APECS Software and Architecture Overview

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

• 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
  ![Diagram of ALSTOM Conventional Steam Plant]

- ALSTOM NGCC (250MWe) with 3D CFD HRSG
  ![Diagram of ALSTOM NGCC HRSG]

- Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC
  ![Diagram of Fuel Cell Auxiliary Power Unit]

- FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor
  ![Diagram of FutureGen Plant]

Performed by collaborators at NETL and ALSTOM Power
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
• 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
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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
Typical Workflow

CFD Engineer

- Develop CFD Model
- Configure CFD model for CO-compliance
- Add CFD Model to Database

Process Engineer

- Develop Process model
- Browse CFD Database and select model
- Set model parameters

- Set up solution strategy
- Map species names
- Conduct integrated simulation
- View CFD results

Indicates Optional Step
• Replace FLUENT model with Reduced Order Model (ROM)

**CFD Engineer**
- Develop CFD Model
- Configure CFD model for CO-compliance
- Add CFD Model to Database
- Run CFD Model and create ROM from results
- Add ROM to Database

**Process Engineer**
- Develop Process model
- Set up solution strategy
- Map species names
- Conduct integrated simulation
- View ROM results

Indicates Optional Step

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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:

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Units</th>
<th>Read Only</th>
<th>Description</th>
<th>Base Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>viscosity-transferred</td>
<td>False</td>
<td></td>
<td>READ ONLY</td>
<td>Whether viscosity should be transferred to the solver.</td>
<td>BOOLEAN</td>
</tr>
<tr>
<td>maximum-iterations</td>
<td>5</td>
<td>UNITLESS</td>
<td>READ-WRITE</td>
<td>Maximum number of FLUENT iterations</td>
<td>INTEGER</td>
</tr>
<tr>
<td>molecular-weight-transferred</td>
<td>False</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>Whether molecular-weight should be transferred to the solver.</td>
<td>BOOLEAN</td>
</tr>
<tr>
<td>density-transferred</td>
<td>False</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>Whether density should be transferred to the solver.</td>
<td>BOOLEAN</td>
</tr>
<tr>
<td>converted</td>
<td>False</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>Whether FLUENT converted or not at the end of a given n</td>
<td>BOOLEAN</td>
</tr>
<tr>
<td>temperature-maximum</td>
<td>400</td>
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<td>READ-WRITE</td>
<td>Maximum temperature for temperature dependent property</td>
<td>DOUBLE</td>
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<tr>
<td>geometry parameter 2</td>
<td>3</td>
<td>UNITLESS</td>
<td>READ-WRITE</td>
<td>length of pipe</td>
<td>DOUBLE</td>
</tr>
<tr>
<td>temperature-minimum</td>
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<td>READ-WRITE</td>
<td>Minimum temperature for temperature dependent property</td>
<td>DOUBLE</td>
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<tr>
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<td>READ ONLY</td>
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<td>BOOLEAN</td>
</tr>
<tr>
<td>geometry-parameters</td>
<td>True</td>
<td>UNITLESS</td>
<td>READ-WRITE</td>
<td>indicates if parameterization is enabled</td>
<td>BOOLEAN</td>
</tr>
<tr>
<td>thermal-conductivity-transferred</td>
<td>False</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>Whether thermal-conductivity should be transferred to the solver.</td>
<td>BOOLEAN</td>
</tr>
<tr>
<td>public-species</td>
<td>ch5oh</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>public species names</td>
<td>STRING</td>
</tr>
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<td>geometry scale factor</td>
<td>1</td>
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<td>READ ONLY</td>
<td>meshing scale factor</td>
<td>DOUBLE</td>
</tr>
<tr>
<td>geometry model name</td>
<td>pipe</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>base name of gmbit journal file</td>
<td>STRING</td>
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<td>geometry parameter 1</td>
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<td>radius of pipe</td>
<td>DOUBLE</td>
</tr>
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<td>file system</td>
<td>pipe</td>
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<td>READ ONLY</td>
<td>Files Required to run the case</td>
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</tr>
<tr>
<td>model views</td>
<td>pipe</td>
<td>UNITLESS</td>
<td>READ ONLY</td>
<td>The equipment views for post-processing</td>
<td>STRING</td>
</tr>
<tr>
<td>archive-onm-data</td>
<td>False</td>
<td>UNITLESS</td>
<td>READ-WRITE</td>
<td>Whether to archive data for reduced order modeling</td>
<td>BOOLEAN</td>
</tr>
</tbody>
</table>
Cₚ for Ethanol
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Remote FLUENT Execution

**Server Configuration**

- **Solver:** Pipe model
- **Server:** linux_1
- **FLUENT specific:**
  - **Number of Processors:** 4
  - **Communicator:** smpi
  - **FLUENT Host File or Compute Nodes:** linux_1, linux_2, linux_2, linux_2

**Solution Step Details**

- **Solver:** Pipe model

**Options:**
- Delete Solution Step
- Reset Iterations
- Add Solution Step
- Iteration Step 0

**Buttons:**
- OK
- Cancel

**Note:**
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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
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Reduced Order Models (ROMs)

- Build inexpensive ROMs from FLUENT results
- ROMs can be run within the PME
Reduced Order Models (2)

- APECS provides methods to evaluate the accuracy of the ROM
• ROMs with post-processing capabilities
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• Permits the process modeler to view CFD or PCA ROM results from within the PME
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VE-Suite Coupling

- Virtual Reality capabilities being developed by partners at Ames Laboratory
Future APECS Architecture
• 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