



**NETL 2009  
Workshop on  
Advanced  
Process  
Engineering  
Co-Simulation  
(APECS)**

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**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**



**APECS**

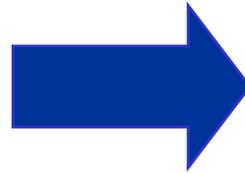
# What is CAPE-OPEN?

- **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](http://www.colan.org))



# CAPE-OPEN Unit Operations

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



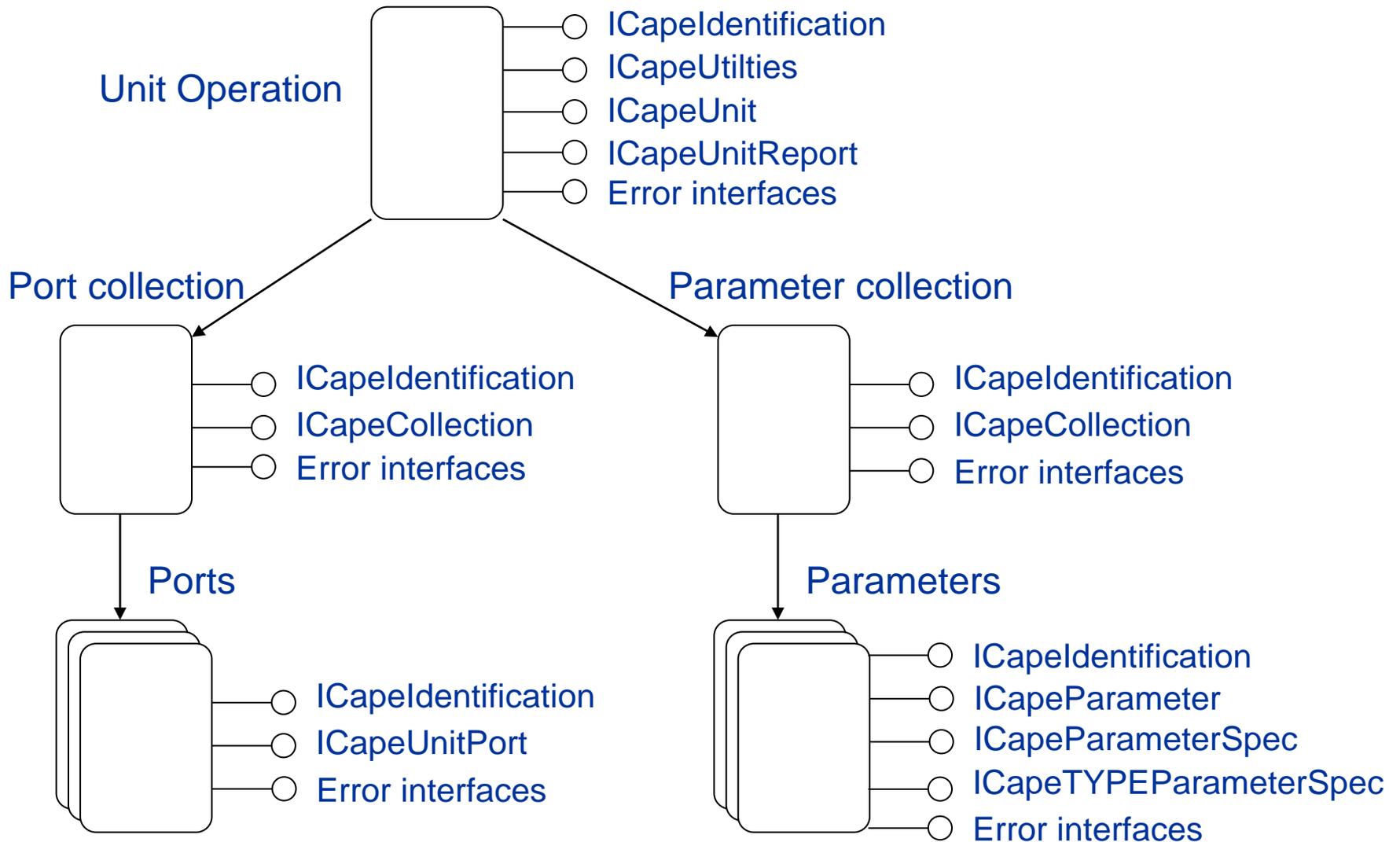
## CO-Compliant Unit Operations

- **APECS**
- ChemSep
- COUSCOUS, GLCC
- gO:CAPE-OPEN
- SolidSim
- TUWAX
- XChanger Suite ...

## CO-Compliant Simulators

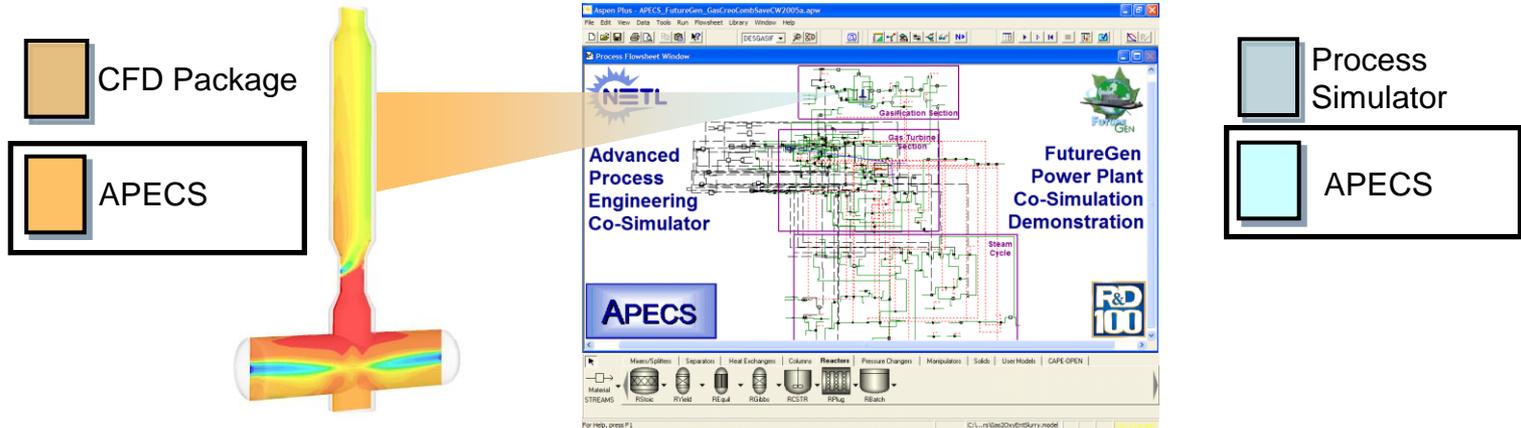
- Aspen Plus
- Aspen Hysys
- COFE
- gPROMS
- INDISS
- Petro-Sim
- ProSim Plus
- UniSim Design ...

# CAPE-OPEN Unit Operation Interface

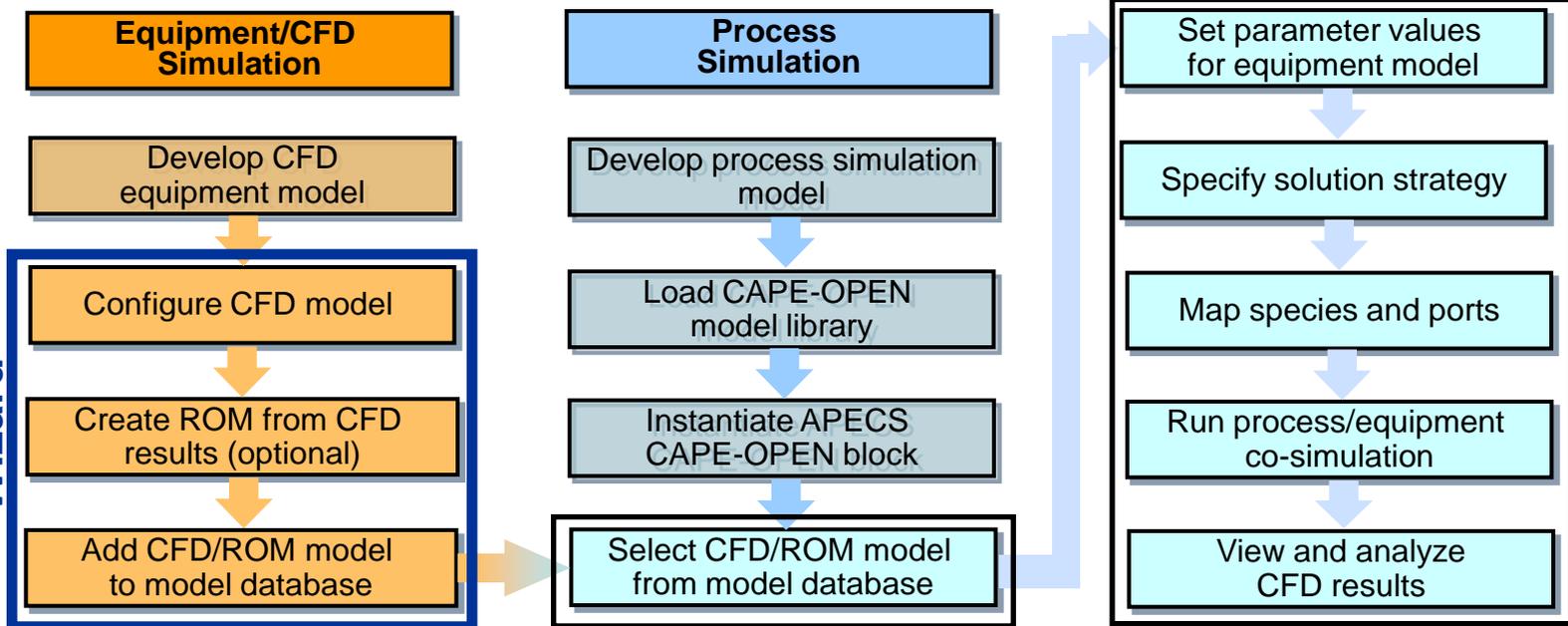


# APECS Co-Simulation Workflow

## Seamless Integration of CFD and Process Simulation Tasks



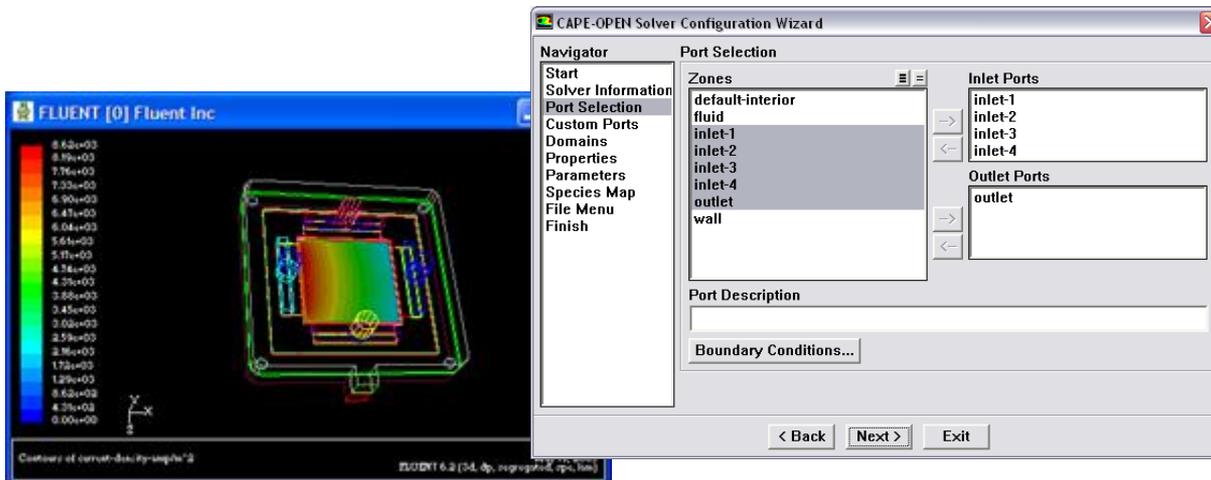
**CAPE-OPEN Configuration Wizard**



# Use of CAPE-OPEN in APECS

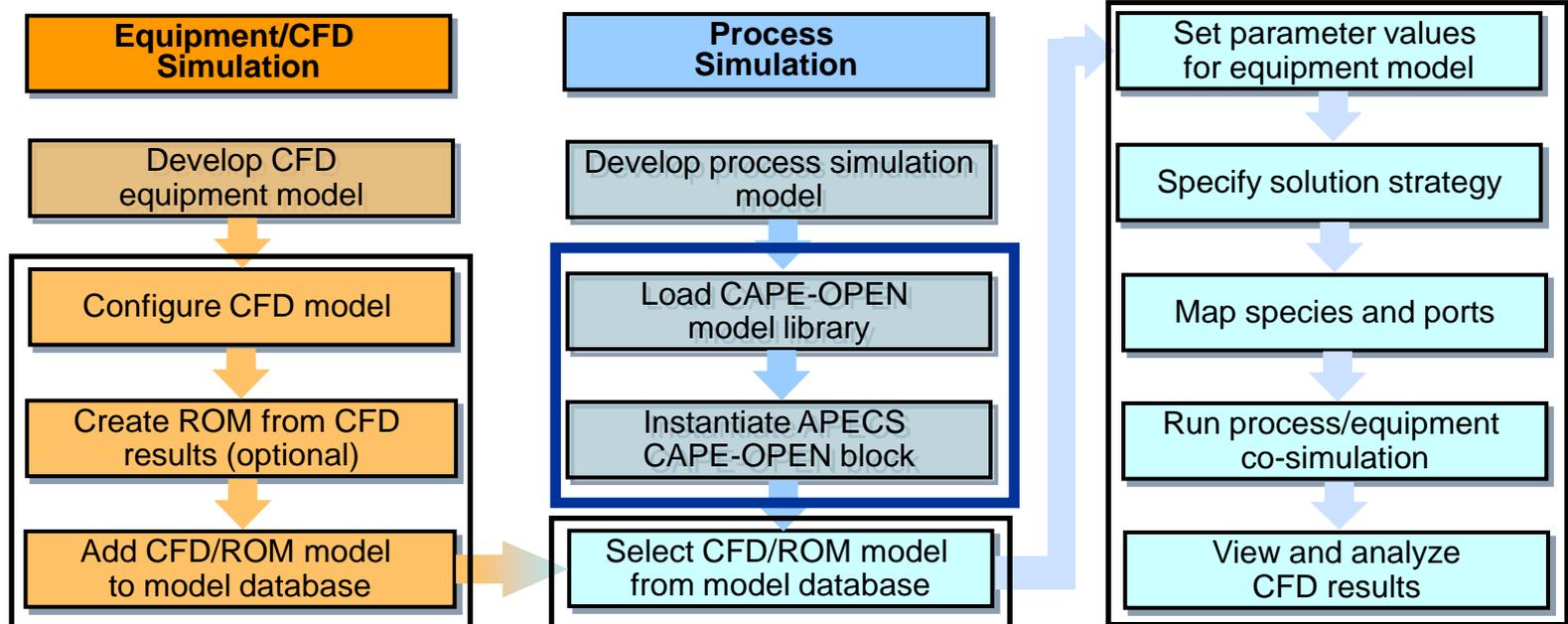
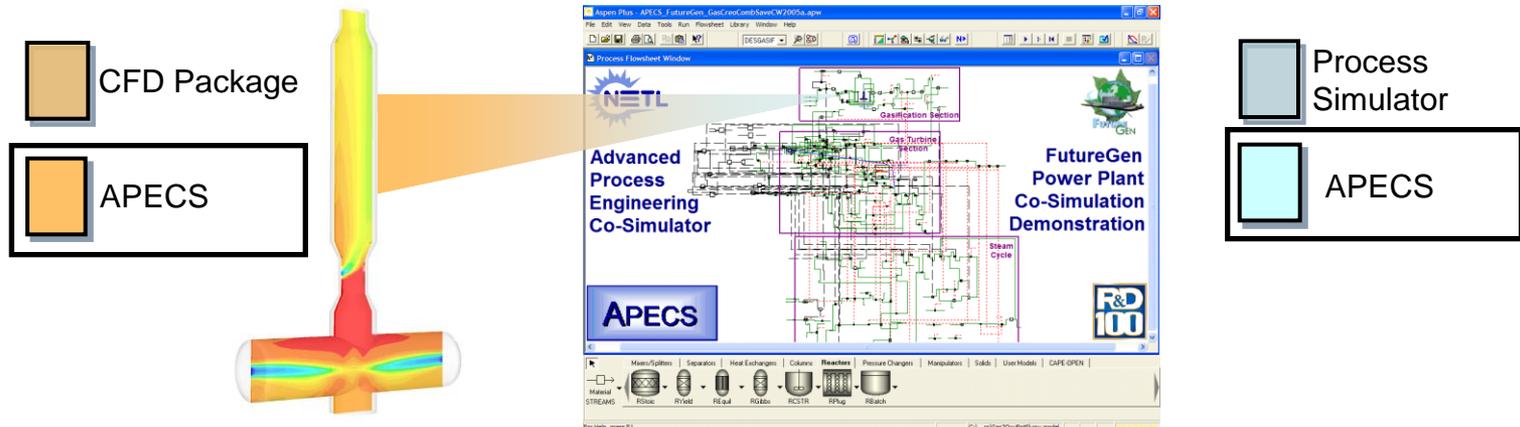
## Unit Operation: Configuration Wizard

- Prepare equipment/CFD models as CAPE-OPEN (CO) models for use in CO-compliant simulators
- Invoke from within FLUENT<sup>®</sup> 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<sup>™</sup>)



# APECS Co-Simulation Workflow

## Seamless Integration of CFD and Process Simulation Tasks

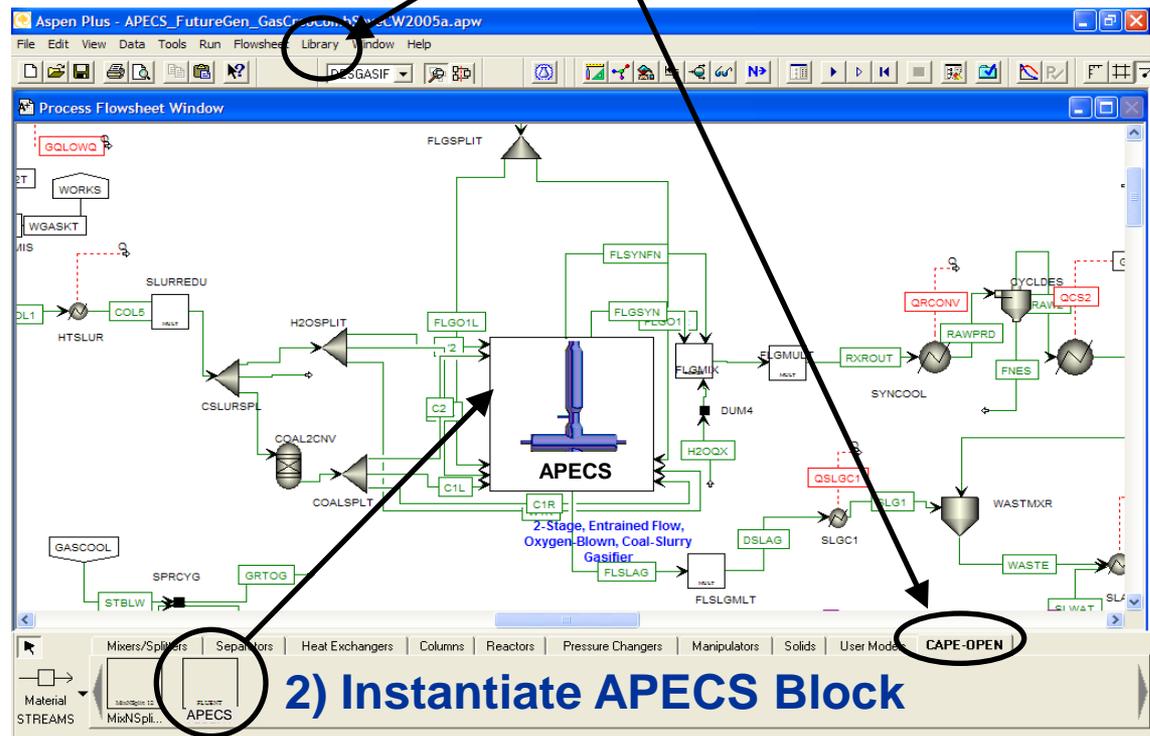


# Use of CAPE-OPEN in APECS

## 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

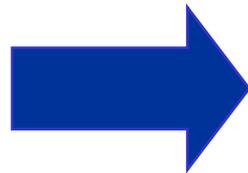


2) Instantiate APECS Block

Process Simulator GUI

# CAPE-OPEN Thermodynamics/Properties

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



## CO-Compliant Simulators

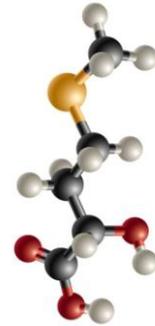
- Aspen Plus
- Aspen Hysys
- COFE
- COMSOL
- gPROMS
- INDISS
- ProSim Plus
- PRO/II
- UniSim Design
- Simulis Thermodynamics
- SolidSim
- TUWAX
- Xchanger Suite

## External CO Property Package

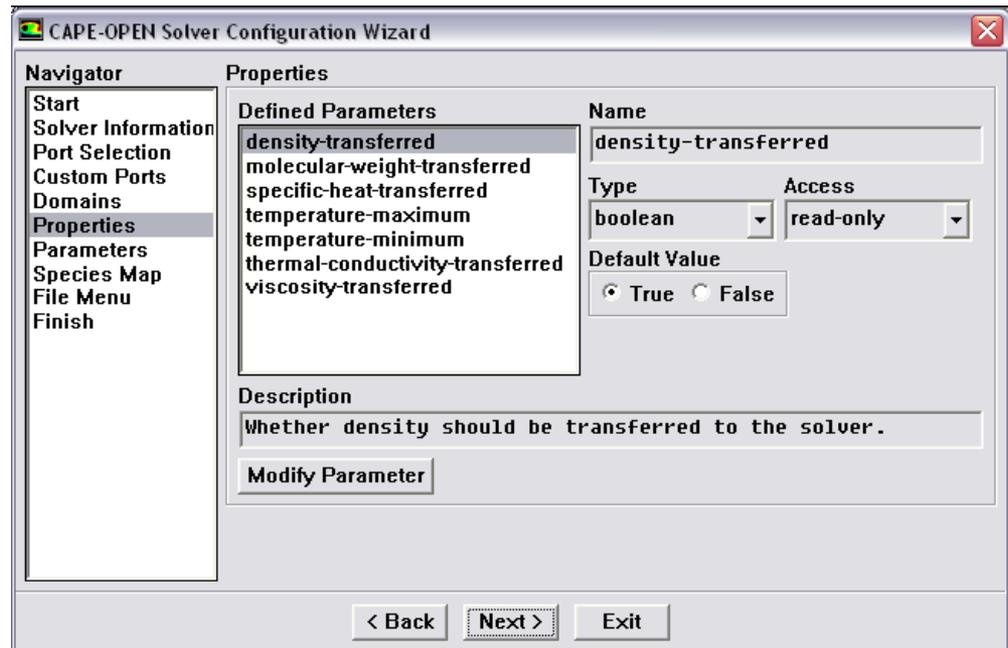
- Aspen Properties
- PPDS
- UniSim COMThermo
- Aspen Hysys COMThermo
- Simulis Thermodynamics
- MultiFlash
- CO-SPPTS, TEA, GERG, ...

# Use of CAPE-OPEN in APECS

## *Physical Properties*

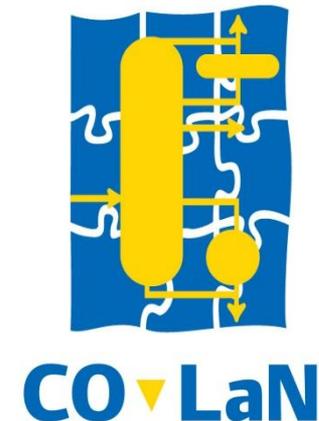


- Automatic transfer of pure component physical properties (limited to a single phase) from process simulator to CFD equipment model
- Temperature-dependent properties
  - Density
  - Specific Heat
  - Thermal Conductivity
  - Viscosity
- Mixture properties are calculated using the mixing rules in FLUENT®



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**APECS**

# CO-LaN: The CAPE community behind CAPE-OPEN

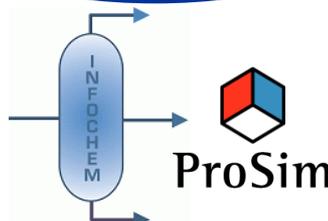
## Process Industries



## Simulation Software Vendors



## Research, Consulting, Government, Universities



# 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](http://capeopen.forumer.com))**
- **Website ([www.colan.org](http://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**

