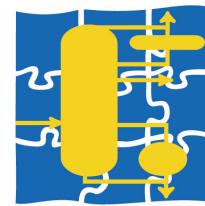


CAPE-OPEN



CO▼LaN

Michel PONS

Chief Technology Officer

Akzo Nobel Chemicals, Arnhem, November 17, 2005



Outline

▼ What is CAPE-OPEN?

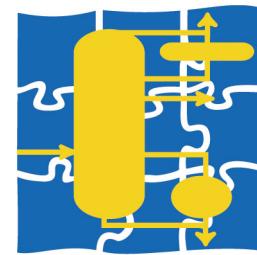
▼ What CAPE-OPEN permits for end-users?

▼ What is the CAPE-OPEN Laboratories Network?

▼ Conclusions



What is CAPE-OPEN?



CO▼LaN

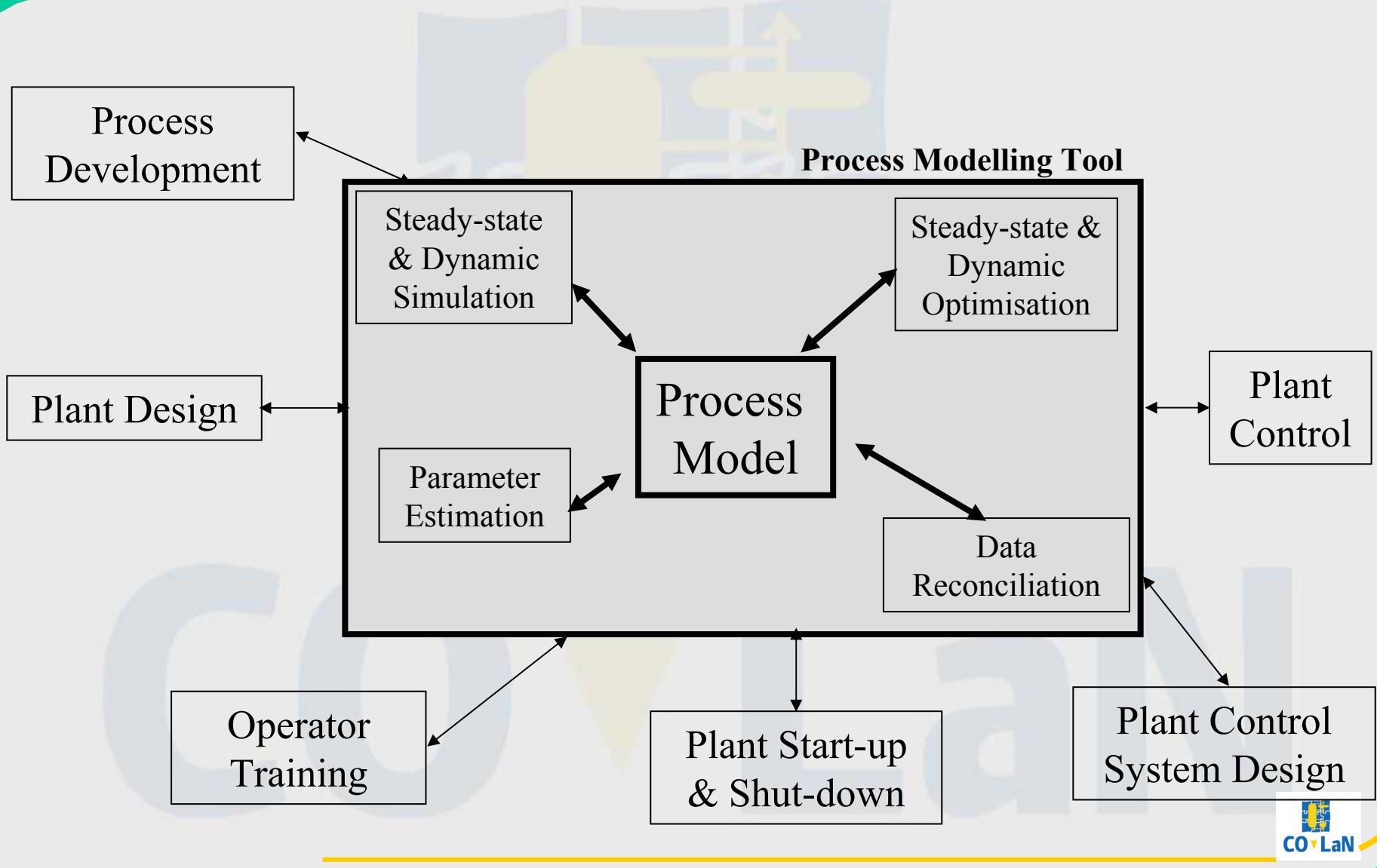


CAPE-OPEN: a technology for integration

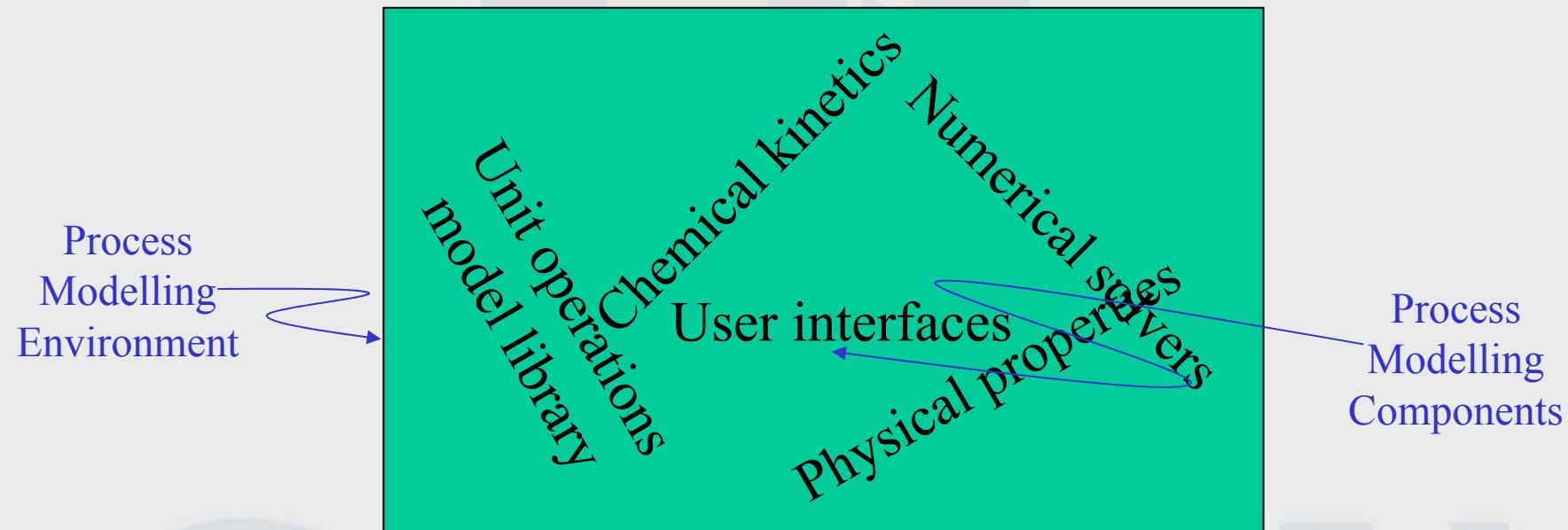
- ▼ A freely available industry standard for interfaces between software components making up process simulation tools
- ▼ The success of a collaboration between software vendors, end-users and academics
- ▼ A proven technology implemented in most process simulation tools
- ▼ A growing adhesion by process simulation market leaders



General-purpose process modelling tools



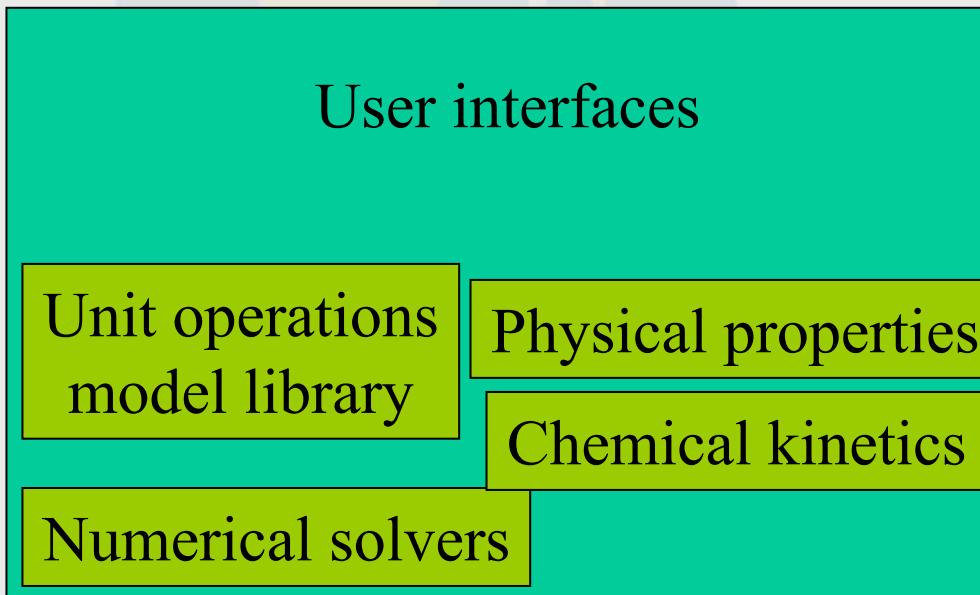
The anatomy of process modelling tools – a (somewhat) confusing reality



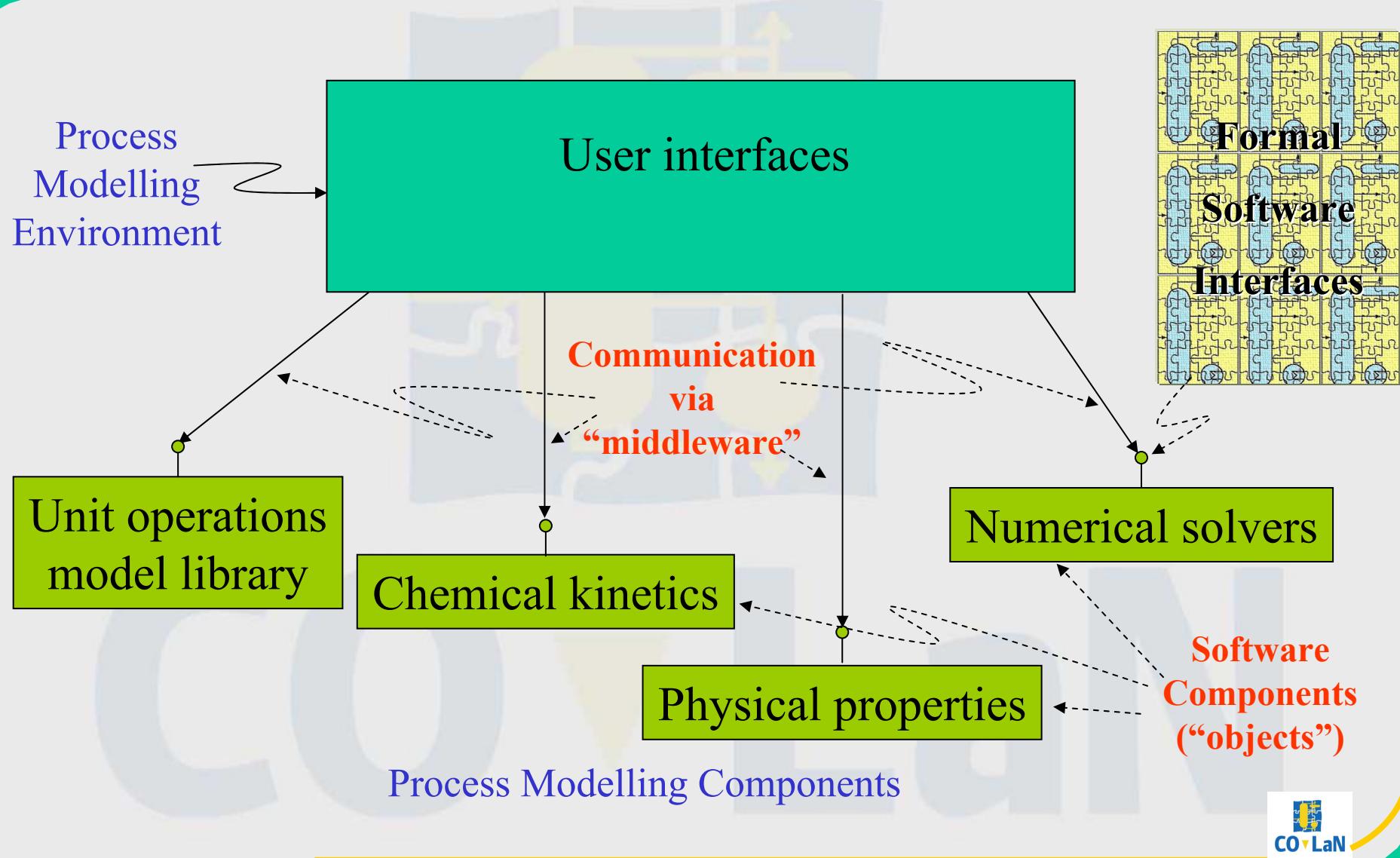
- Many interacting components...
- ...all tightly coupled with each other
- Component boundaries not always clearly delineated



Clarify boundaries between key components



...and break tool into 1 PME & multiple PMCs



Process modelling: components & environments

▼ Process Modelling Components (PMCs)

- ↪ Well-defined pieces of software, relatively narrow function
- ↪ Wide range of applications
 - Physical properties
 - Unit operation modules
 - Numerical solvers
 -



Process modelling: components & environments

▼ Process Modelling Components (PMCs)

▼ Process Modelling Environments (PMEs)

⇒ Support construction of process model

- From first-principles and/or library of unit operation models

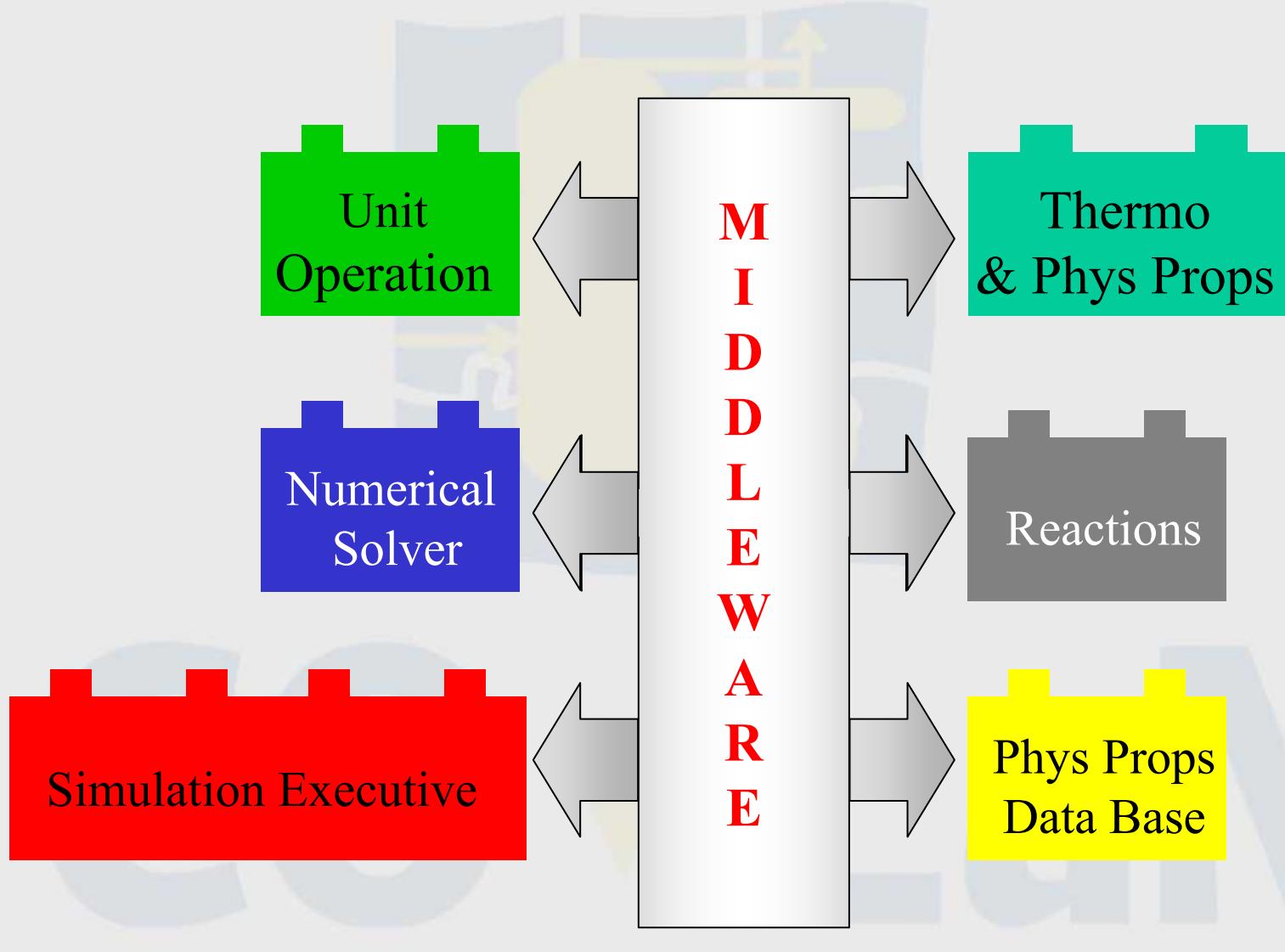
⇒ Support a number of model-based applications

- Simulation, optimisation, ...

⇒ May make use of one or more PMCs



CAPE-OPEN Components



CAPE-OPEN Documentation Set

▼ Abstract CO Interface specification

- ➲ Textual requirements
- ➲ Use Cases
- ➲ UML Diagrams
- ➲ List of interfaces/Methods/Arguments

▼ COM/CORBA implementations

- ➲ Interface Definition Language files
- ➲ Type library



CAPE-OPEN architecture

▼ Business interfaces

- Domain-specific interfaces for CAPE application domain: define interfaces to CO components involved in a CO process simulation application.

▼ PME Interfaces

- Interfaces for CO simulator executives: services of general use are defined such as diagnostics and material systems in order to be called by any CO component.

▼ Common interfaces

- Interfaces for handling services that may be required by any Business and COSE/PME interfaces: support basic functions and are always independent of Business and COSE/PME Interfaces.



CO interfaces releases

0.9 (CAPE-OPEN)
0.93 (GCO 2001)
1.0 (GCO 2002)

Other
Services

Planning
& Scheduling

PME Services

SMST

Numeric

PEDR

Optimisation
MILP, MINLP

PDAE
Solvers

Solvers
LAE, NLAE, DAE

Unit
Operations

Unit Operations

Physical
Properties

Petroleum
Fractions

Thermodynamic and Physical
Properties

Physical Properties
Data Bases

Electrolytes
Reactions

Parameters Collections

Persistence

Common Interfaces

Error Handling

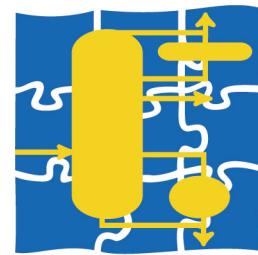
Identification

Utilities

Types and undefined values



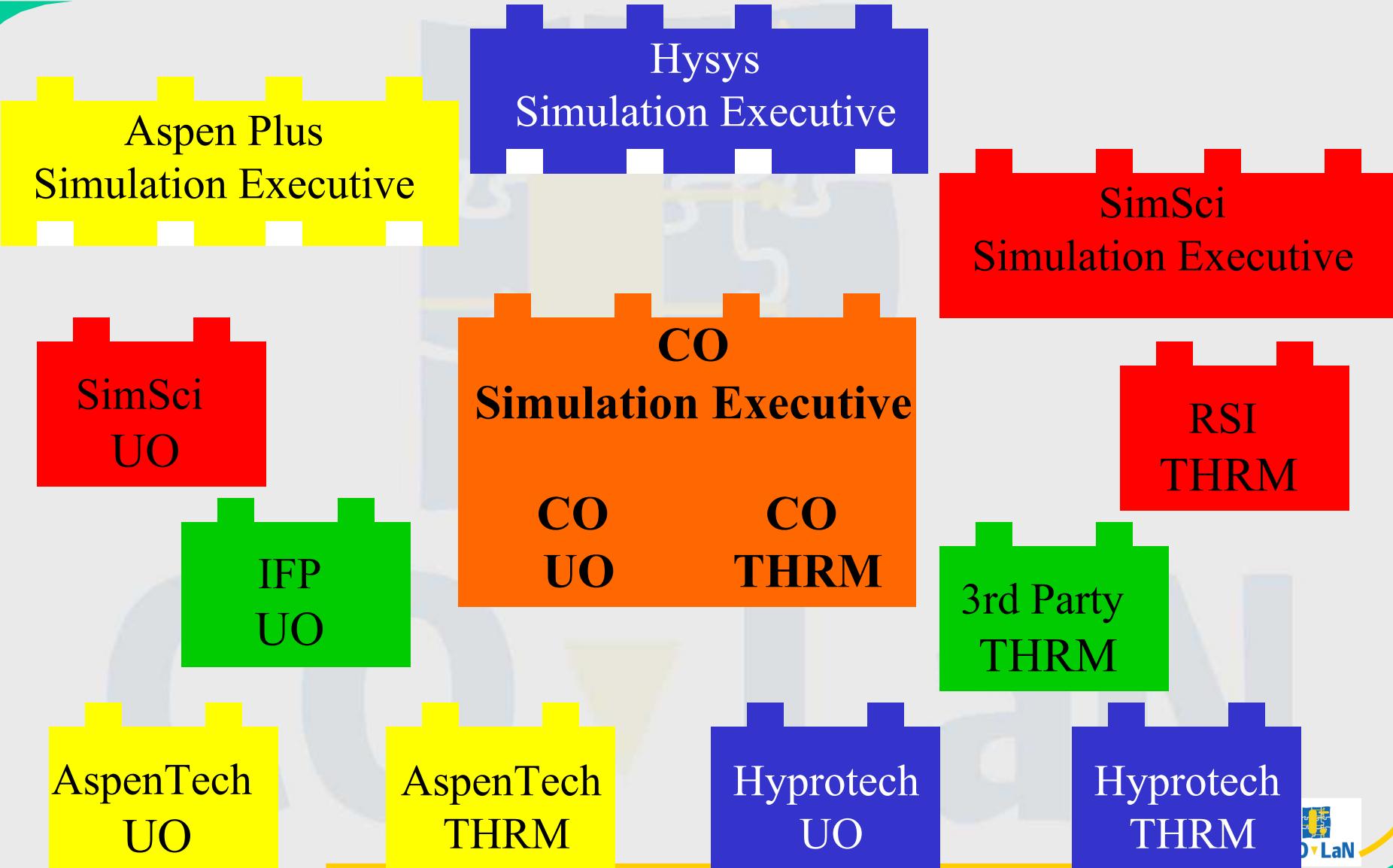
What CAPE-OPEN permits for end-users?



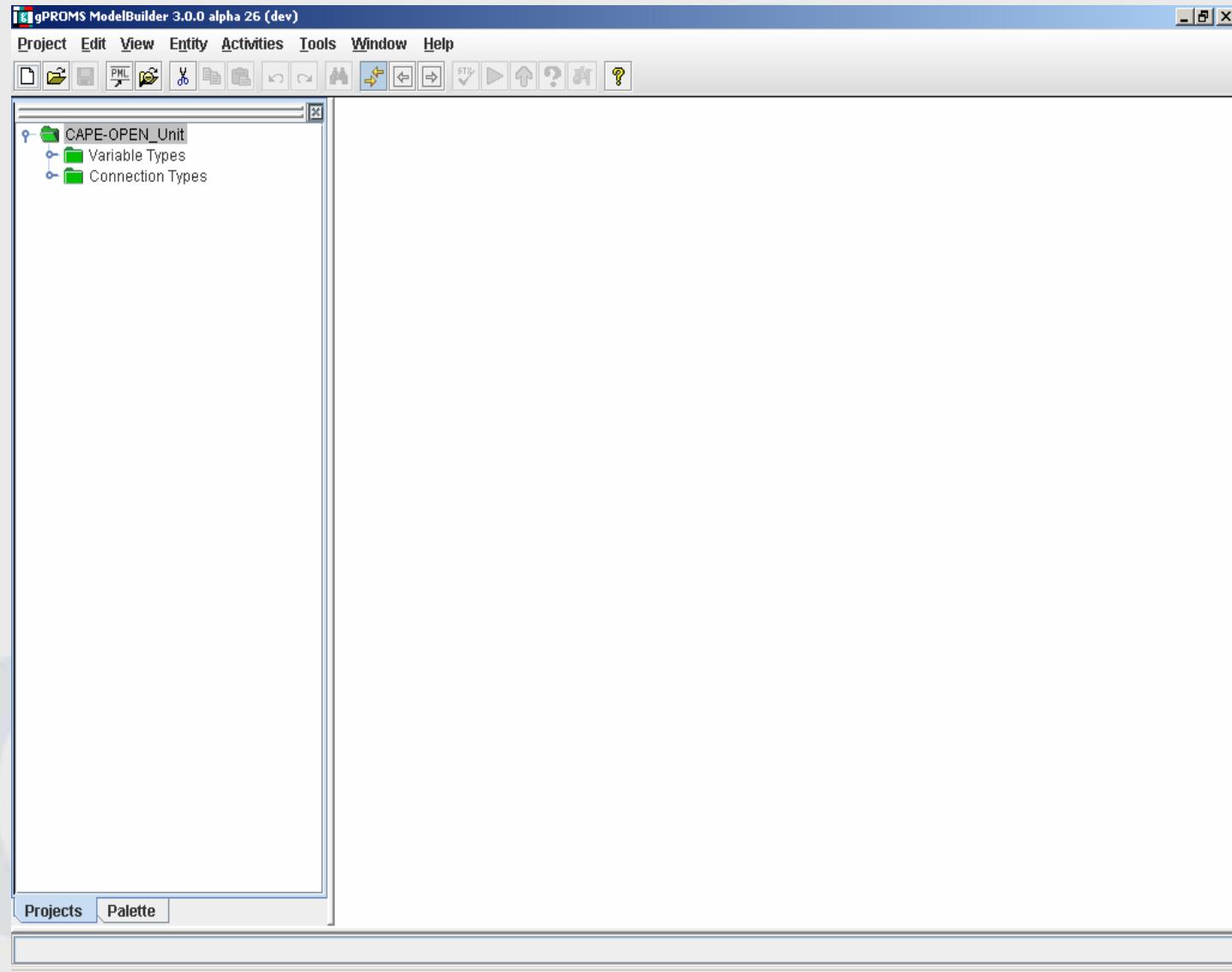
CO▼LaN



Interoperability



Load CAPE-OPEN library in ModelBuilder



Load/Create Mixer Model

The screenshot shows the gPROMS ModelBuilder interface with a project titled "PHJunction (PHMixer2)". The left pane displays a tree view of the project structure, including CAPE-OPEN Unit, Variable Types, Connection Types, and a PHMixer2 folder containing Variable Types, Stream Types, Connection Types, Models (with PHJunction selected), Tasks, Processes, Optimisations, Parameter Estimations, Experiment Designs, Experiments, Saved Variable Sets, and Miscellaneous Files.

The main pane contains the source code for the PHJunction model:

```
3
4 PORT
5   MidInlet AS CO_Material
6   TopInlet AS CO_Material
7   TopOutlet AS CO_Material
8
9 VARIABLE
10  junction_mass_specific_enthalpy    AS mass_specific_enthalpy
11  junction_mass_fraction           AS ARRAY(TopOutlet.no_components) OF mass_fraction
12  outFlow                         AS ARRAY(TopOutlet.no_components, 1) OF mass_flow
13  pressure                         AS no_type
14  DeltaP                           AS no_type
15  input_energy_rate                AS energy_rate
16 # flashResult AS ARRAY(TopOutlet.no_components*3 + 11) of no_type
17
18 EQUATION
19
20  FOR i := 1 TO TopOutlet.no_components DO
21    0 = TopInlet.mass_flowrate      * TopInlet.mass_fraction(i)
22    + MidInlet.mass_flowrate      * MidInlet.mass_fraction(i)
23    - ( TopOutlet.mass_flowrate * TopOutlet.mass_fraction(i) );
24
25  END
26
27  TopOutlet.enthalpy_flow * TopOutlet.mass_flowrate = TopInlet.enthalpy_flow
28    * TopInlet.mass_flowrate + MidInlet.enthalpy_flow * MidInlet.mass_flowrate
29    + input_energy_rate ;
30
31 # Out flows
32  TopOutlet.mass_flowrate = TopInlet.mass_flowrate + MidInlet.mass_flowrate;
33
34  TopOutlet.mass_fraction = junction_mass_fraction ;
35
```

Annotations with callouts point to specific parts of the code:

- A speech bubble labeled "Mass balance" points to the variable declarations for `junction_mass_specific_enthalpy` and `junction_mass_fraction`.
- A speech bubble labeled "Energy balance" points to the equation block where mass fractions are multiplied by enthalpy flow rates to calculate the outlet enthalpy flow.

Launch CAPE-OPEN export

No need to change model for CAPE-OPEN exportation

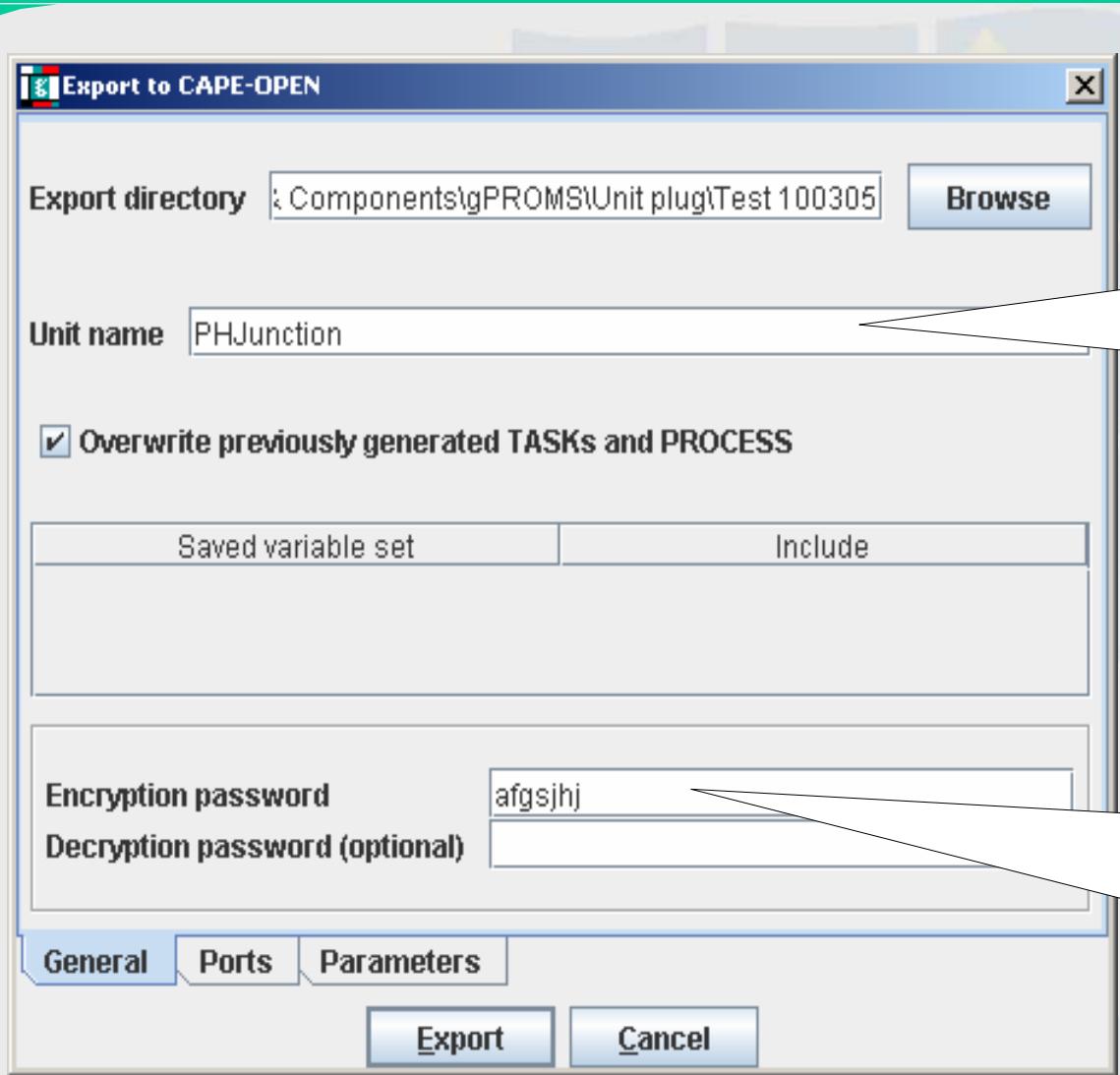
gPROMS supports CAPE-OPEN Material Object

The screenshot shows the gPROMS ModelBuilder interface. The left sidebar displays a project tree with nodes like CAPE-OPEN_Unit, PHMixer2, and various process models. The main area shows a table of stream ports:

Port	Connection type	Dimensions	Direction	X	Y	Port set
MidInlet	CO_Material		Inlet	0	0,524	MidInlet
TopInlet	CO_Material		Inlet	0	0,238	TopInlet
TopOutlet	CO_Material			1	0,231	TopOutlet

At the bottom, there are buttons for Add..., Edit..., and Delete.

Crypt gCO file

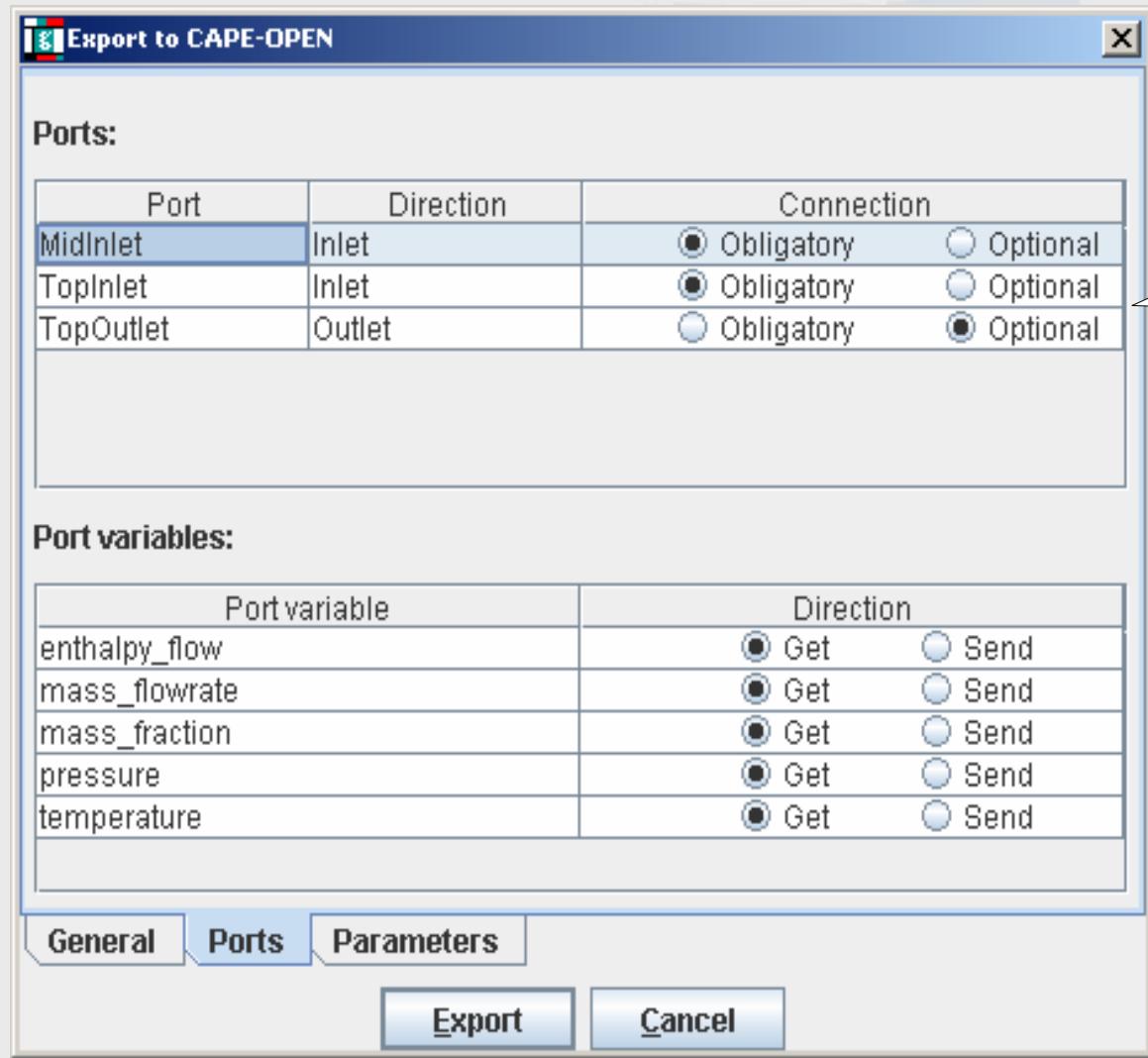


Exportation leads to a single file being created (extension gCO). Easily deployable.

Encrypting the gCO file enables deployment to other parties and ensures consistency



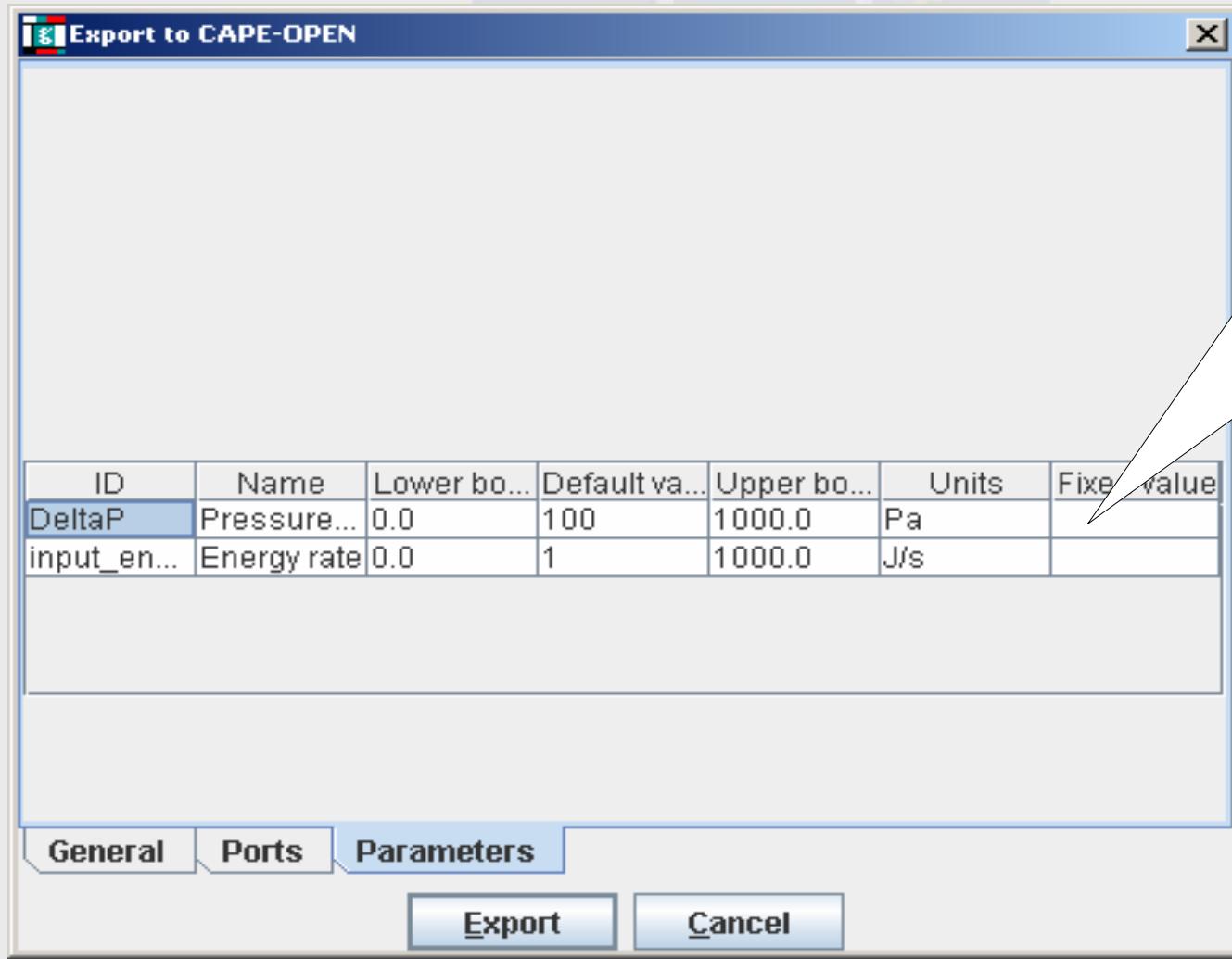
Define ports options and parameters settings



Ports connection may be mandatory or optional



Parameter default settings



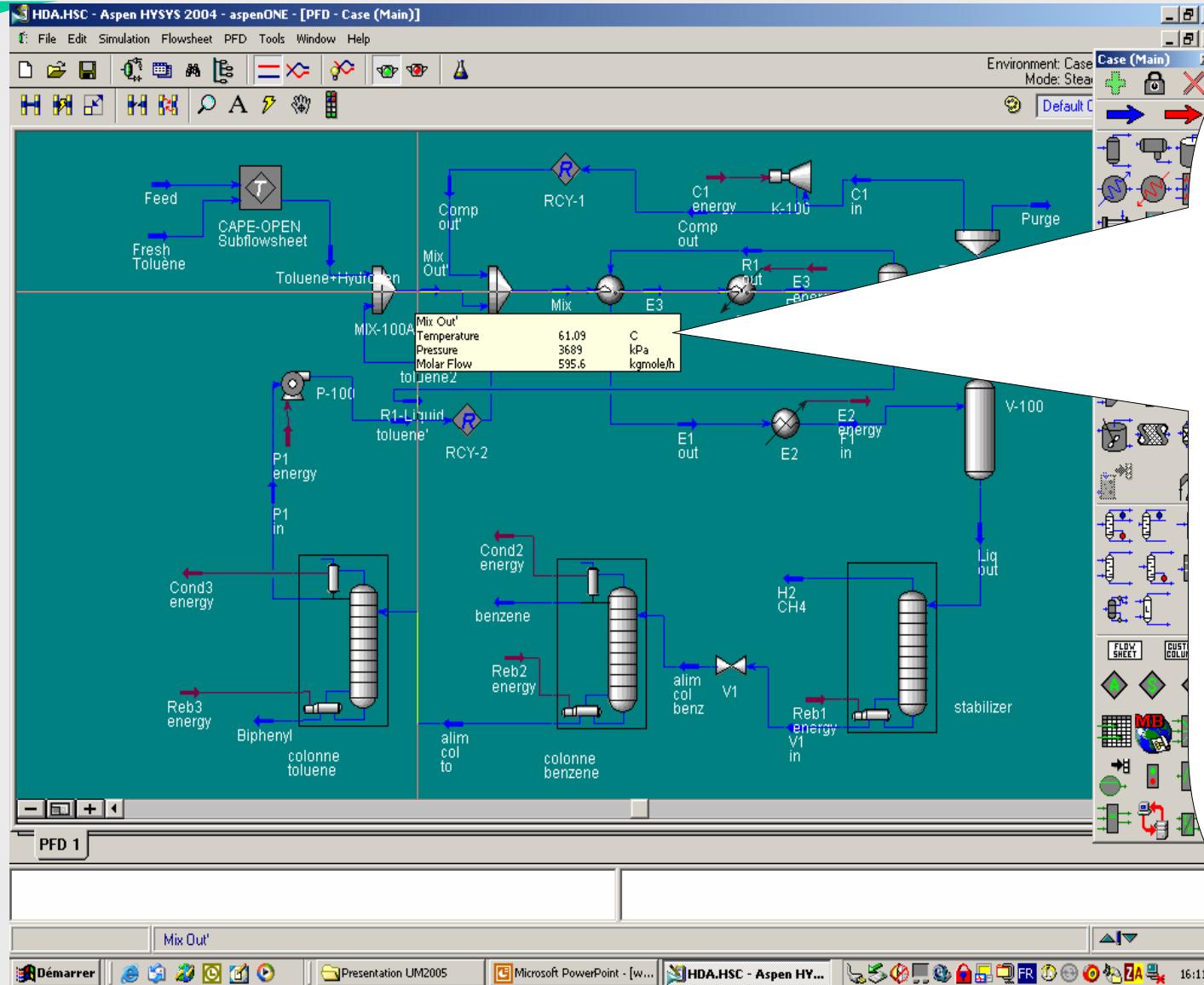
Each parameter is provided with a lower and upper bound as well as a default value.



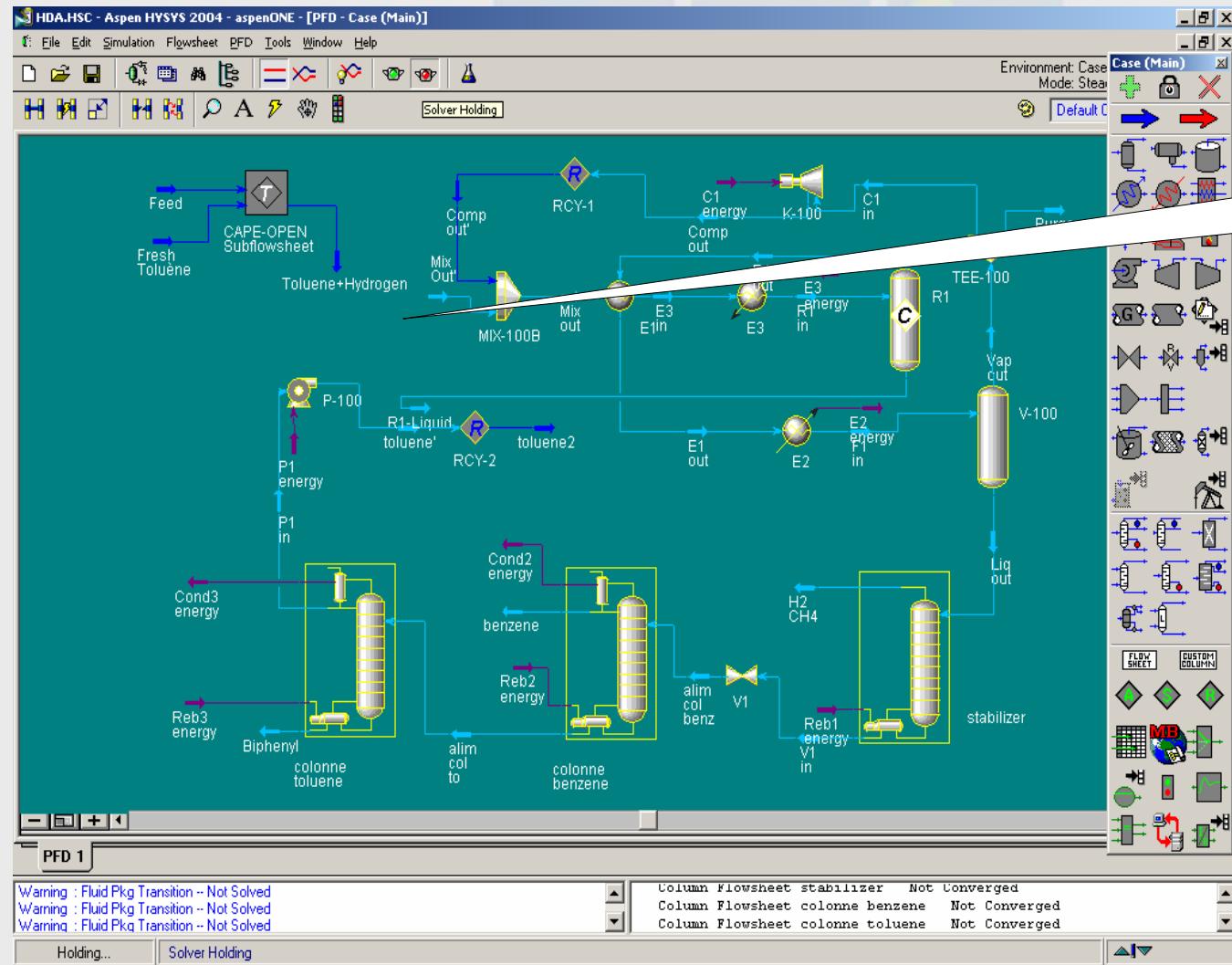
Running gPROMS model in HYSYS.Process



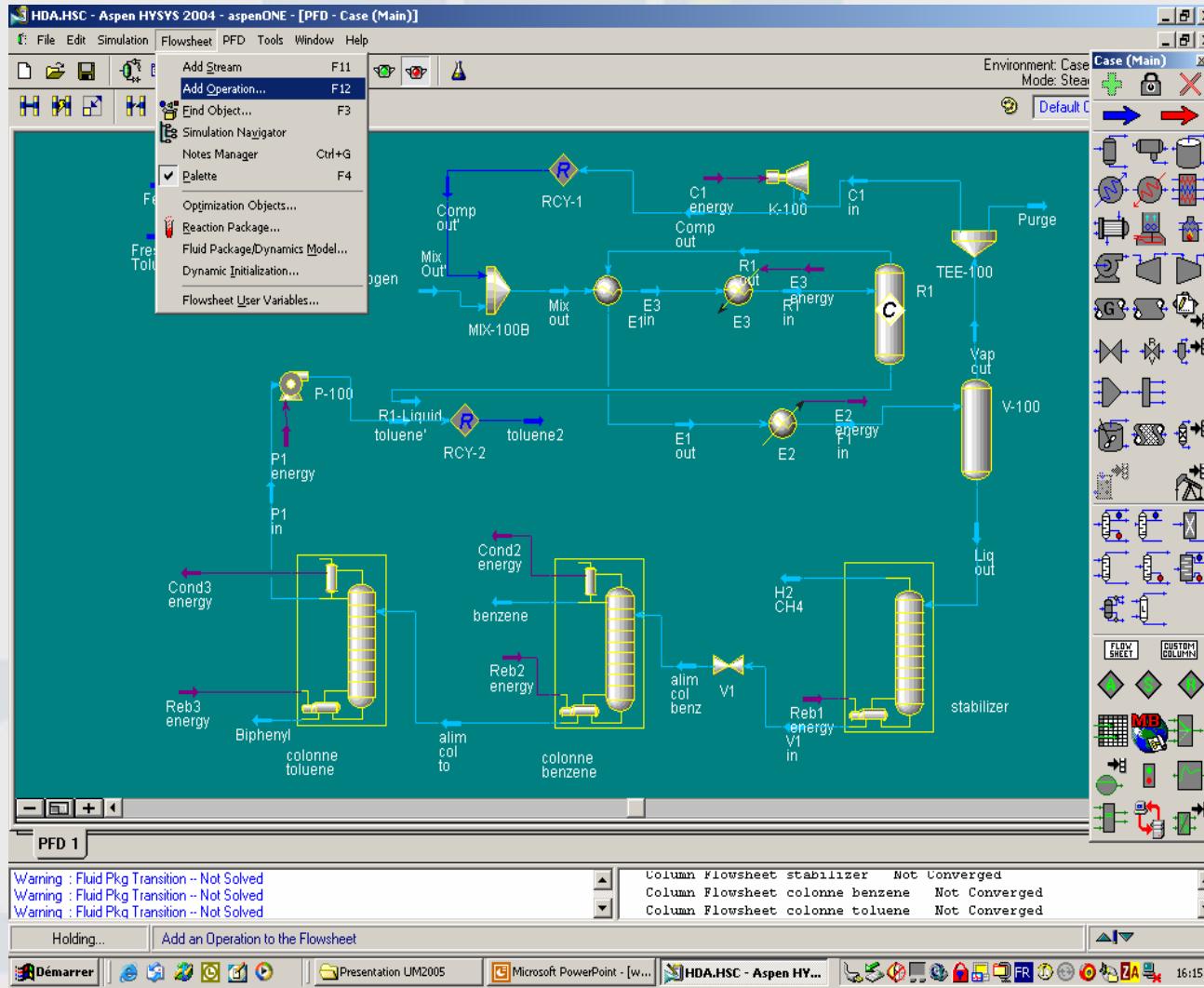
HDA process model in Aspen HYSYS 2004



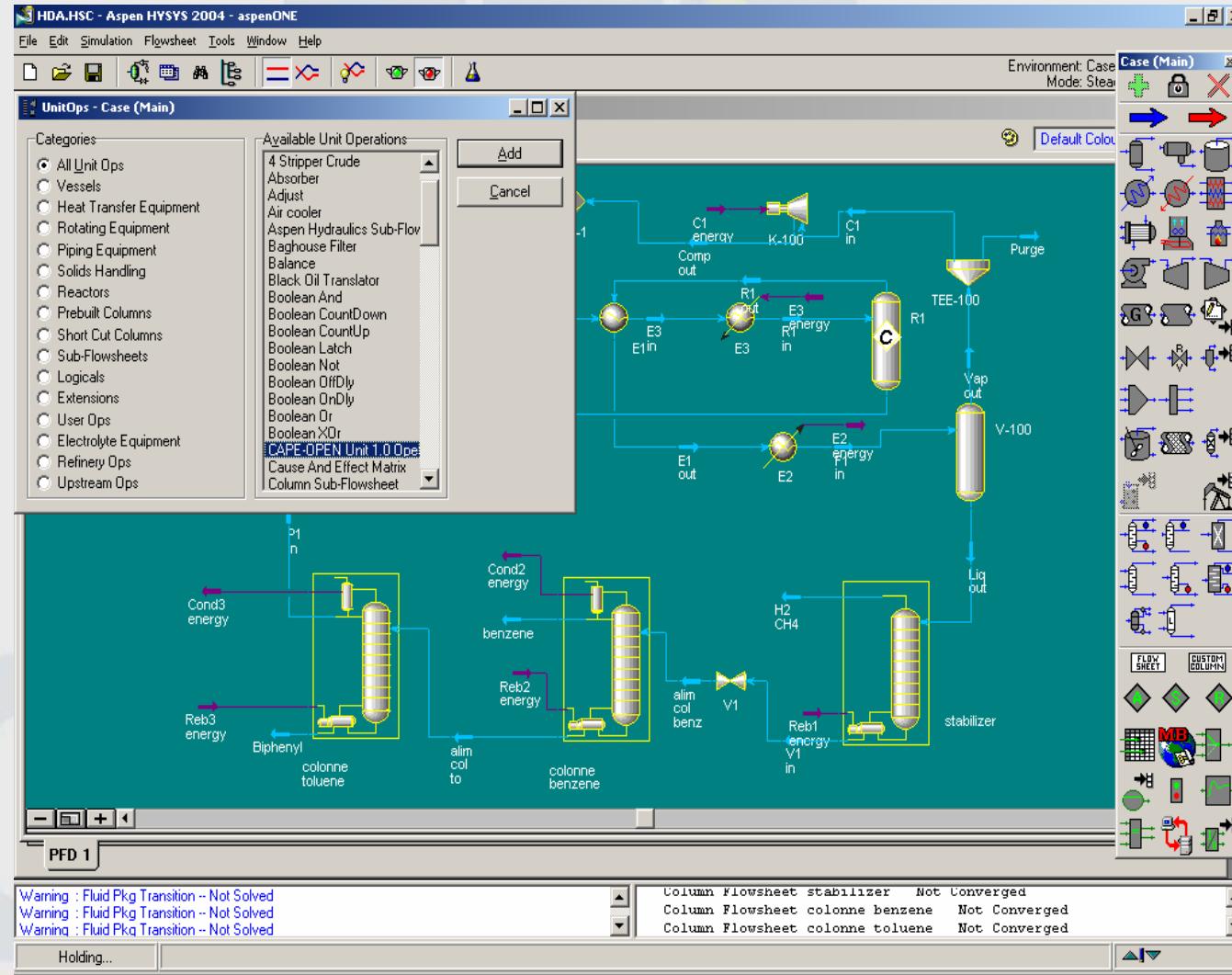
Native mixer deleted and solver on hold



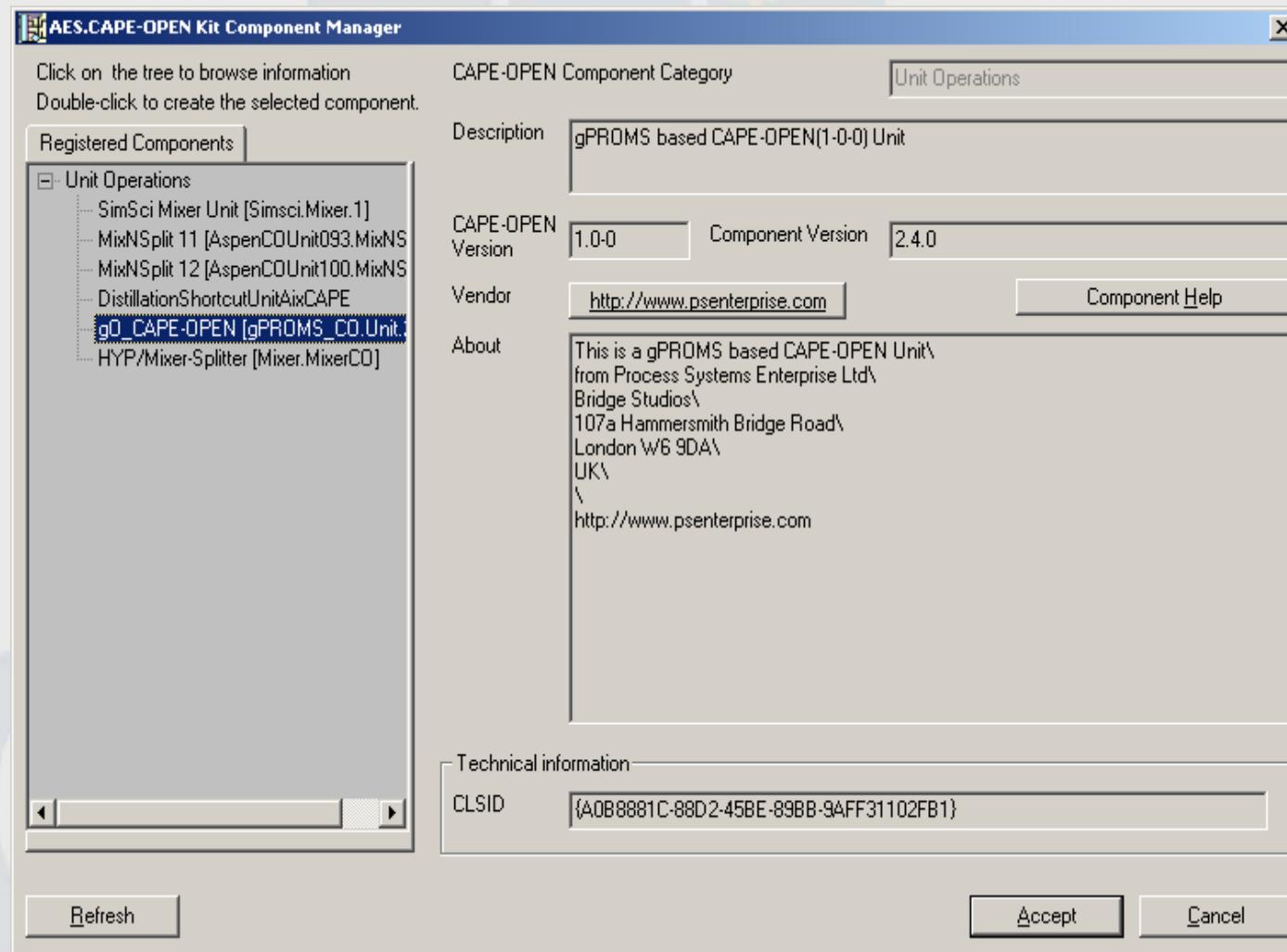
Replace native Mixer



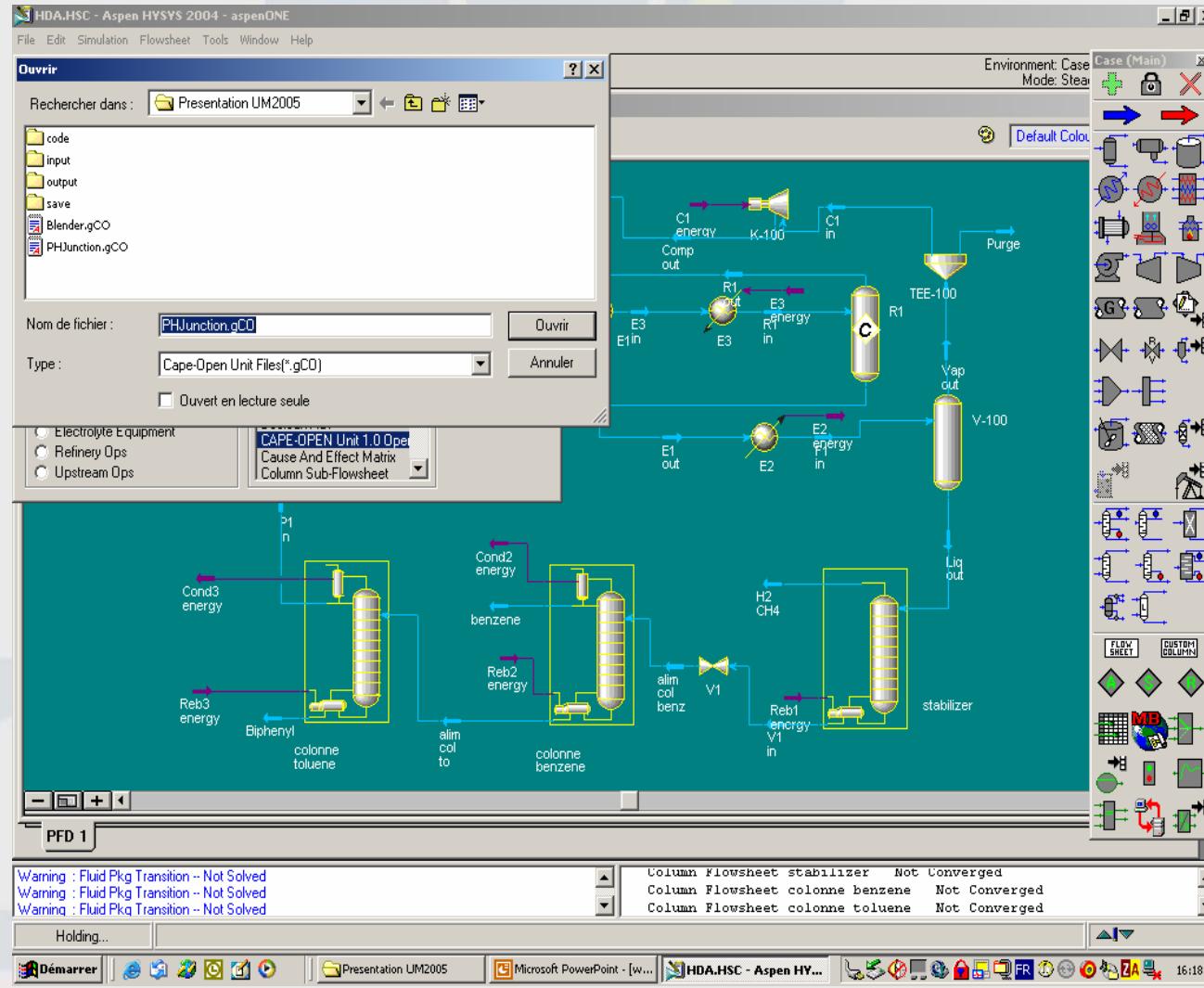
Select CAPE-OPEN 1.0 UNIT Ops



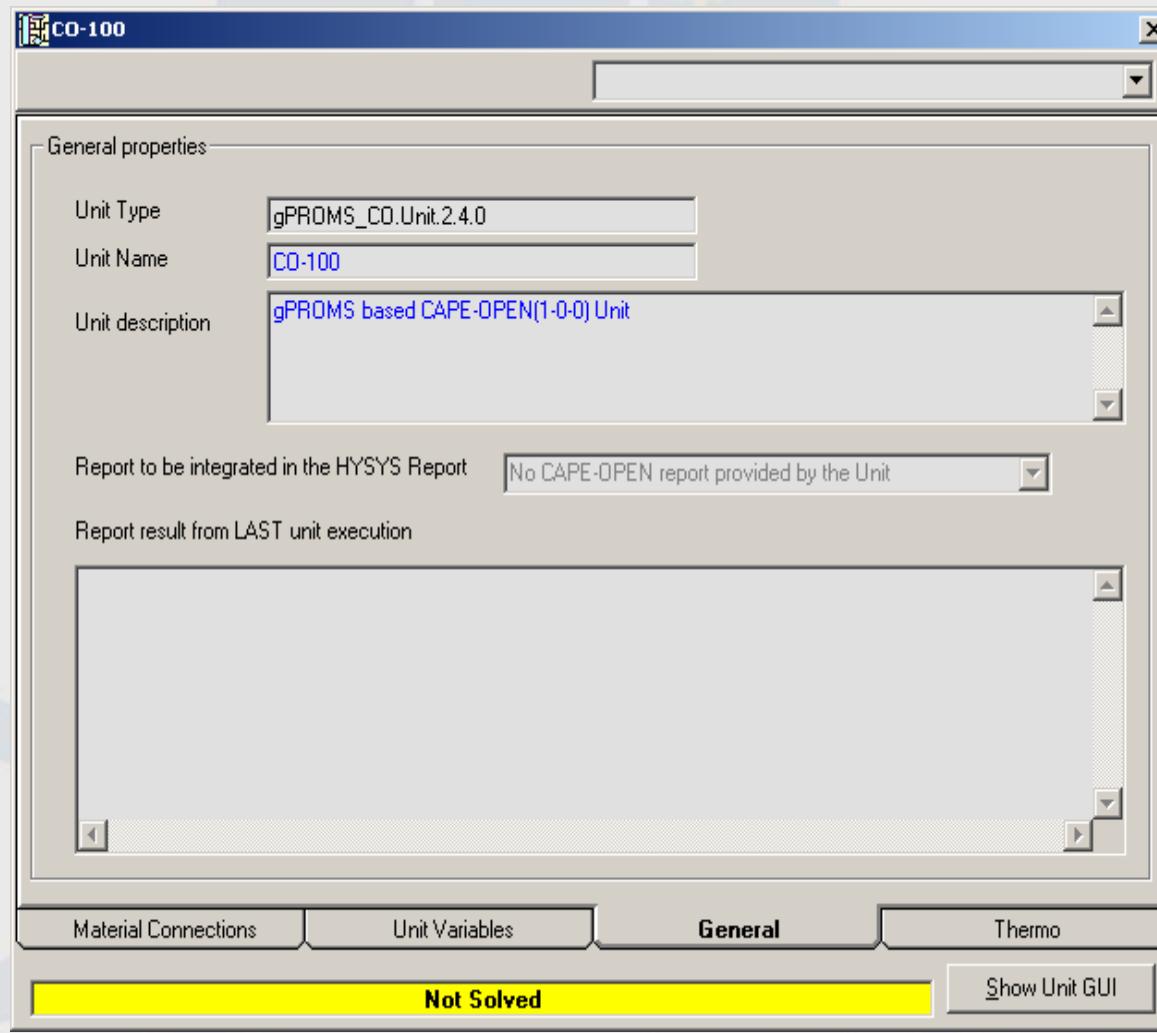
Select gO:CAPE-OPEN wrapper



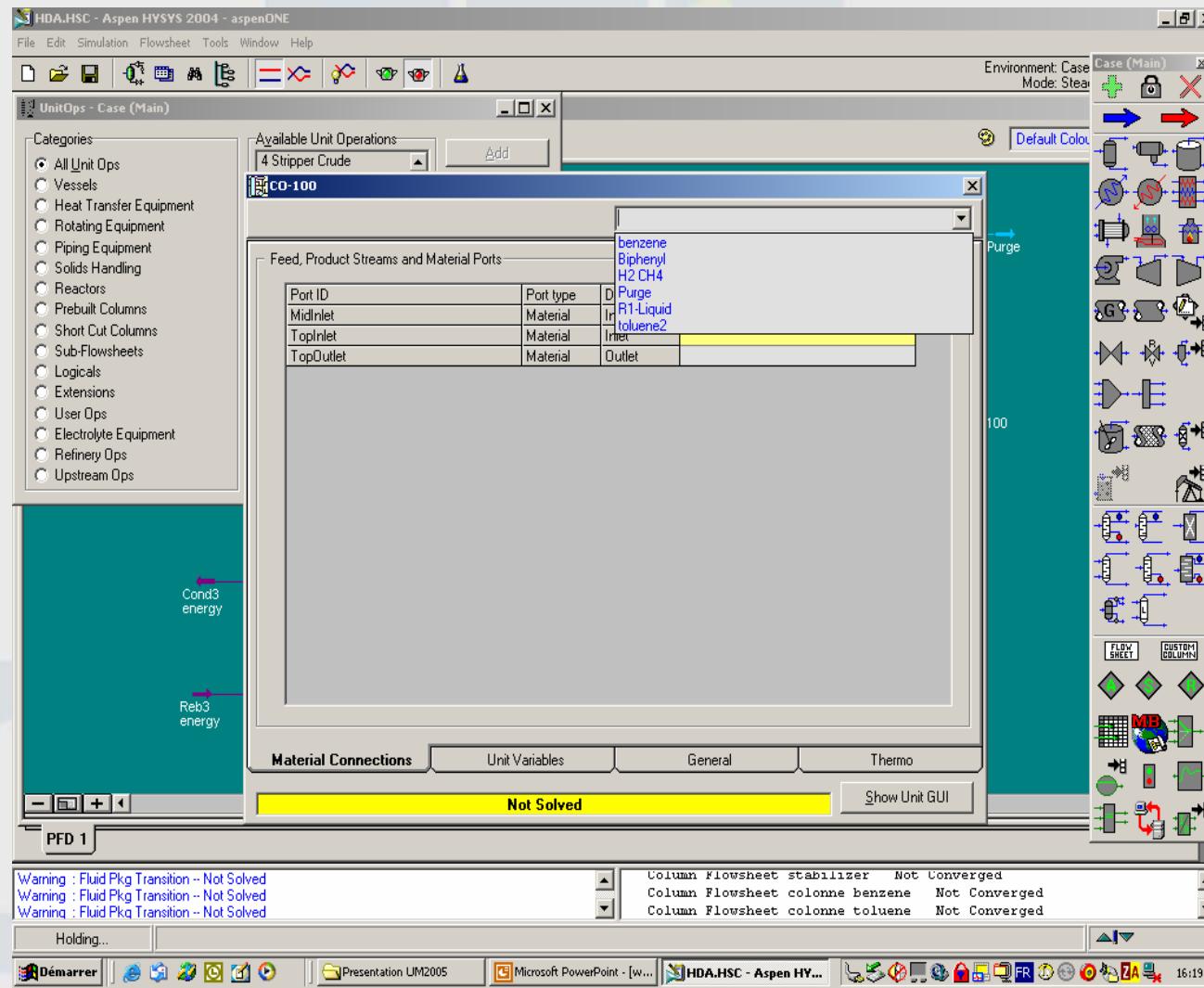
Select the gCO file to be used



Enter generic GUI provided by HYSYS



Connect inlet and outlet ports to streams



Set up the gPROMS model

The image displays two windows of the CO-100 software, which is used for setting up gPROMS models.

Left Window (Material Ports):

- Title Bar:** CO-100
- Panel:** Mix Out'
- Table:** Feed, Product Streams and Material Ports

Port ID	Port type	Direction	Material name
MidInlet	Material	Inlet	Toluene+Hydrogen
TopInlet	Material	Inlet	toluene2
TopOutlet	Material	Outlet	Mix Out'

- Buttons:** Material Connections, Unit Variables, General, Thermo, Show Unit GUI, Not Solved

Right Window (Unit Parameters):

- Title Bar:** CO-100
- Panel:** Unit Specific Data and Public Variables
- Table:** Name, Type, Mode, Lower bound, Upper bound, Value, Validated

Name	Type	Mode	Lower bound	Upper bound	Value	Validated
Energy rate	Real	IN	0	1000	1	
Pressure Drop	Real	IN	0	1000	100	

- Buttons:** Material Connections, Unit Variables, Thermo, Show Unit GUI, Reset Parameters, Not Solved

Annotations:

- A callout bubble points to the "All ports connected" status in the left window.
- A callout bubble points to the "Initial parameter settings" status in the right window.

Set energy input / pressure drop to zero

The screenshot shows two instances of the "gPROMS Cape-Open Unit Object" interface and two associated dialog boxes for modifying parameters.

Top Left Window: Shows the "Input Parameters" tab selected. A table lists parameters with their current values, lower bounds, upper bounds, and units:

Parameter	Type	Value	Lower bound	Upper bound	Units
Energy rate	Real	1	0	1000	J/s
Pressure Drop	Real	100	0	1000	Pa

Top Right Dialog: Energy rate

Value: J/s
Lower Bound:
Upper Bound:

OK Cancel

Bottom Left Window: Shows the "Input Parameters" tab selected. The "Energy rate" value has been changed to 0, and the "Pressure Drop" value has been changed to 0.

Parameter	Type	Value	Lower bound	Upper bound	Units
Energy rate	Real	0	0	1000	J/s
Pressure Drop	Real	0	0	1000	Pa

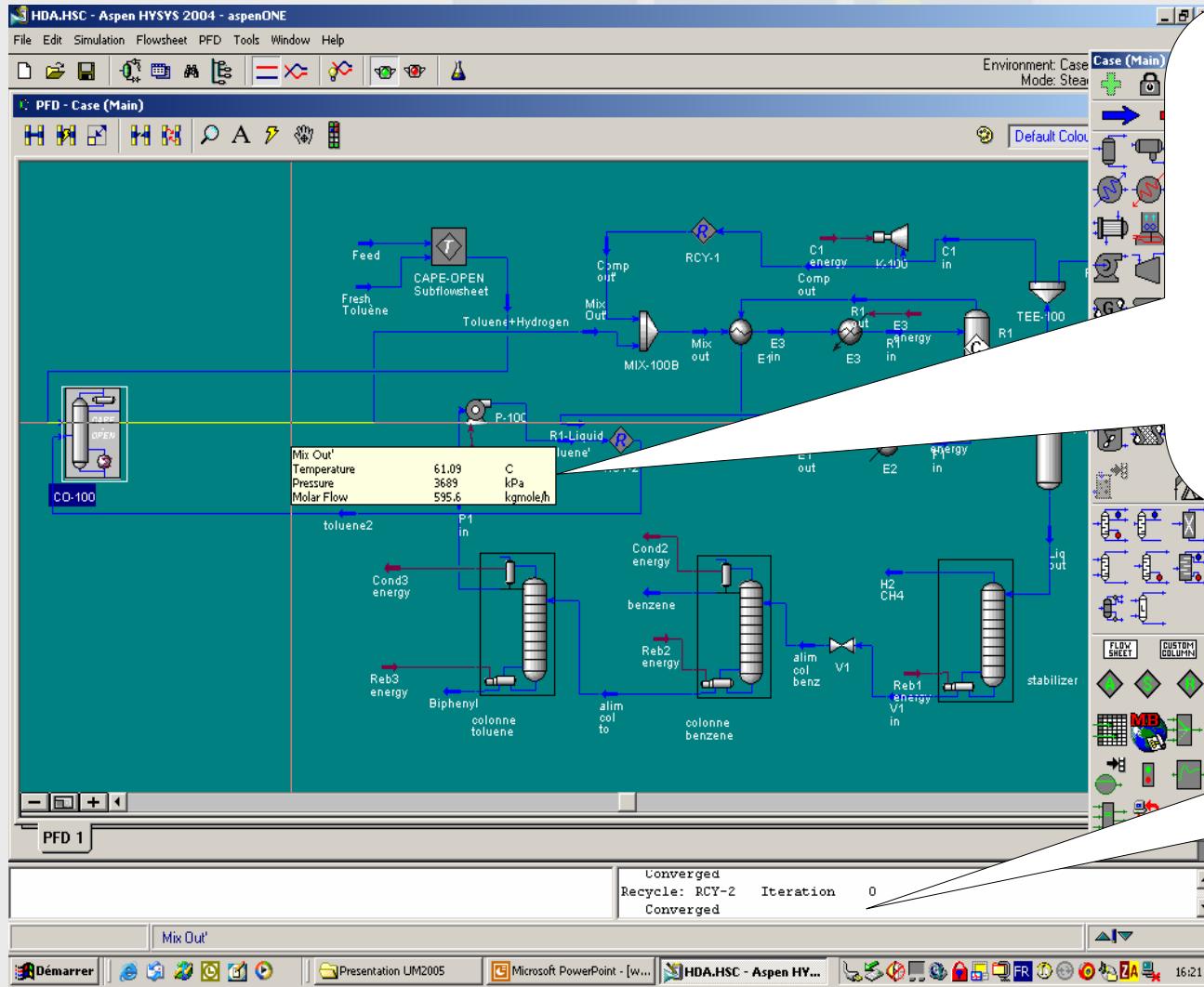
Bottom Right Dialog: Pressure Drop

Value: Pa
Lower Bound:
Upper Bound:

OK Cancel



gPROMS Mixer output results



Results obtained are strictly the same as with native Aspen HYSYS 2004 mixer model.

Simulation converged.



Direct Benefits

Cheaper, better and faster design, operation and control of processes

↪ Plug-and-play

- Ability to seamlessly integrate a component from the library of foreign objects (unit operations, thermo models, solvers etc.).
- Ability to seamlessly integrate in-house proprietary components in commercial environments.

↪ Niche software

- Ability to link specific niche modules to the simulators. Small and niche software vendors will provide CO-compliant components.

↪ Return On Investment

- Individual studies will cost less because of the technical advantages of being able to mix-and-match.
- Plug-and-play capacity will stimulate the market and create new opportunities.



Plug and Play

▼ SASOL

- ⇒ Reactor models made CAPE-OPEN compliant:
 - to be independent from process simulators in which they are used.

▼ SHELL

- ⇒ In-house thermo server (SPPTS) made CAPE-OPEN compliant:
 - same code accessible in all process simulators Shell is using.

▼ US DOE and Alstom Power

- ⇒ Fluent CFD models embedded in 0D process simulators through CAPE-OPEN interfaces



Niche software

▼ Already available

- ↪ MultiFlash (Infochem): thermodynamic server
- ↪ ChemSep: rate-based distillation model

▼ To be made available

- ↪ CosmoTherm (Cosmologic): thermodynamics
- ↪ TACITE dynamic pipe: unit operation



Return on Investment

▼ HTRI

- ↪ Xchanger Suite will need to support only one type of interface in order to be pluggable in all process simulators

▼ SIMULIS Thermodynamics

- ↪ Marketed on internet as an affordable thermodynamic component



CoSPPTS

Cape/Open - Shell Physical Properties and Thermodynamic Software

- Motivation

- Use of existing Shell methods and data in commercial programs
 - Consistent and fast implementation of results of own research

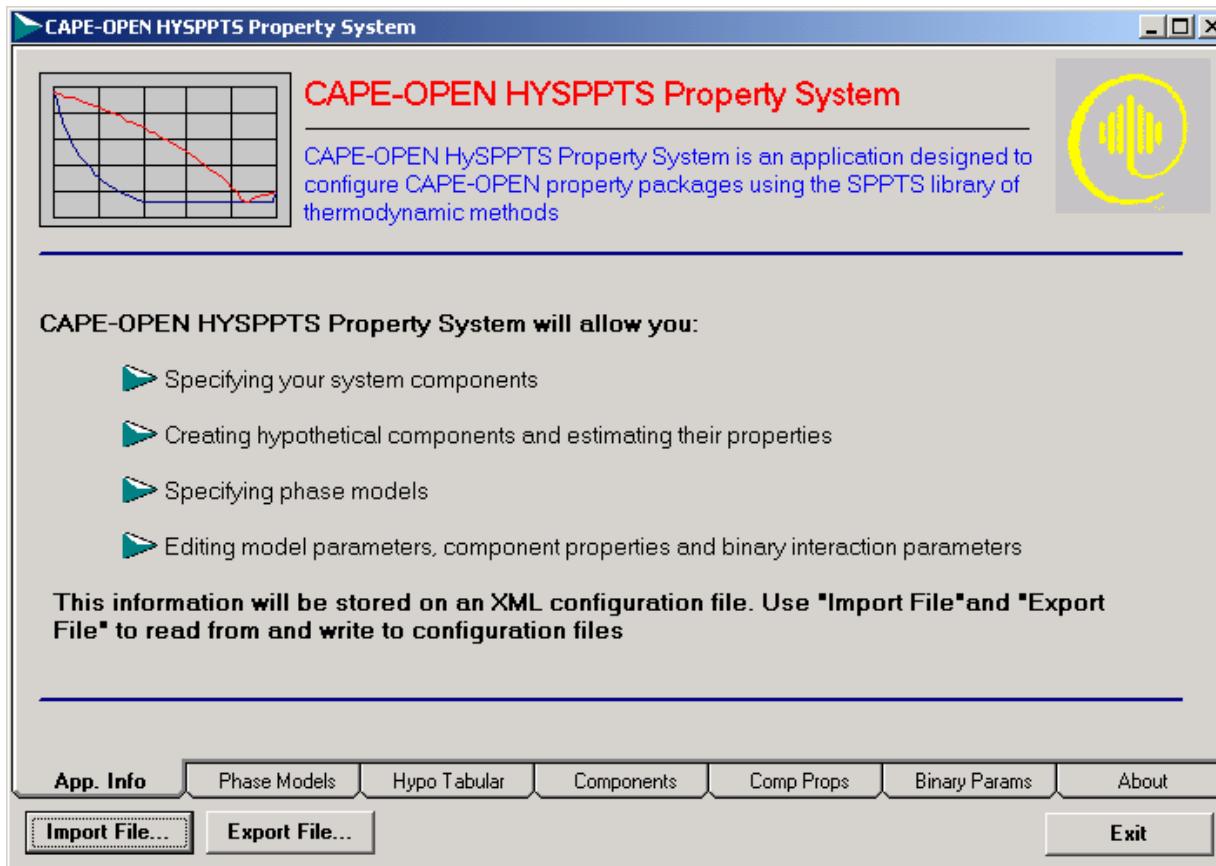
- Functionality

- Access to main Shell methods
 - Equations of state: SMIRK and CPA
 - Activity model Shell-NRTL/Henry
 - Shell pure component and binary database
 - COSPPTS front end (GUI)
 - Selection of models and components
 - Data entry for pseudo components and model parameters (overwrite)



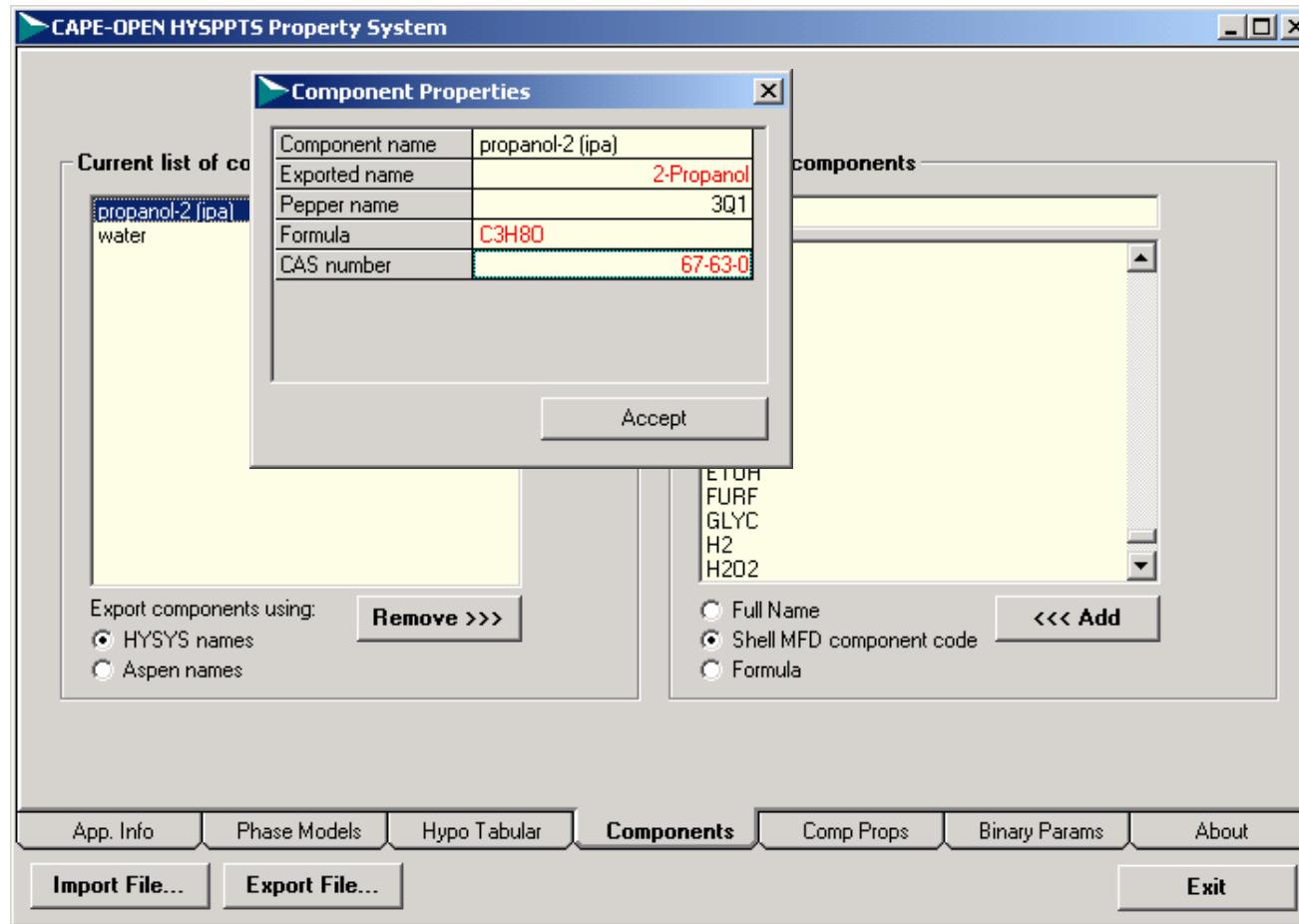
CoSPPTS

GUI of the tool – start up window



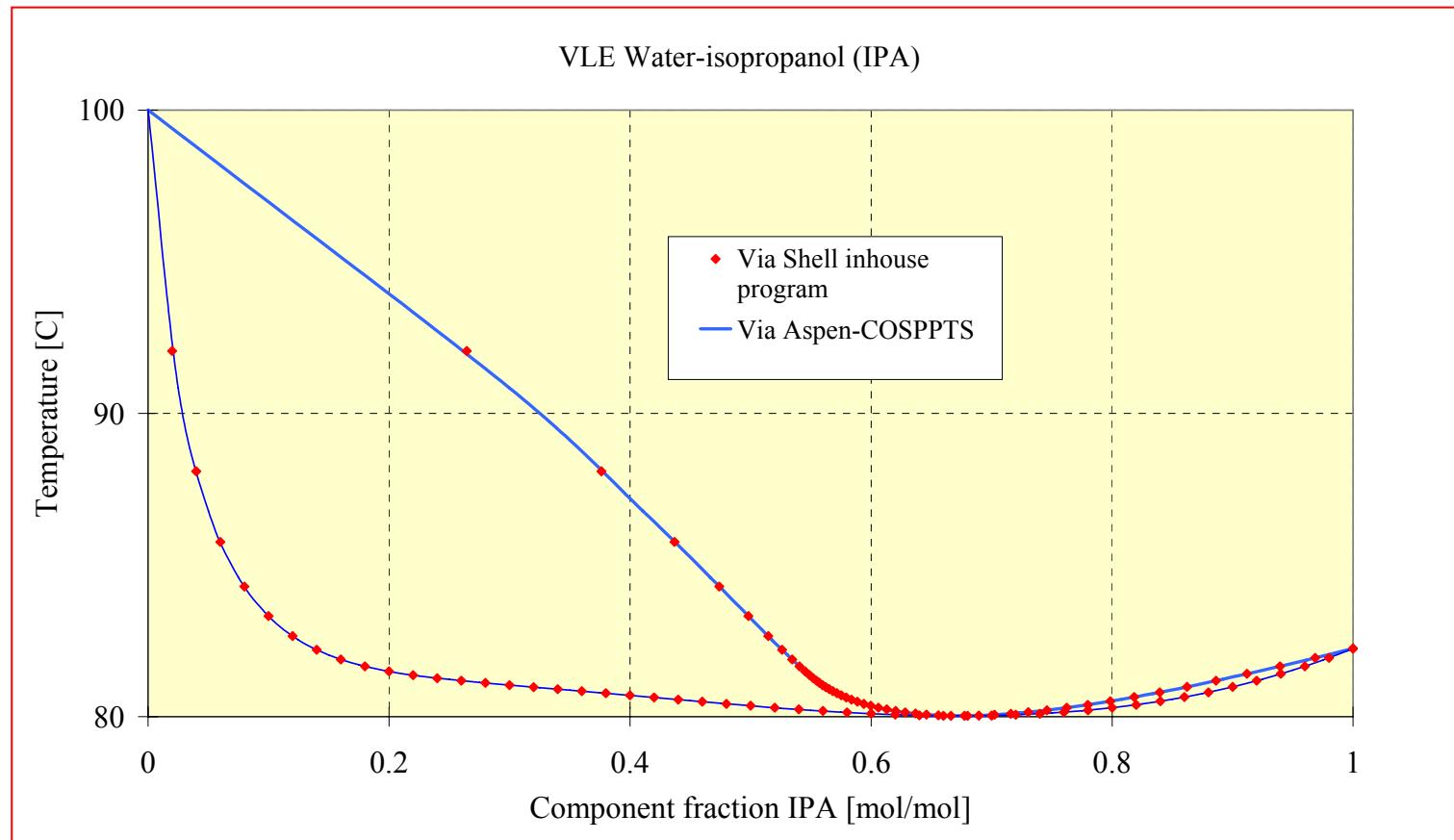
CoSPPTS

GUI of the tool – selection of components



CoSPPTS

Consistency check: own program versus AspenPlus



National Energy Technology Laboratory

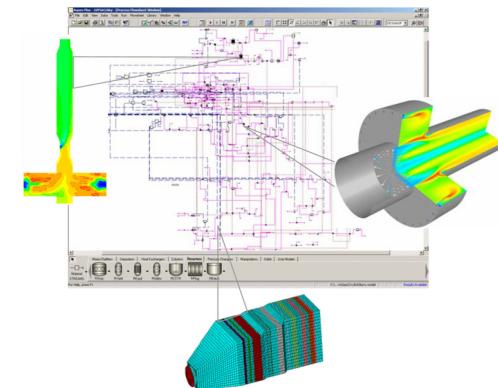
Office of Science, Technology & Analysis

- **Goal**

- Reduce the time, cost, and technical risk of developing advanced power generation systems

- **Objectives**

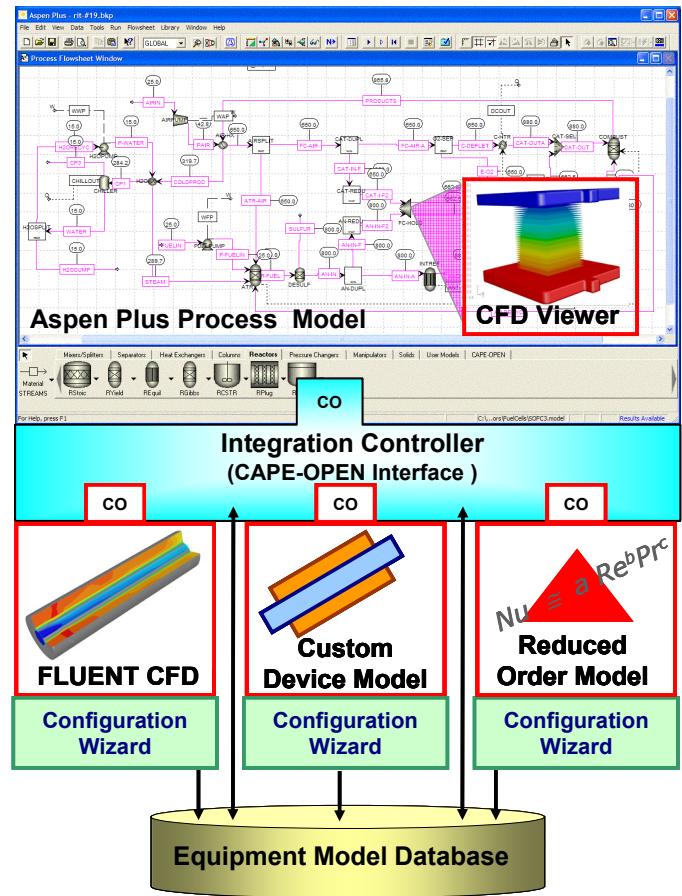
- Apply wide range of modeling and simulation technology
 - Computational chemistry, CFD, process simulation
 - Develop integrated, multiscale simulation capabilities
 - Use co-simulation frameworks
 - Exploit open standards
 - Couple with advanced visualization and high-performance computing
 - Demonstrate virtual power plant simulations





Advanced Process Engineering Co-Simulator (APECS)

- Combines process simulation with custom engineering models and computational fluid dynamics (CFD)
- Complies with the process industry CAPE-OPEN software standard
- Offers fast reduced order models (ROMs) and parallel computing for improved performance
- Exploits advanced visualization for equipment and process analysis
- First of a kind development by NETL and its R&D technology partners
- Recognized with 2004 R&D 100 Award



APECS Software Integration Framework



ALSTOM

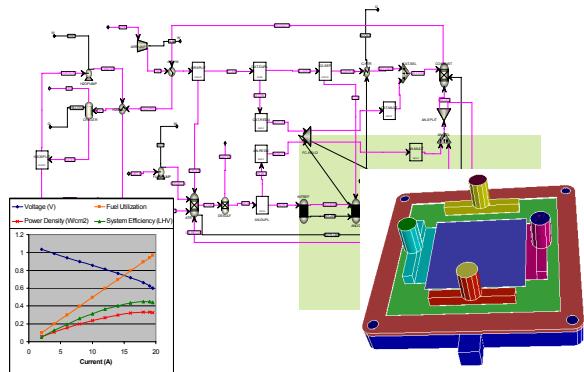
Carnegie Mellon

IOWA STATE UNIVERSITY

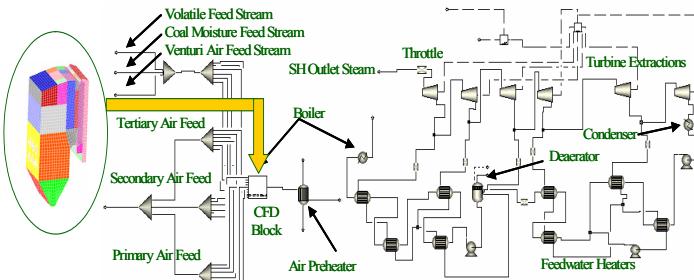
CAPE-OPEN Meeting SEZ/NETL/August 24-25, 2004

APECS Power Generation Applications

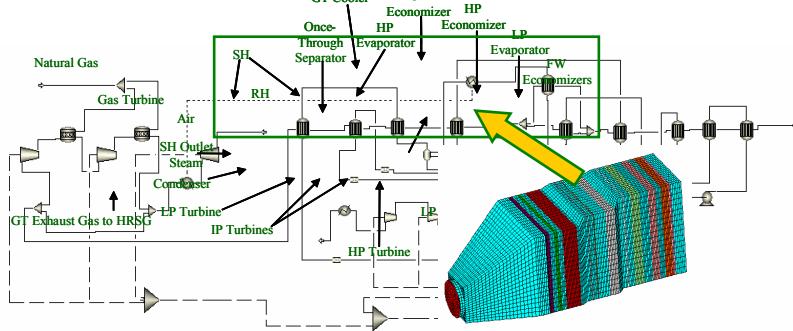
- Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC



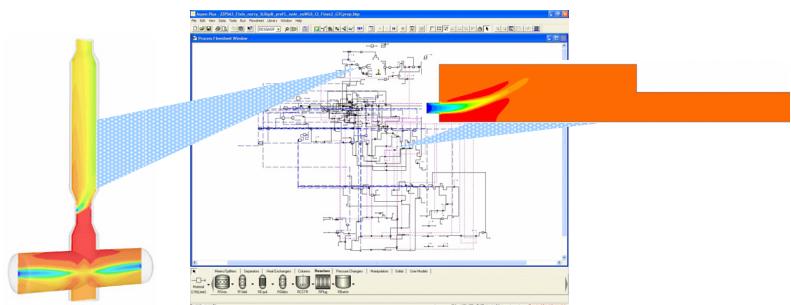
- ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler



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

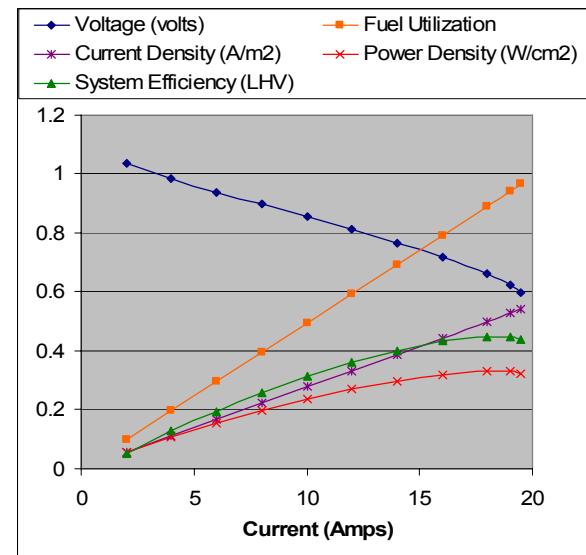
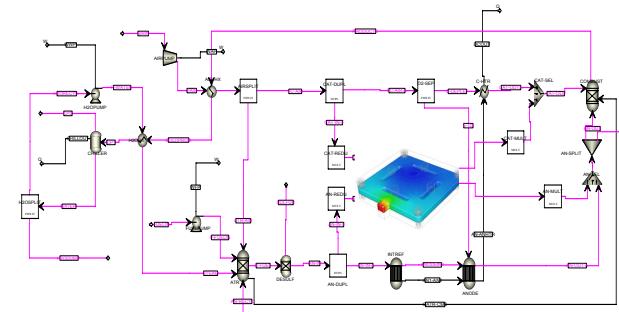


- FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor



APECS Application - SECA Fuel Cell APU System

- Aspen Plus process model of Auxiliary Power Unit (APU)
- FLUENT 3D CFD model of SECA solid oxide fuel cell
- Optimize process efficiency by varying CFD parameter (fuel cell current)
- Maximum system efficiency (LHV) of 45% at 18 amps
- Maximum system power of 4.3 kW
- Convergence in 6-10 Aspen Plus iterations requiring 45-60 minutes of CPU time

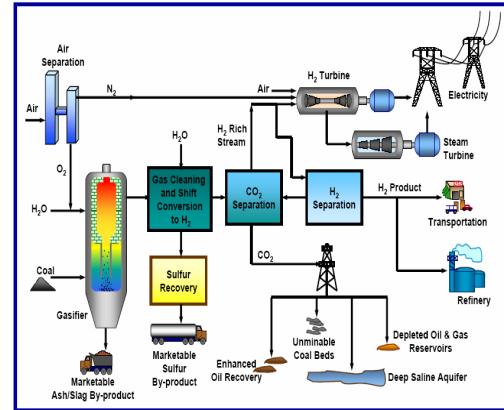


Zitney, S.E., Prinkey, M.T., Shahnam, M., and Rogers, W.A. (2004), "Coupled CFD and Process Simulation of a Fuel Cell Auxiliary Power Unit," In *Proc. of the ASME Second International Conference on Fuel Cell Science, Engineering, and Technology*, Eds. R. Shah and S.G. Kandlikar, Rochester NY, June 13-16, 2004, Paper 2490, pp. 339-345.

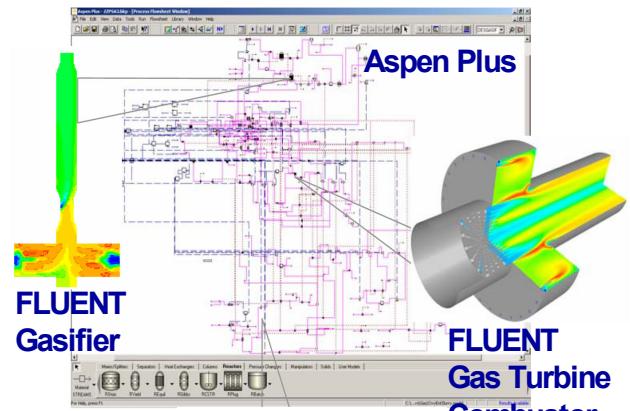
APECS Application - FutureGen Power Plant



- FutureGen Power Plant
 - IGCC with CO₂ capture and H₂ production (275 MWe)
 - Large, integrated plant with aggressive design goals
 - New, innovative equipment with lack of design data
- APECS Application
 - Process model
 - Aspen Plus steady-state
 - Over 250 equipment items
 - CFD models
 - FLUENT 3D Gasifier
 - FLUENT 2D GT Combustor



FutureGen Process Diagram



FutureGen APECS





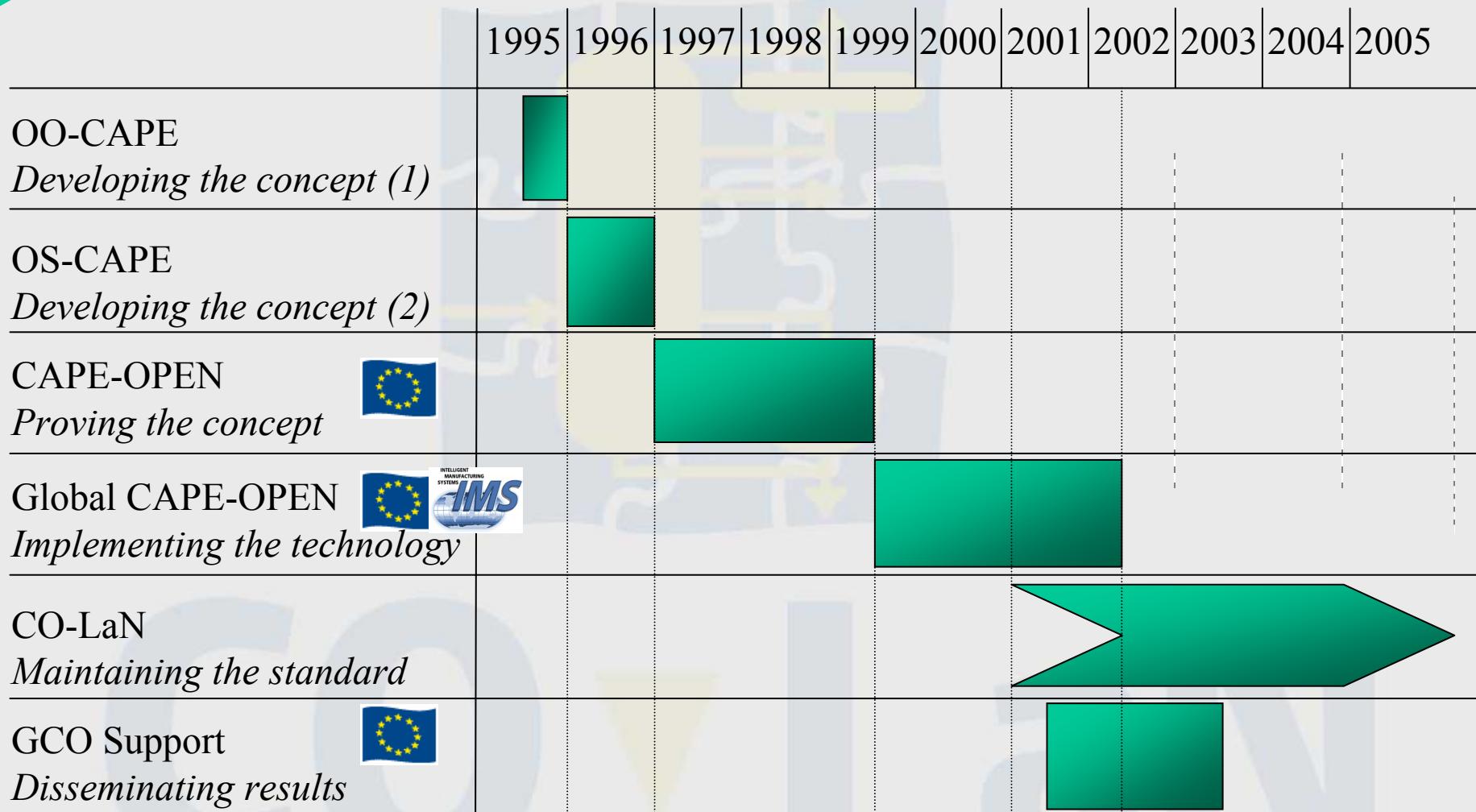
CO-LaN

CAPE-OPEN Laboratories Network

A group of end users taking responsibility
for putting resources together to support
ongoing work on the standard



Making a visionary idea a reality



Need for an organization

▼ A standard can't live by itself

▼ A standard needs to be

↪ **Distributed**

- Dissemination, free distribution, accompanying software, training programs

↪ **Supported**

- Information, documentation

↪ **Maintained**

- Corrections, debugging

↪ **Improved**

- Upgrade, extensions

▼ **Not-for-profit organisation open to all CAPE actors**

⇒ Established on February 8, 2001 (www.colan.org).

▼ **Full Members: pay fees**

⇒ End user organisations: operating companies, process licensing companies, engineering companies.

▼ **Associate Members: pay no fees**

⇒ All others: software suppliers, universities, government, other non for profit institutions.



CO-LaN missions

▼ User priorities for CAPE-OPEN interface standard

- ↪ Work with software vendors to clarify user priorities for process modelling software component/environment interoperability and also promote communication and co-operation among CAPE software vendors to insure that the CAPE-OPEN standard actually translates into commercially valuable interoperability.

▼ Dissemination

- ↪ Promote the CAPE-OPEN interface standard to end-users and distribute CAPE-OPEN information and technology internationally.



CO-LaN missions (cont.)

▼ CAPE-OPEN specifications life cycle management

- ↪ Organise the maintenance, evolution, and expansion of the specifications following user priorities.

▼ Testing, interoperability facilitation

- ↪ Supply compliance testers to support development of components, organise interoperability tests between suppliers of Process Modelling Components and Process Modelling Environments, sponsor consultancy services on CAPE-OPEN.

▼ Training/Migration facilitation

- ↪ Ensure that training module guidelines and tools to facilitate component wrapping are developed and available.



Activities

▼ Disseminate

- ↪ Web site, documents, CO Update Newsletter.
- ↪ « CAPE-OPEN Tour » days.

▼ Develop independent testers and software

- ↪ CO-LaN Tester suite, wizards, logger.

▼ Facilitate Interoperability

- ↪ Use software made available in any combination.
- ↪ Sponsor consultancy by CAPE-OPEN experts.

▼ Organize targeted Special Interest Groups on standards

- ↪ Trigger projects.
- ↪ Open to all members.



CO-LaN SIGs as of November 2005

▼ Thermo: specification upgrade

- Leader: Werner Drewitz, BASF AG
- Development of revision 1.1 as well as extension to solids

▼ Unit: Unit Operation extension

- Leader: Marcel van Maasdam, Shell Global Solutions
- Extension to dynamic simulation

▼ Interoperability support

- Leader: Peter Banks, BP
- Further progress on interoperability



CO-LaN progress over the last 2 years

▼ Membership

- ⇒ Number of members doubled

▼ Adoption of the technology

- ⇒ Commercial, academia, in-house

▼ Support actions for CAPE-OPEN implementation

- ⇒ Endorsement by major organizations



Full Members (as of November 2005)

- ▼ Air Liquide (Philippe Arpentinier)
- ▼ BASF AG (Ronald-Alexander Klein)
- ▼ BP International Ltd. (Peter Banks/Malcolm Woodman)
- ▼ Institut Français du Pétrole (Bertrand Braunschweig)
- ▼ The Dow Chemical Company (Werner Merk)
- ▼ Shell Global Solutions (Ray Dickinson)
- ▼ TOTAL (Jacques Bousquet)



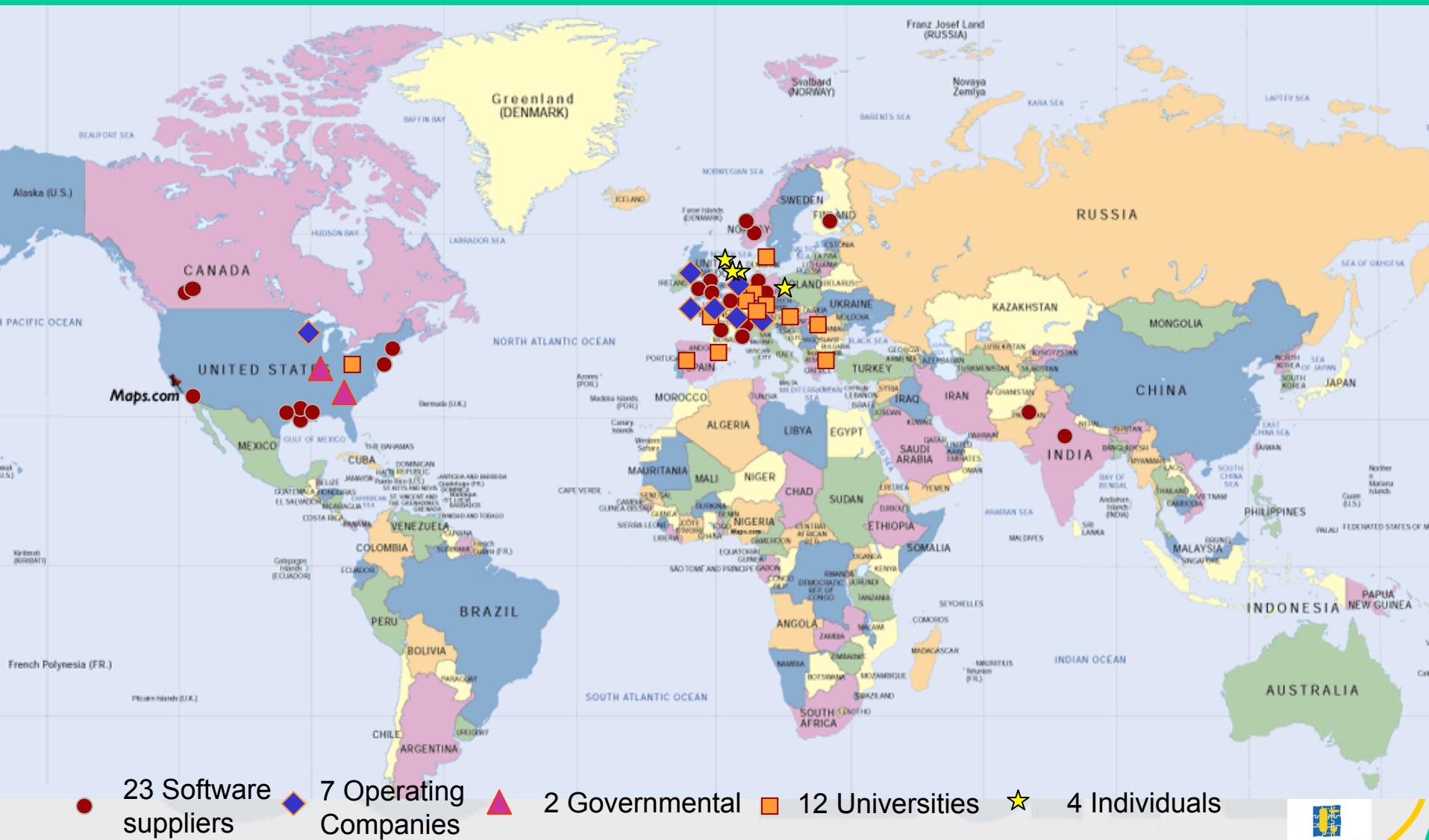
Associate Members (as of November 2005)

- ▼ Chemstations
- ▼ Belsim SA
- ▼ SHMA Pvt Ltd.
- ▼ SINTEF
- ▼ US EPA
- ▼ US DOE/NETL
- ▼ ProtechSoft
- ▼ Valladolid Univ.
- ▼ Bucarest Univ.
- ▼ Peter Banks
- ▼ Hans-Horst Mayer
- ▼ Richard Baur
- ▼ Jasper van Baten
- ▼ Honeywell

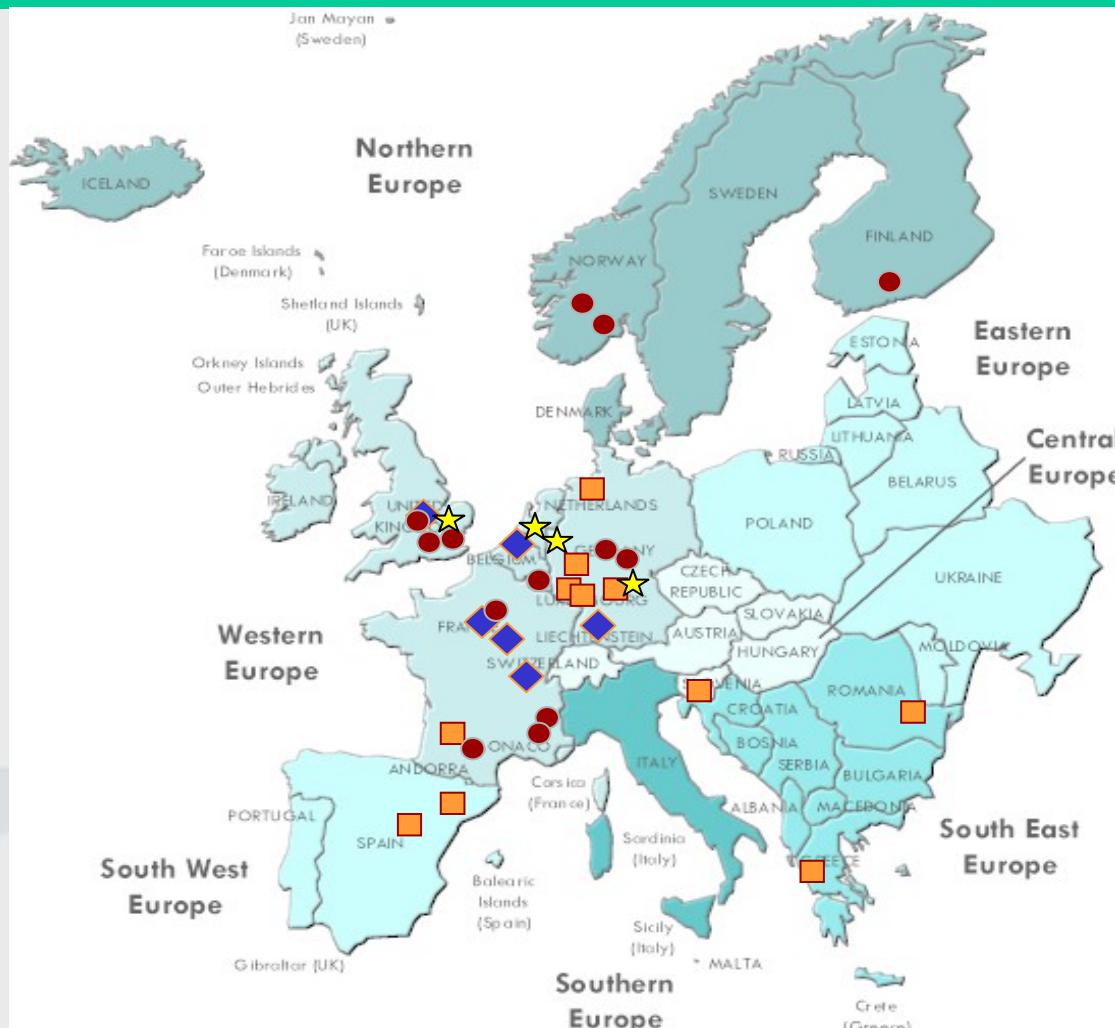
- ▼ Infochem
- ▼ Univ. Polyt. Catal.
- ▼ ProSim SA
- ▼ HTRI Inc.
- ▼ Fantoft Process
- ▼ SIMSCI-ESSCOR
- ▼ RWTH LPT
- ▼ DIPPR
- ▼ University of Maribor
- ▼ Dechema e.V.
- ▼ AspenTech
- ▼ Carnegie Mellon
- ▼ RWTH I5
- ▼ RSI
- ▼ EPCON
- ▼ CPERI
- ▼ Cosmologic
- ▼ CAPEC-DTU
- ▼ PSE Ltd
- ▼ Virtual Mat. Group
- ▼ TUHH
- ▼ Fluent
- ▼ TUV NEL Ltd
- ▼ INP Toulouse
- ▼ Processium
- ▼ VTT
- ▼ ChemSep.org



48 Members worldwide in November 2005



European membership



What does CO-LaN bring?

▼ CO-LaN members are at the “learning edge”, acquiring the ability to create business and technology architectures that take full advantage of transparent access to CAPE resources.

- ⇒ Web site with public and private access
- ⇒ Repository of specification documents
 - Supports standards dissemination and development
- ⇒ CO Tester Suite for validation and testing
- ⇒ CO wizards



Network of Experts

- ▼ The best CAPE-OPEN Experts contribute to CO-LaN SIGs
- ▼ Meet in CO-LaN activities
- ▼ Meet at CAPE Conferences and Software vendors Users meetings
- ▼ Ask any question!

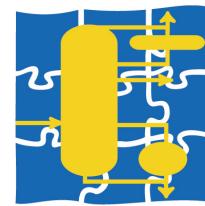


Conclusion

- ▼ Significant results obtained
- ▼ Commercial implementations available
- ▼ Proven technology
- ▼ Major benefits already from Unit and Thermo
- ▼ Use it!



CAPE-OPEN



CO▼LaN

Michel PONS

Chief Technology Officer

Akzo Nobel Chemicals, Arnhem, November 17, 2005

