Process-Industry CAPE-OPEN Software Standard Overview

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Outline of Presentation

• Introduction
  – What is CAPE-OPEN?
  – Brief History

• CAPE-OPEN Interfaces
  – Unit Operations
    • Use in APECS
  – Thermodynamics/Properties
    • Use in APECS

• CAPE-OPEN Laboratories Network (CO-LaN)
  – Missions

• Concluding Remarks
What is CAPE-OPEN?

• CAPE-OPEN (CO) defines open standard interfaces that allow CAPE (Computer-Aided Process Engineering) software components to interoperate
  – Unit Operations  – Numerical Solvers
  – Physical Properties  – Reaction Kinetics

• European CAPE-OPEN Project (1997-99)
  – 15 partners, including Aspen Technology

• Global CAPE-OPEN (1999-2001)
  – 30 partners in Europe, USA, Canada, Japan

• CAPE-OPEN Laboratories Network (CO-LaN)
  – > 80 partners from process industries, software vendors, research and consulting entities, universities, and government labs
  – Contributing resources to support ongoing work on the CO standard
  – Interface specifications and software download (www.colan.org)
CAPE-OPEN Unit Operations

• End-user can plug any CO-compliant Unit Operation into any CO-compliant Simulator (socket)

CO-Compliant Unit Operations
• APECS
• ChemSep
• COUSCOUS, GLCC
• gO:CAPE-OPEN
• SolidSim
• TUWAX
• XChanger Suite  …

CO-Compliant Simulators
• Aspen Plus
• Aspen Hysys
• COFE
• gPROMS
• INDISS
• Petro-Sim
• ProSim Plus
• UniSim Design  …
CAPE-OPEN Unit Operation Interface

Unit Operation
- ICapelIdentification
- ICapeUtilities
- ICapeUnit
- ICapeUnitReport
- Error interfaces

Port collection
- ICapelIdentification
- ICapeCollection
- Error interfaces

Parameter collection
- ICapelIdentification
- ICapeCollection
- Error interfaces

Ports
- ICapelIdentification
- ICapeUnitPort
- Error interfaces

Parameters
- ICapelIdentification
- ICapeParameter
- ICapeParameterSpec
- ICapeTYPEParameterSpec
- Error interfaces
APECS Co-Simulation Workflow
Seamless Integration of CFD and Process Simulation Tasks

**Equipment/CFD Simulation**
- Develop CFD equipment model
- Configure CFD model
- Create ROM from CFD results (optional)
- Add CFD/ROM model to model database

**Process Simulation**
- Develop process simulation model
- Load CAPE-OPEN model library
- Instantiate APECS CAPE-OPEN block
- Select CFD/ROM model from model database

**APECS Co-OPEN Configuration Wizard**
- Set parameter values for equipment model
- Specify solution strategy
- Map species and ports
- Run process/equipment co-simulation
- View and analyze CFD results

**APECS CFD Package**
- Process Simulator

**APECS**
- CAPE-OPEN Configuration Wizard
Use of CAPE-OPEN in APECS

Unit Operation: Configuration Wizard

- Prepare equipment/CFD models as CAPE-OPEN (CO) models for use in CO-compliant simulators
- Invoke from within FLUENT® or as standalone tool
- Define CO ports (e.g., BCs, custom 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 Model Database (EKM™)
APECS Co-Simulation Workflow
**Seamless Integration of CFD and Process Simulation Tasks**

**Equipment/CFD Simulation**
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**Process Simulation**
- Develop process simulation model
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**Integration Steps**
- Set parameter values for equipment model
- Specify solution strategy
- Map species and ports
- Run process/equipment co-simulation
- View and analyze CFD results
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

1) Load CAPE-OPEN Library

2) Instantiate APECS Block

Process Simulator GUI
CAPE-OPEN Thermodynamics/Properties

- End-user can plug any CO-compliant Property Package into a CO-compliant Simulator

**External CO Property Package**
- Aspen Properties
- PPDS
- UniSim COMThermo
- Aspen Hysys COMThermo
- Simulis Thermodynamics
- MultiFlash
- CO-SPPTS, TEA, GERG, ...

**CO-Compliant Simulators**
- Aspen Plus
- Aspen Hysys
- COFE
- COMSOL
- gPROMS
- INDISS
- ProSlm Plus
- PRO/II
- UniSim Design
- Simulis Thermodynamics
- SolidSim
- TUWAX
- Xchanger Suite
Use of CAPE-OPEN in APECS

**Physical Properties**

- Automatic transfer of pure component physical properties (limited to a single phase) from process simulator to CFD equipment model
- Temperature-dependent properties
  - Density
  - Specific Heat
  - Thermal Conductivity
  - Viscosity
- Mixture properties are calculated using the mixing rules in FLUENT®
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CO-LaN: The CAPE community behind CAPE-OPEN

Process Industries

Simulation Software Vendors

Research, Consulting, Government, Universities

...And quite a few more

www.colan.org
CAPE-OPEN Laboratories Network

81 members as of October 2009

- 42 Software suppliers
- 8 Operating Companies
- 2 Governmental
- 23 Universities
- 6 Individuals
CO-LaN Missions

• User Priorities
• Exploitation and Dissemination
• Lifecycle Management
• Testing and Interoperability Facilitation
• Training and Migration Facilitation
User Priorities for CAPE-OPEN Standards

• Work with user community to clarify priorities for CO-compliant software components/simulators
  – New CO-compliant Thermo/Properties sockets
    • Matlab and Scilab
  – New CO-compliant Unit Operations
    • Excel, Matlab, and Scilab
  – Upgraded versions of CO-compliant simulators
    • aspenONE v7.1, PRO/II 8.3, ProSim Plus 3.1, COCO 1.15, gPROMS 3.2, …
Exploitation and Dissemination

- Promote CAPE-OPEN standard and distribute information and technology to the international user community
- CAPE-OPEN European Conference Series
  - April 2-3, 2009, Munich, Germany
    - 30+ participants
    - Skopau, Germany (2004); Como, Italy (2005); Cannes, France (2006); Heidelberg, Germany (2007), Cambridge, UK (2008)
- CAPE-OPEN U.S. Conference series
  - November 11, 2009, Nashville, Tennessee
    - EPA, Cincinnati (2004); NETL, Morgantown (2005); AIChE, San Francisco (2006); Salt Lake City (2007); Philadelphia (2008)
- Forum (capeopen.forumer.com)
- Website (www.colan.org)
  - Interface specifications and software download
Lifecycle Management

• Organize the maintenance, evolution, and expansion of the CAPE-OPEN interface specifications

• Special Interest Groups
  – Hydrodynamic SIG
    • Design of interface specification for hydrodynamic point model
  – Thermo SIG
    • Revision of Thermodynamic and Physical Properties interface specification 1.0 and 1.1 to clear them up
  – Methods & Tools SIG
    • Flowsheeting monitoring interface design
Testing and Interoperability Facilitation

• **Interoperability**
  – Interoperability is the core of CO-LaN
  – Large set of interoperability tests performed and reported in 2008:
    • Around 165 documented tests
    • Continued effort on specific tests prioritized by full members

• **Remote access to CO-LaN laptop**
  – Equipped with 13 PMEs and 20+ PMCs

• **Logging and Testing Tools**
  – COLTT (v1.07) maintained by CO-LaN
    • Works in process. Open source (SourceForge)
  – OATS maintained by AmsterCHEM
    • Works out of process
Training and Migration Facilitation

- Ensure that training modules, guidelines, and tools to facilitate component wrapping are developed and available
- CO-LaN can advise on training options and facilitate contacts for training providers
- Wizards
  - Automatically creates most of the code needed to make a CAPE-OPEN Unit Operation
  - Visual Basic 6.0, C++, Fortran 90, Delphi
- Code examples
  - Unit Operation: heat exchanger (M&T SIG)
  - Property Package 1.1 (Thermo SIG)
Concluding Remarks

• CAPE-OPEN is recognized as THE non-proprietary software interface standard in process simulation

• CO-LaN is the internationally recognized user-driven organization for testing and managing the CO standard

• Key process simulation software providers are developing CAPE-OPEN solutions and ensuring full compliance
  – CO-compliant simulators with sockets for unit operations and thermodynamics packages
  – CO-compliant unit operation and thermodynamic/property package plugs
  – Push made by end-user organizations

• End users are developing proprietary CO-compliant unit operations and thermodynamics packages

• CAPE-OPEN standard facilitates interoperability for process/equipment co-simulation in APECS