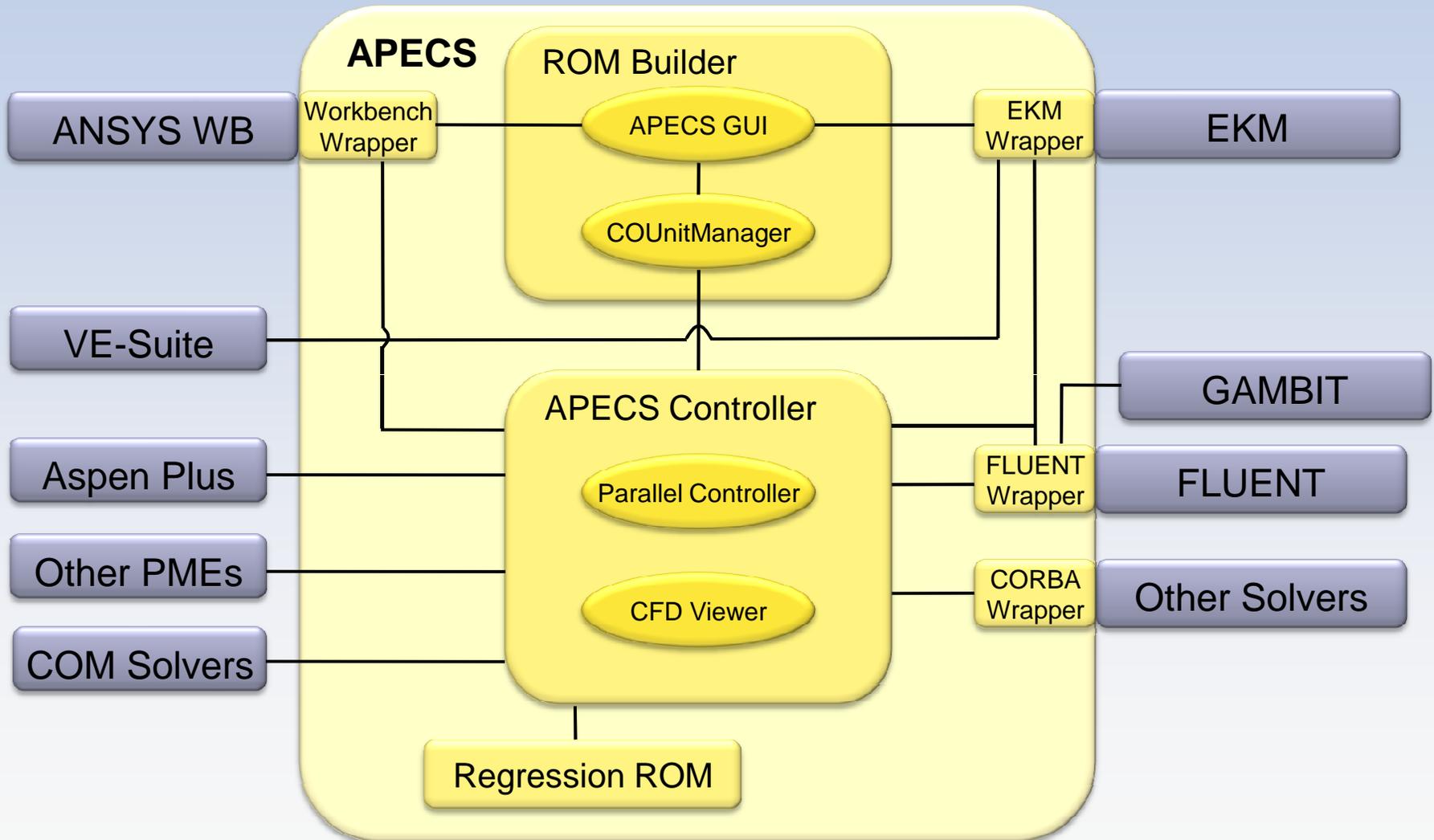
- Virtual Reality capabilities being developed by partners at Ames Laboratory



APECS Architecture



Future APECS Architecture



Summary



- APECS is *enabling* software being developed to couple Process Modeling and CFD for improved process design
- APECS permits process engineers to include high fidelity models in simulations of the overall plant performance
 - predict spatial variations in temperature, species concentrations, phases, etc.
 - reduce empiricism in predicting mixing, heat transfer, etc.
 - visualize the three-dimensional distributions within your equipment
 - model with greater realism, by including particle size distributions, turbulence/chemistry interaction, multiphase flow, thermal radiation, ...
 - more reliably predict off-design conditions
 - virtual scale-up capability based on first-principles simulation
- A variety of features are being implemented in APECS to maximize the utility and ease of use