CAPE-OPEN

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Chief Technology Officer

Akzo Nobel Chemicals, Arnhem, November 17, 2005

Outline

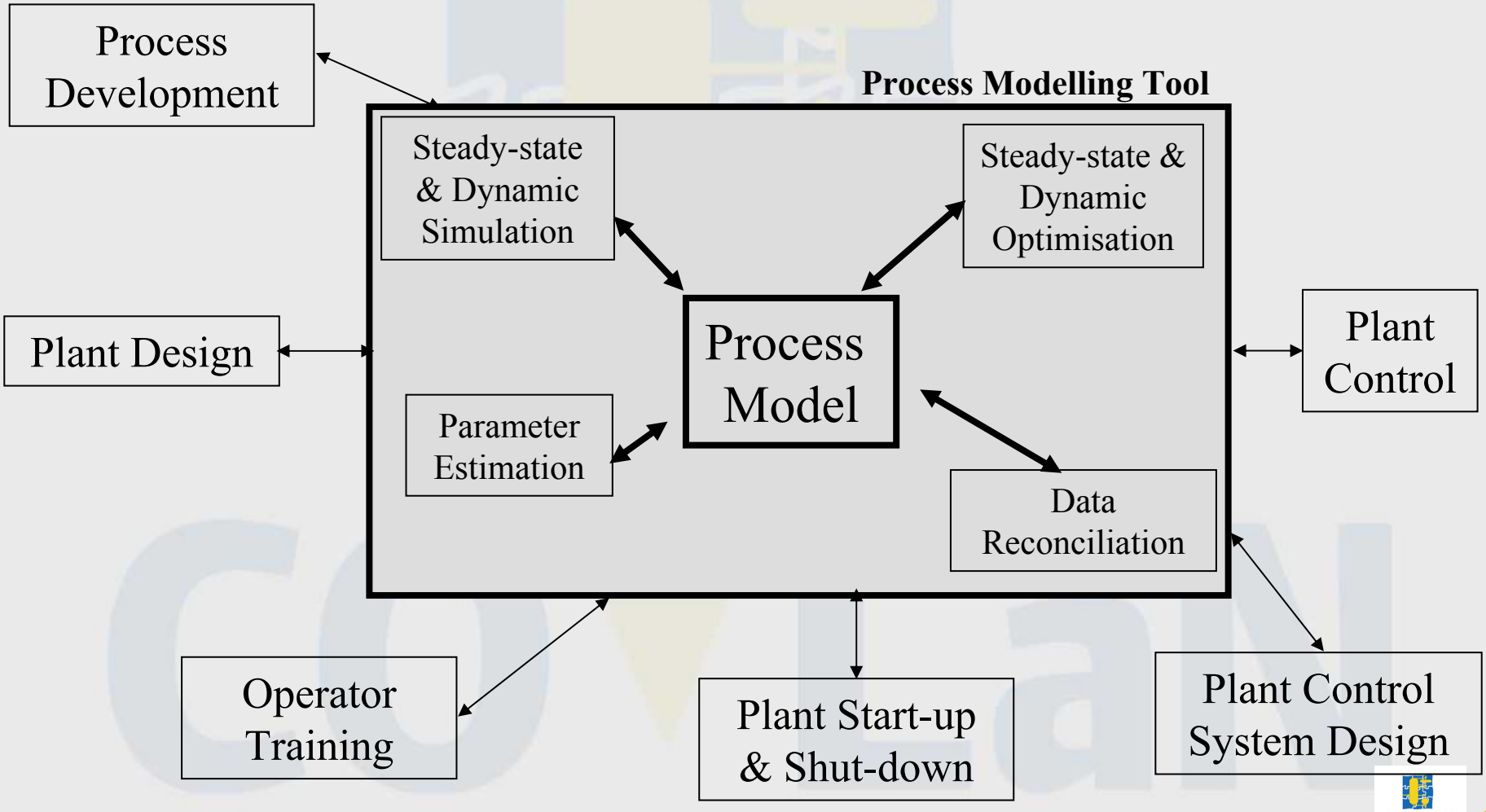
- What is CAPE-OPEN?
- What CAPE-OPEN permits for end-users?
- What is the CAPE-OPEN Laboratories Network?
- Conclusions

What is CAPE-OPEN?

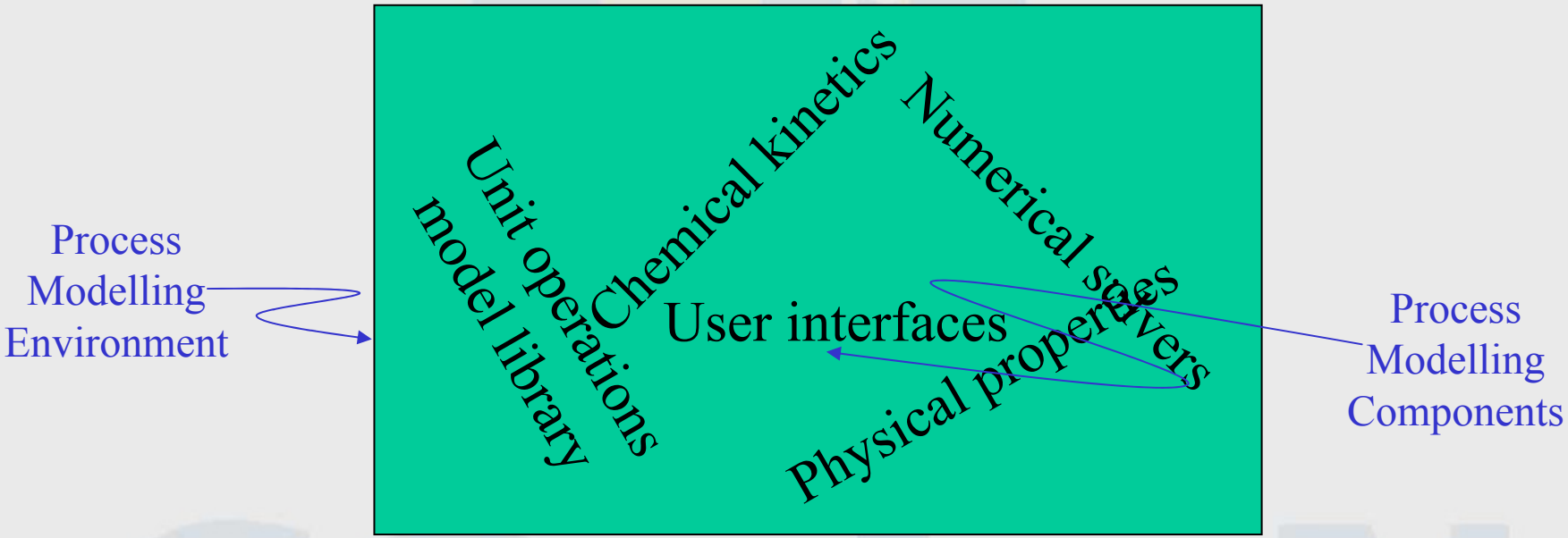
CAPE-OPEN: a technology for integration

- 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

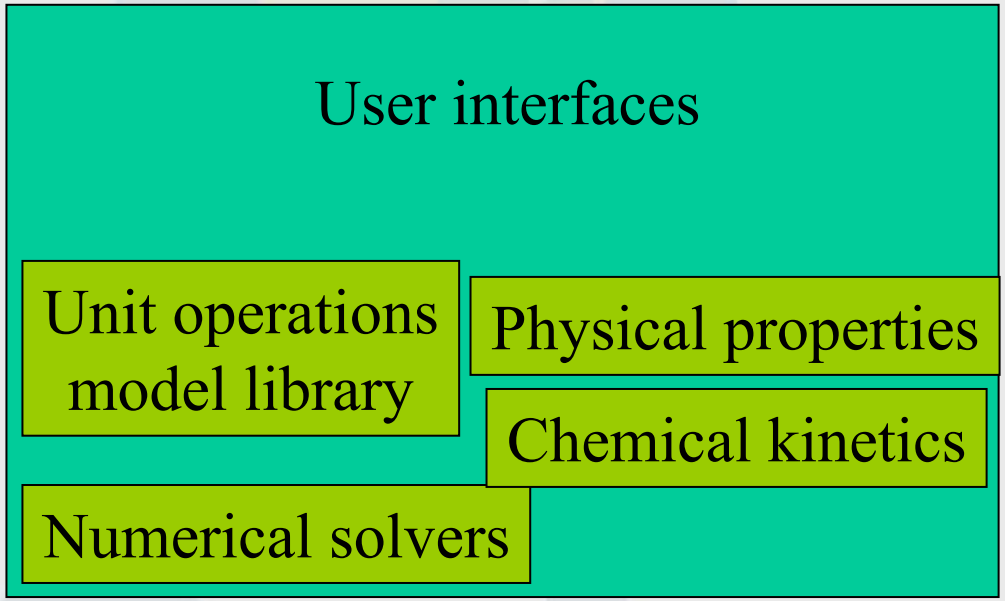


The anatomy of process modelling tools – a (somewhat) confusing reality

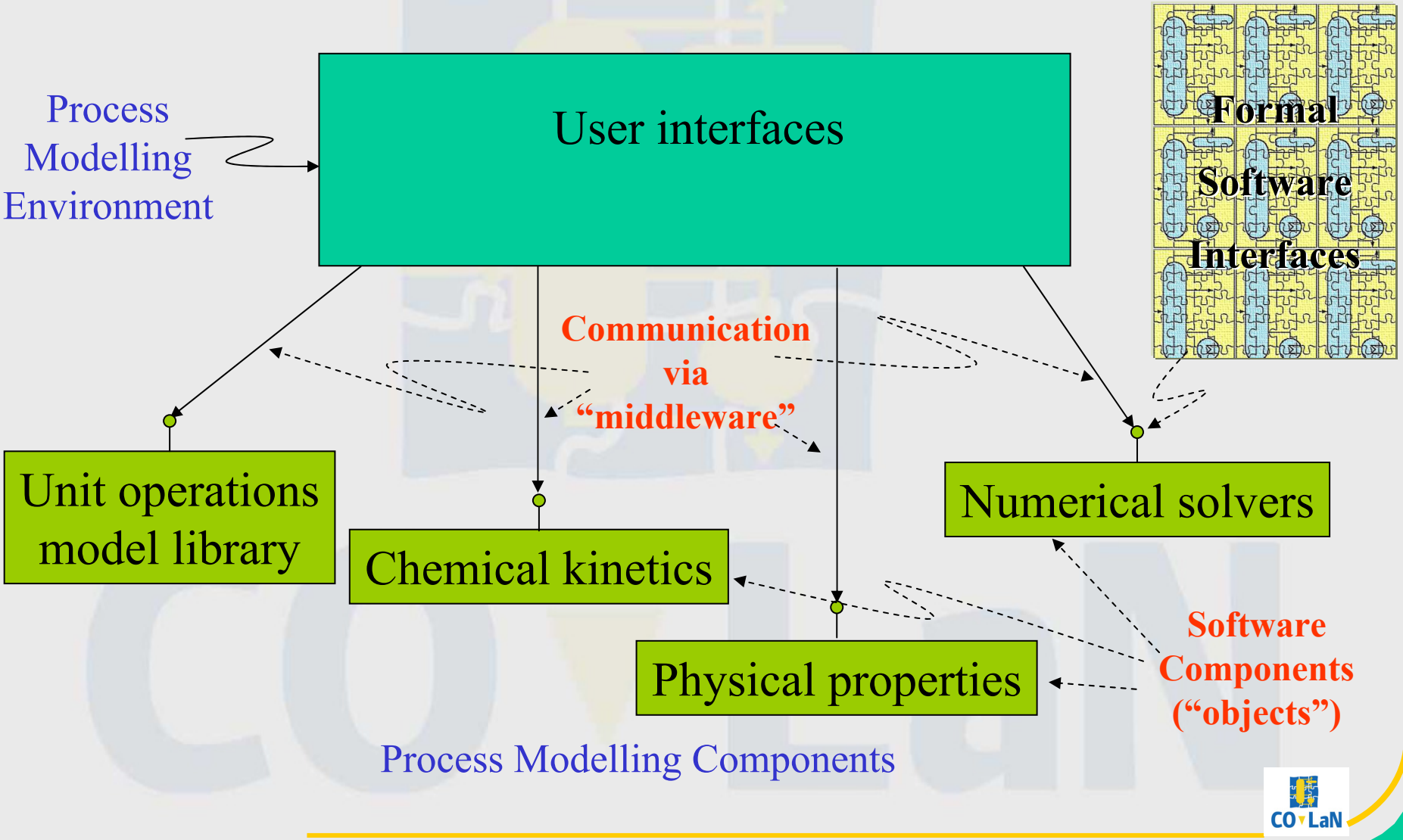


- Many interacting components…
- …all tightly coupled with each other
- Component boundaries not always clearly delineated

Clarify boundaries between key components



…and break tool into 1 PME & multiple PMCs



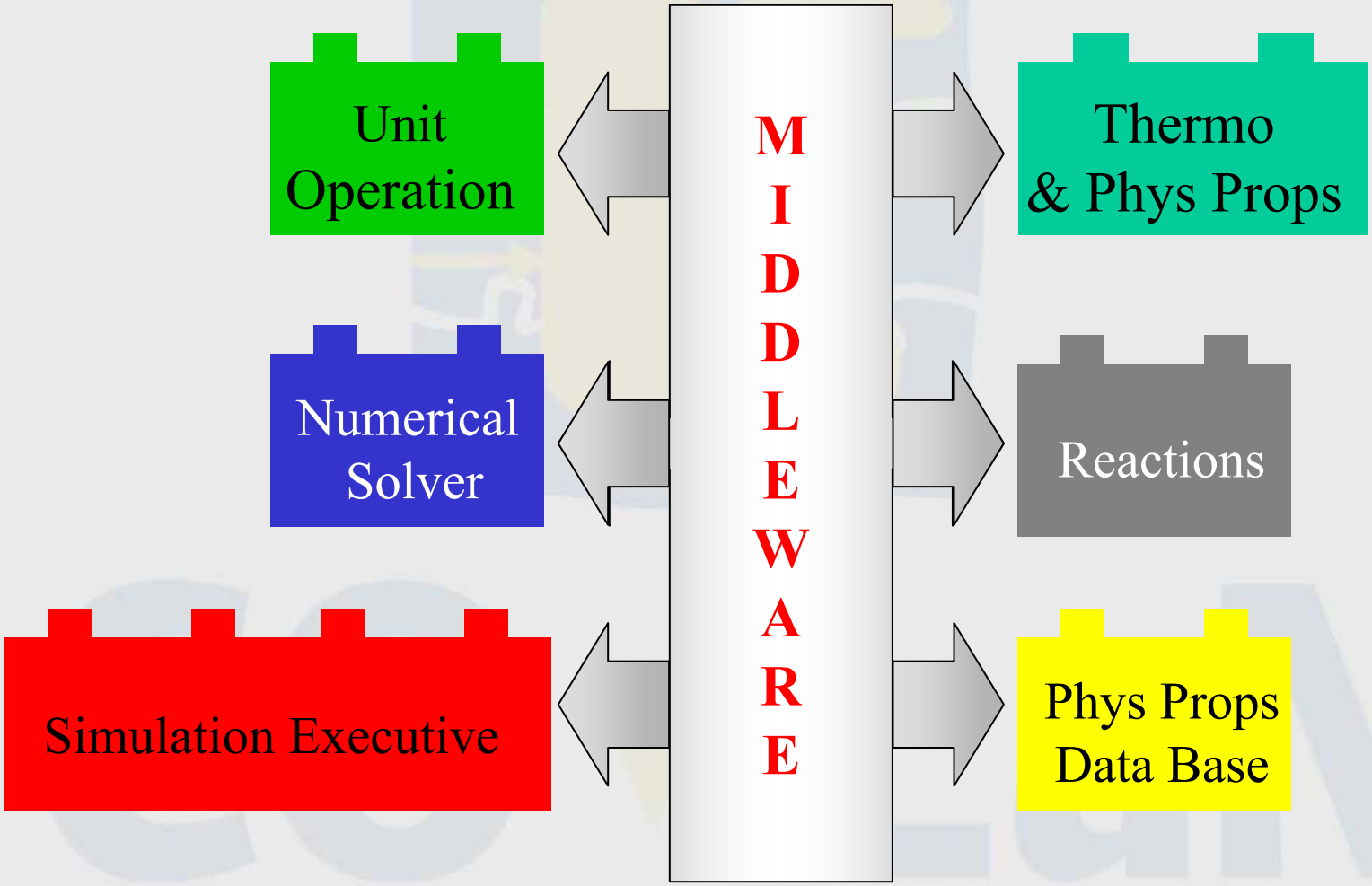
Process modelling: components & environments

- **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

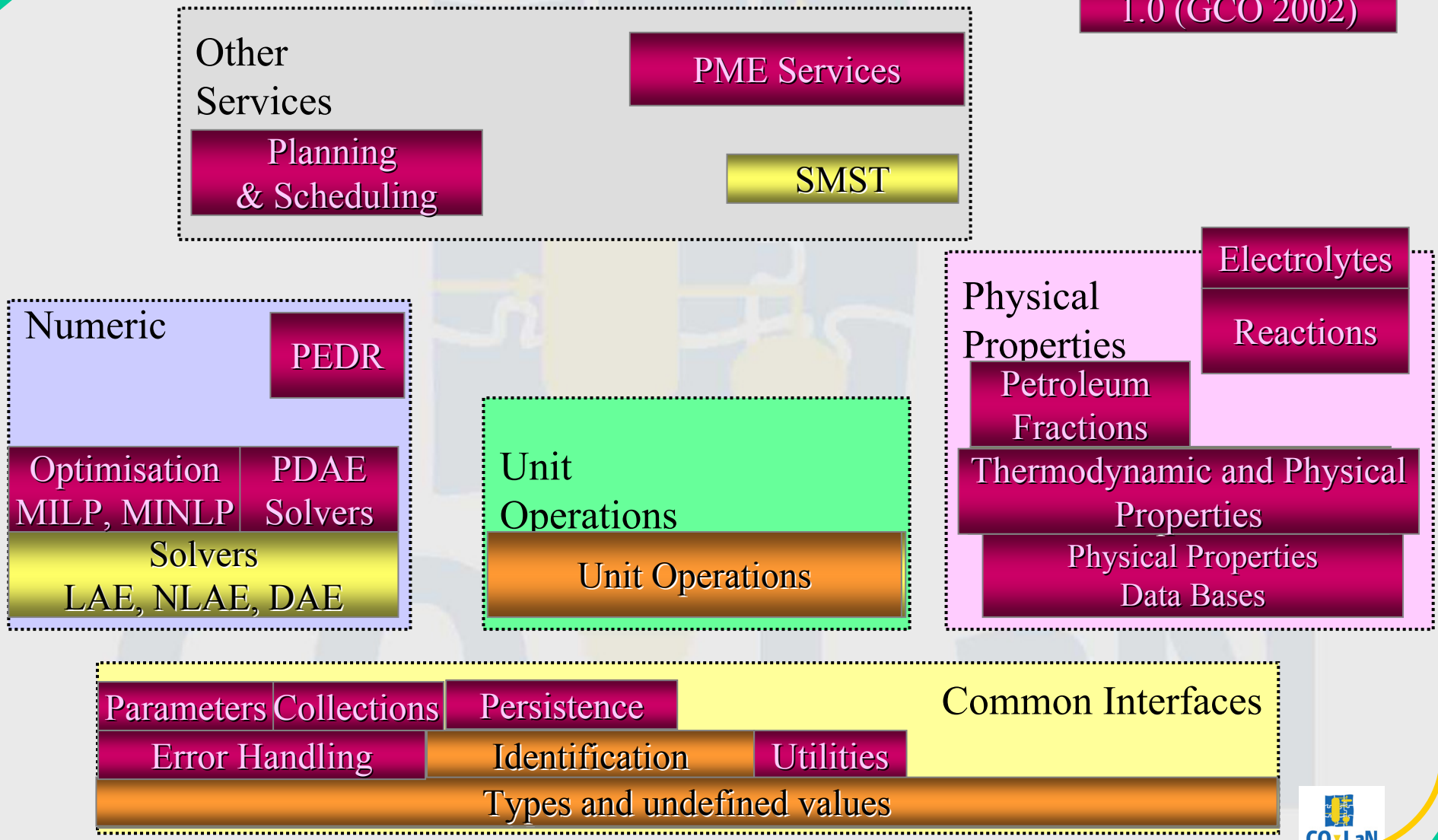
- Interfaces for CO simulator executives: services of general use are defined such as diagnostics and material systems in order to be called by any CO component.

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.

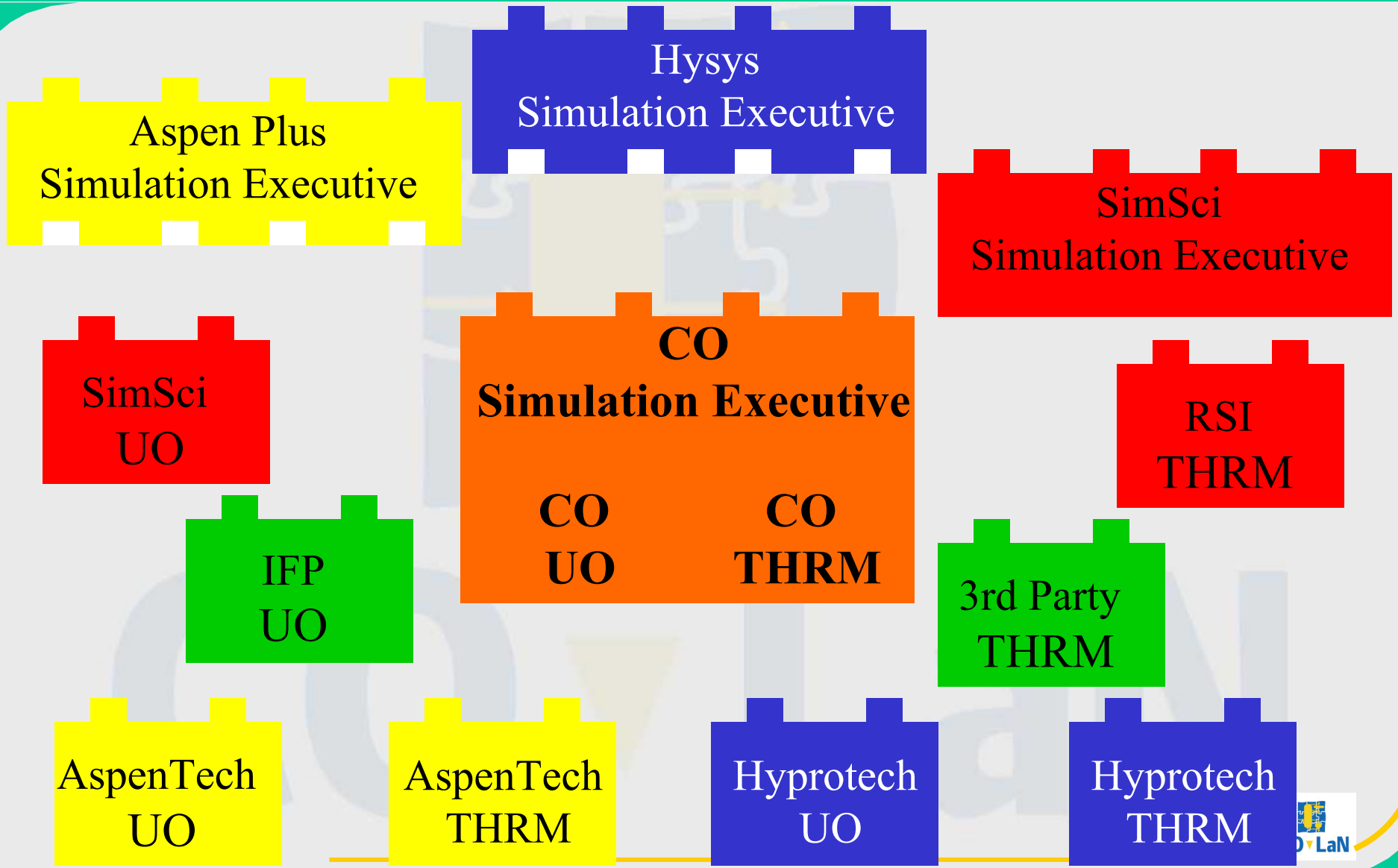
CO interfaces releases

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

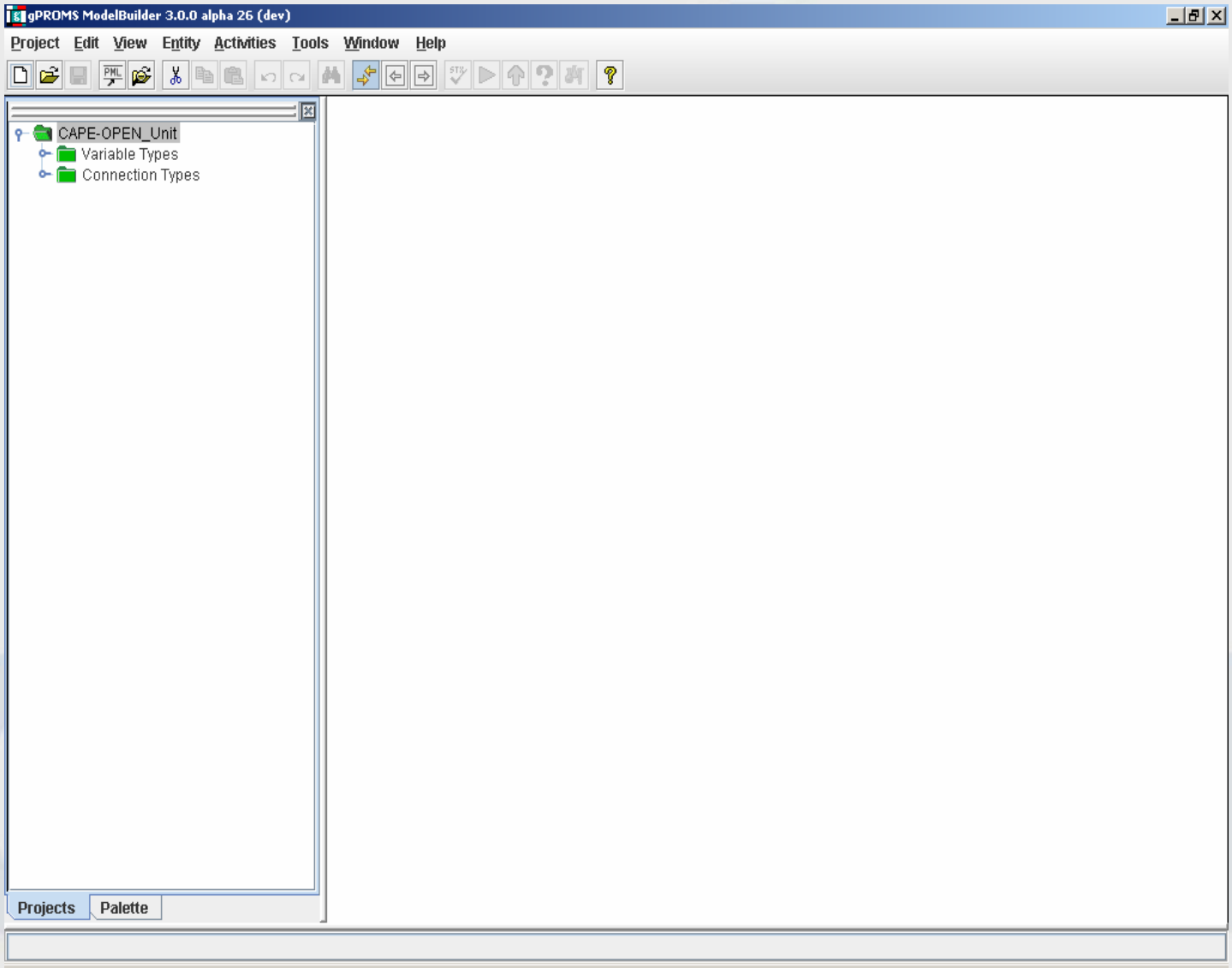


What CAPE-OPEN permits for end-users?

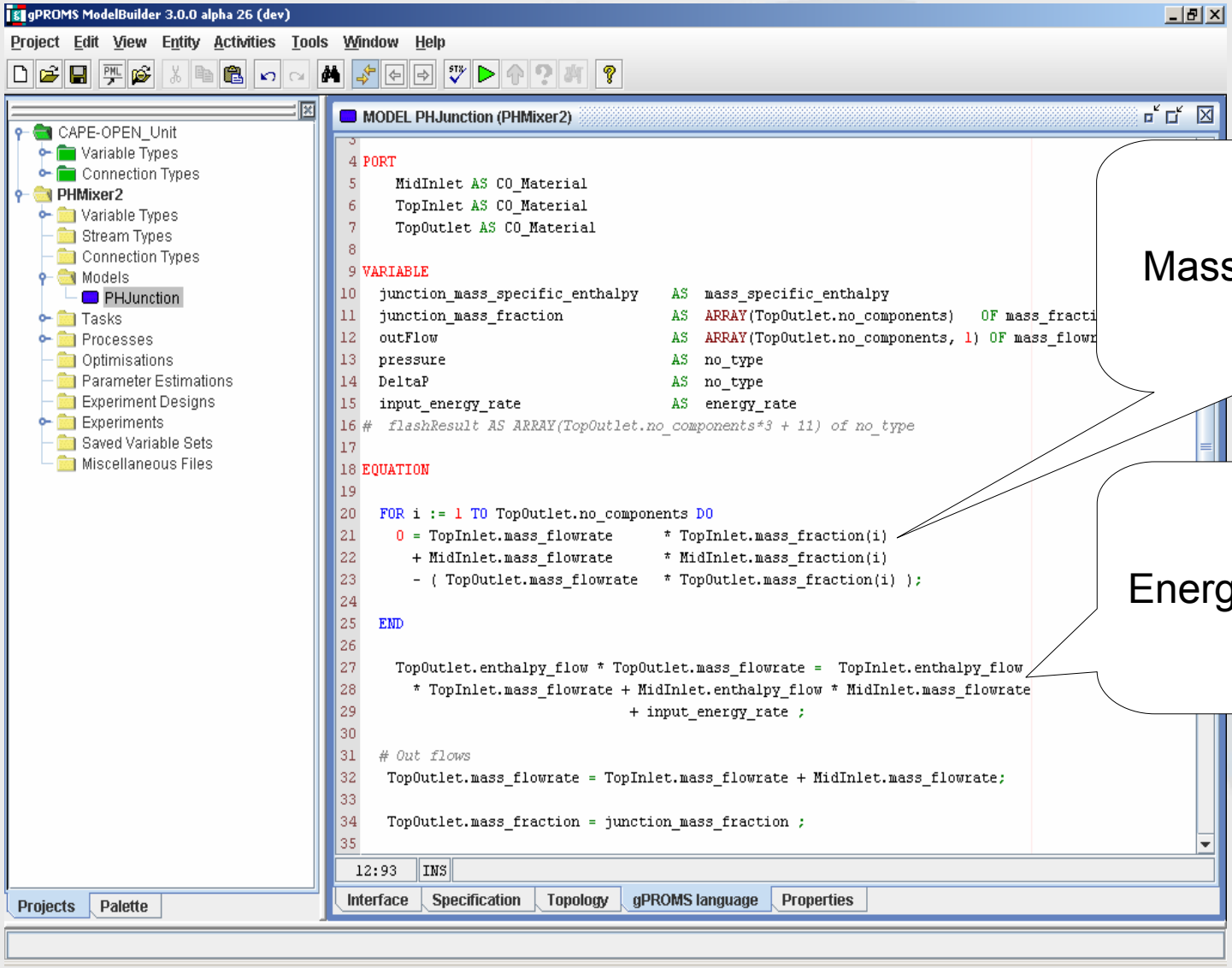
Interoperability



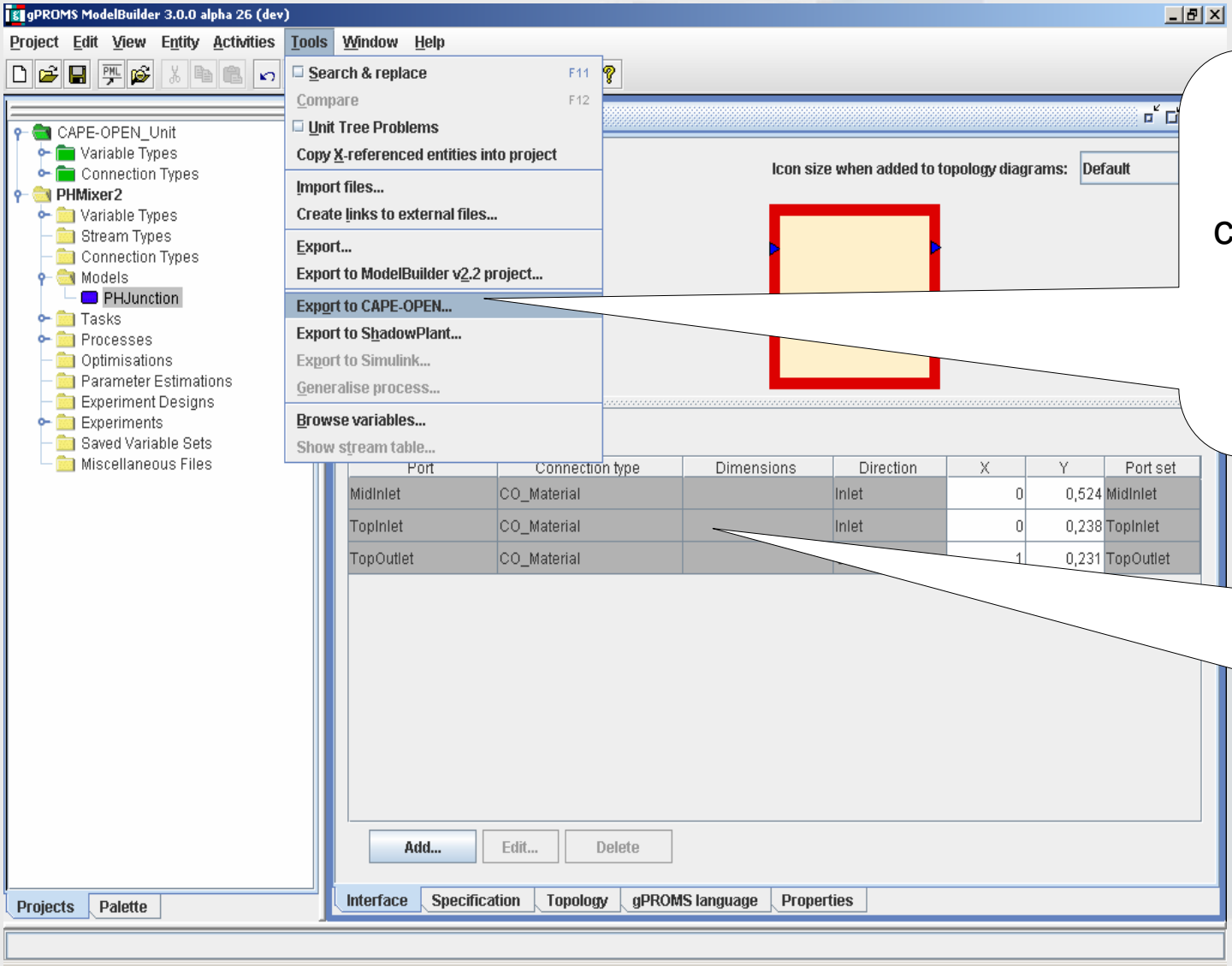
Load CAPE-OPEN library in ModelBuilder



Load/Create Mixer Model



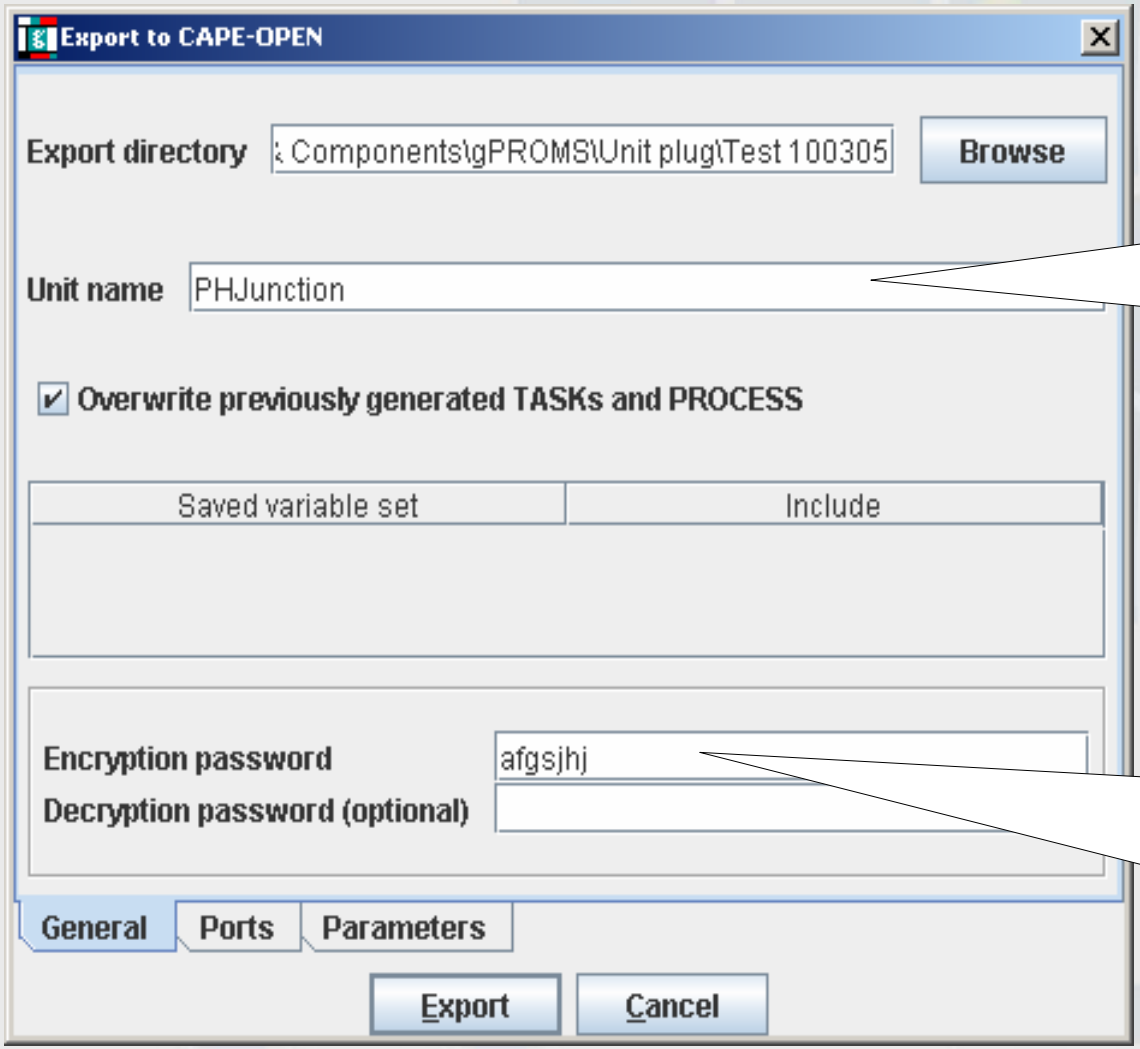
Launch CAPE-OPEN export



No need to change model for CAPE-OPEN exportation

gPROMS supports CAPE-OPEN Material Object

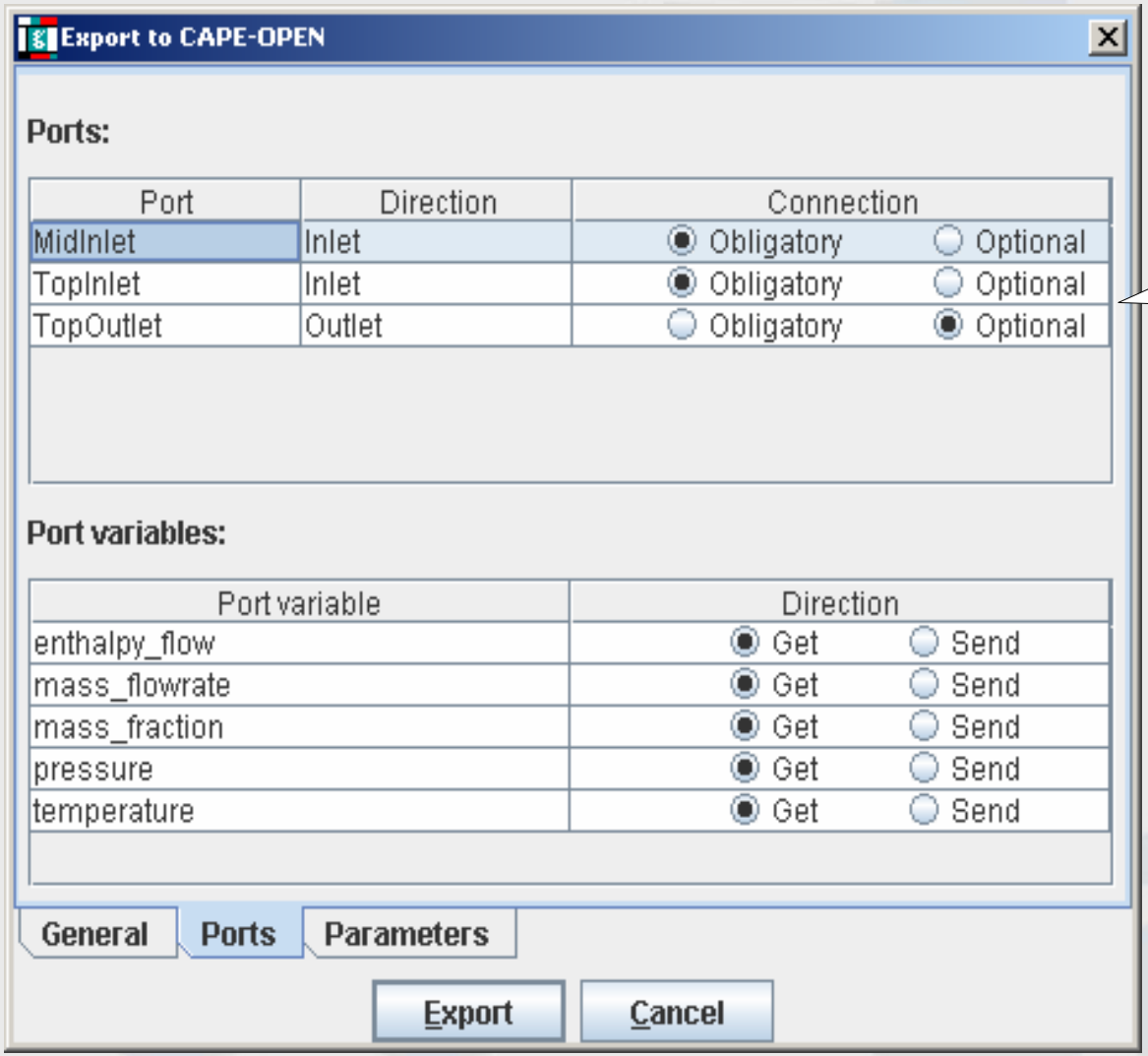
Crypt gCO file



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

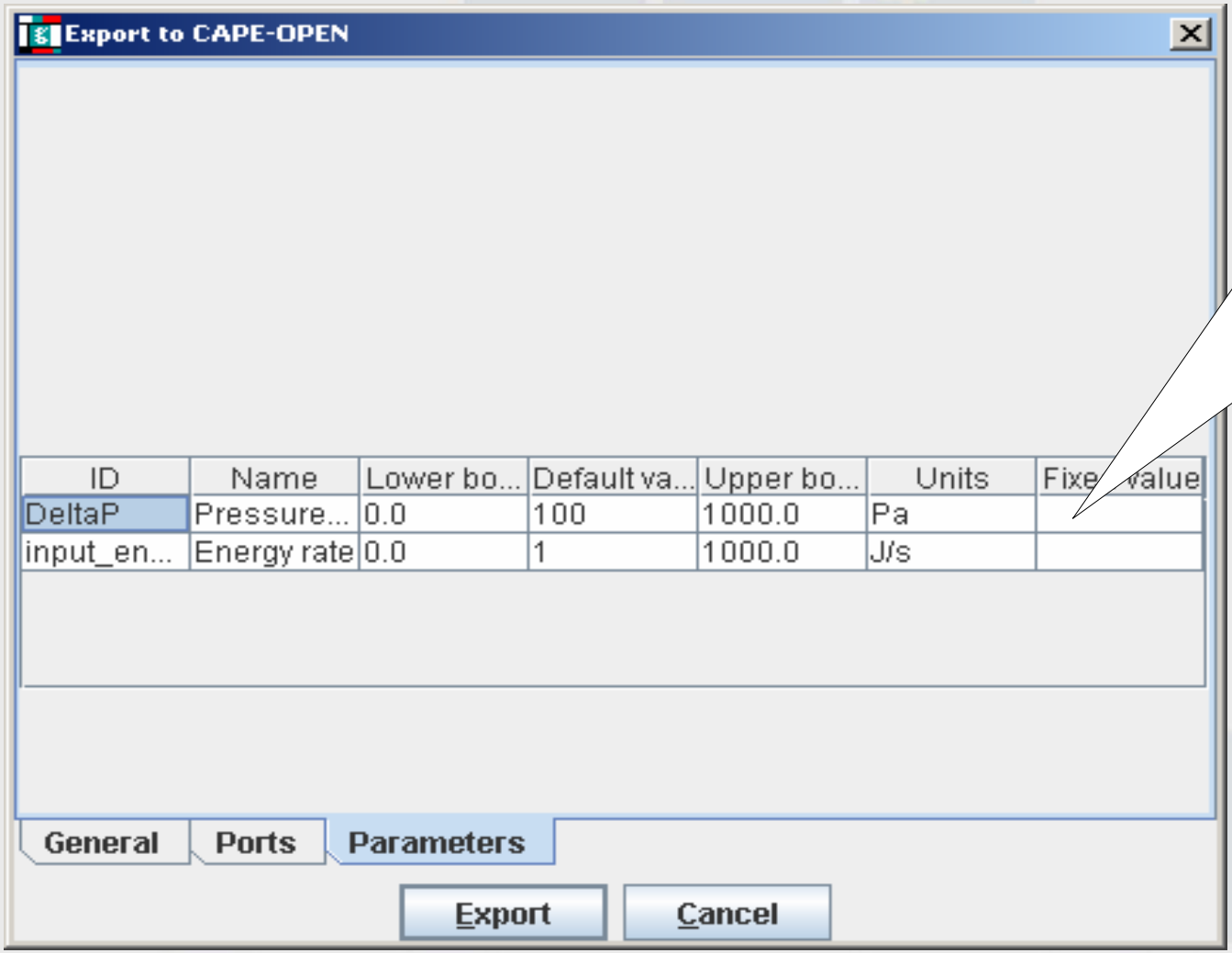
Encrypting the gCO file enables deployment to other parties and ensures consistency

Define ports options and parameters settings



Ports connection may be mandatory or optional

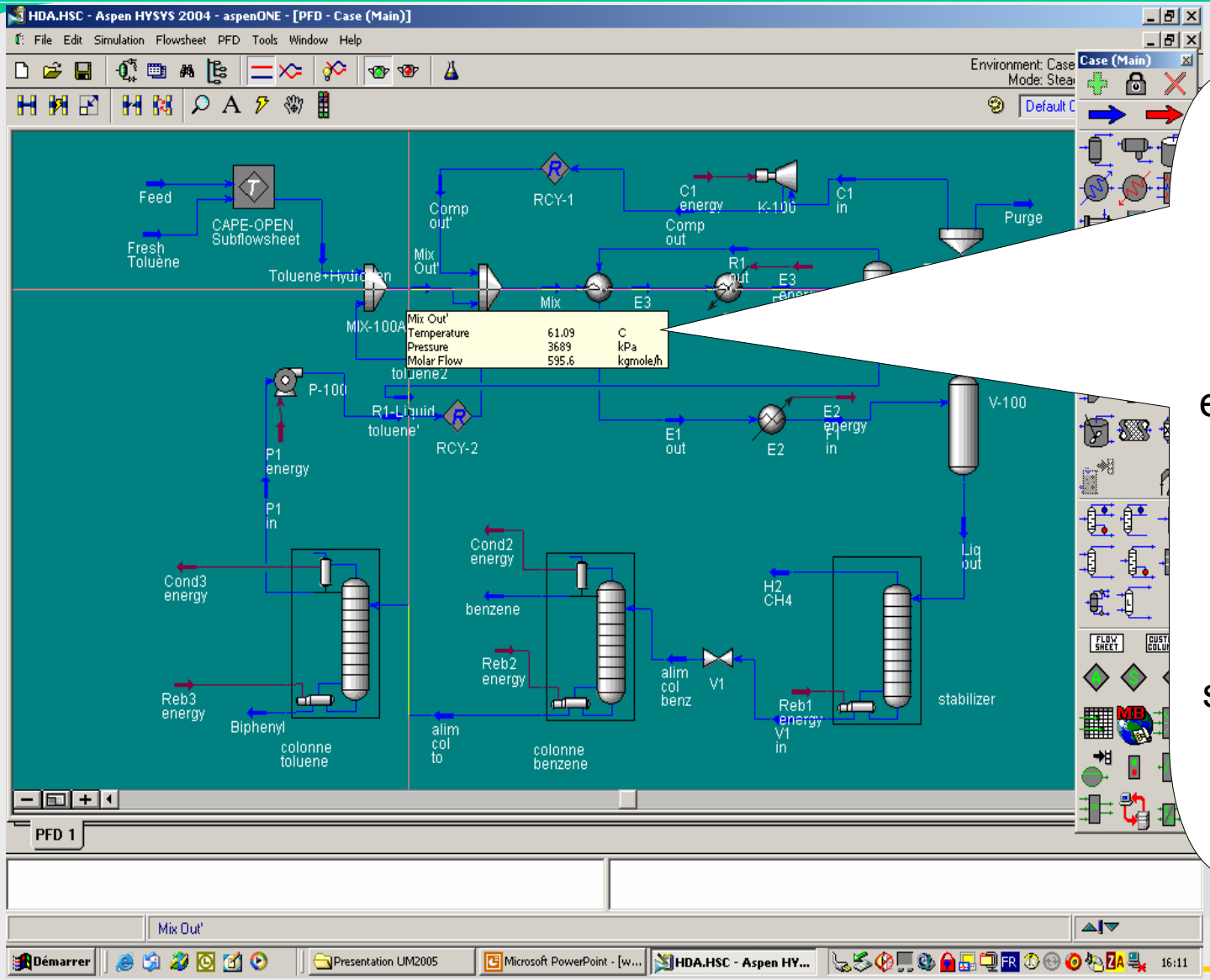
Parameter default settings



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

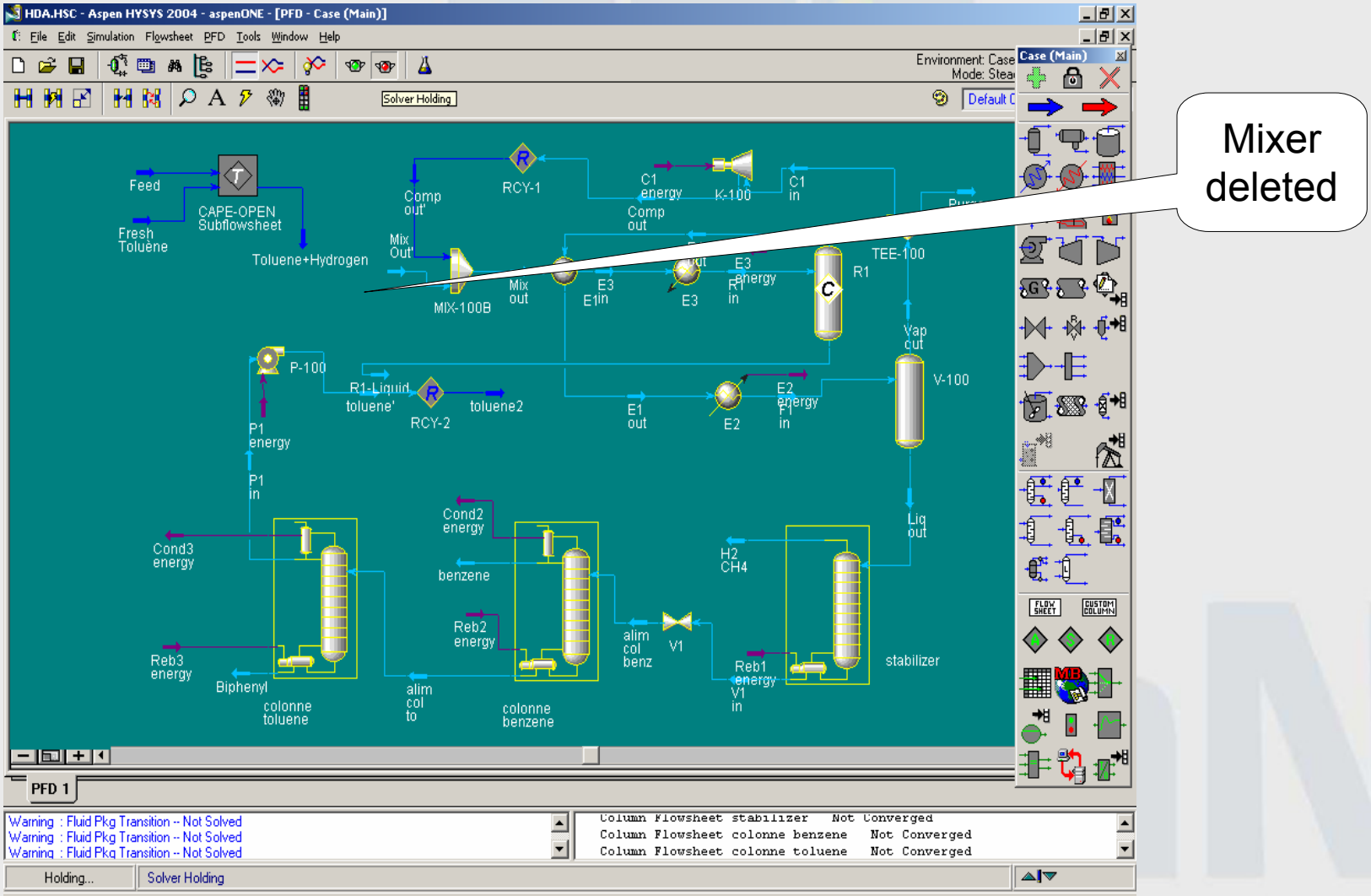
Running gPROMS model in HYSYS.Process

HDA process model in Aspen HYSYS 2004



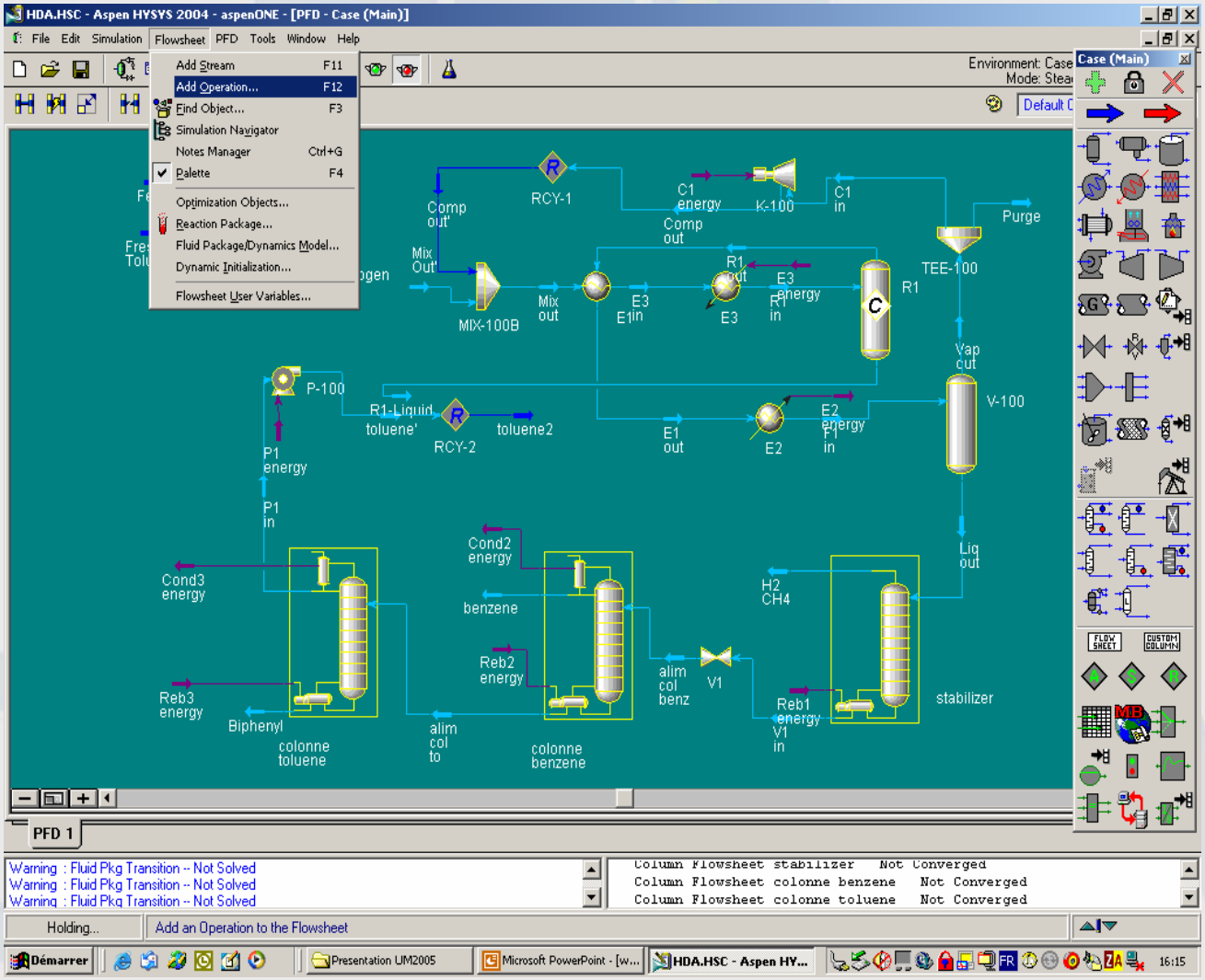
Since gPROMS mixer model involves basic material and energy balances, results with Aspen HYSYS 2004 native mixer and gPROMS mixer should be strictly the same.

Native mixer deleted and solver on hold

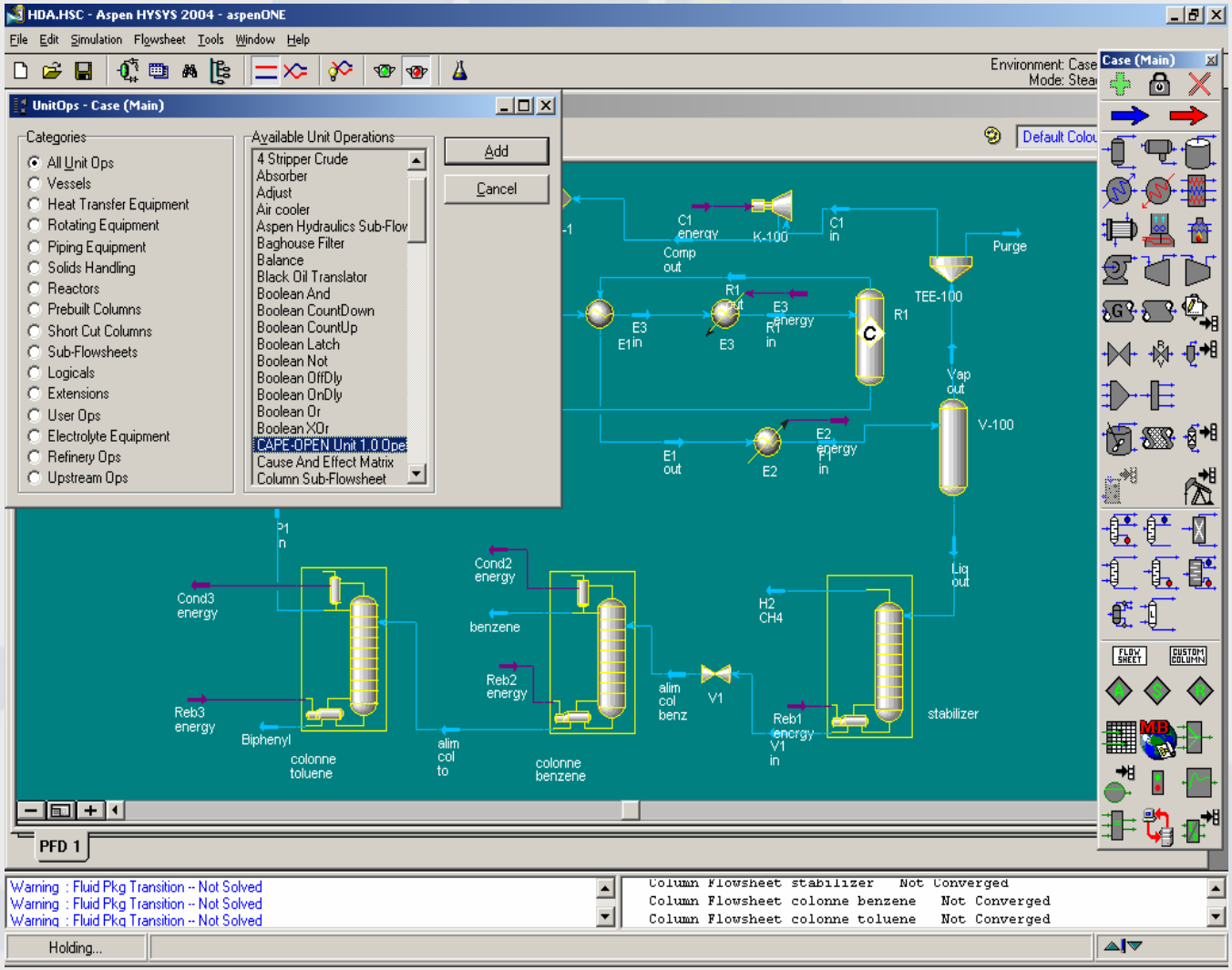


Mixer deleted

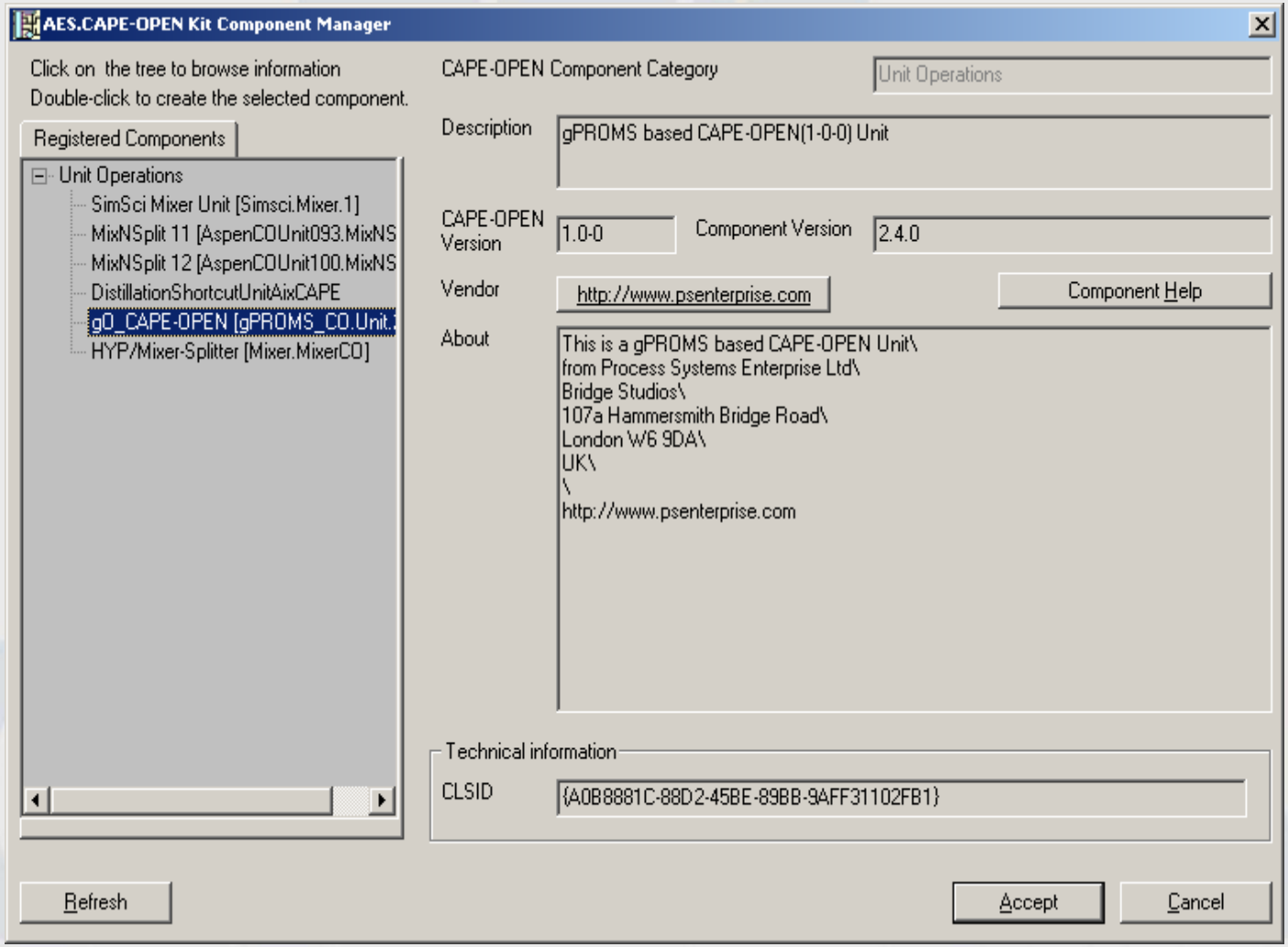
Replace native Mixer



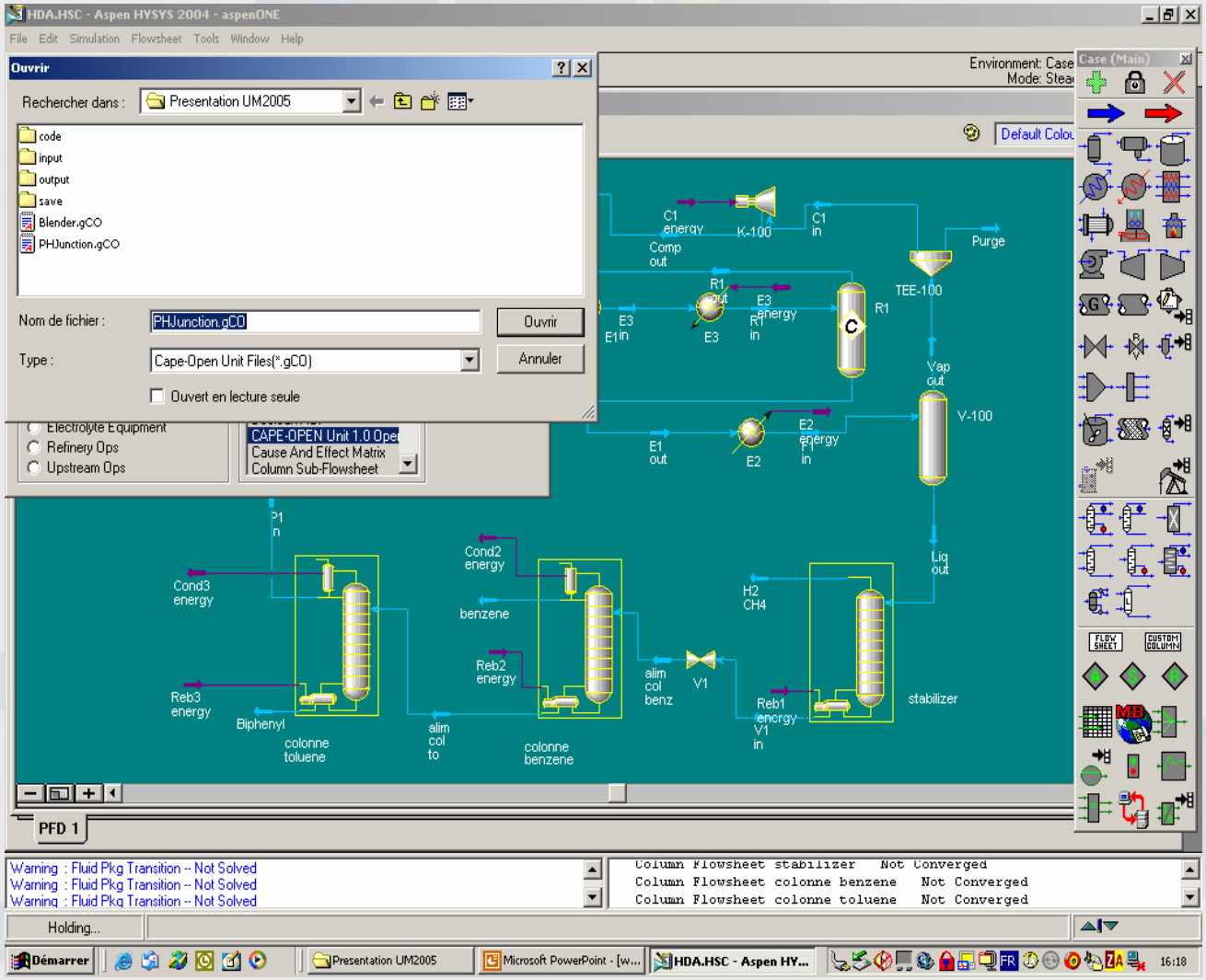
Select CAPE-OPEN 1.0 UNIT Ops



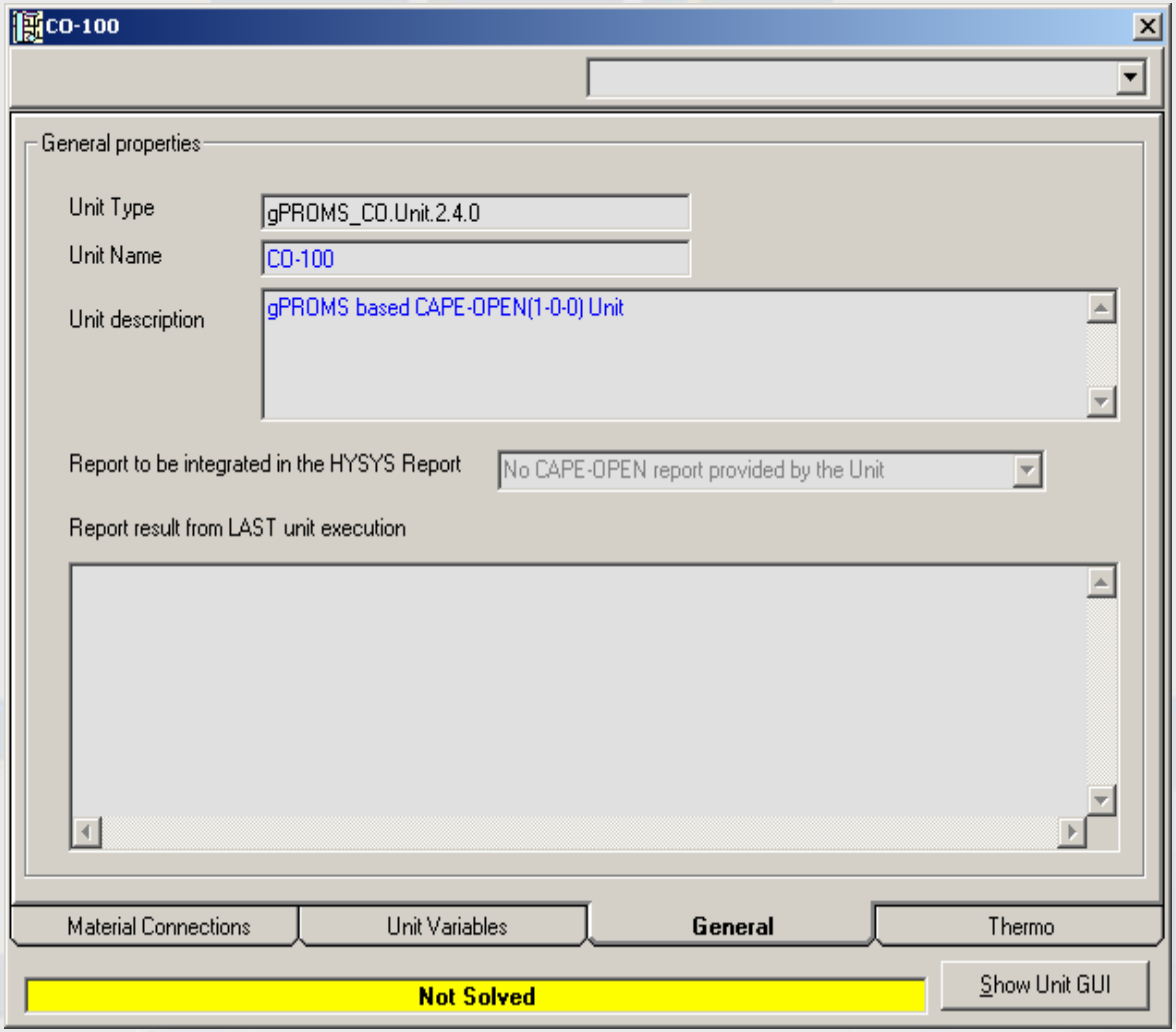
Select gO:CAPE-OPEN wrapper



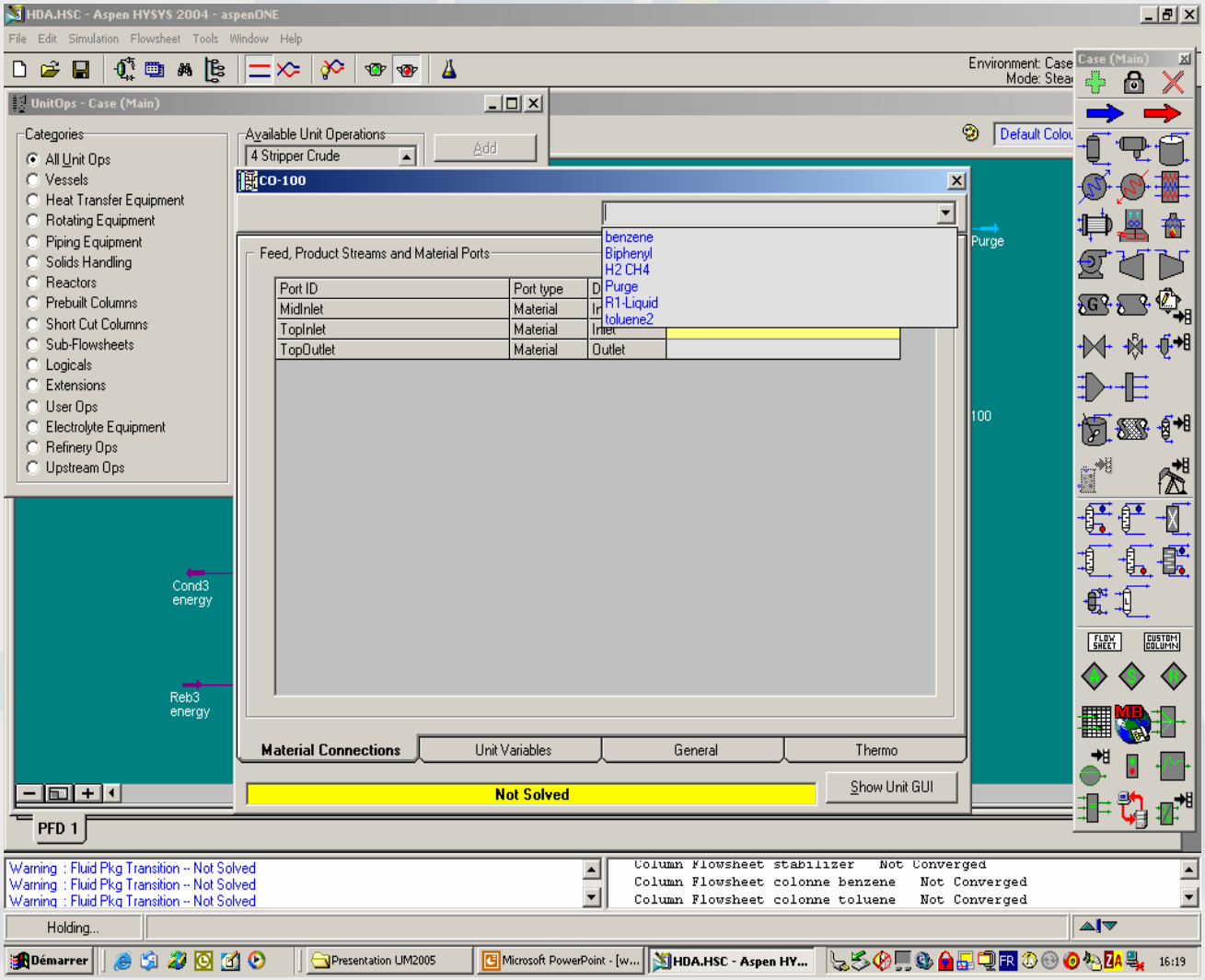
Select the gCO file to be used



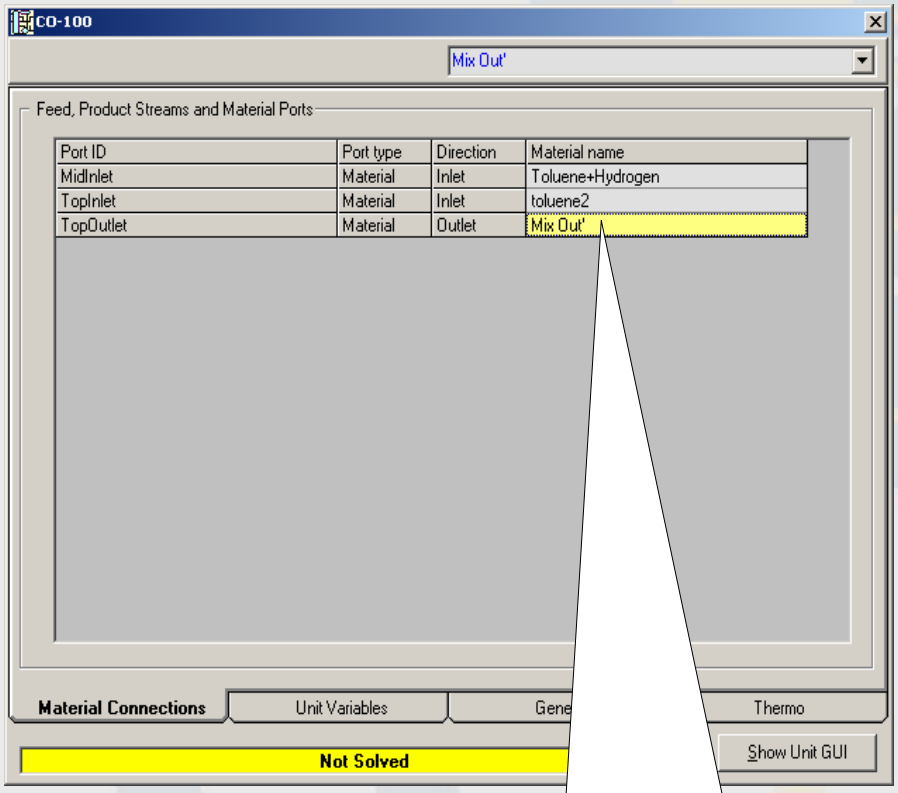
Enter generic GUI provided by HYSYS



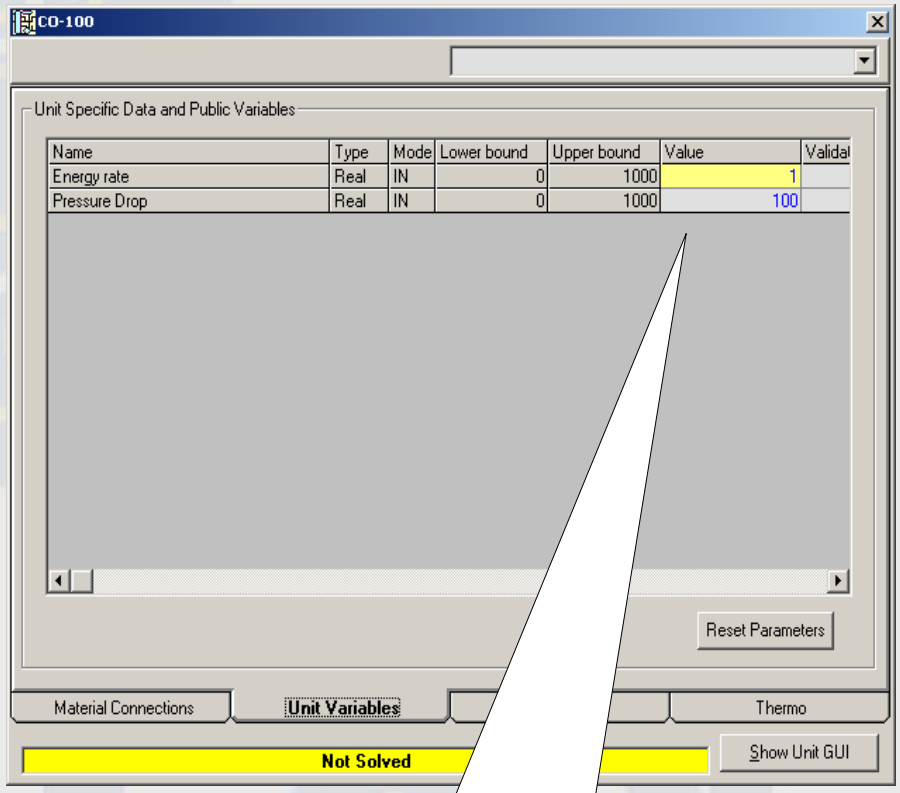
Connect inlet and outlet ports to streams



Set up the gPROMS model

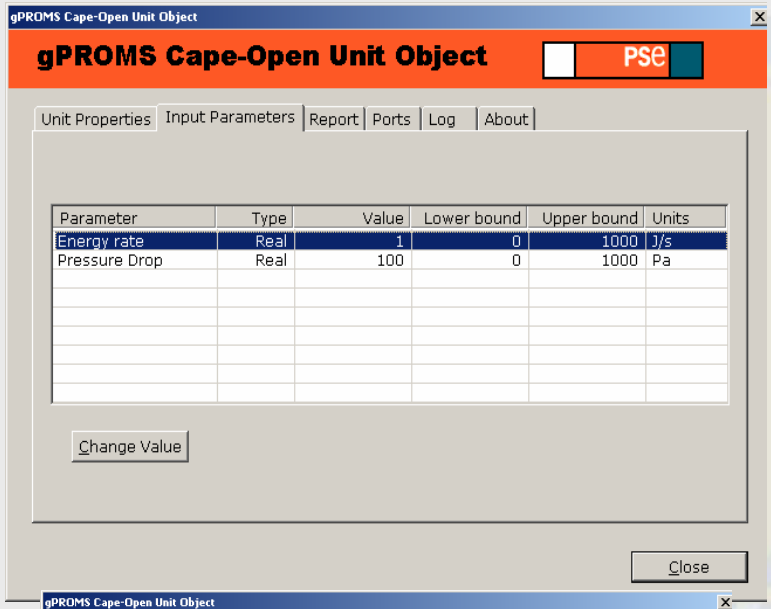


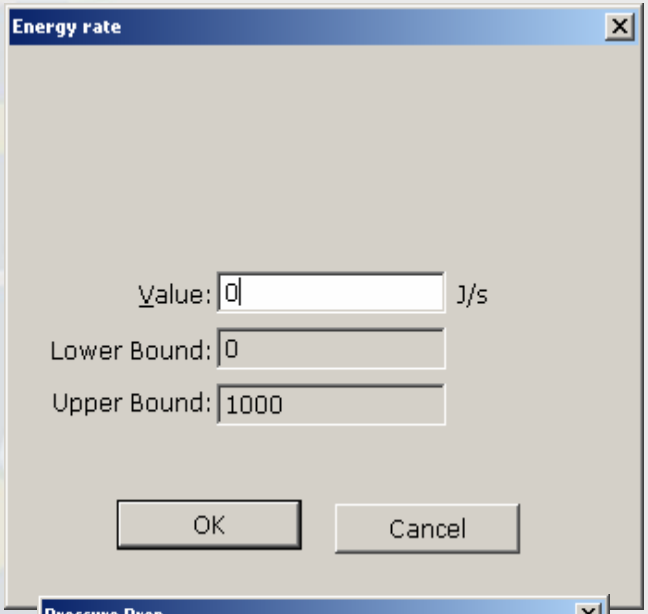
All ports connected

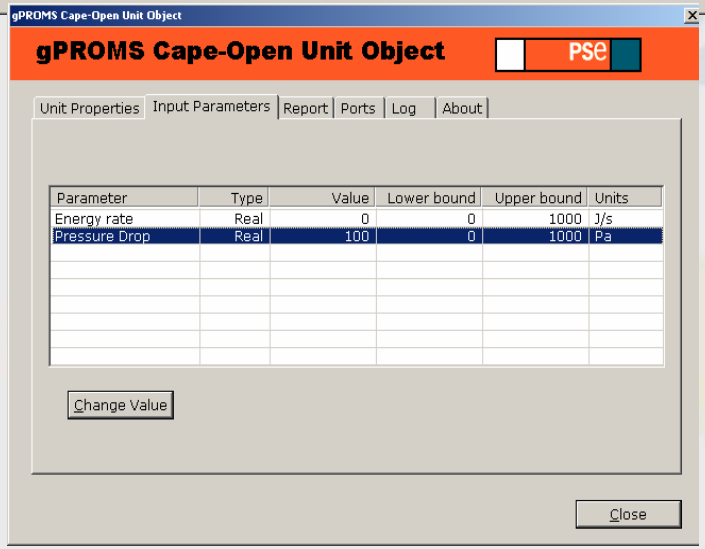


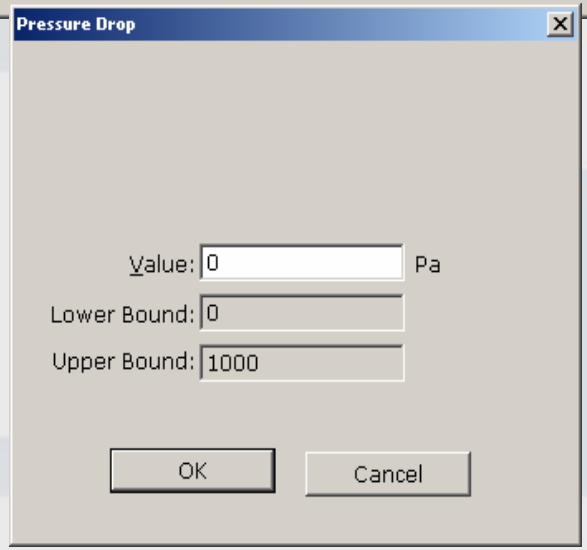
Initial parameter settings

Set energy input / pressure drop to zero

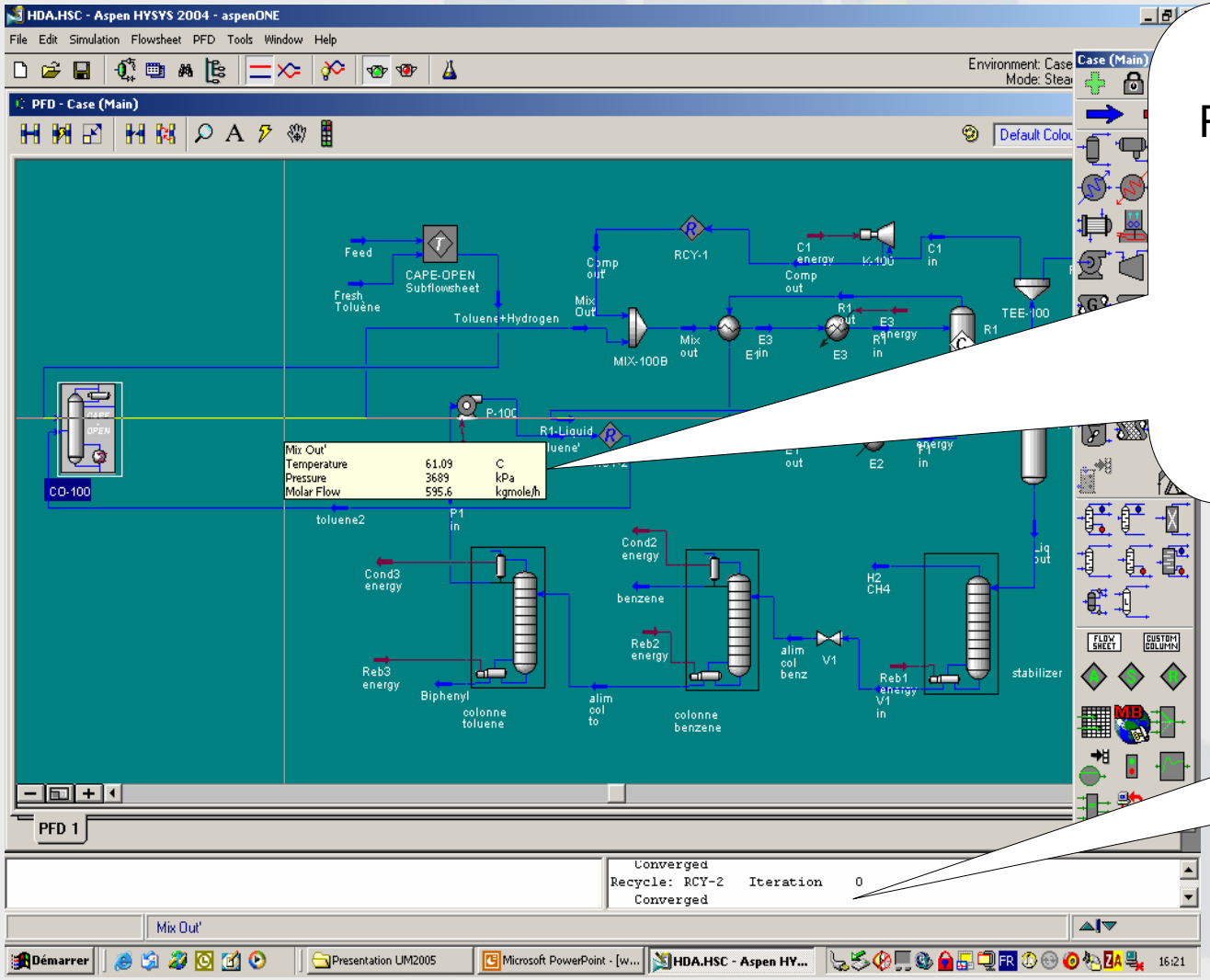








gPROMS Mixer output results



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

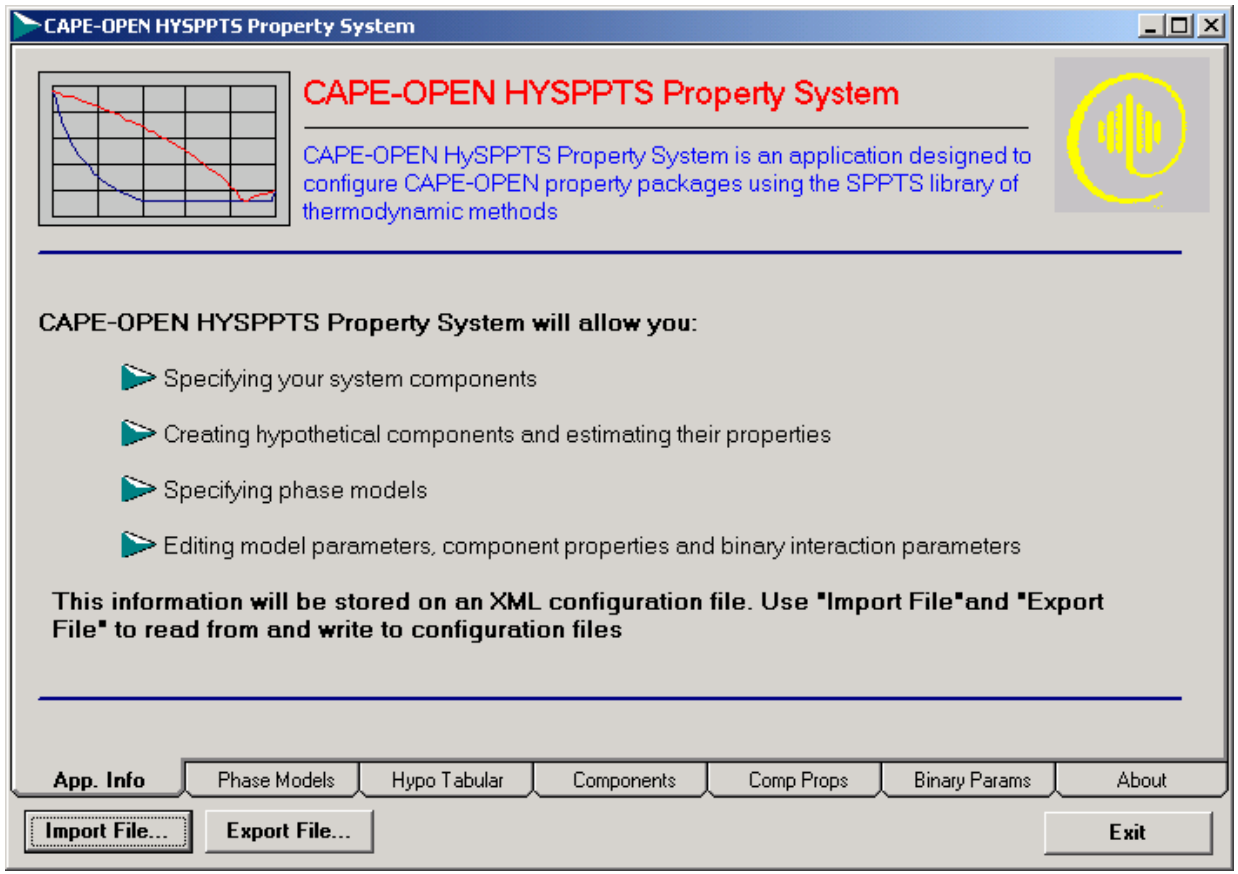
CoSPPTS

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)

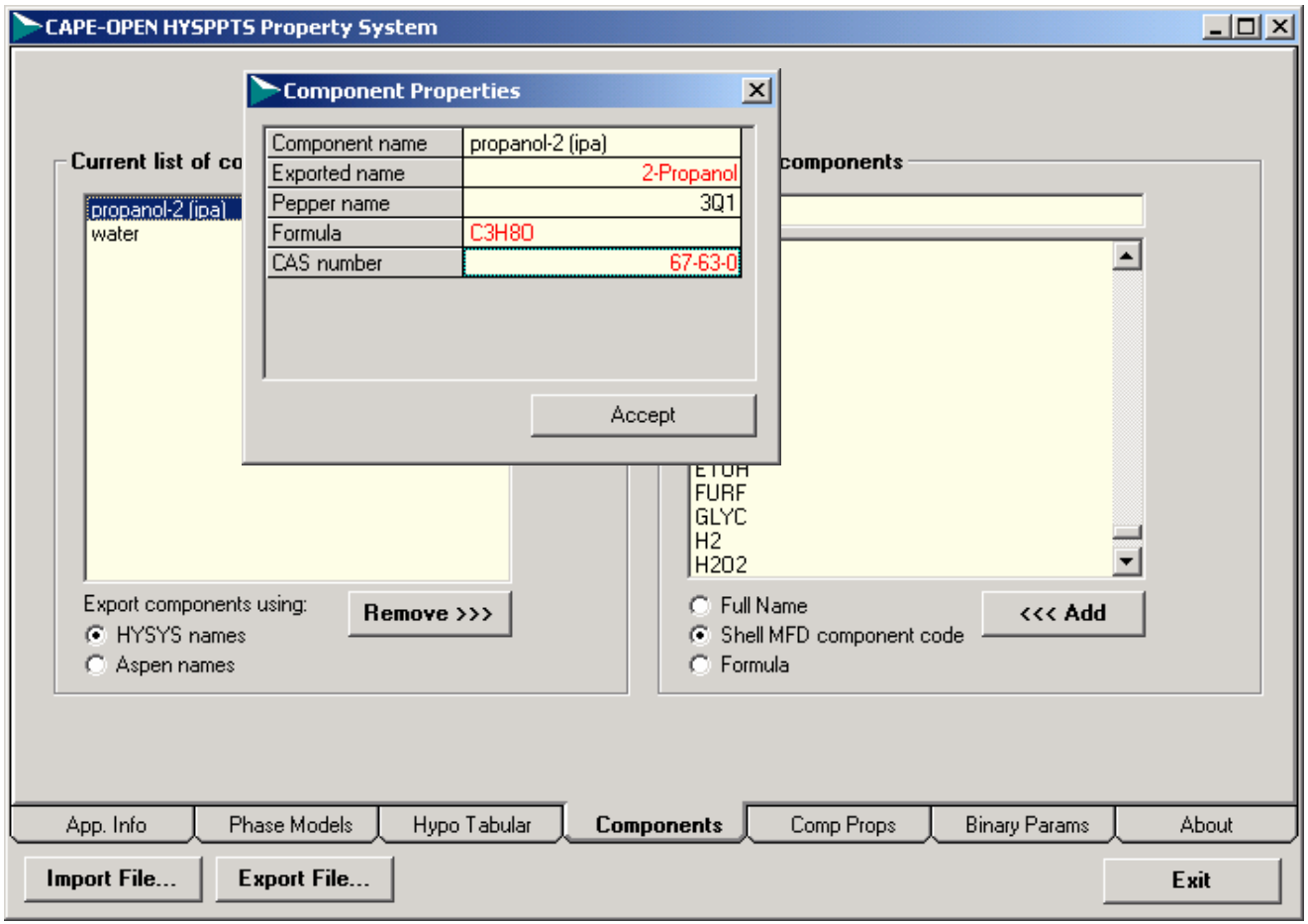
CoSPPTS

GUI of the tool – start up window



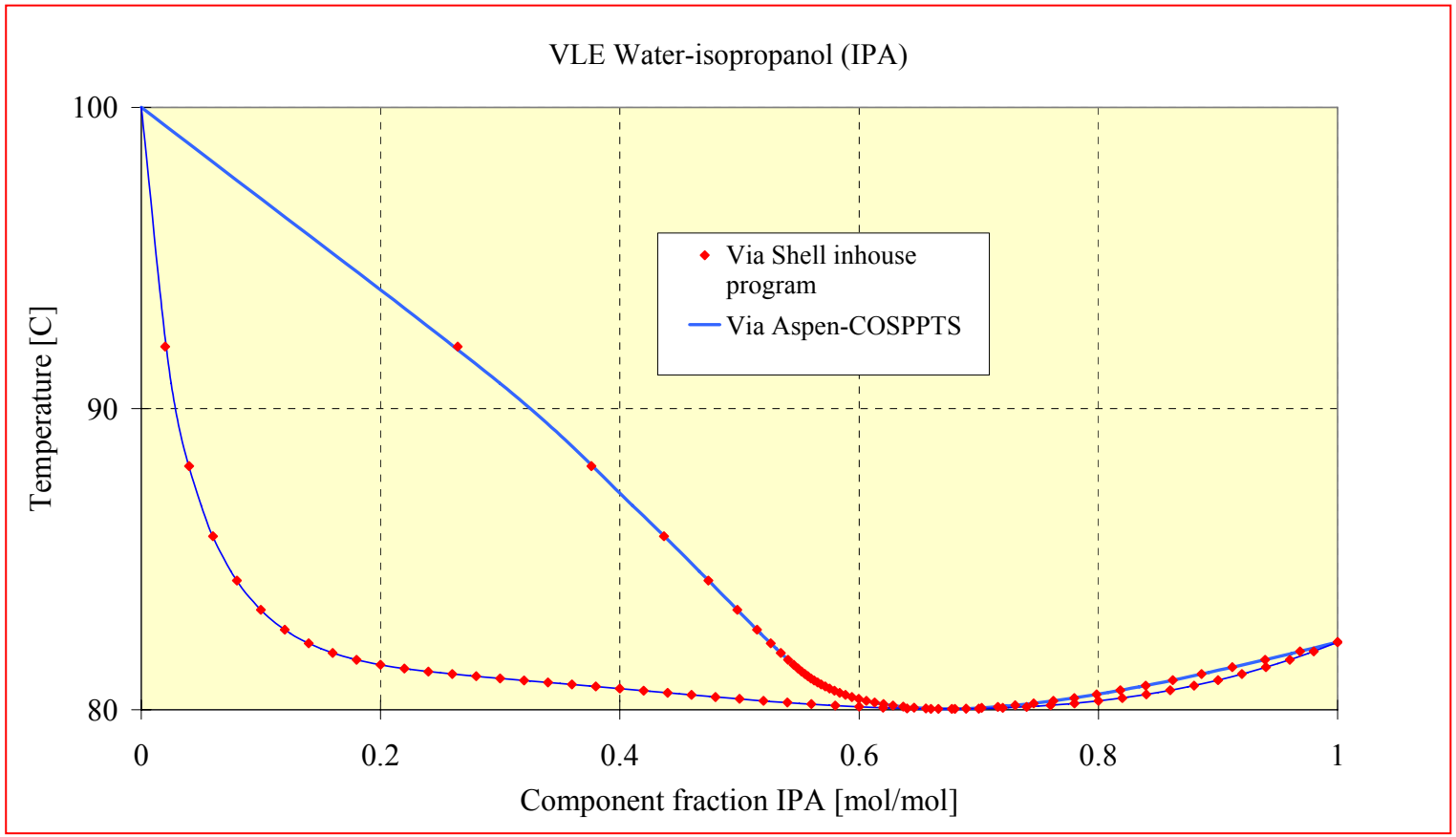
CoSPPTS

GUI of the tool – selection of components



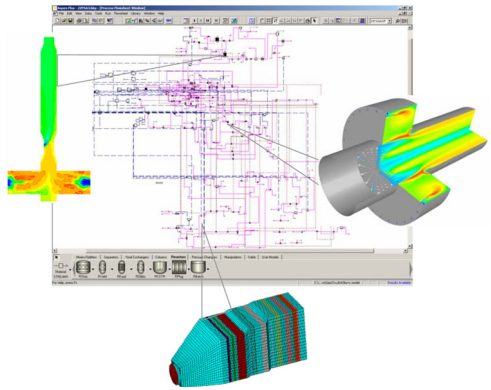
CoSPPTS

Consistency check: own program versus AspenPlus



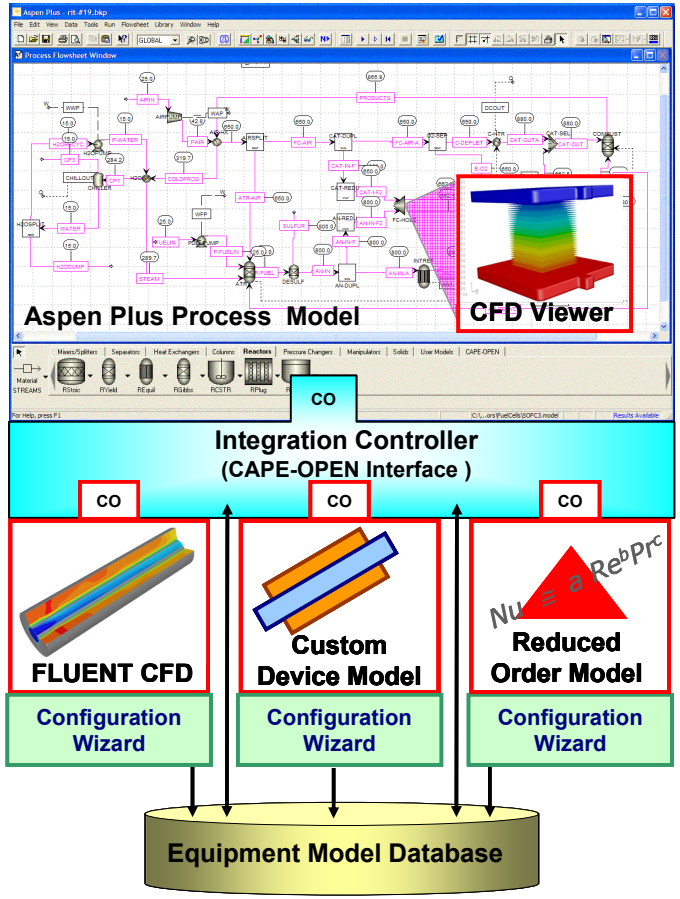
National Energy Technology Laboratory
Office of Science, Technology & Analysis

- **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)

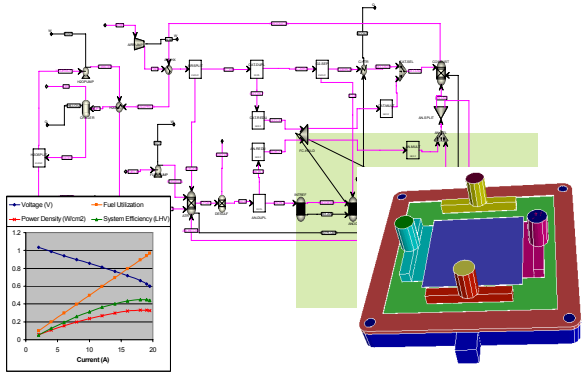
- Combines process simulation with custom engineering models and computational fluid dynamics (CFD)
- Complies with the process industry CAPE-OPEN software standard
- Offers fast reduced order models (ROMs) and parallel computing for improved performance
- Exploits advanced visualization for equipment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



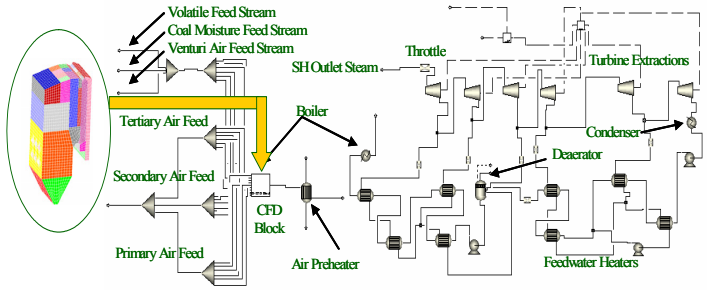
APECS Software Integration Framework

APECS Power Generation Applications

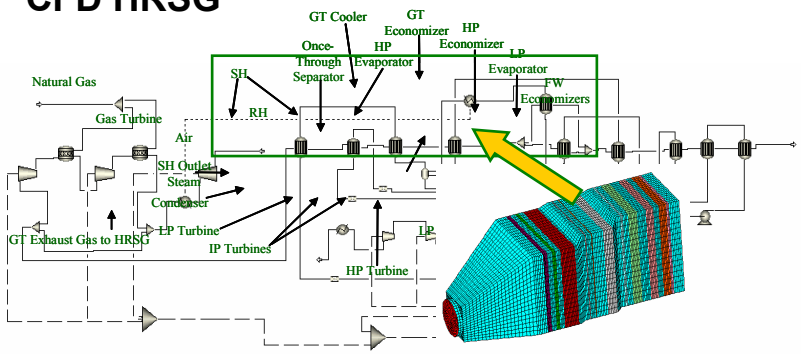
- **Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC**



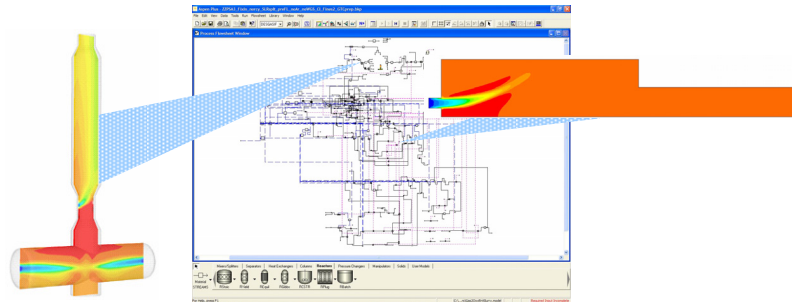
- **ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler**



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

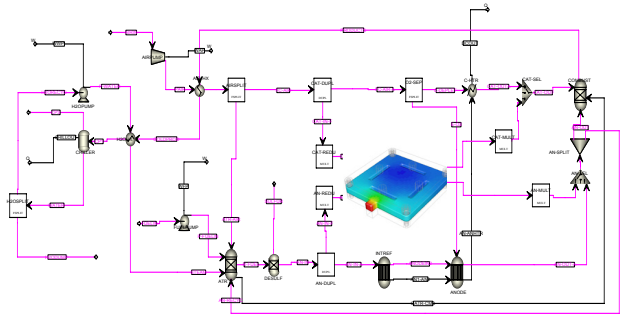


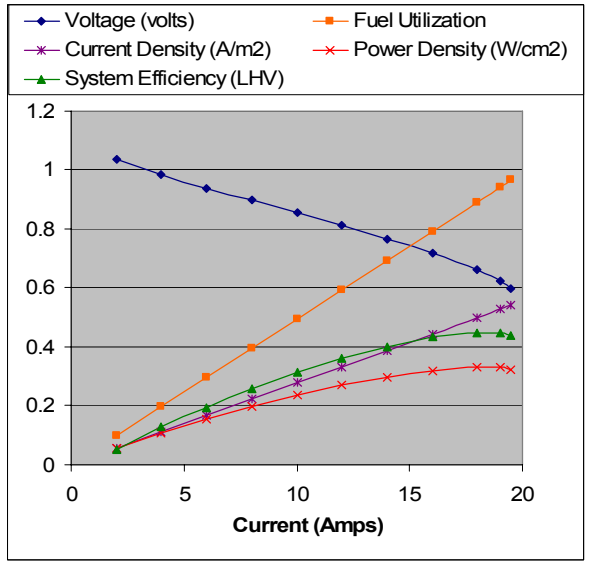
- **FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor**



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

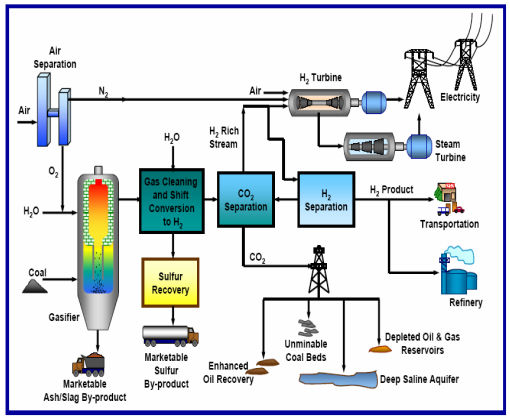




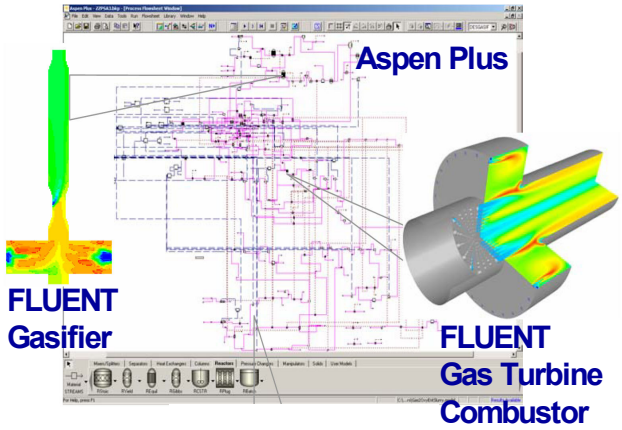
Zitney, S.E., Prinkey, M.T., Shahnam, M., and Rogers, W.A. (2004), "Coupled CFD and Process Simulation of a Fuel Cell Auxiliary Power Unit," In *Proc. of the ASME Second International Conference on Fuel Cell Science, Engineering, and Technology*, Eds. R. Shah and S.G. Kandlikar, Rochester NY, June 13-16,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

APECS Application - FutureGen Power Plant

- **FutureGen Power Plant**
  - IGCC with CO_2 capture and H_2 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

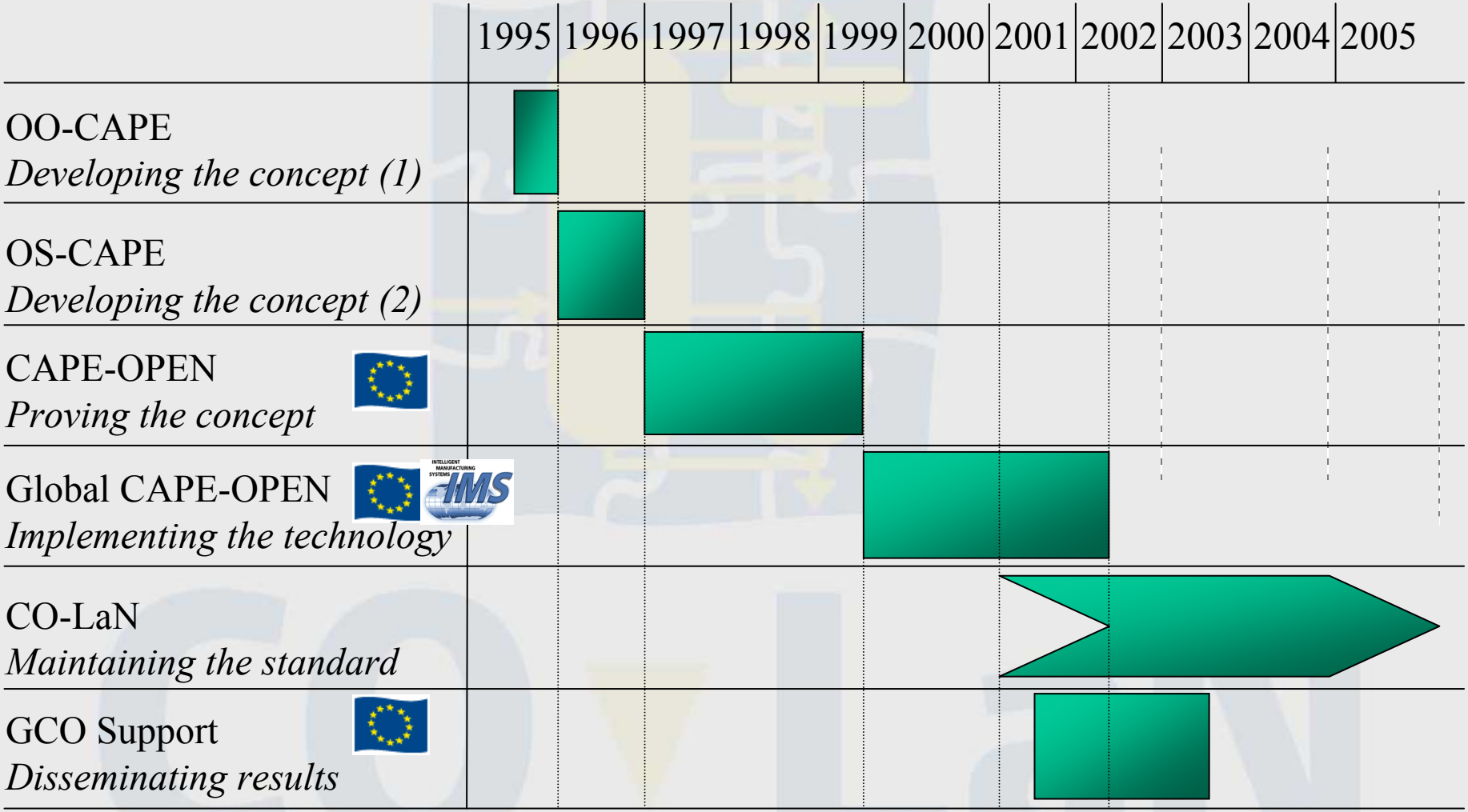


FutureGen APECS

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

CO-LaN

- **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
- HTRInc.
- 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

23 Software suppliers

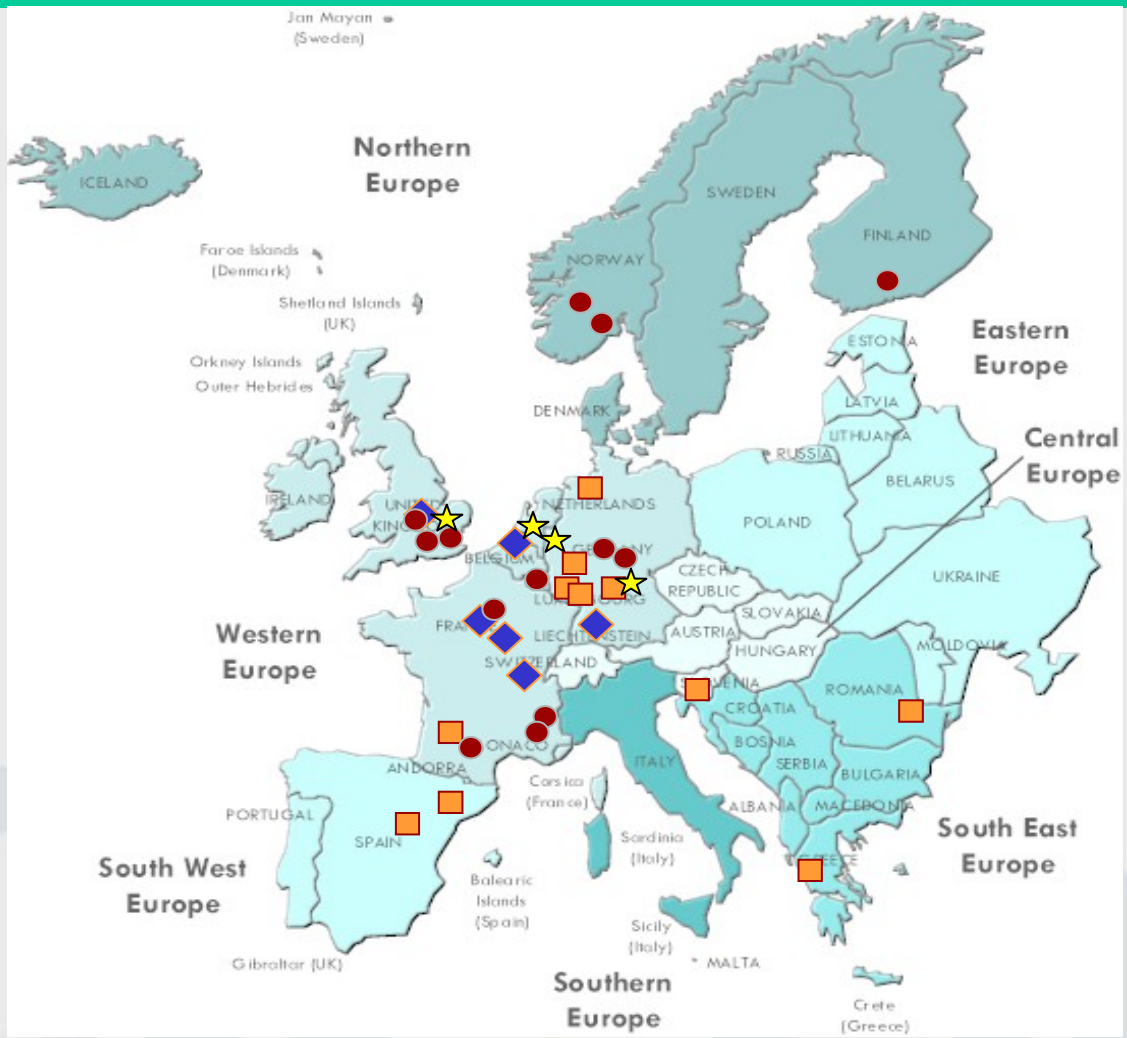
7 Operating Companies

2 Governmental

12 Universities

4 Individuals

European membership



23 Software suppliers | 7 Operating Companies | 2 Governmental | 12 Universities | 4 Individuals

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

Michel PONS

Chief Technology Officer

Akzo Nobel Chemicals, Arnhem, November 17, 2005