Applications of CAPE-OPEN standards to reactor and kinetic modeling

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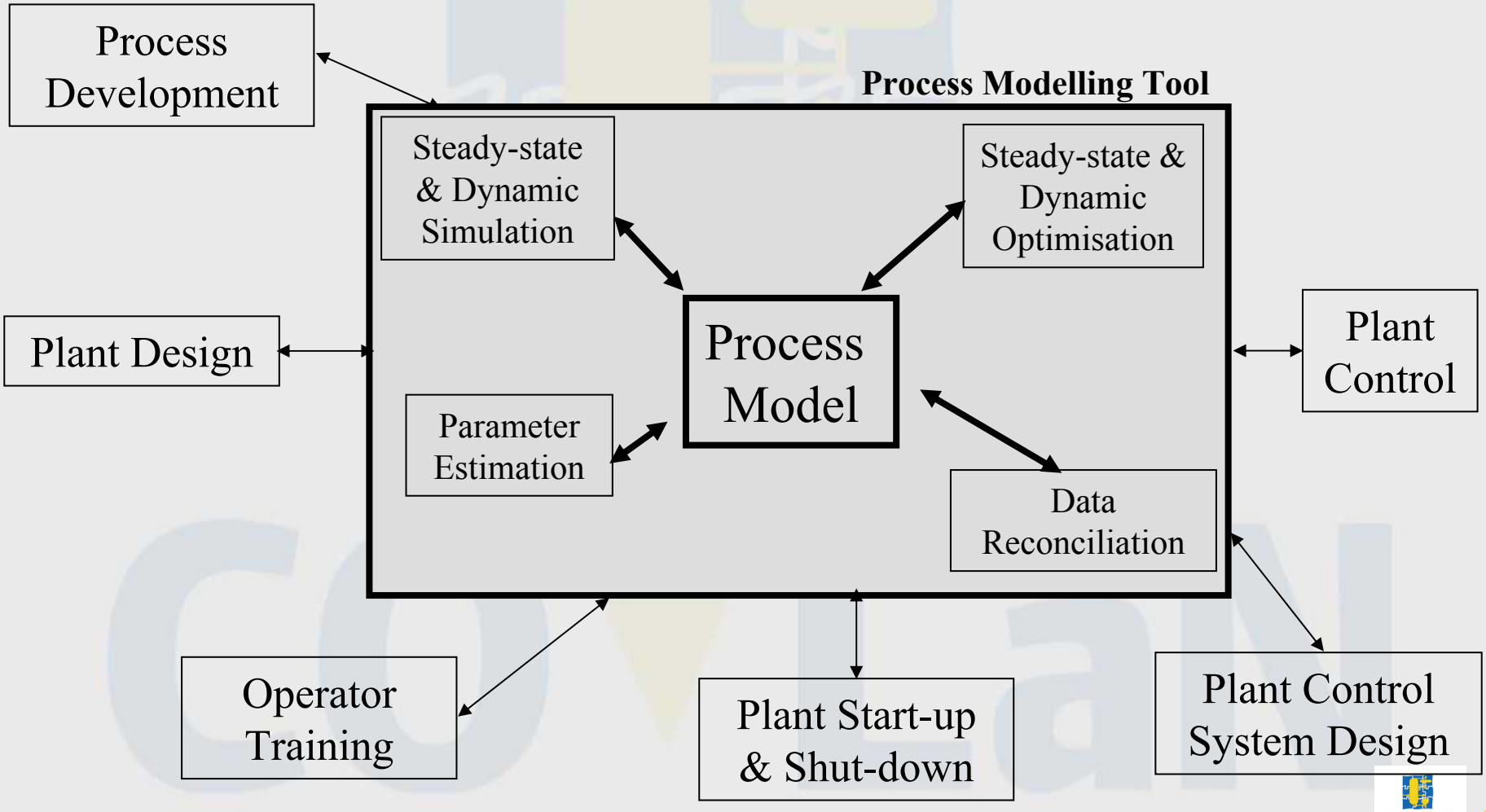
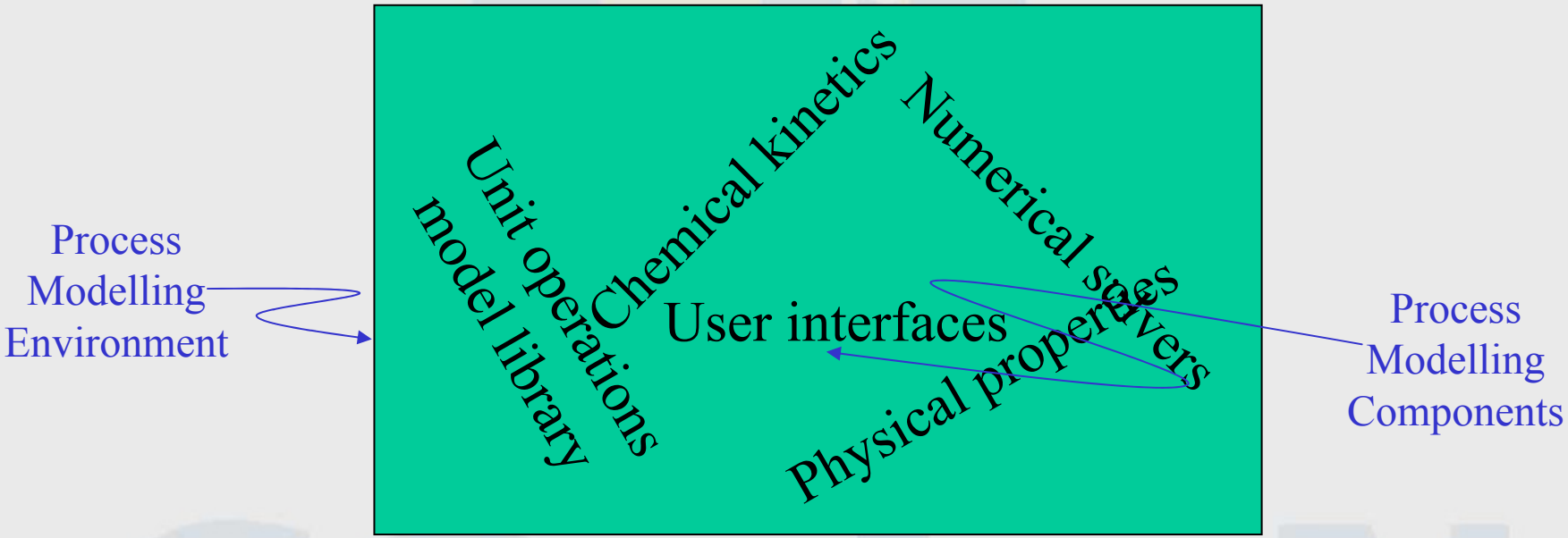
EUROKIN Workshop, October 20, 2005

What is CAPE-OPEN?

General-purpose process modelling tools

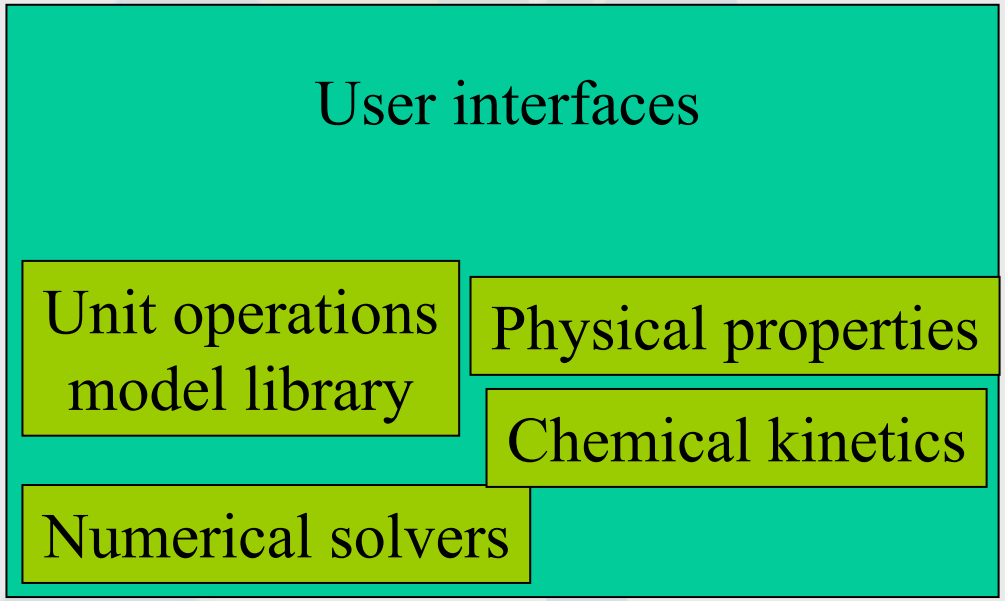


The anatomy of process modelling tools – a (somewhat) confusing reality

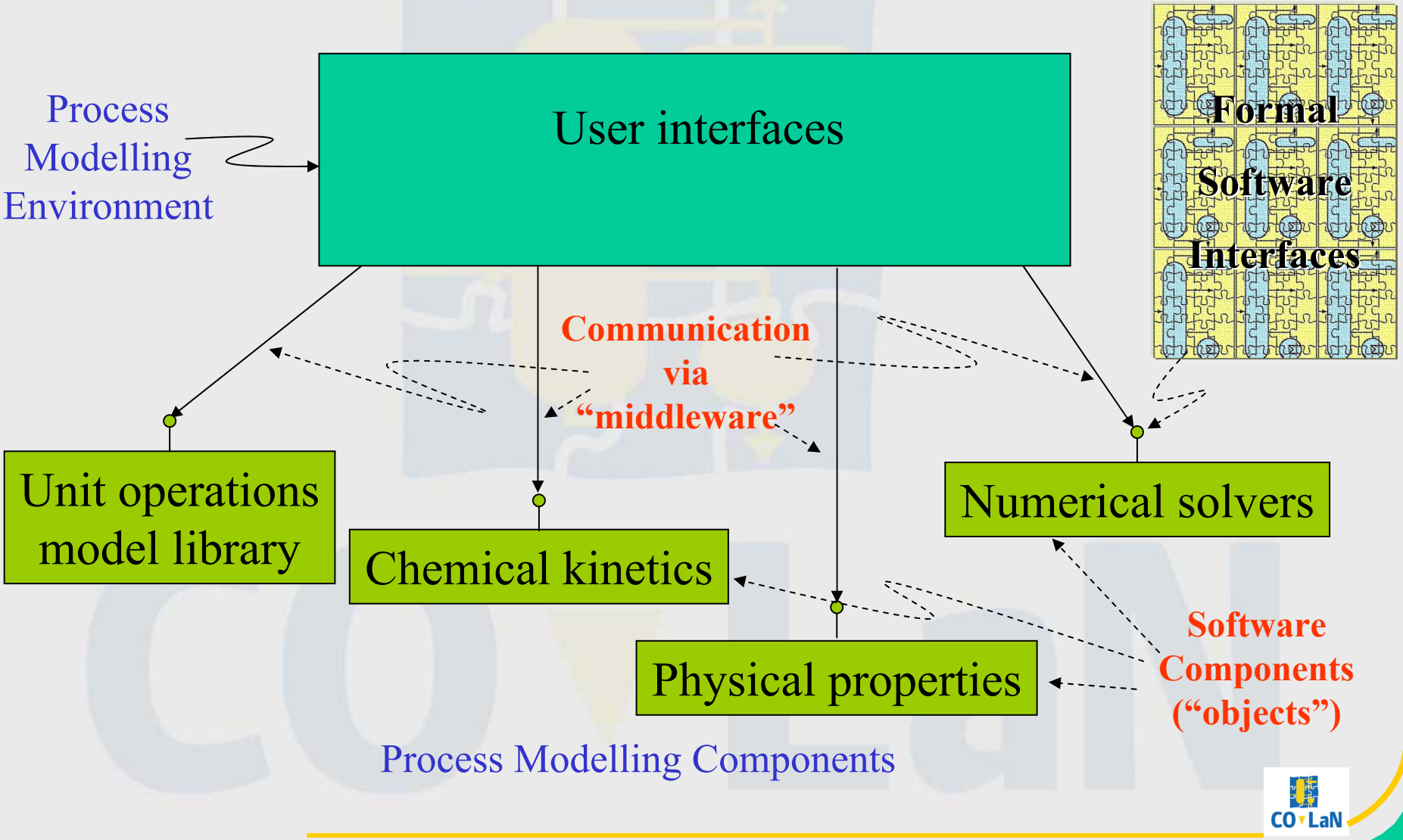


- Many interacting components…
- …all tightly coupled with each other
- Component boundaries not always clearly delineated

Clarify boundaries between key components



…and break tool into 1 PME & multiple PMCs

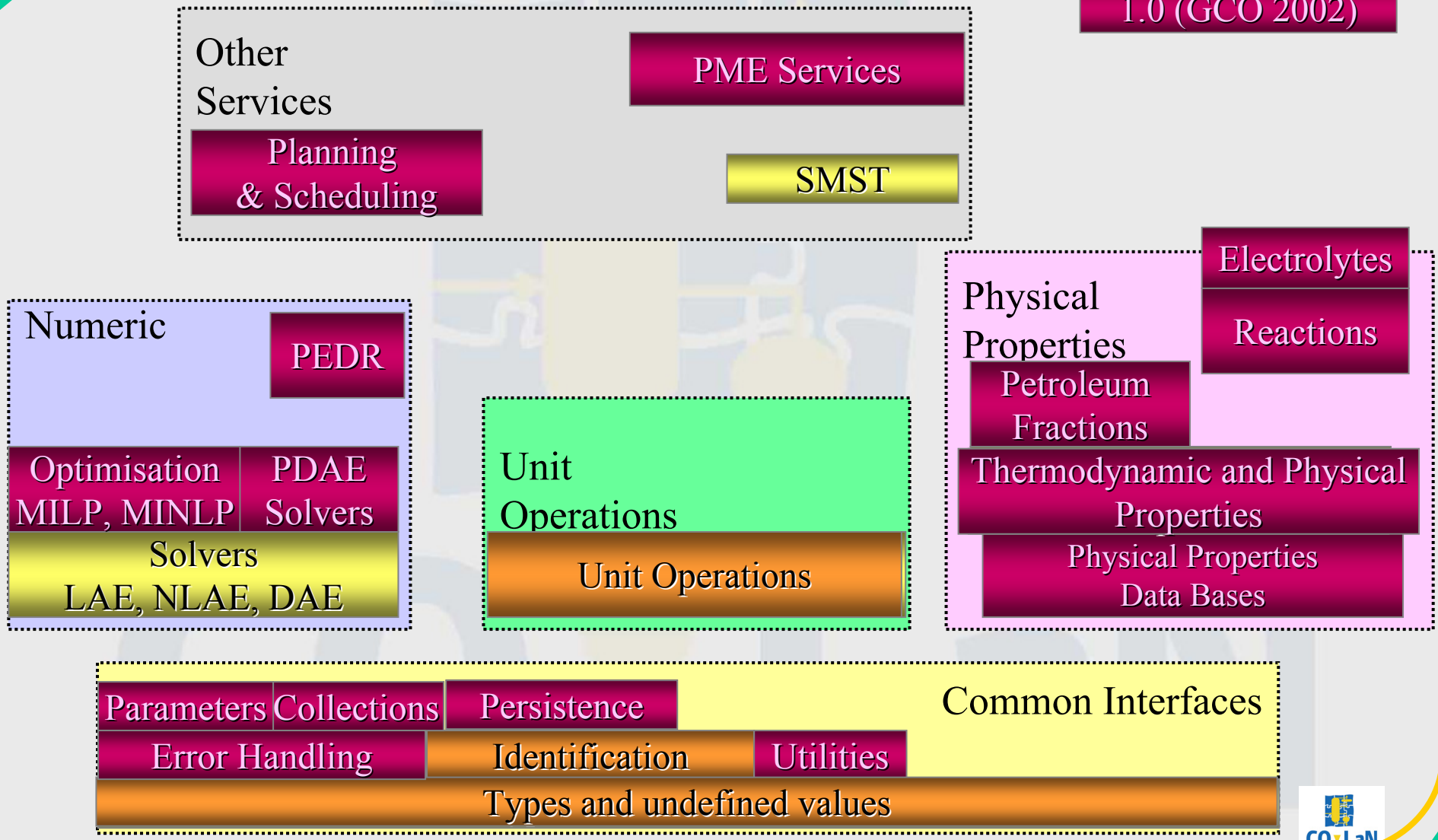


CAPE-OPEN: a technology for integration

- 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

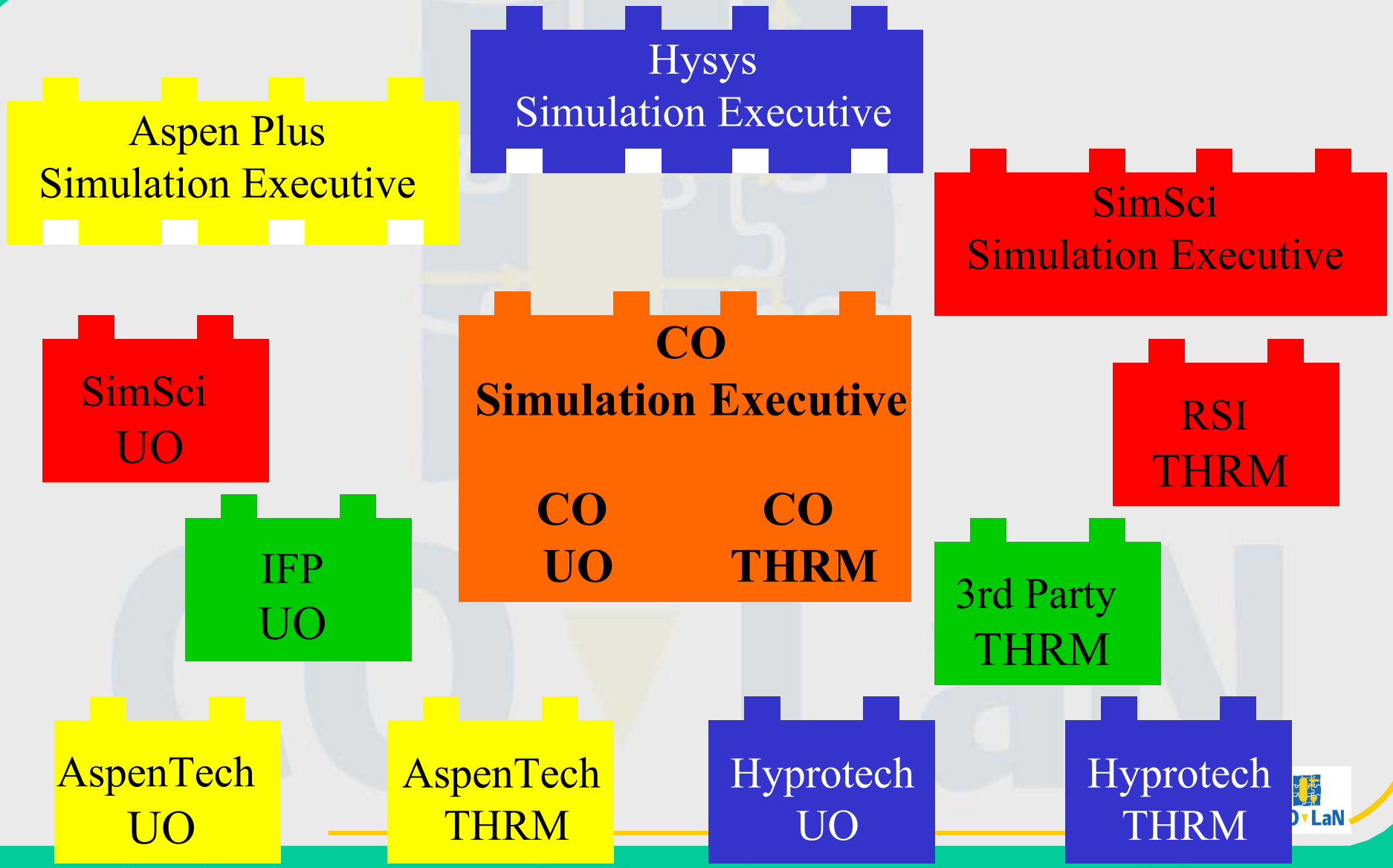
CO interfaces releases

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

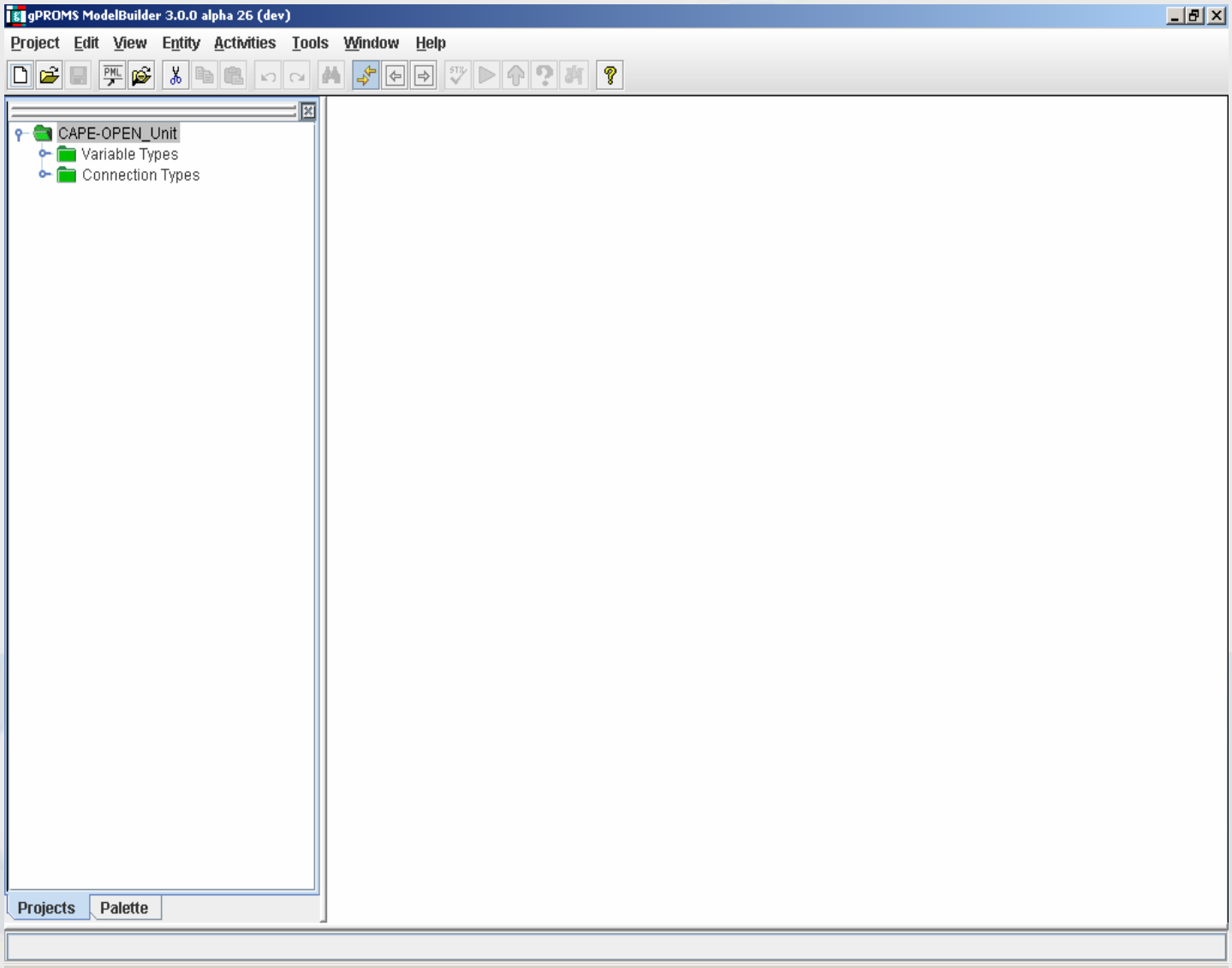


What CAPE-OPEN permits?

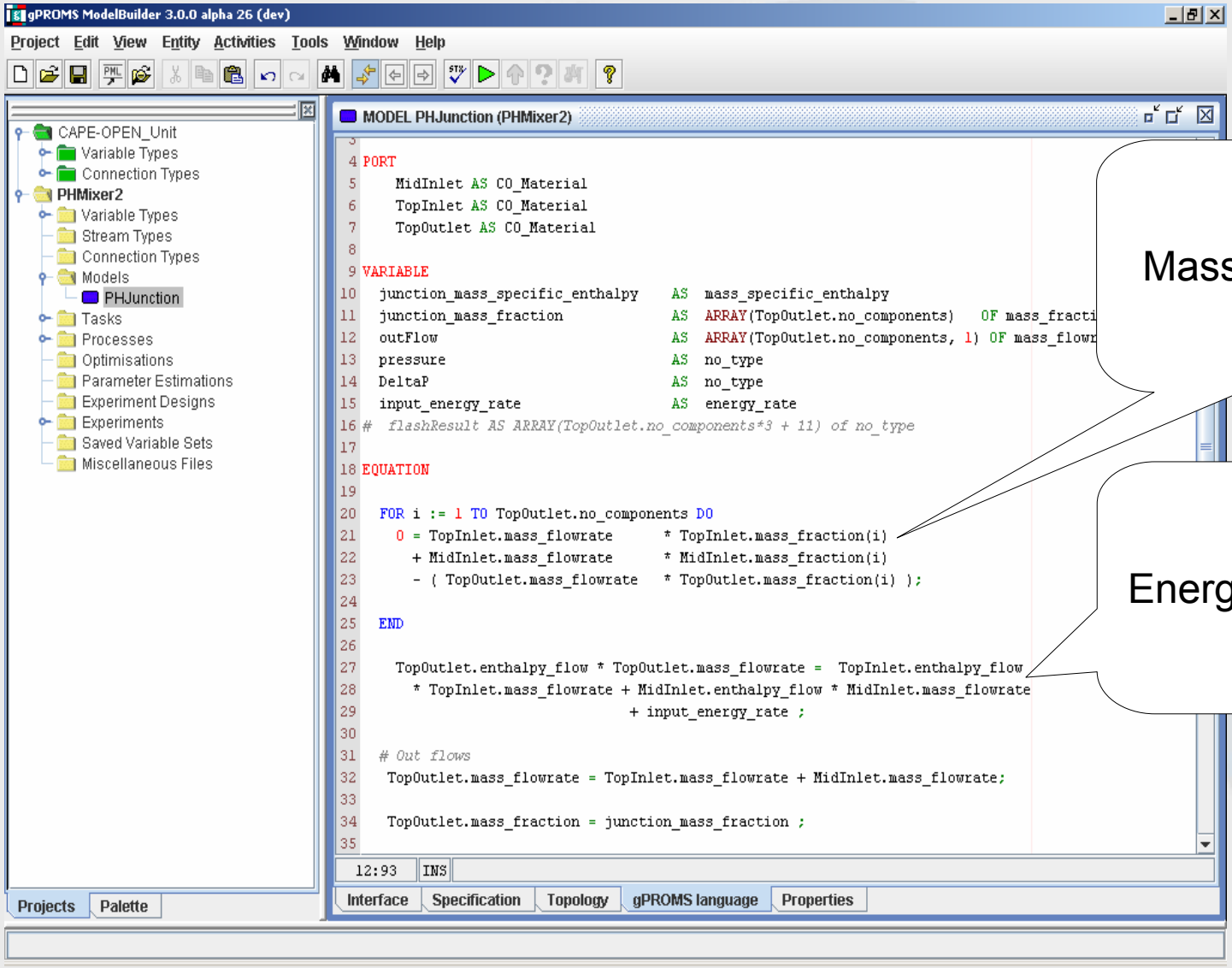
CAPE-OPEN supports all combinations of components



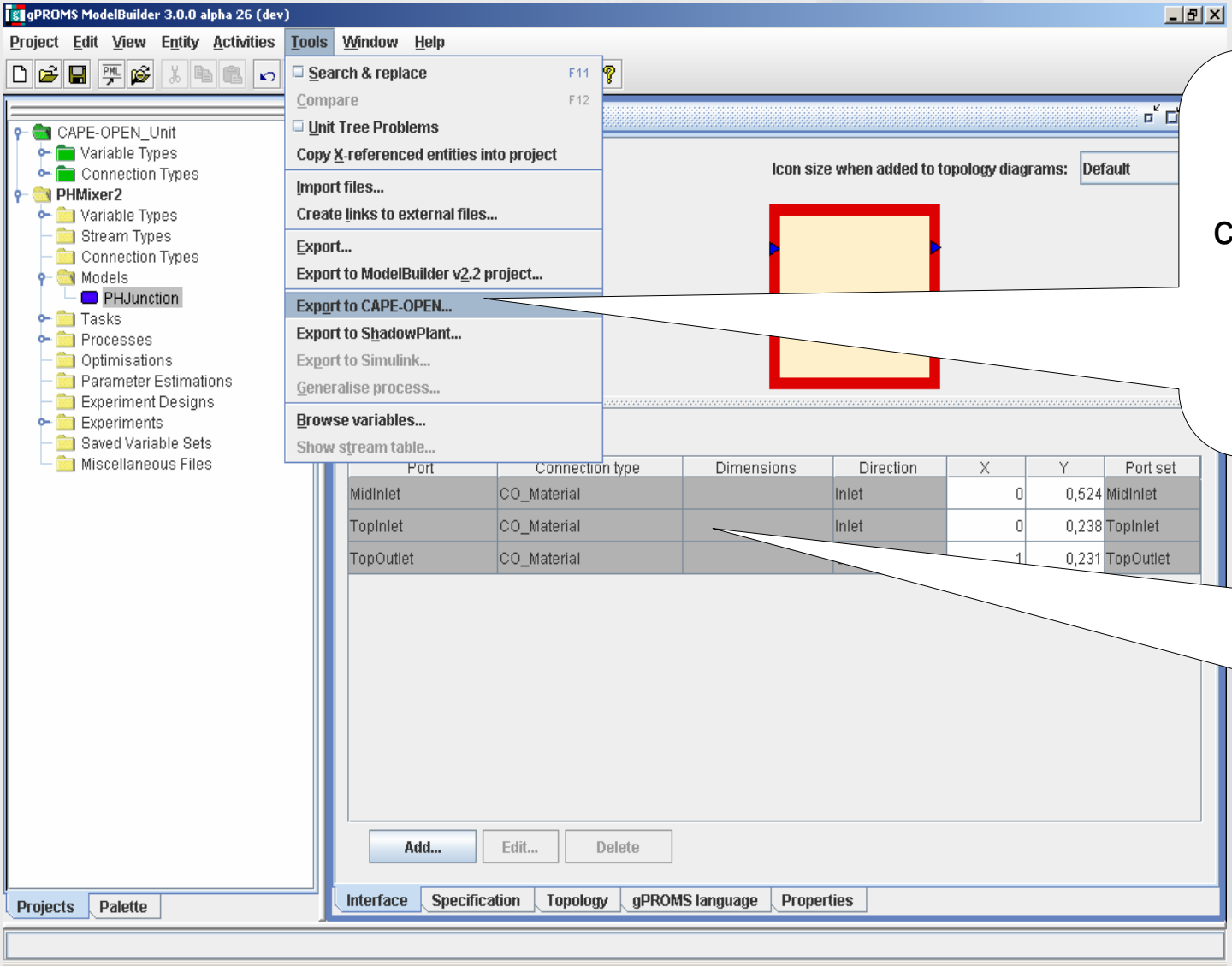
Load CAPE-OPEN library in ModelBuilder



Load/Create Mixer Model



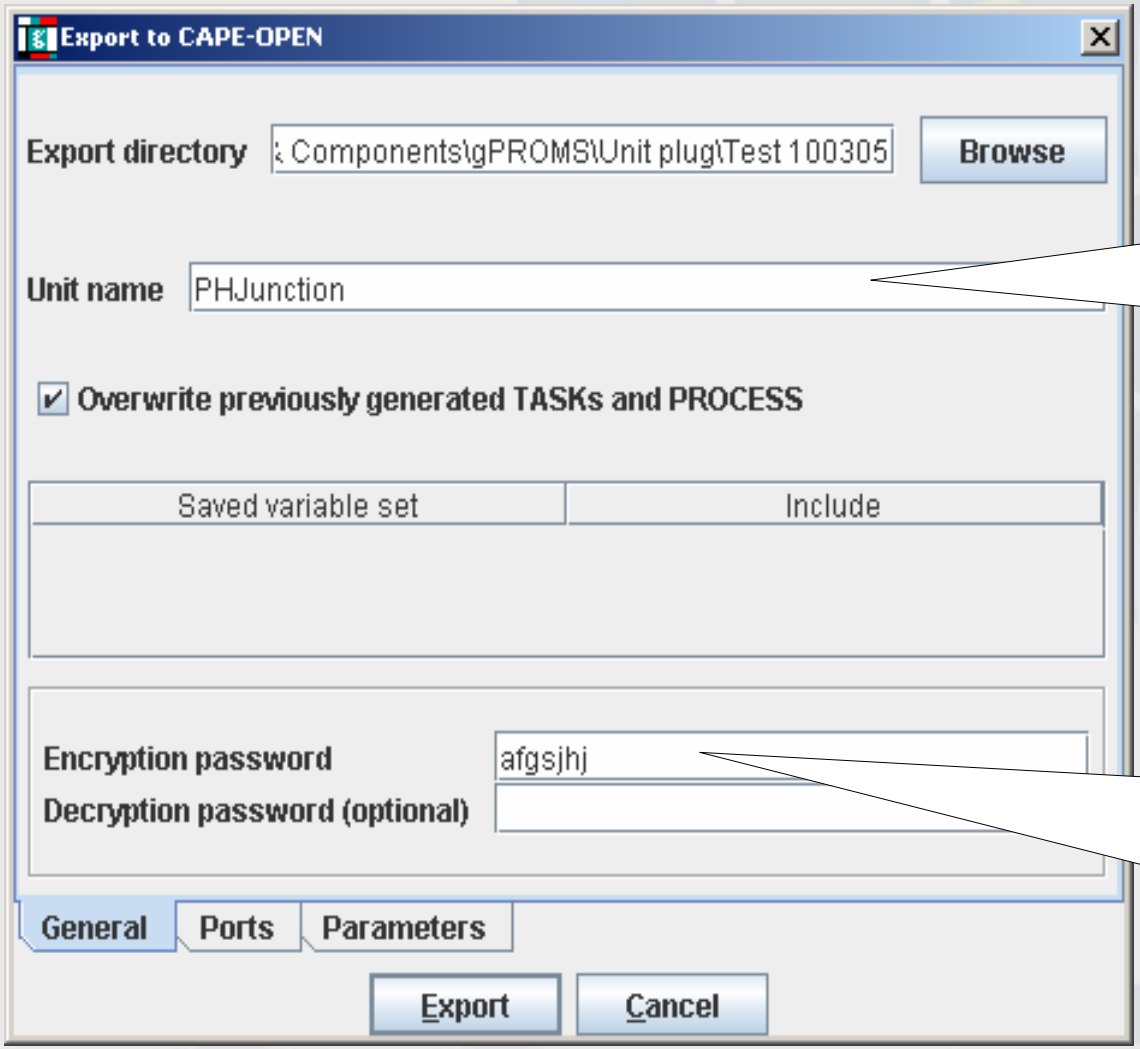
Launch CAPE-OPEN export



No need to change model for CAPE-OPEN exportation

gPROMS supports CAPE-OPEN Material Object

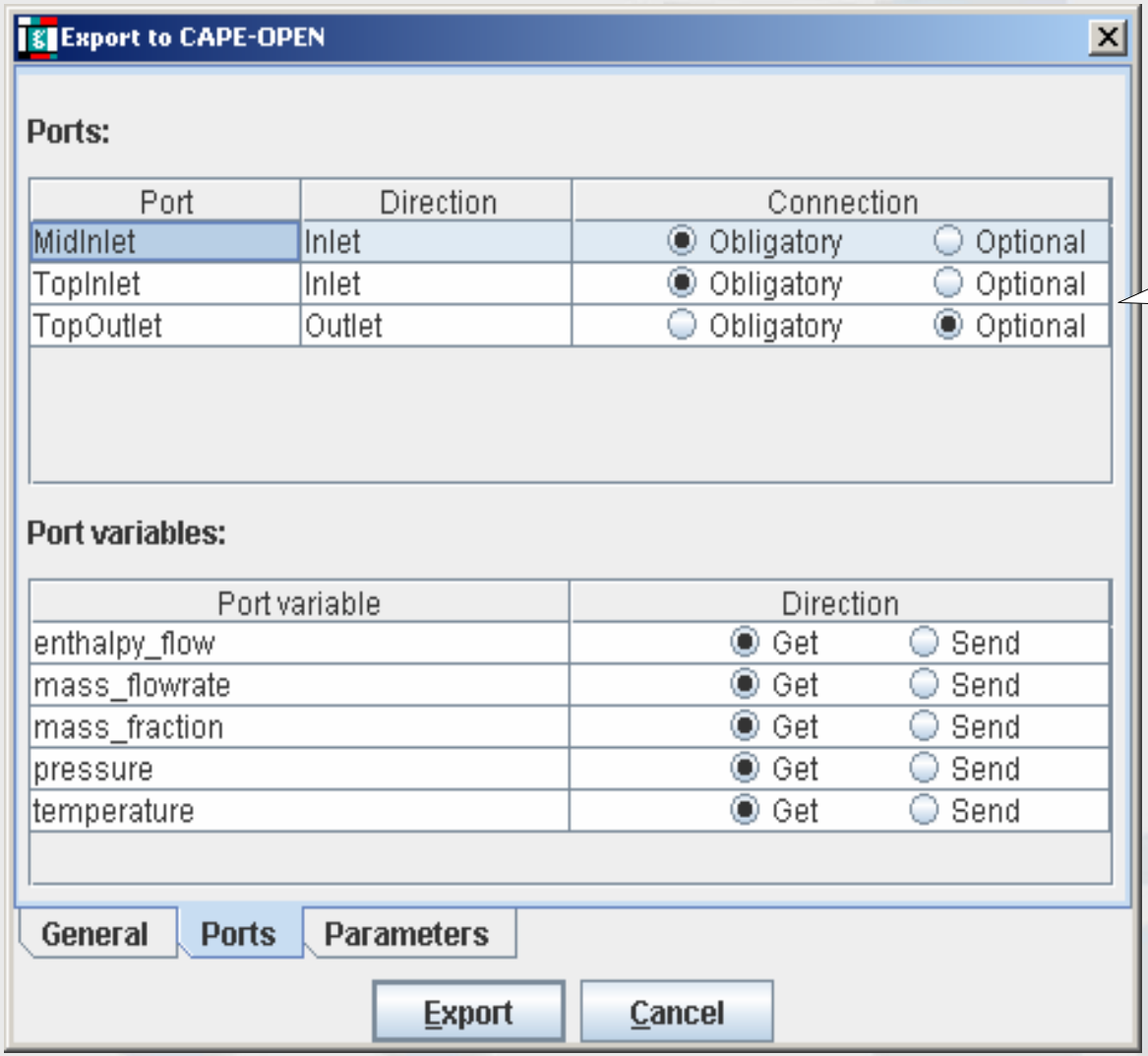
Crypt gCO file



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

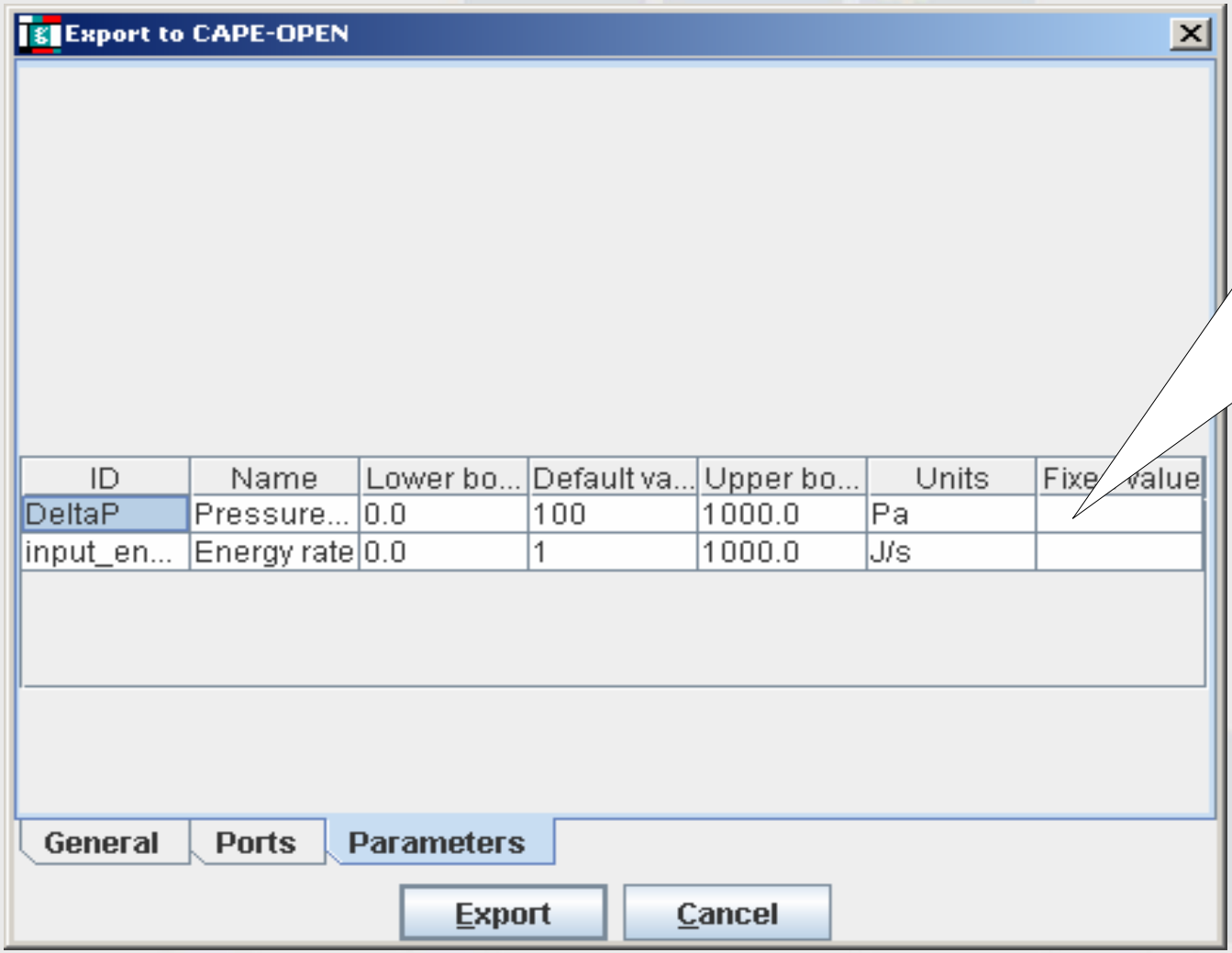
Encrypting the gCO file enables deployment to other parties and ensures consistency

Define ports options and parameters settings



Ports connection may be mandatory or optional

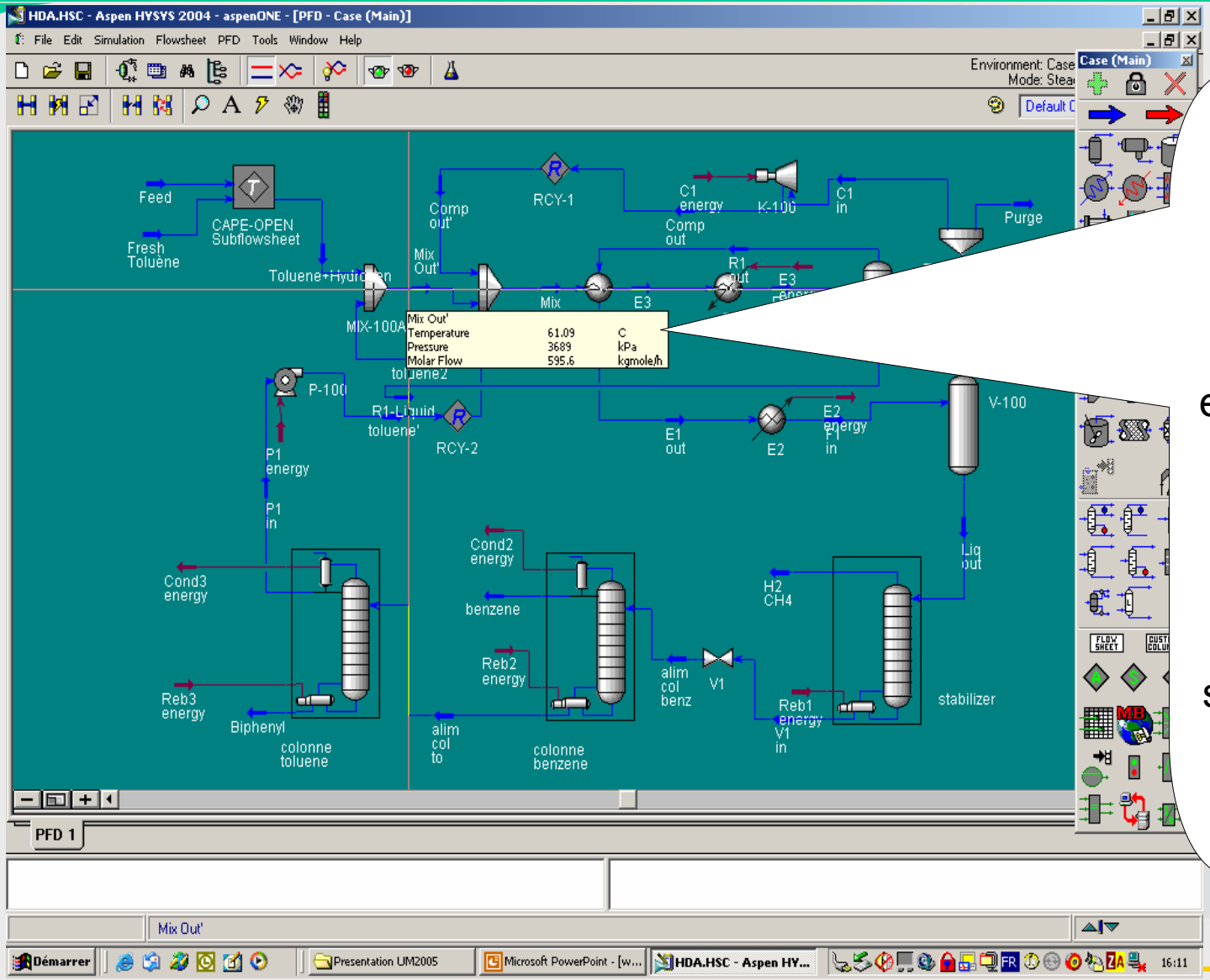
Parameter default settings



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

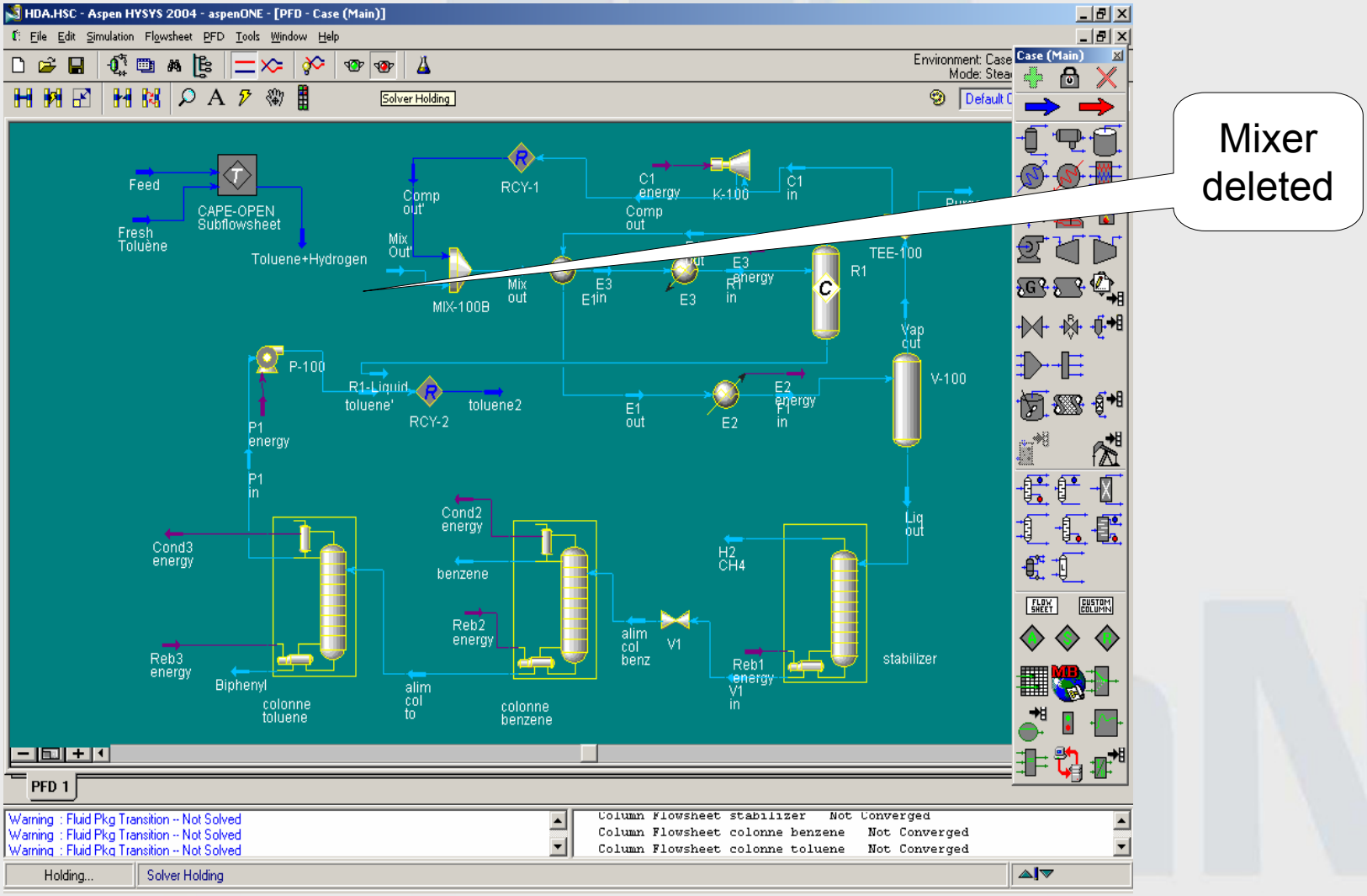
Running gPROMS model in Aspen HYSYS

HDA process model in Aspen HYSYS 2004



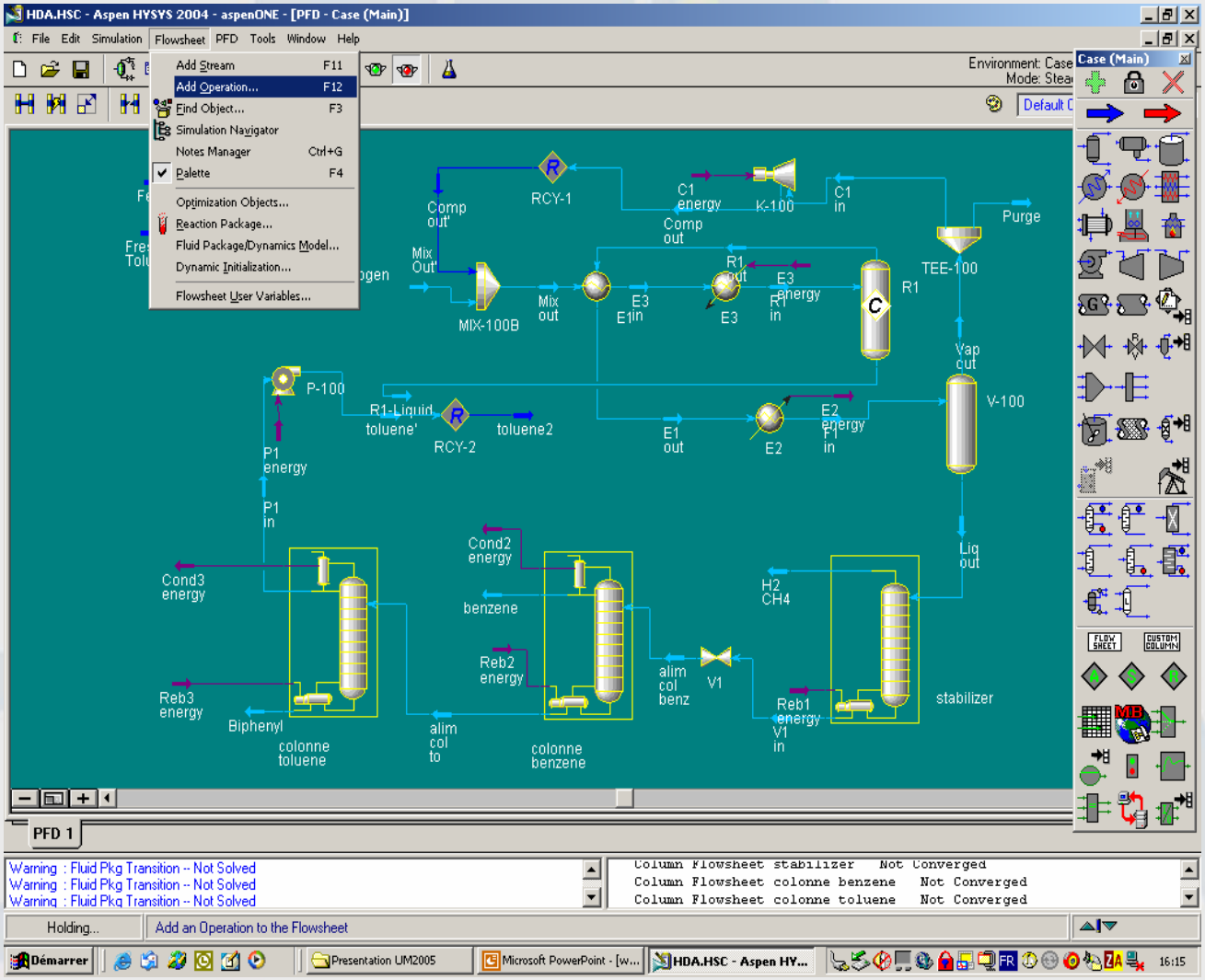
Since gPROMS mixer model involves basic material and energy balances, results with Aspen HYSYS 2004 native mixer and gPROMS mixer should be strictly the same.

Native mixer deleted and solver on hold

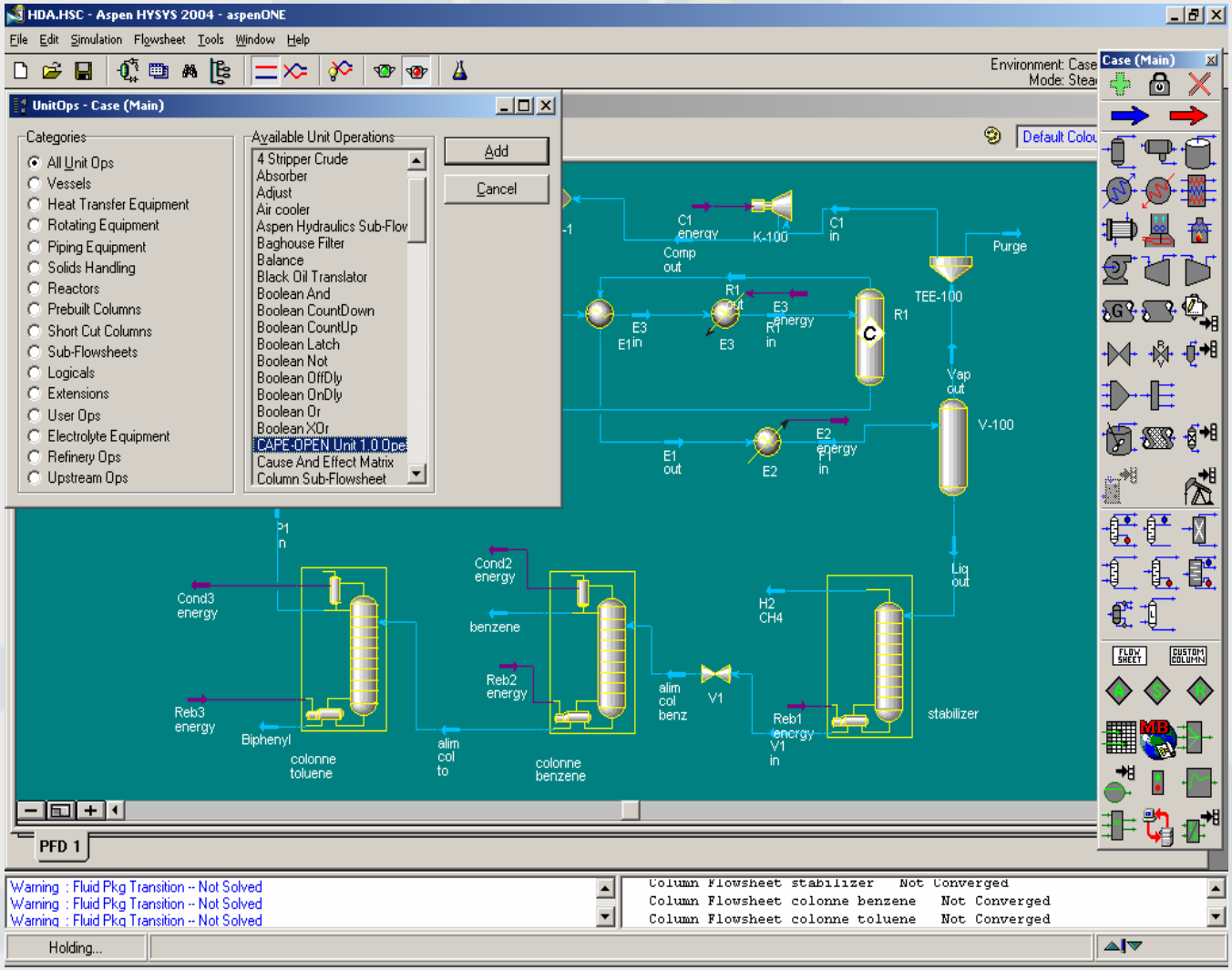


Mixer deleted

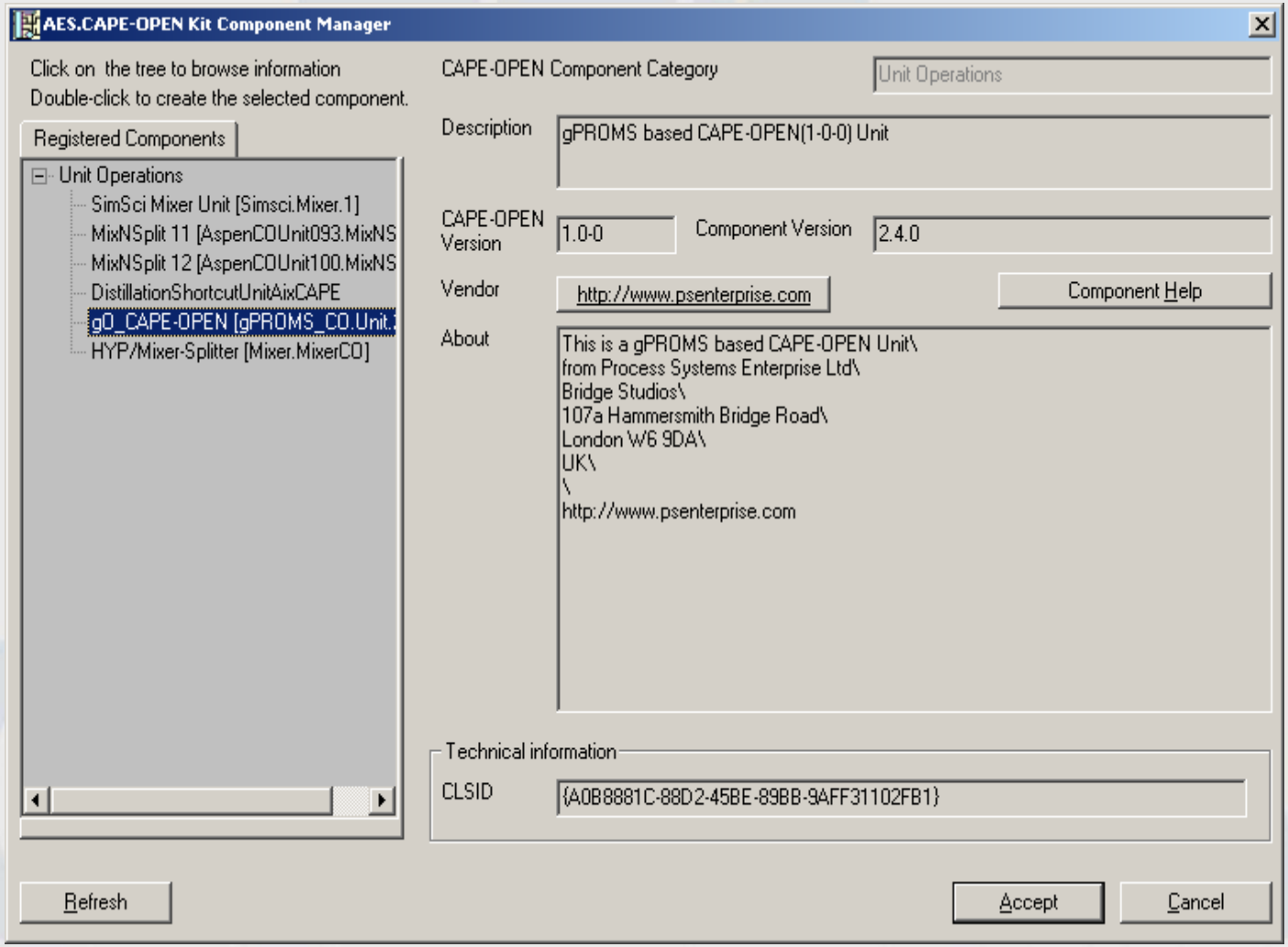
Replace native Mixer



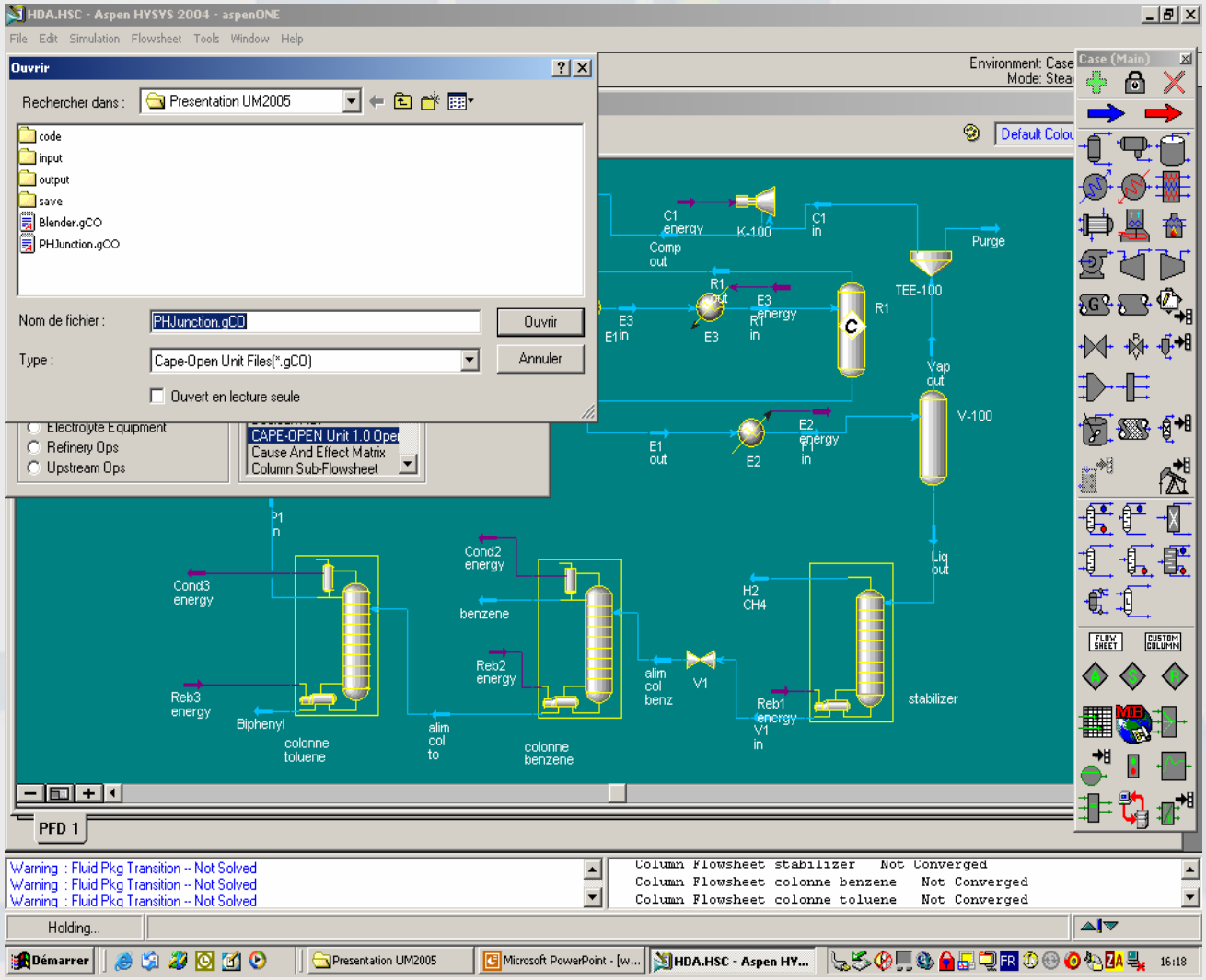
Select CAPE-OPEN 1.0 UNIT Ops



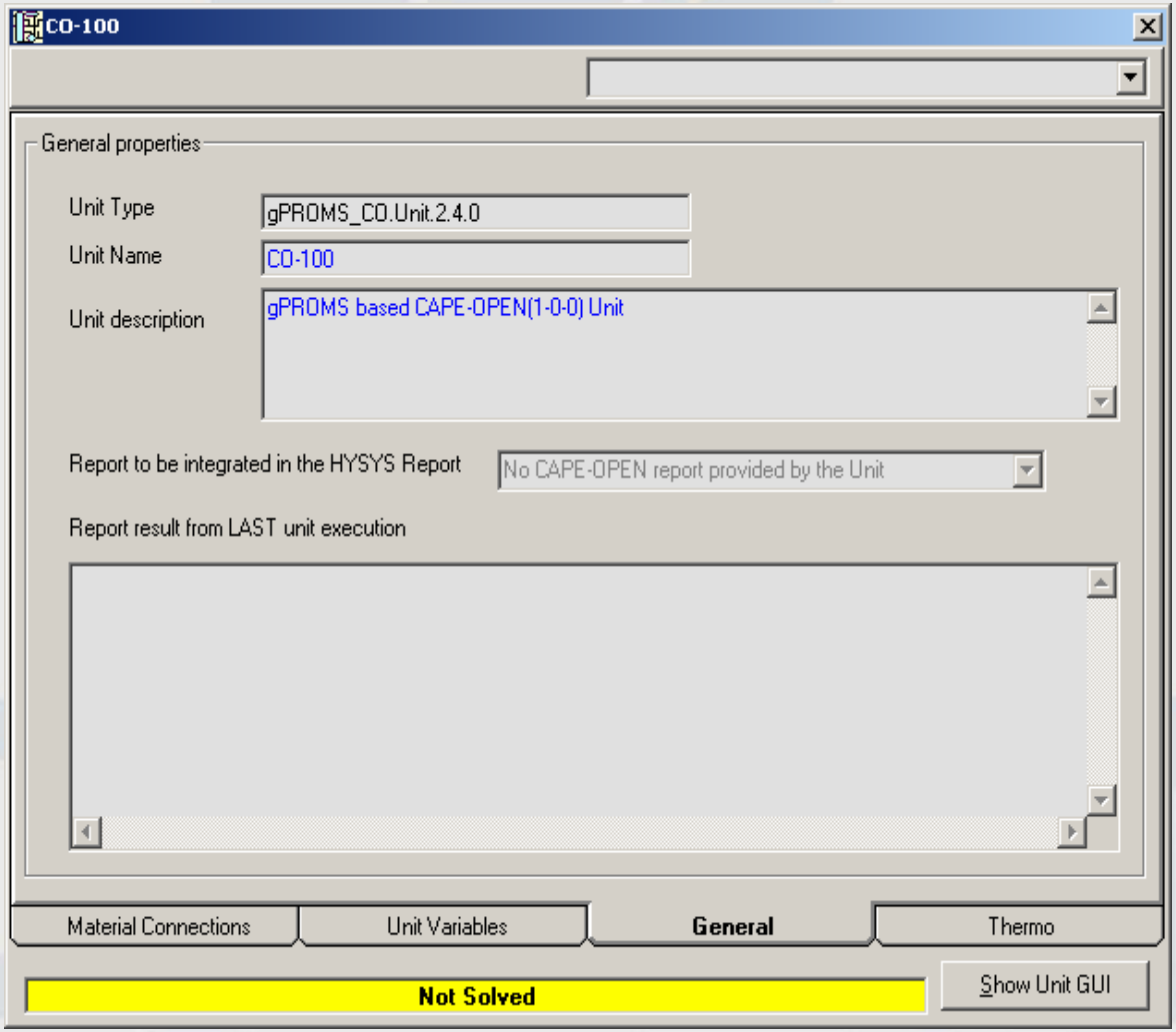
Select gO:CAPE-OPEN wrapper



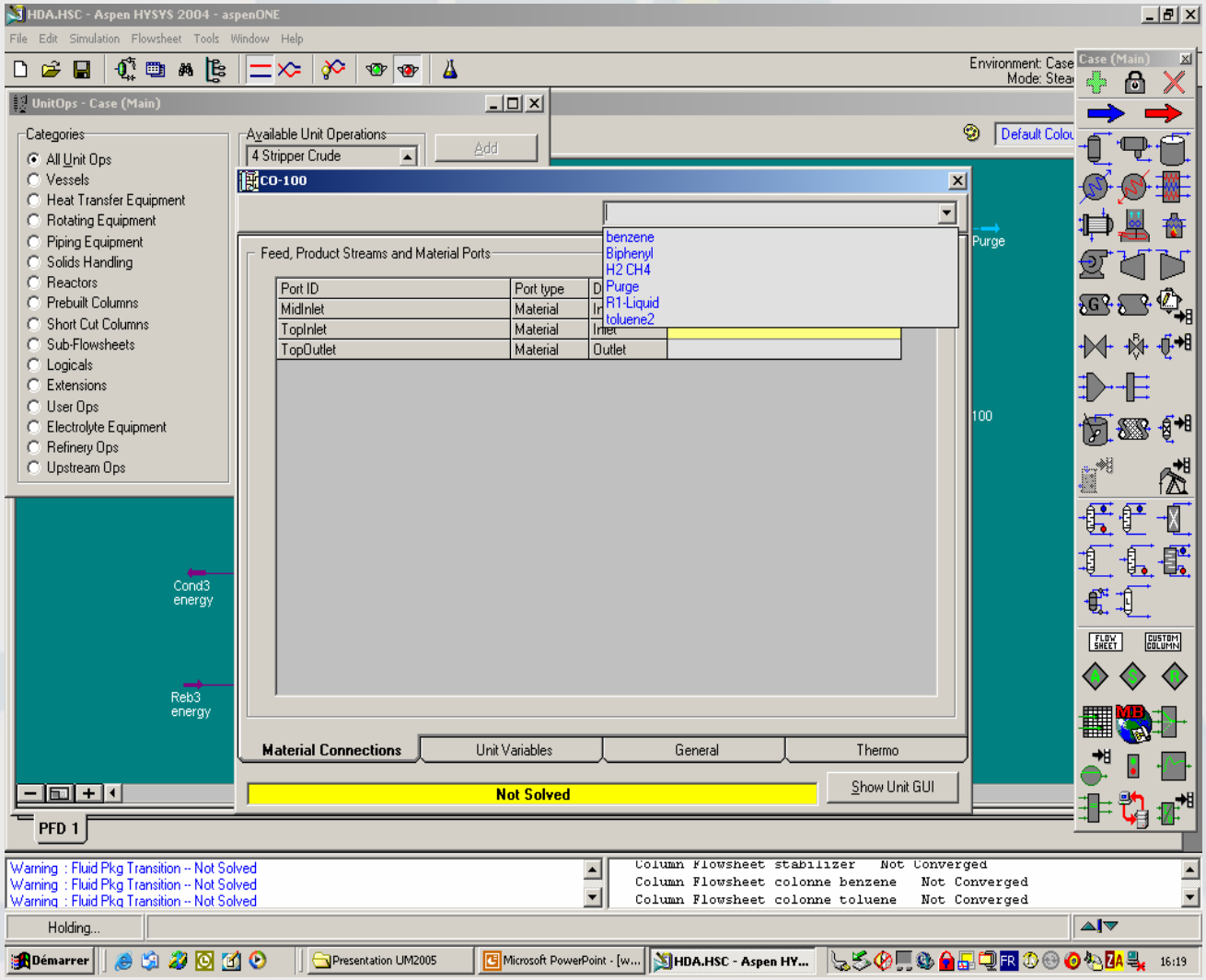
Select the gCO file to be used



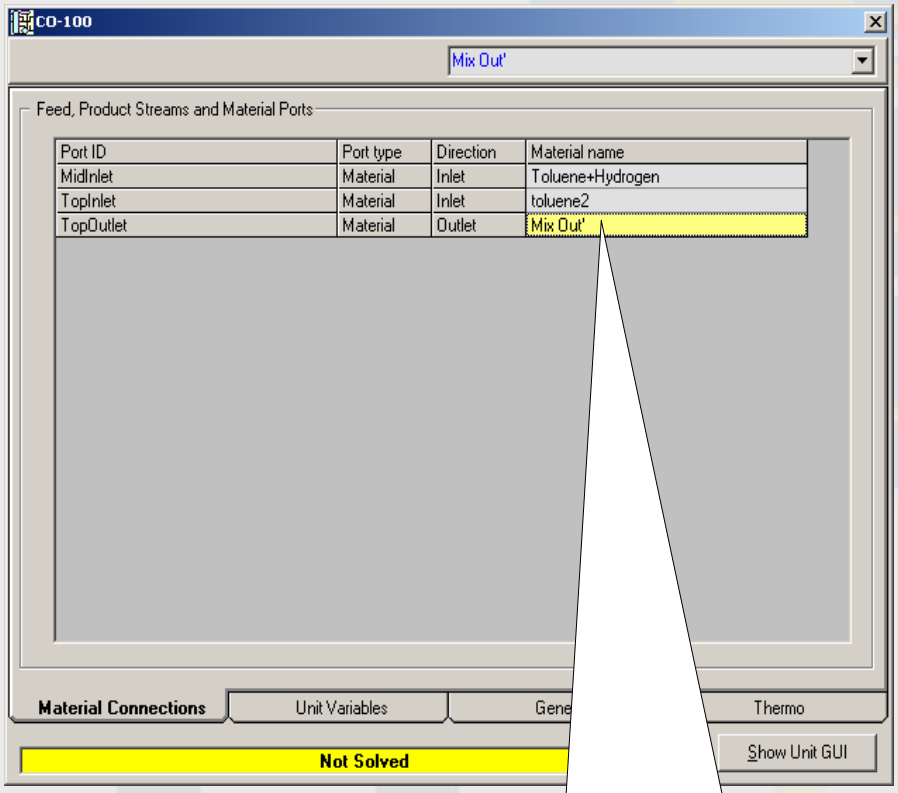
Enter generic GUI provided by HYSYS



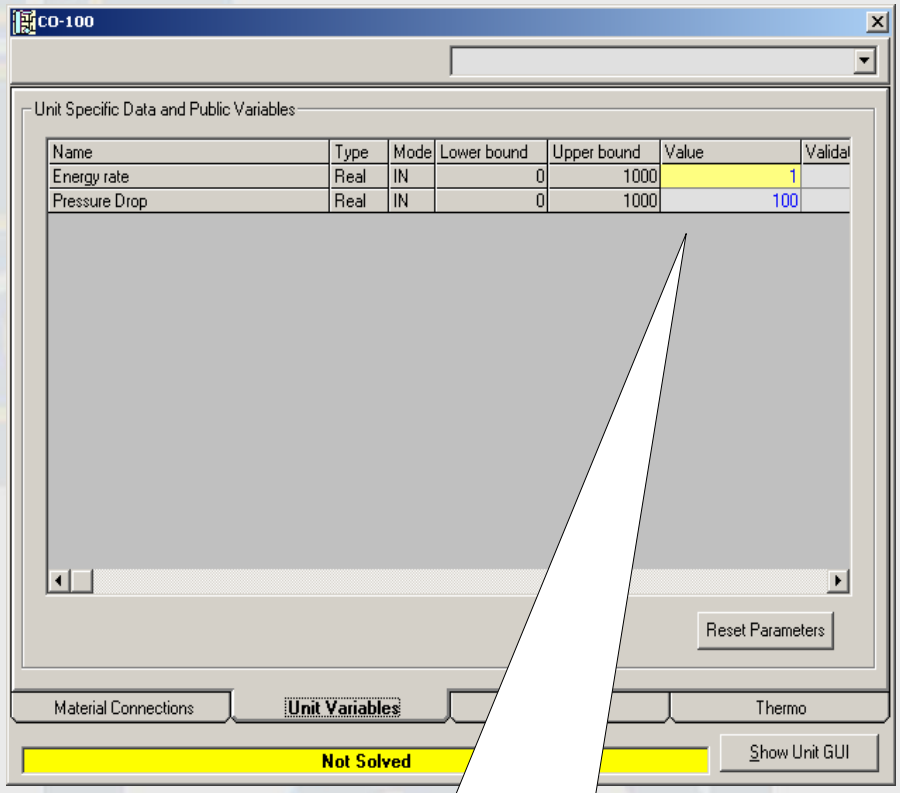
Connect inlet and outlet ports to streams



Set up the gPROMS model

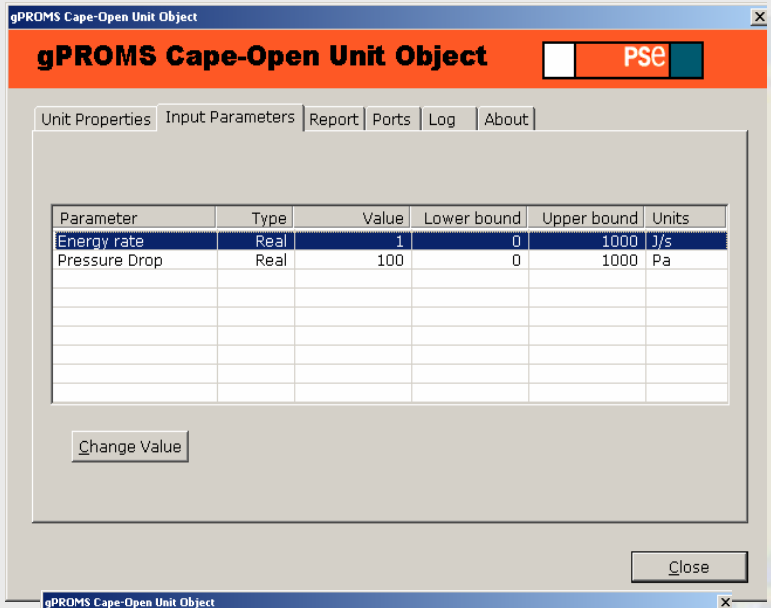


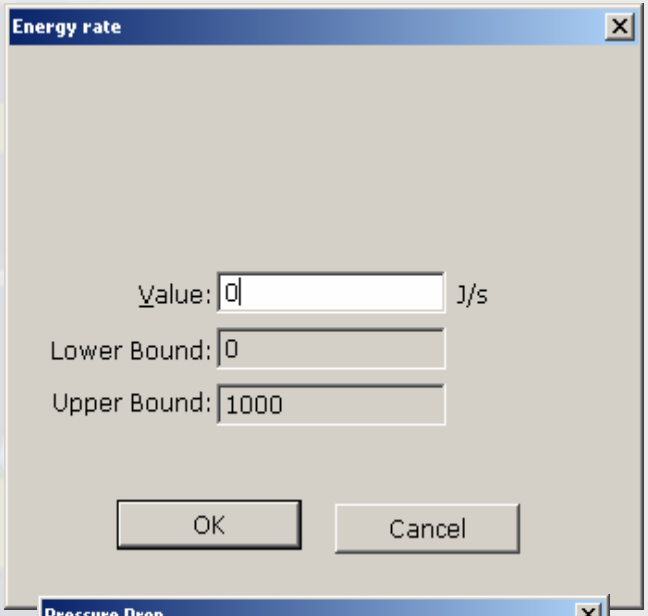
All ports connected

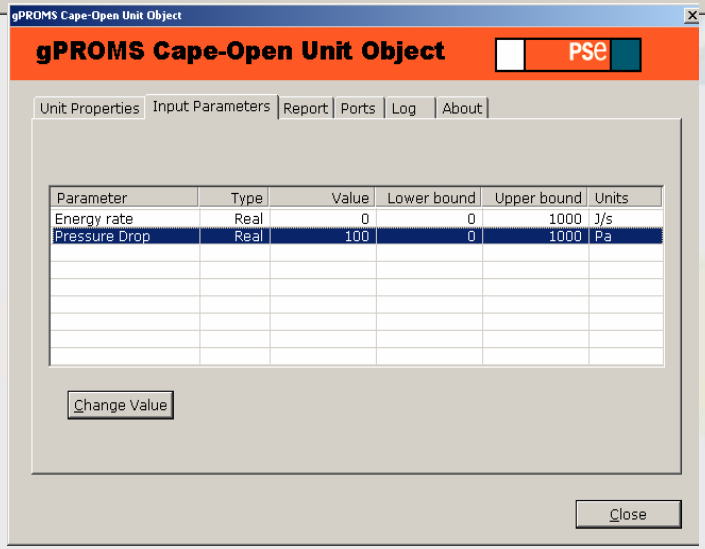


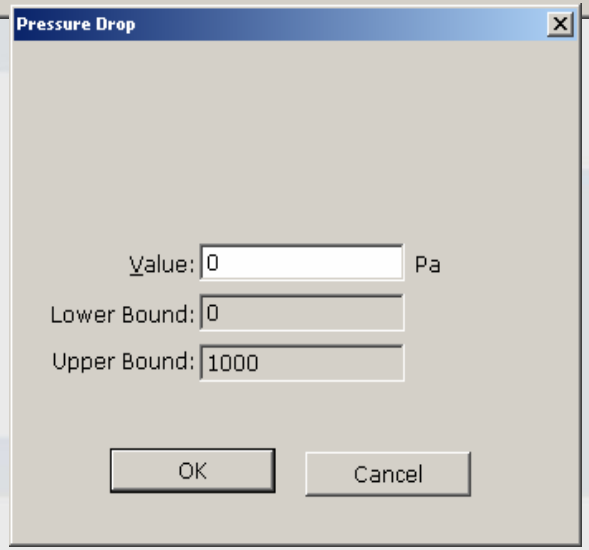
Initial parameter settings

Set energy input / pressure drop to zero

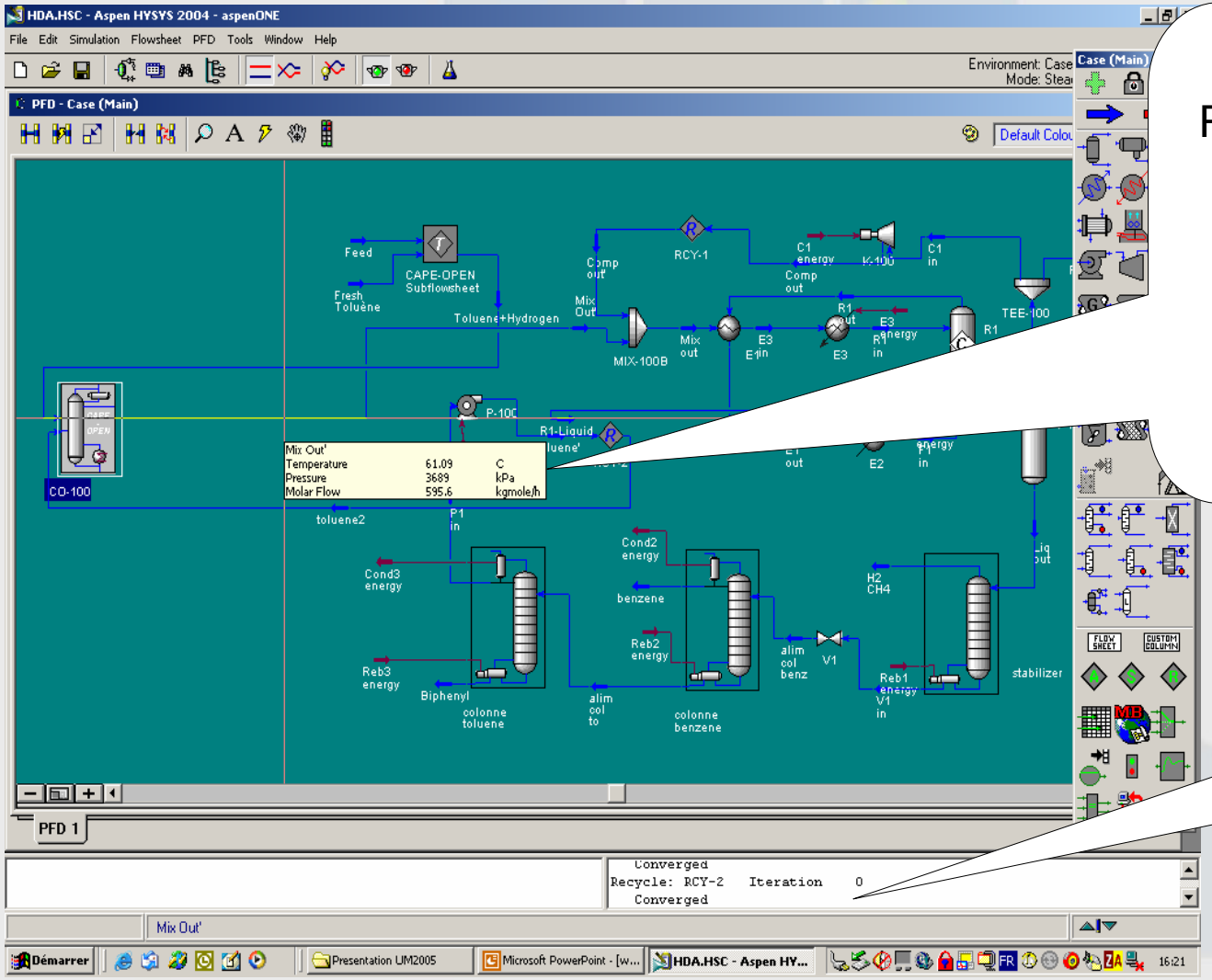








gPROMS Mixer output results



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

Simulation converged.

Other generic uses

- Same mixer model can be run as well in Aspen Plus or in PRO/II

- Same applies to thermodynamic components:
  - A CAPE-OPEN Property Package out of Multiflash (Infochem) runs the same in Aspen Plus, Pro/II, Aspen Hysys, Simulis, gPROMS…

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.

The CAPE-OPEN Standard: End-user applications

Examples

ATOFINA

- Detailed model of a reactive absorption column: very limited knowledge of CAPE-OPEN needed

IFP

- Detailed model of a catalytic reactor: advanced knowledge of CAPE-OPEN needed

US DOE / Alstom Power

- Detailed (CFD) model of a combustor: very limited knowledge of CAPE-OPEN needed

Rate-based model of absorbers

ATOFINA

- **Situation**
  - Current tool no longer developed by AspenTech
  - Model embedded can't cope with fast liquid film reactions
    - CO_2 absorption by NaOH aqueous solutions
- **Solution developed**
  - gPROMS modeling
    - Rigorous handling of Maxwell-Stefan equations
    - Appropriate model for fast kinetics in liquid film
- **Limitations**
  - gPROMS requires a thermodynamic server
    - OLI linked to gPROMS but OLI not licensed by ATOFINA

CO-LaN

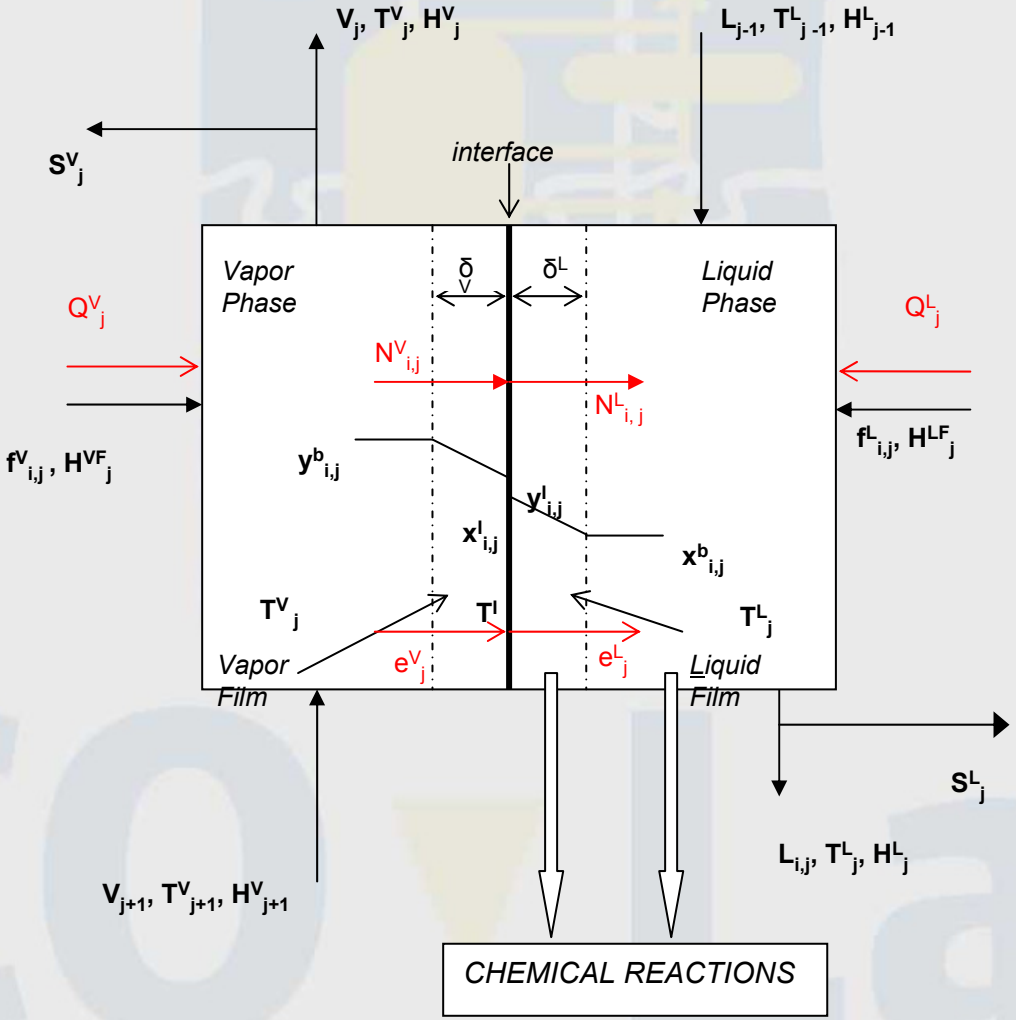
Rate-based model of absorbers

- User requirements
  - gPROMS model using an Aspen Plus thermo
    - Typically ELECNRTL
  - gPROMS model used within an Aspen Plus model
    - To be used just as any Ratefrac unit model
- Technical solutions applied
  - Make a CAPE-OPEN Property Package out of Aspen Plus based on ELECNRTL
  - Call this CO PP within gPROMS model through CO Thermodynamics and Physical Properties interfaces
  - Include the gPROMS model as a CO Unit Operation within an Aspen Plus flowsheet

Making a CO Property Package

- Within Aspen Plus (no need to know any CO specific)
  - Define chemical compounds
  - Define methods to be used for each property
  - Export as a CO Property Package (CO PP)
- Requires Aspen Plus license when being called upon
- Referenced through the name given to the CO PP file
- Registered in the Windows registry as a CO PP within the CO Thermo System supplied by AspenTech

System modeled



10 species
50000 variables
Steady-state
6 min to converge

Thermodynamic calls

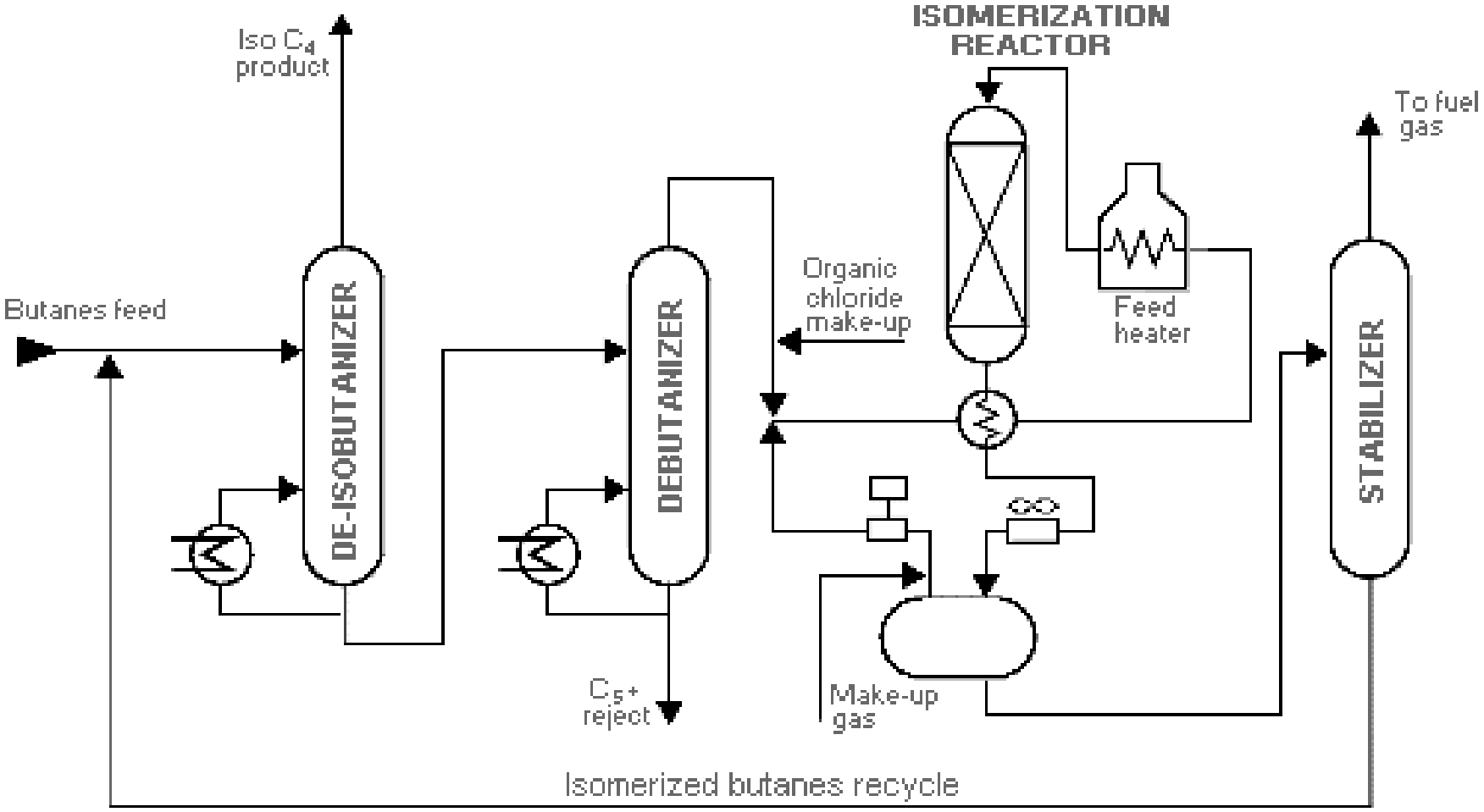
- gPROMS model calling A+ CO Property Package
  - Properties requested from Aspen Plus
    - Vapor Heat Capacity
    - Vapor Thermal Conductivity
    - Vapor Enthalpy
    - Liquid Activity Coefficient
    - Liquid Enthalpy
    - Liquid Volume
    - Liquid Thermal Conductivity
    - Surface Tension
    - Liquid Fugacity Coefficient
    - Liquid Viscosity

    (note: flash equations within the gPROMS model)

Calls to CO Property Package

```
UNIT
      Plant AS Column
SET
      WITHIN Plant DO
        PhysProps := "(PS)ATCOProperties.COPropertySystem.1<gPROMS121new>";
……….
FOR y := 0 TO 1 DO
    FOR z := 0 TO 1 DO
        FOR i := 1 TO 4 DO
              Molarfrac_aux(i, y, z) = Molarfrac(i, y, z) ;
        END
        FOR i := 5 TO 11 DO
          Molarfrac_aux(i, y, z) = 0 ;
        END
        FOR i := 1 TO NoVapSpecies DO
          VapHeatCapacity(i, y, z) = PhysProps.VapourHeatCapacity(T(y, z), P, frac(i, )) ;
        END
          Lambda_vapour(y, z) = PhysProps.VapourThermalConductivity(T(y, z), P,
                                Molarfrac_aux(, y, z)) ;
     END
END
```

C4 isomerization flow diagram

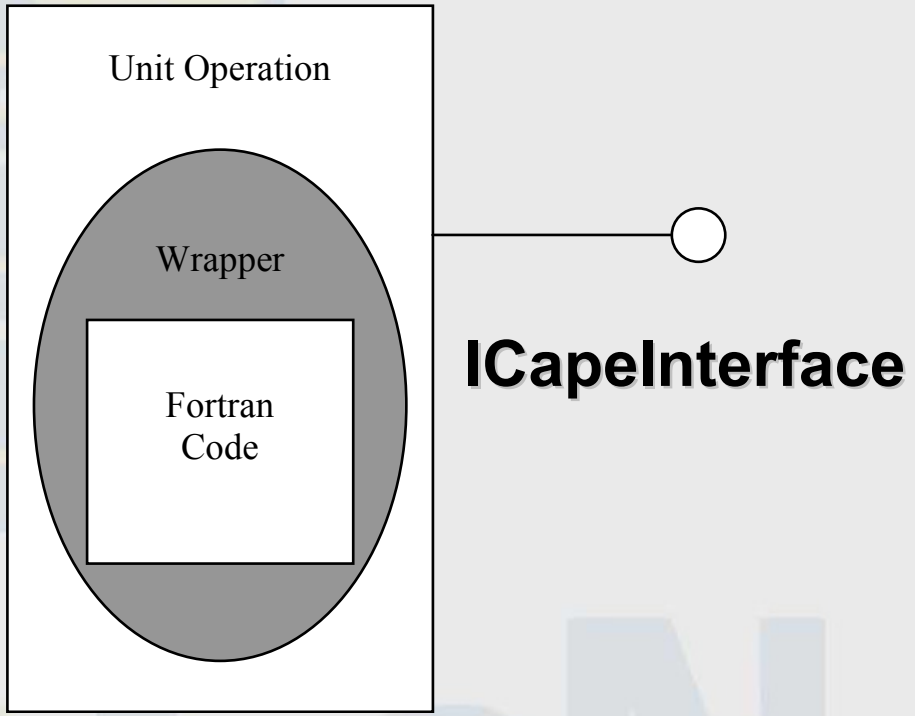


Process technical description

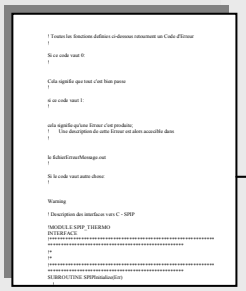
- **Thermodynamic**
  - Isobutane formation is promoted at low temperature
  - Catalyst to work at low temperature
- **Catalyst**
  - Butane is less reactive than long paraffins
  - Catalyst must provide important acidity
  - No zeolith catalyst
- **Reaction mechanism**
  - A bimolecular mechanism is modelled:
    - a reaction intermediate C8 produces i-butane
    - cracking product (C1- C3)
    - disproportionation product as C5 i-C5

CO compliant component development

- **Introduction**
  - **Migrating a FORTRAN 90 Reactor Model to the CAPE-OPEN standard.**
- **Description**
  - **IFP / CAPE-OPEN BIP Reactor architecture:**



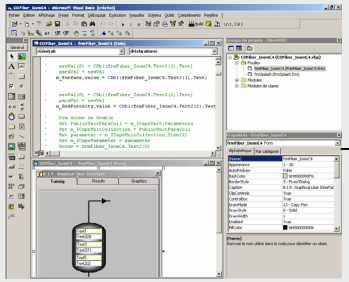
Implementation description



Fortran

Flat DLL

1. Create a Fortran DLL with Source file of the standalone Model.



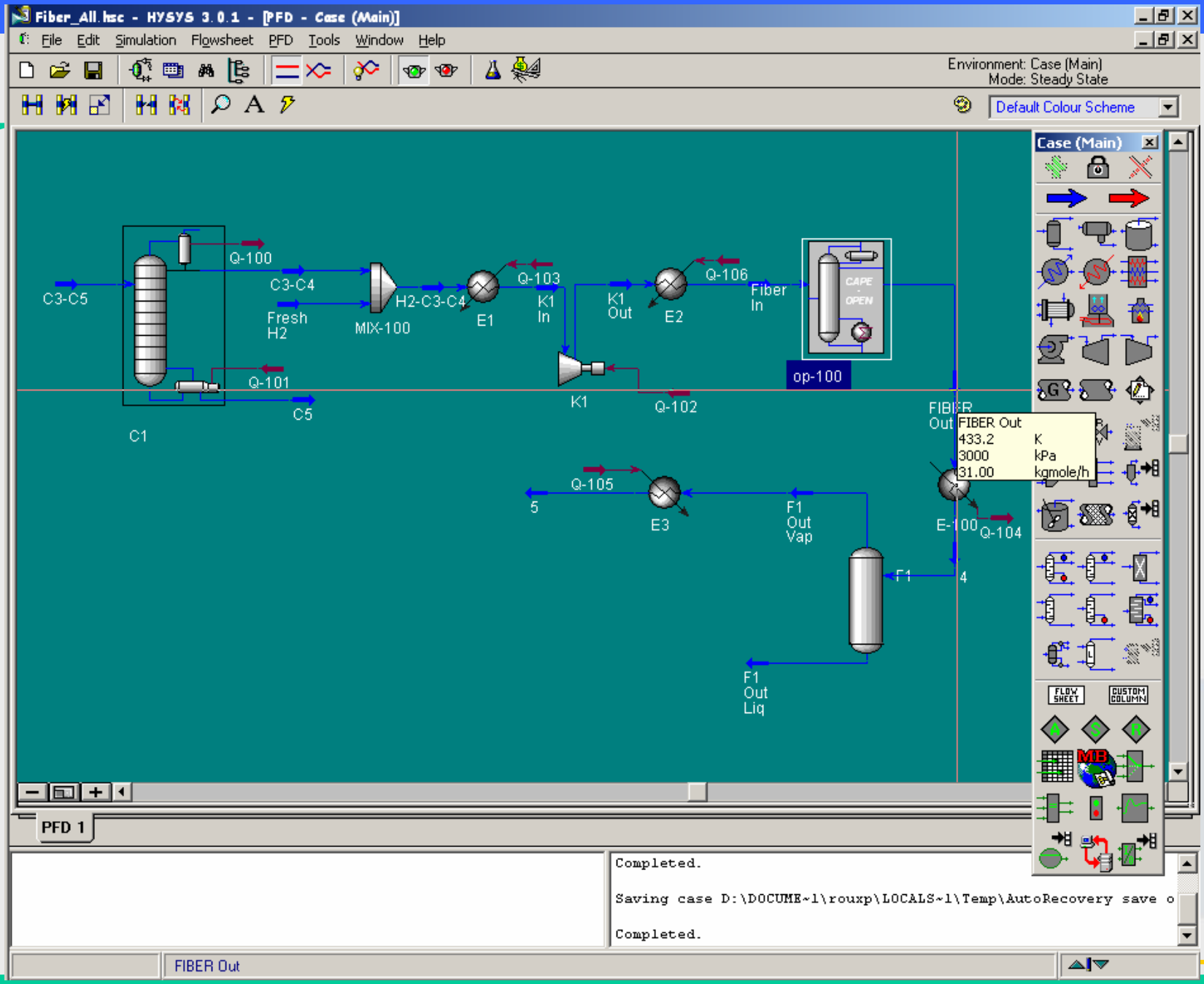
VB

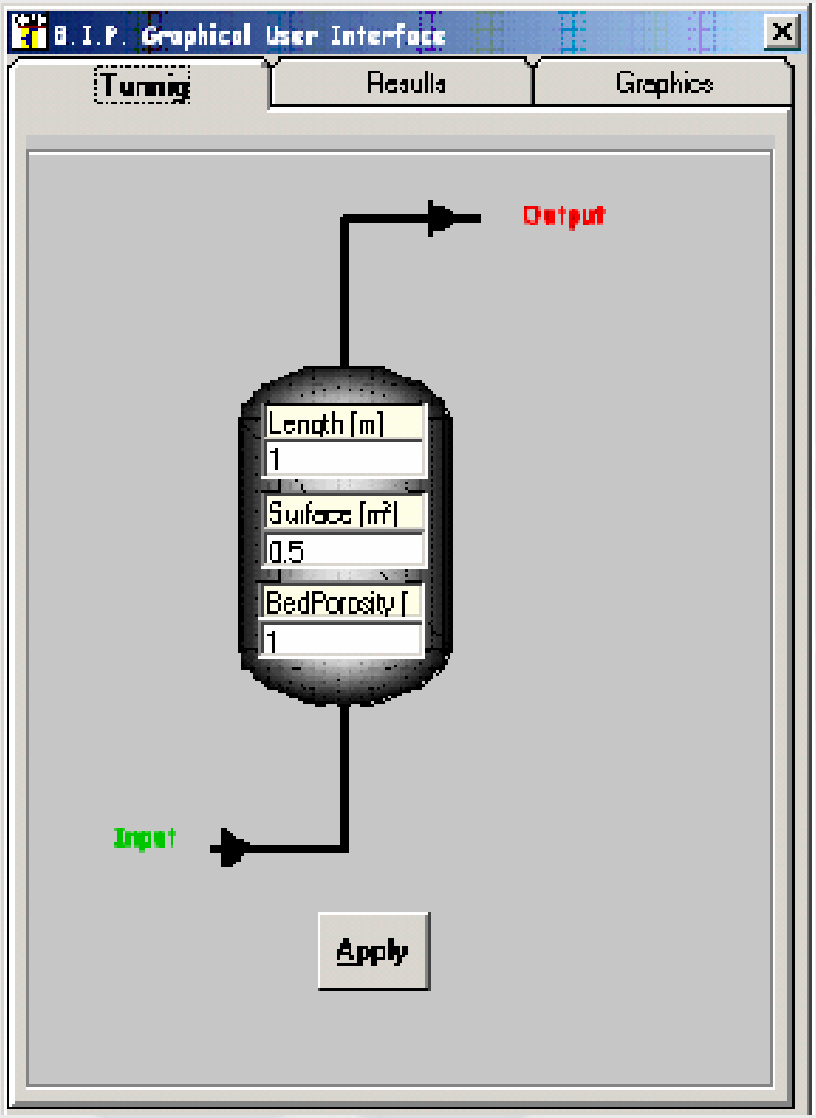
COM

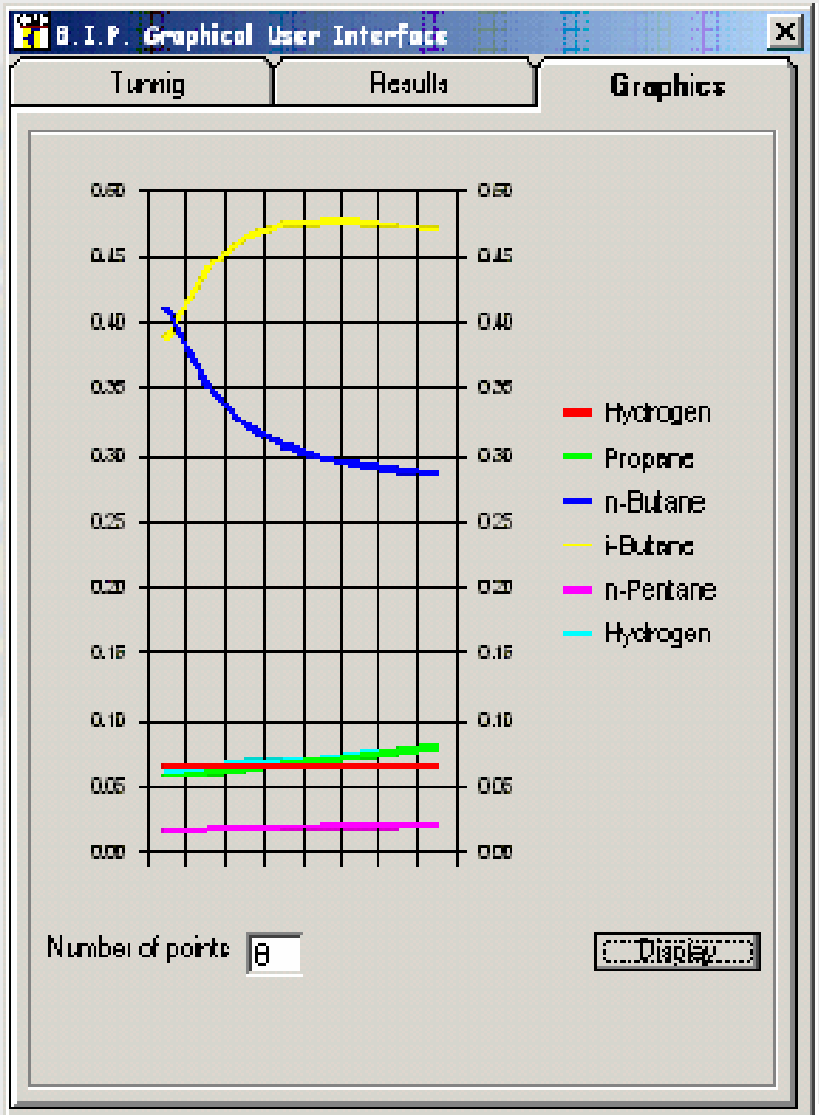
DLL

2. Create a COM DLL using CO Unit Wizard

3. Connect these two DLLs


Fiber_All.hsc - HYSYS 3.0.1 - [PFD - Case (Main)]
File Edit Simulation Flowsheet PFD Tools Window Help
Environment: Case (Main)
Mode: Steady State
Default Colour Scheme
Case (Main)
C3-C5
Q-100
C3-C4
Fresh H2
H2-C3-C4
MIX-100
E1
Q-103
K1 In
K1 Out
E2
Q-106
Fiber In
CAPE - OPEN
op-100
Q-101
C5
C1
K1
Q-102
FIBER Out
FIBER Out
433.2 K
3000 kPa
31.00 kgmole/h
Q-105
5
E3
F1 Out Vap
E-100
Q-104
4
F1
F1 Out Liq
FLOW SHEET
CUSTOM COLUMN
PFD 1
Completed.
Saving case D:\DOCUME~1\rouxp\LOCALS~1\Temp\AutoRecovery save o
Completed.
FIBER Out


B.I.P. Graphical User Interface
Tunnig
Results
Graphics
Output
Length [m]
1
Surface [m²]
0.5
BedPorosity [
1
Input
Apply


B.I.P. Graphical User Interface
Tunnig
Results
Graphics
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Hydrogen
Propane
n-Butane
i-Butane
n-Pentane
Hydrogen
Number of points
8
Display

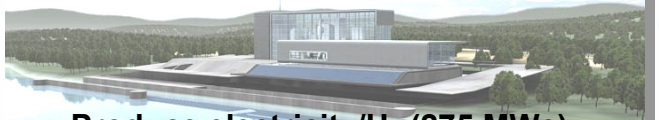
DOE Fossil Energy R&D Programs

SECA

Fuel Cells

FutureGen

- $1B, 10-year demonstration project
- Coal-fired, gasification-based plant

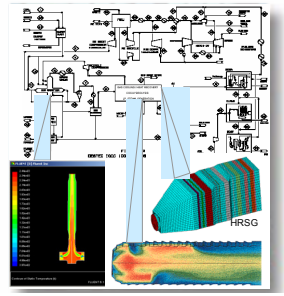


- Produce electricity/H_2 (275 MWe)
- Generate near-zero air emissions
- Capture/sequester > 90% of CO_2

Carbon Sequestration

Gasification with Cleanup & Separation

Gas Turbines



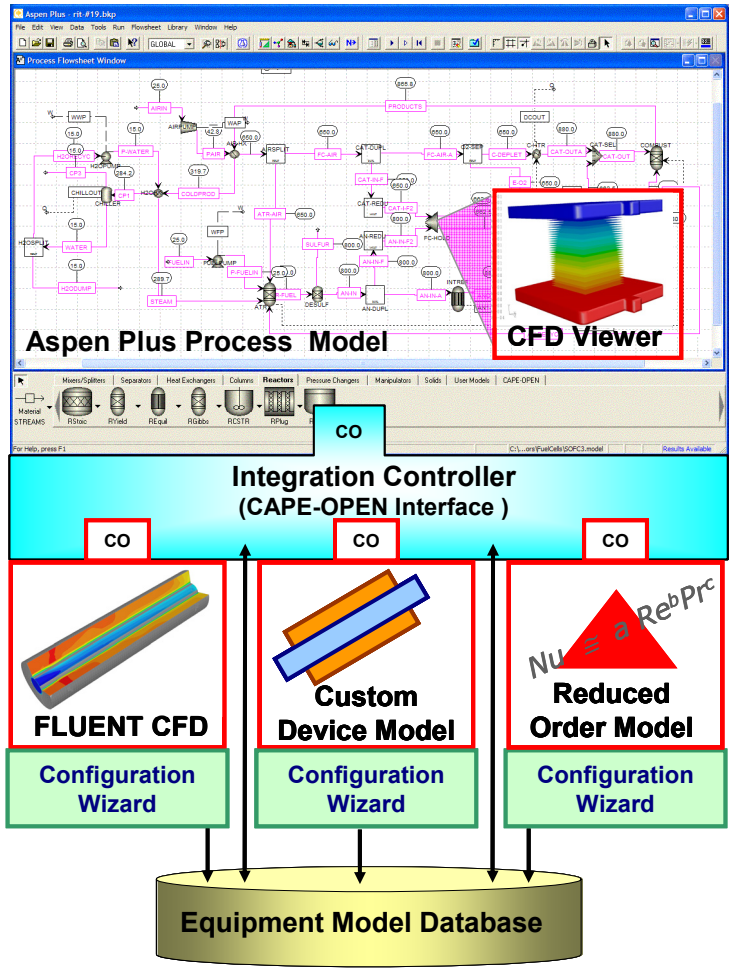
Systems Analysis & Integration

NETL

NETL's Advanced Power and Energy Co-Simulation (APECS)

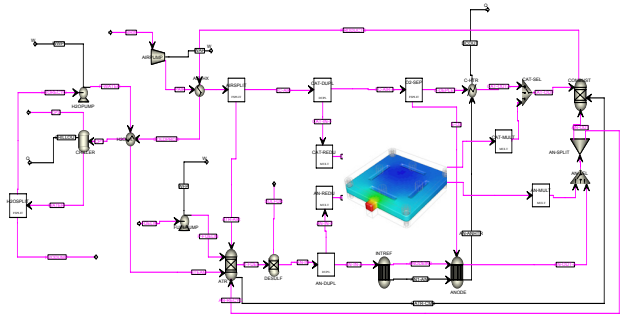
Major Components and Features

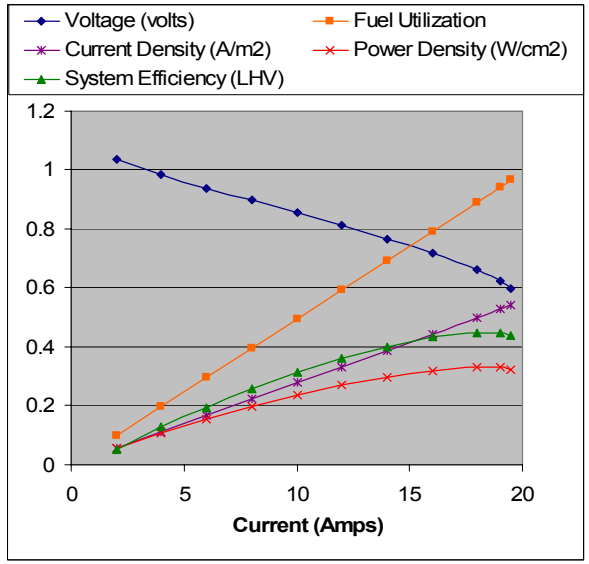
- **Process Models**
  - Aspen Plus®
- **Equipment Models**
  - FLUENT®
  - Custom Device Models
  - Reduced-Order Models (ROM)
- **Integration Controller**
  - CAPE-OPEN (CO) Interfaces
  - Unit Operations, Physical Properties, Reactions
- **Configuration Wizards**
  - FLUENT*
  - Custom Model** and ROM**
- **Model Database**
- **CFD Viewer**
- **Solution Strategies**
  - Speed (ROM)
  - Accuracy (CFD)
- **Remote Execution**
  - Windows/Linux
  - Serial/Parallel



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

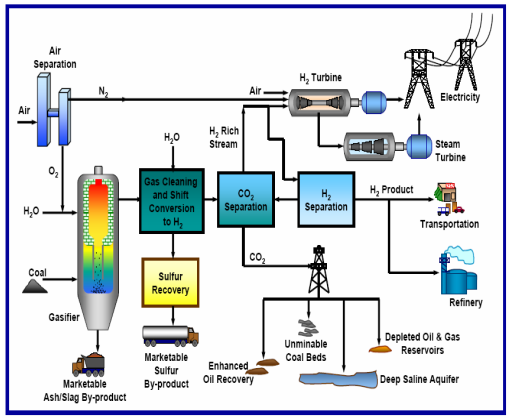




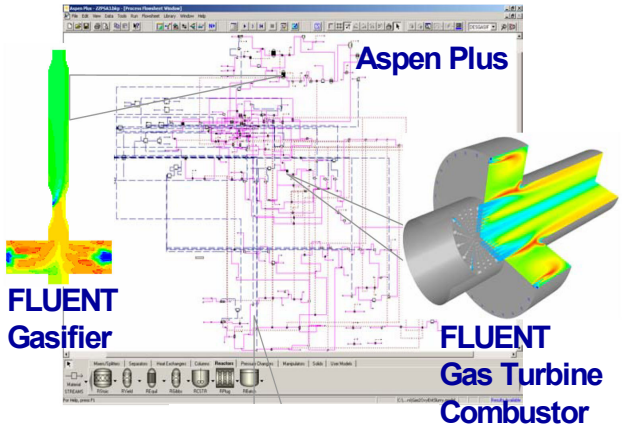
Zitney, S.E., Prinkey, M.T., Shahnam, M., and Rogers, W.A. (2004), "Coupled CFD and Process Simulation of a Fuel Cell Auxiliary Power Unit," In *Proc. of the ASME Second International Conference on Fuel Cell Science, Engineering, and Technology*, Eds. R. Shah and S.G. Kandlikar, Rochester NY, June 13-16,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

Available CO compliant software

- **Software providers**
  - AspenTech: Aspen Plus, Aspen Properties, Aspen Hysys, COM Thermo, Distil
  - SimSci-ESSCOR: PRO/II
  - PSE: gPROMS
  - Belsim, Infochem, ProSim, Dechema, RSI, HTRI, Fluent, ...
- **Operating companies**
  - IFP, Total, BASF, Shell…
- **Universities**
  - INPT, UPC, RWTH.LPT, ChemSep, CMU...
- **Government agencies**
  - US EPA

Conclusion

- CAPE-OPEN provides a “simple” way to:
- Embed tailor-made unit operation models in flowsheeting tools
- Provide access to advanced thermodynamics within tailor-made unit operation models
- Encapsulate reaction packages for use within flowsheeting tools

Applications of CAPE-OPEN standards to reactor and kinetic modeling

Michel Pons
Chief Technology Officer
EUROKIN workshop, October 20, 2005