

## Demonstrating interoperability

**Plugging the same gPROMS Unit  
Operation models in Aspen Plus, Hysys  
and PRO/II process simulators**

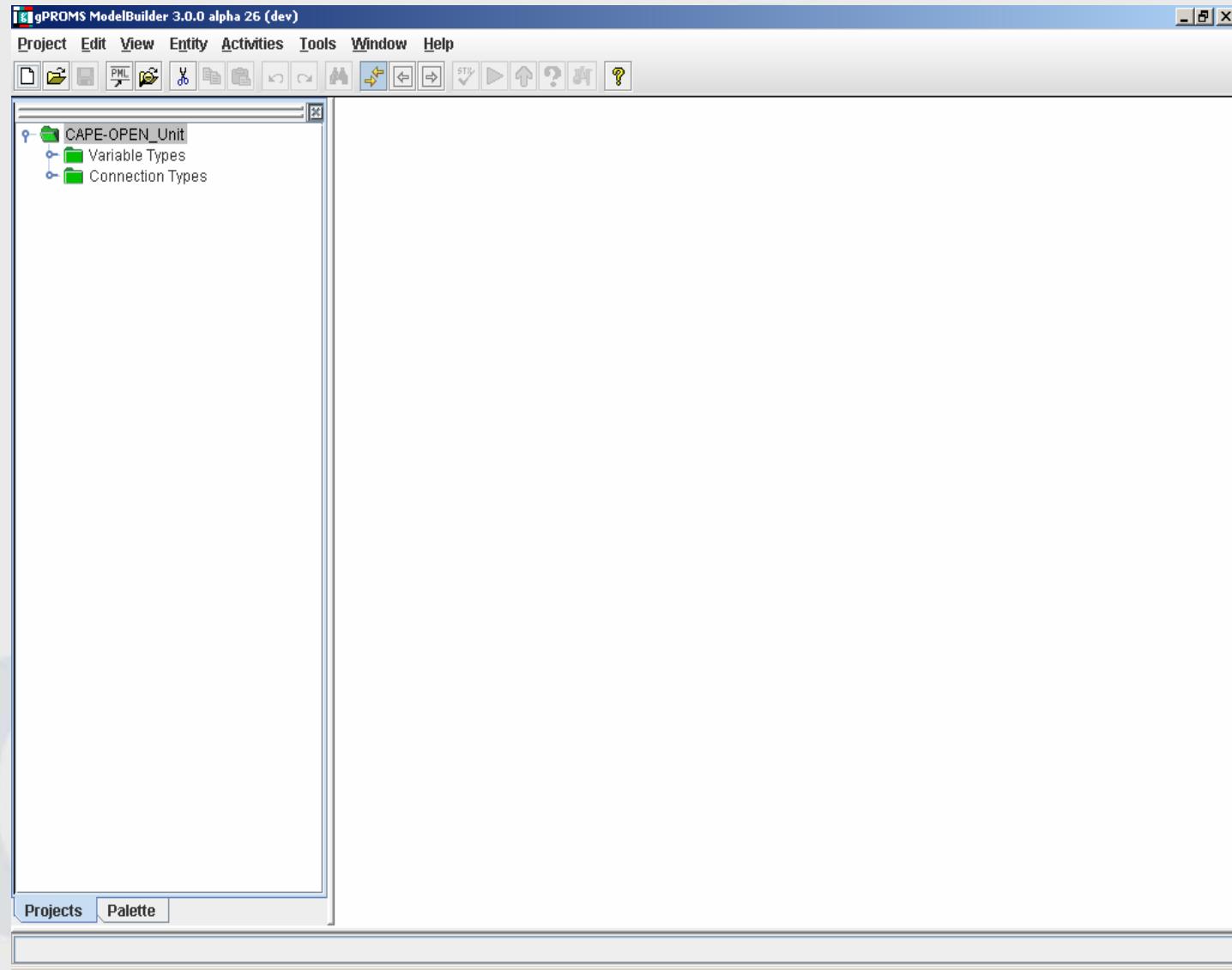


# Objectives

- ▼ Shows how a steady-state unit operation model developed in gPROMS ModelBuilder can be exported as a CAPE-OPEN Unit Operation.
- ▼ Shows how this CAPE-OPEN Unit Operation can be similarly used in a number of steady-state process simulators.
- ▼ Demonstrates the concept of once developed, available for use anywhere.
- ▼ Demonstrates automatic generation of CAPE-OPEN Unit Operation models, limiting the need for specific knowledge by model developers.



# 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 the project structure, and the right pane shows the model code.

```
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 in the code:

- A speech bubble labeled "Mass balance" points to the variable declarations and the first equation block (lines 10-24).
- A speech bubble labeled "Energy balance" points to the enthalpy calculation in the second equation block (line 27).

# Launch CAPE-OPEN export

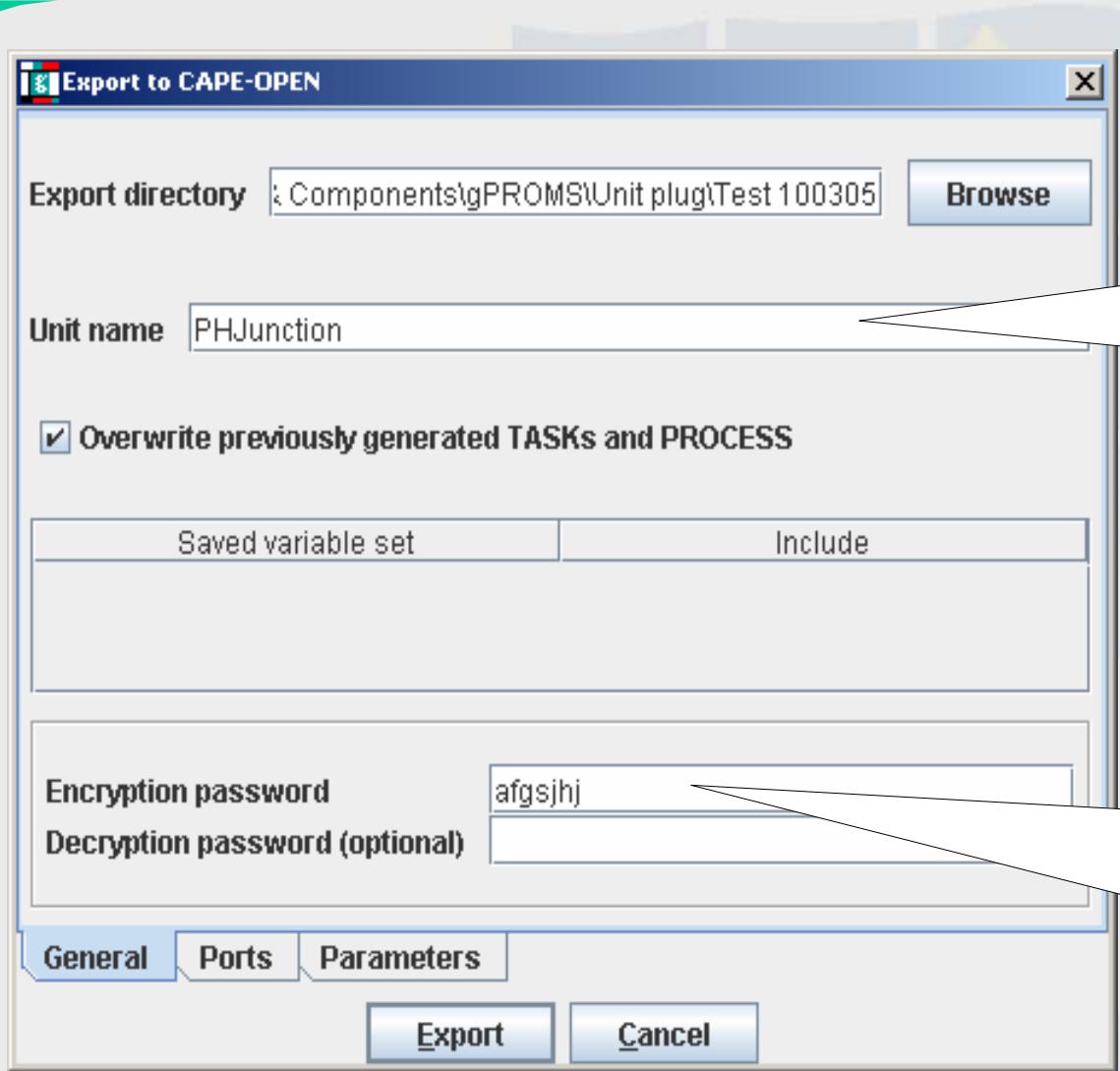
No need to change model for CAPE-OPEN exportation

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 window shows a table of stream ports with columns for Port, Connection type, Dimensions, Direction, X, Y, and Port set. The 'Tools' menu is open, and the 'Export to CAPE-OPEN...' option is highlighted.

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

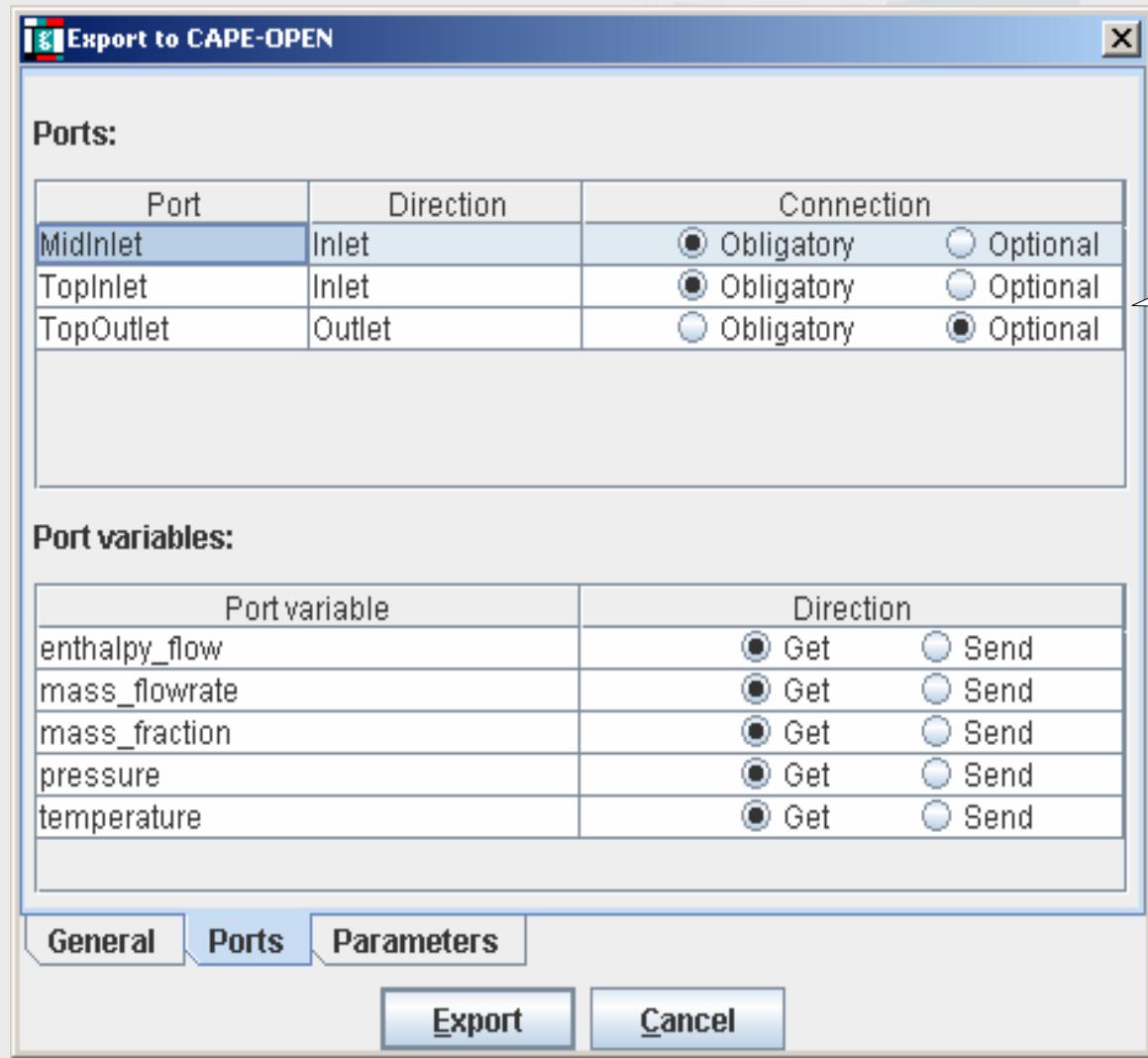
# Crypt gCO file



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

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

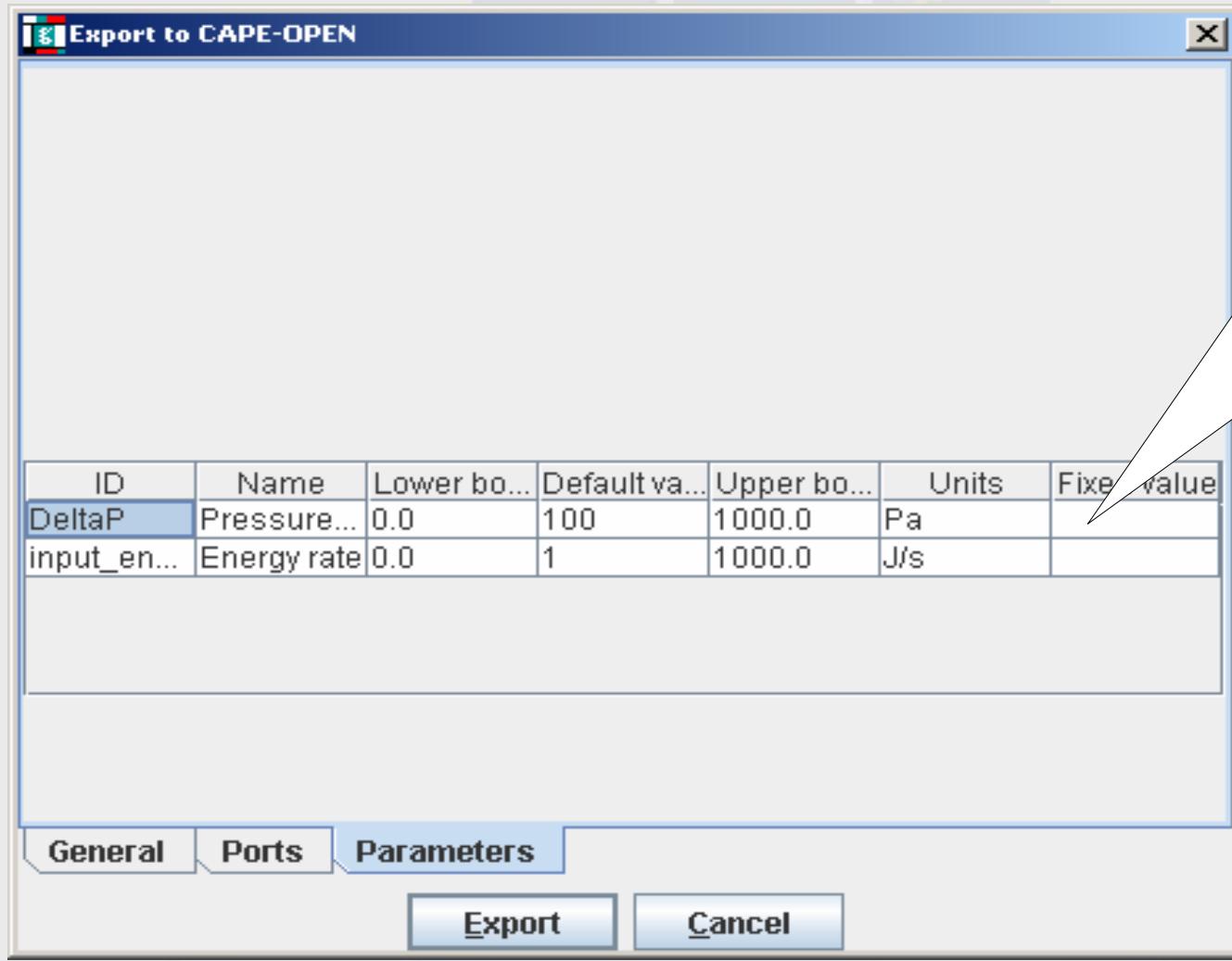
# Define ports options and parameters settings



Ports connection may be mandatory or not



# Parameter default settings



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





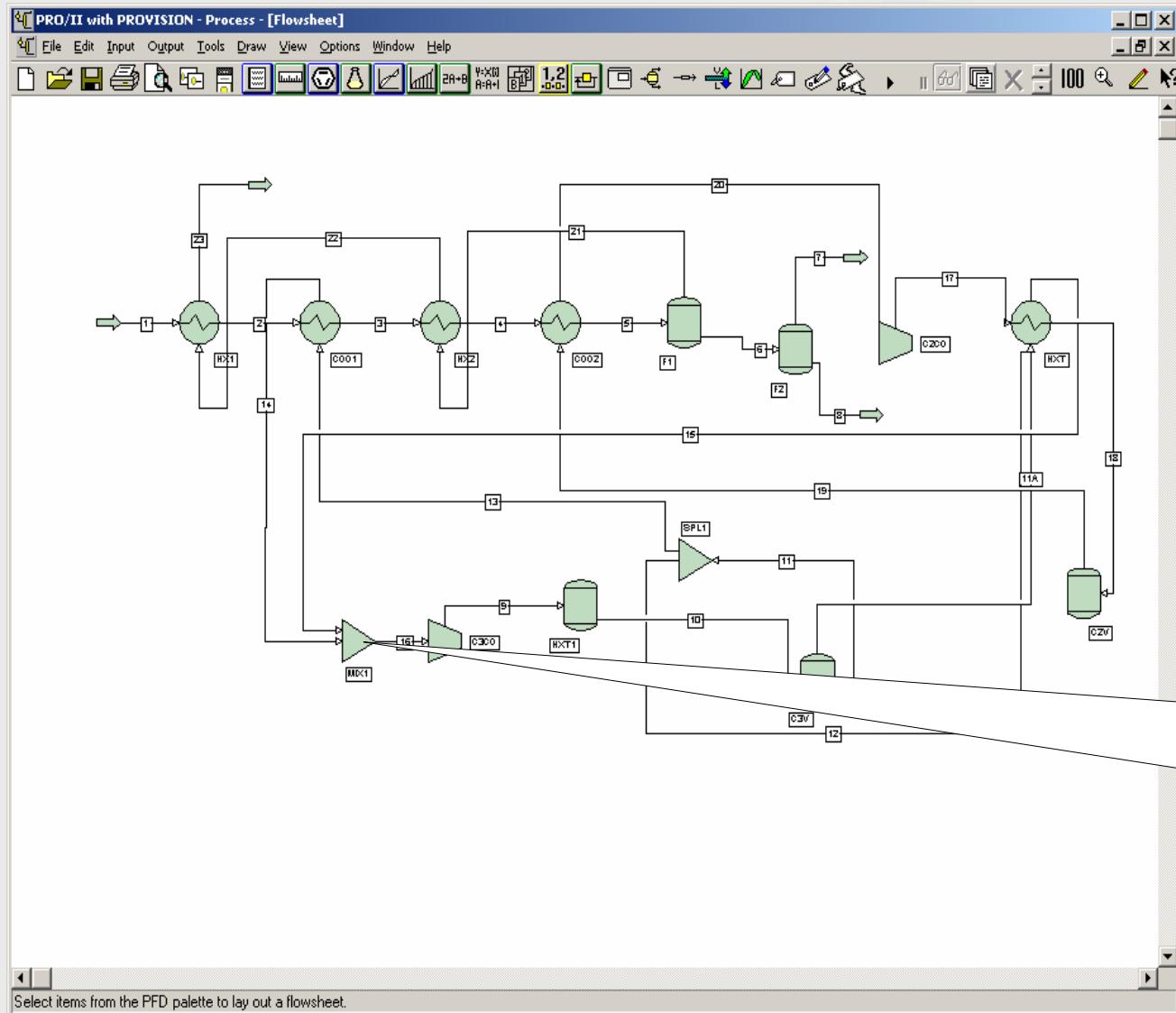
# Running gPROMS Mixer model in PRO/II



CO<sup>2</sup>LaN



# PRO/II 7.1 process model



This native mixer model will be replaced by a gPROMS Mixer model



# Native PRO/II mixer model output

```
Programmer's File Editor
File Edit Options Template Execute Macro Window Help
C:\Documents and Settings\PDONS\Local Settings\TEMP\VW3F.tmp
THERMODYNAMIC SYSTEM PR
STREAM '16'
TOTAL          VAPOR
RATE, LB-MOL/HR    50.0000   50.0000
TEMPERATURE, F      252.95    252.95
PRESSURE, PSIA       11.14     11.14
MOLECULAR WEIGHT    44.0970   44.0970
FRACTION             1.0000
ENTHALPY, BTU/LB-MOL 11690.6862 11690.6862
CP, BTU/LB-F         0.5089    0.5089

MOLAR FLOWRATES, LB-MOL/HR
 1 - C1            0.0000    0.0000
 2 - C2            0.0000    0.0000
 3 - C3            50.0000   50.0000
 4 - IC4           0.0000    0.0000
 5 - NC4           0.0000    0.0000
 6 - IC5           0.0000    0.0000
 7 - NC5           0.0000    0.0000
 8 - NC6           0.0000    0.0000

MOLAR COMPOSITIONS
 1 - C1            0.0000    0.0000
 2 - C2            0.0000    0.0000
 3 - C3            1.0000   1.0000
 4 - IC4           0.0000    0.0000
 5 - NC4           0.0000    0.0000
 6 - IC5           0.0000    0.0000
 7 - NC5           0.0000    0.0000
 8 - NC6           0.0000    0.0000

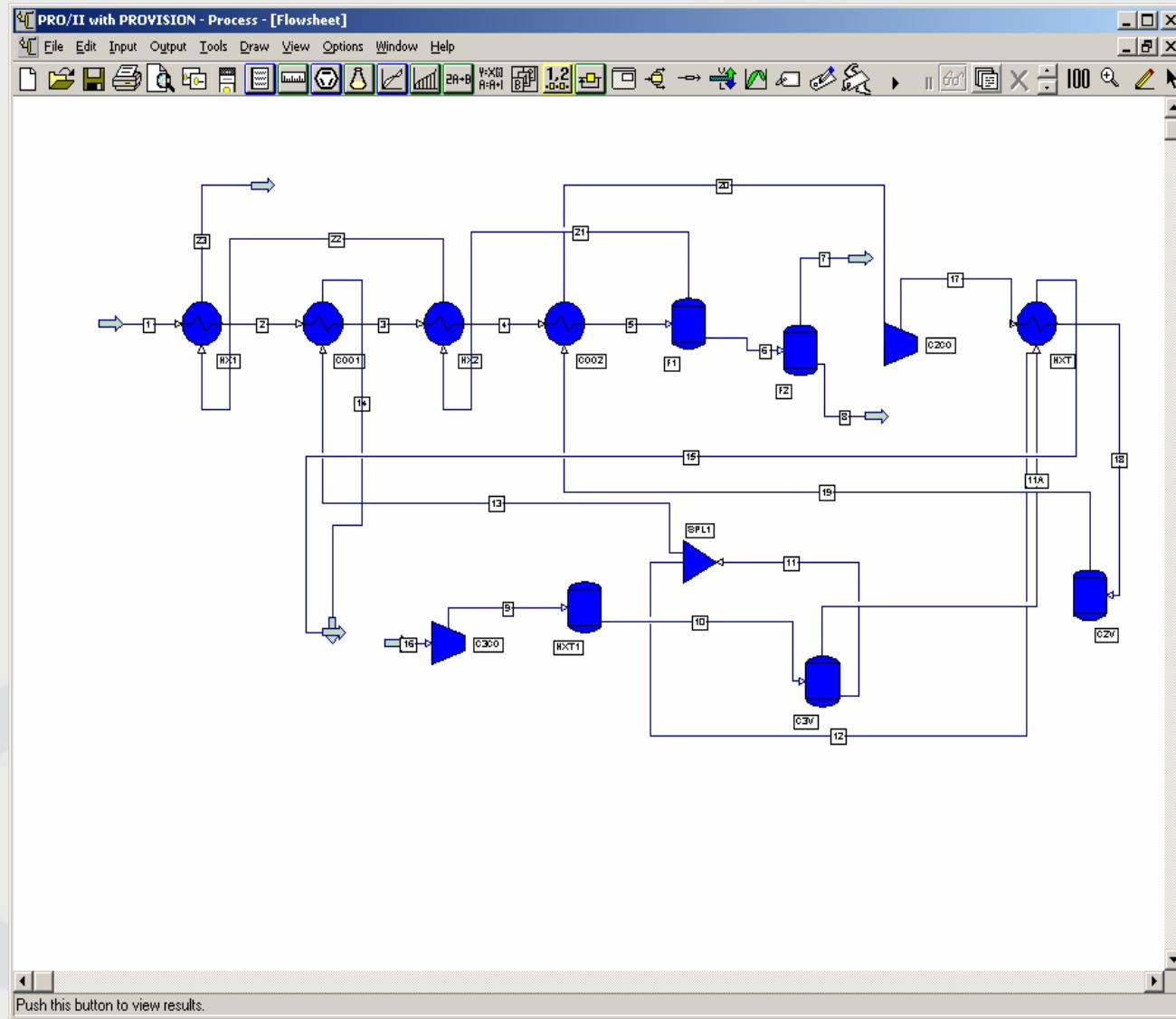
Ln 1 Col 1 33 /WR Rec Off No Wrap DOS INS
```

Mixer outlet  
stream

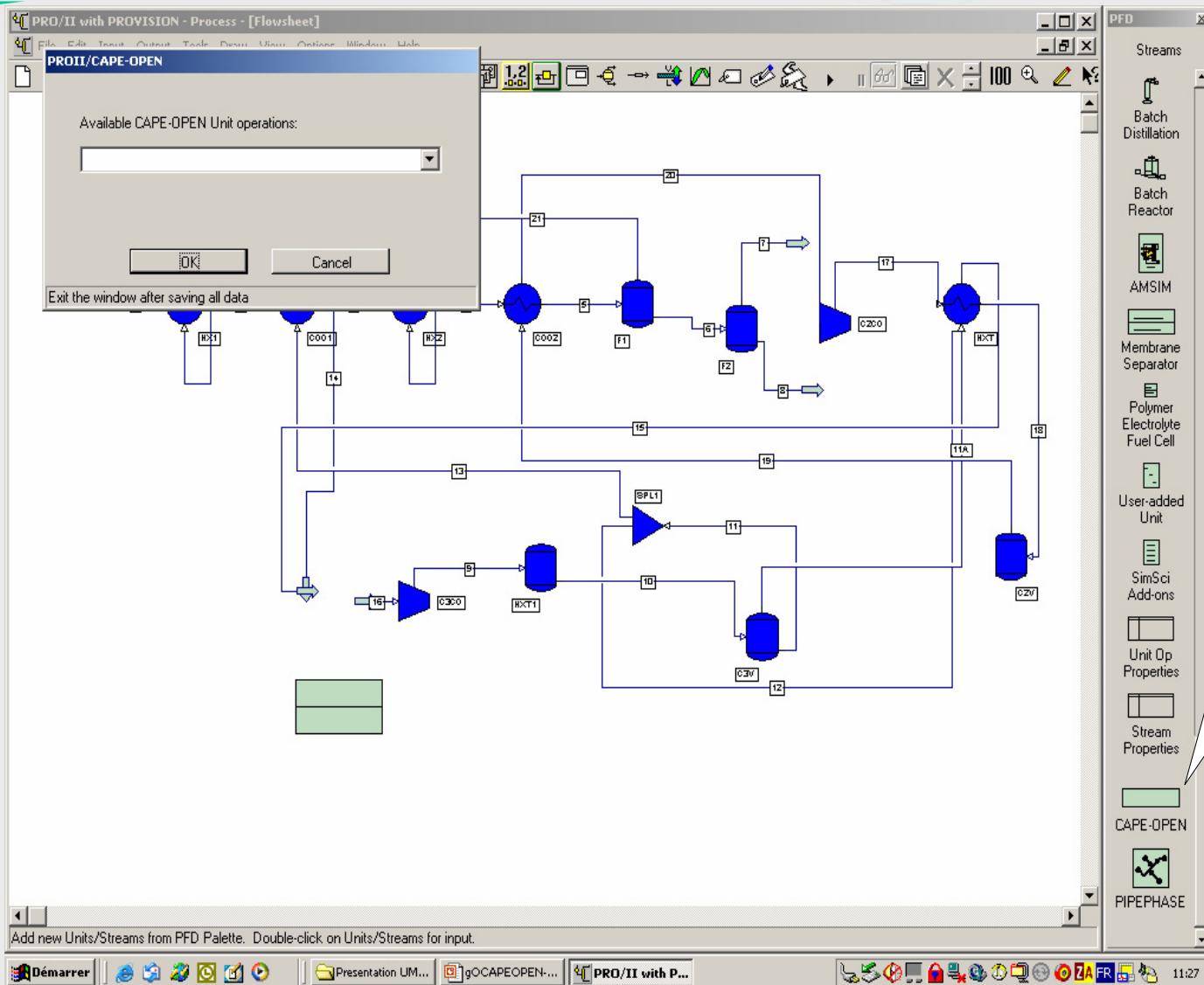
Since gPROMS mixer model involves basic material and energy balances, results with PRO/II native mixer and gPROMS mixer should be strictly the same



# Delete native PRO/II mixer



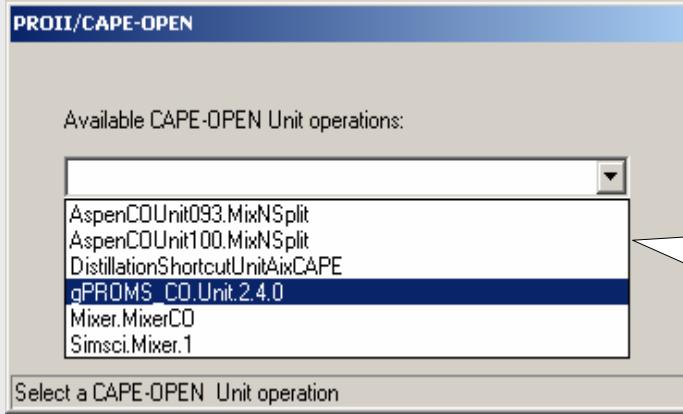
# Add a CAPE-OPEN Unit Operation



PRO/II  
allows for  
CAPE-OPEN  
UNIT  
Operations to  
be inserted in  
any PRO/II  
process  
model  
through the  
palette

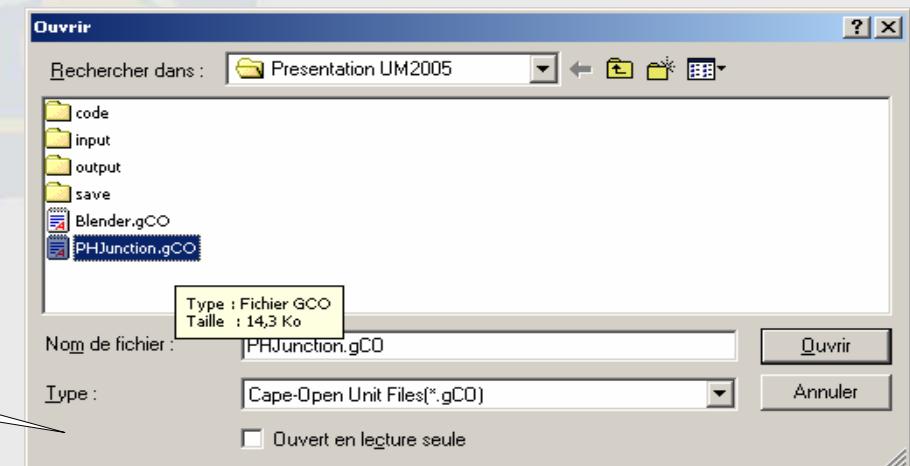


# Select go:CAPE-OPEN UNIT Operation

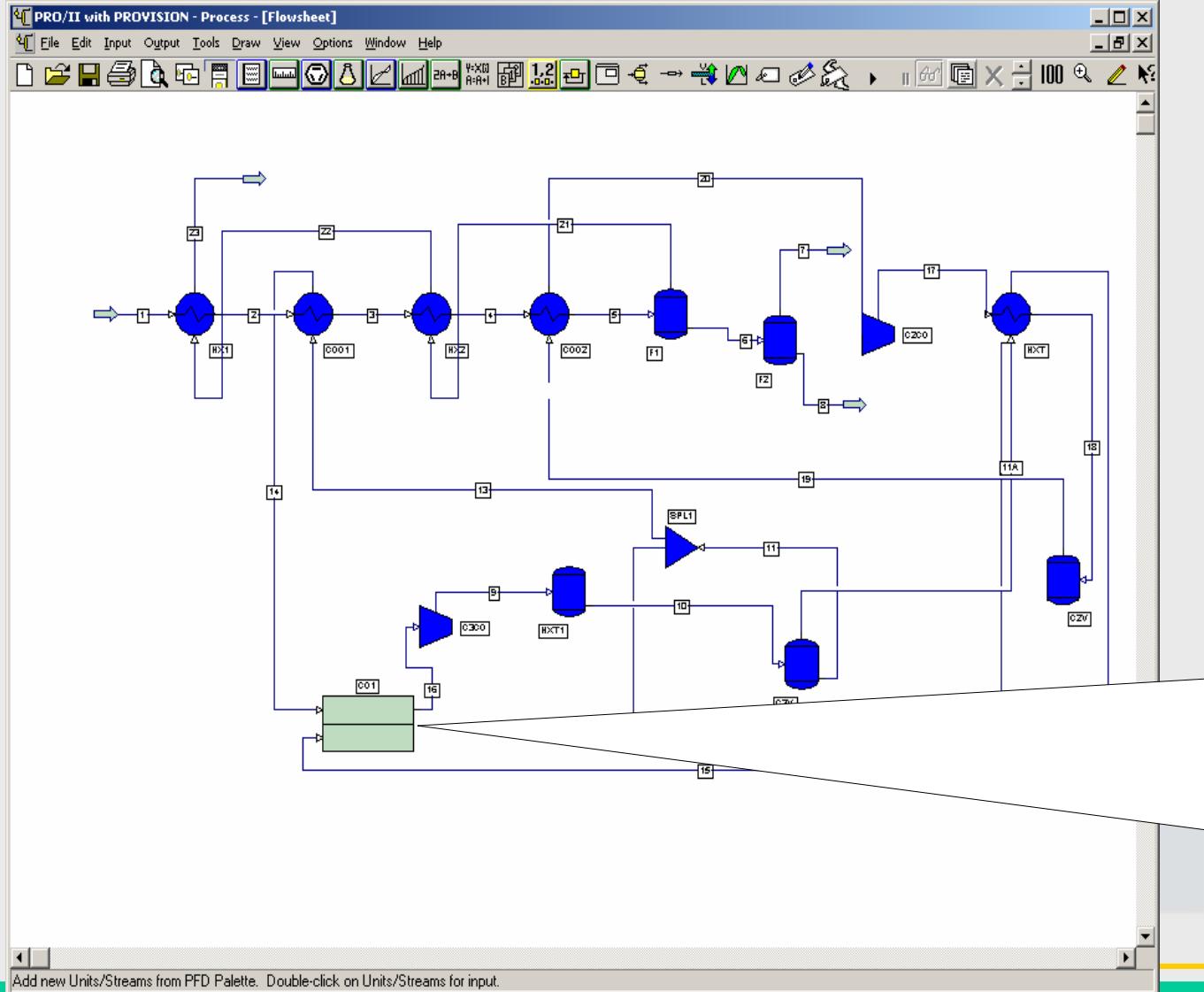


PRO/II lists all CAPE-OPEN  
UNIT operations available on  
the current machine

gO:CAPE-OPEN asks for the  
gCO file to be used within  
the gO:CAPE-OPEN  
wrapper

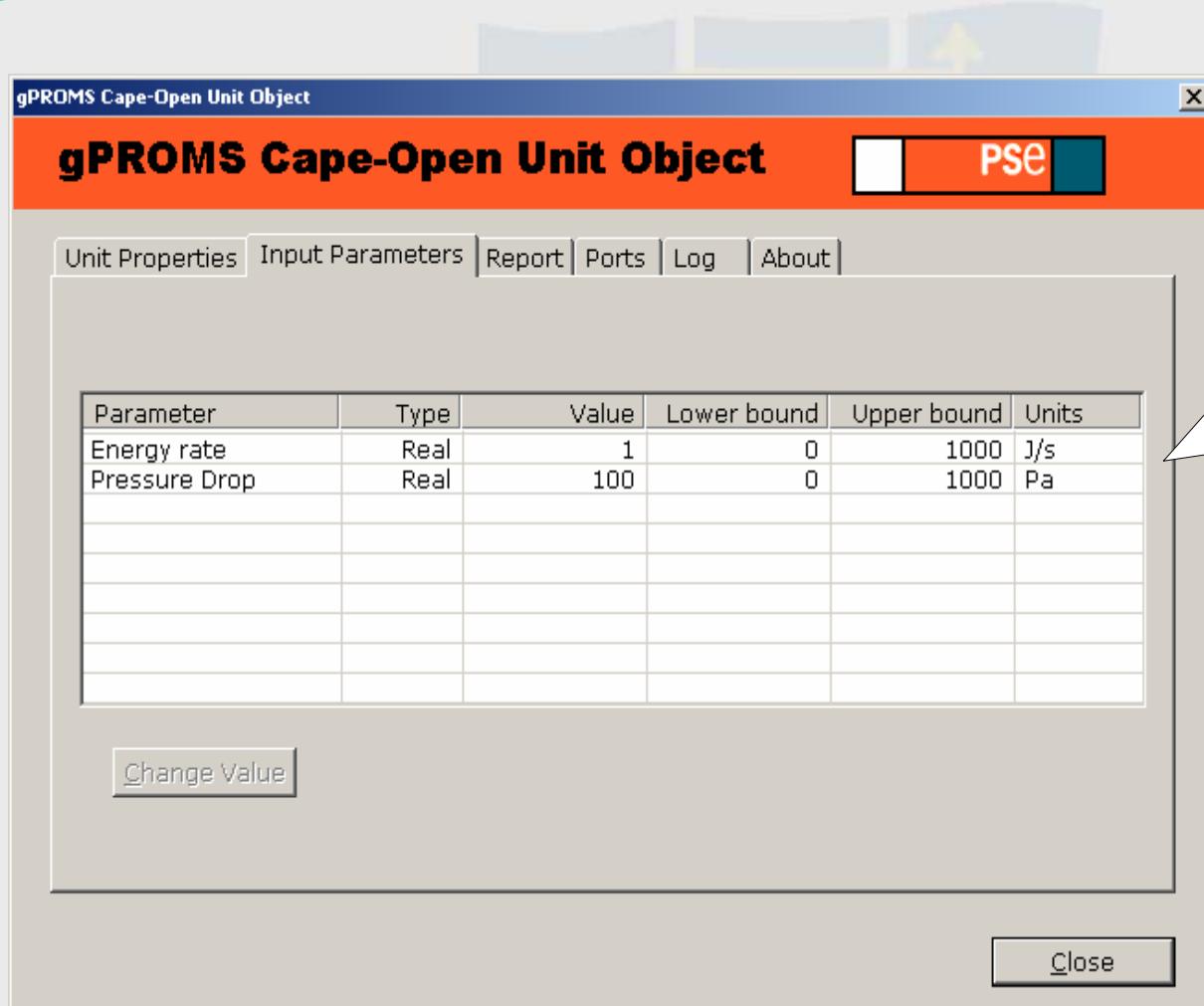


# Connect streams to CO UNIT ports



Streams are connected to the gPROMS UNIT just as to any native PRO/II unit operation

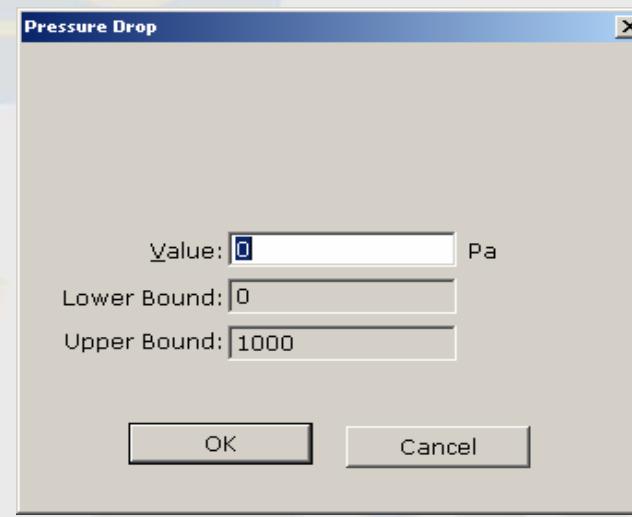
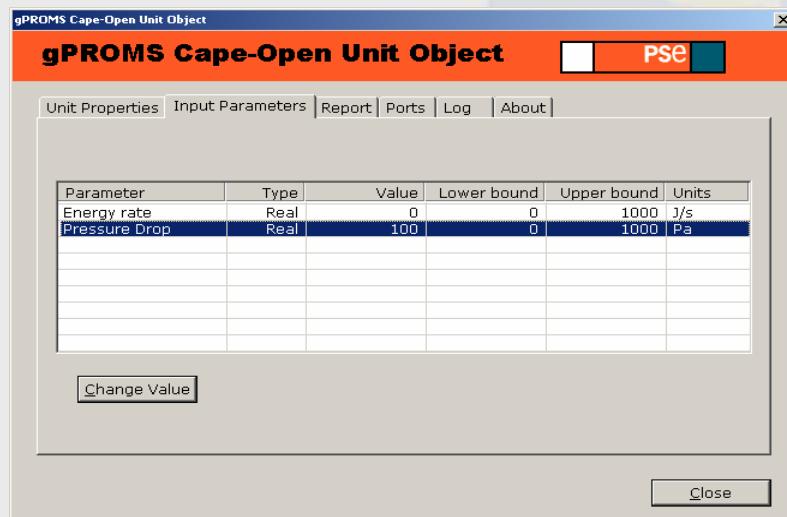
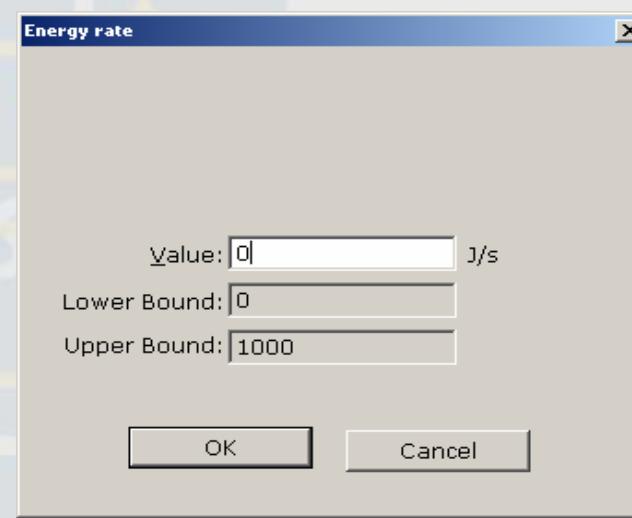
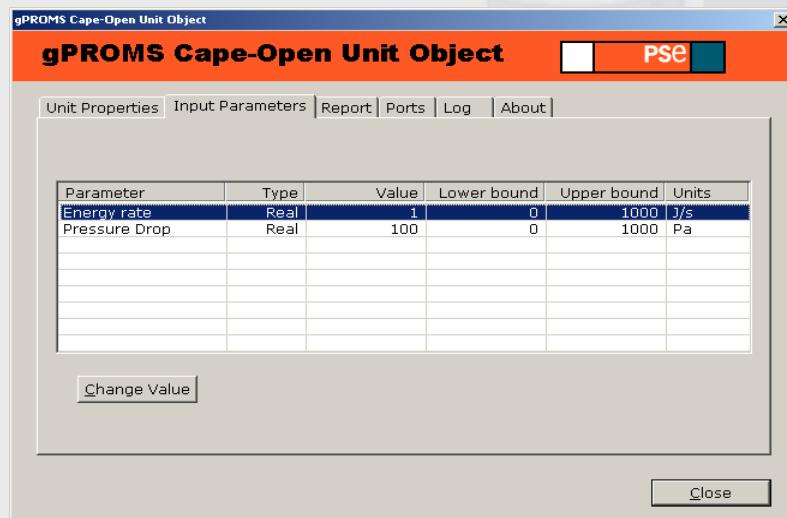
# Display parameter values



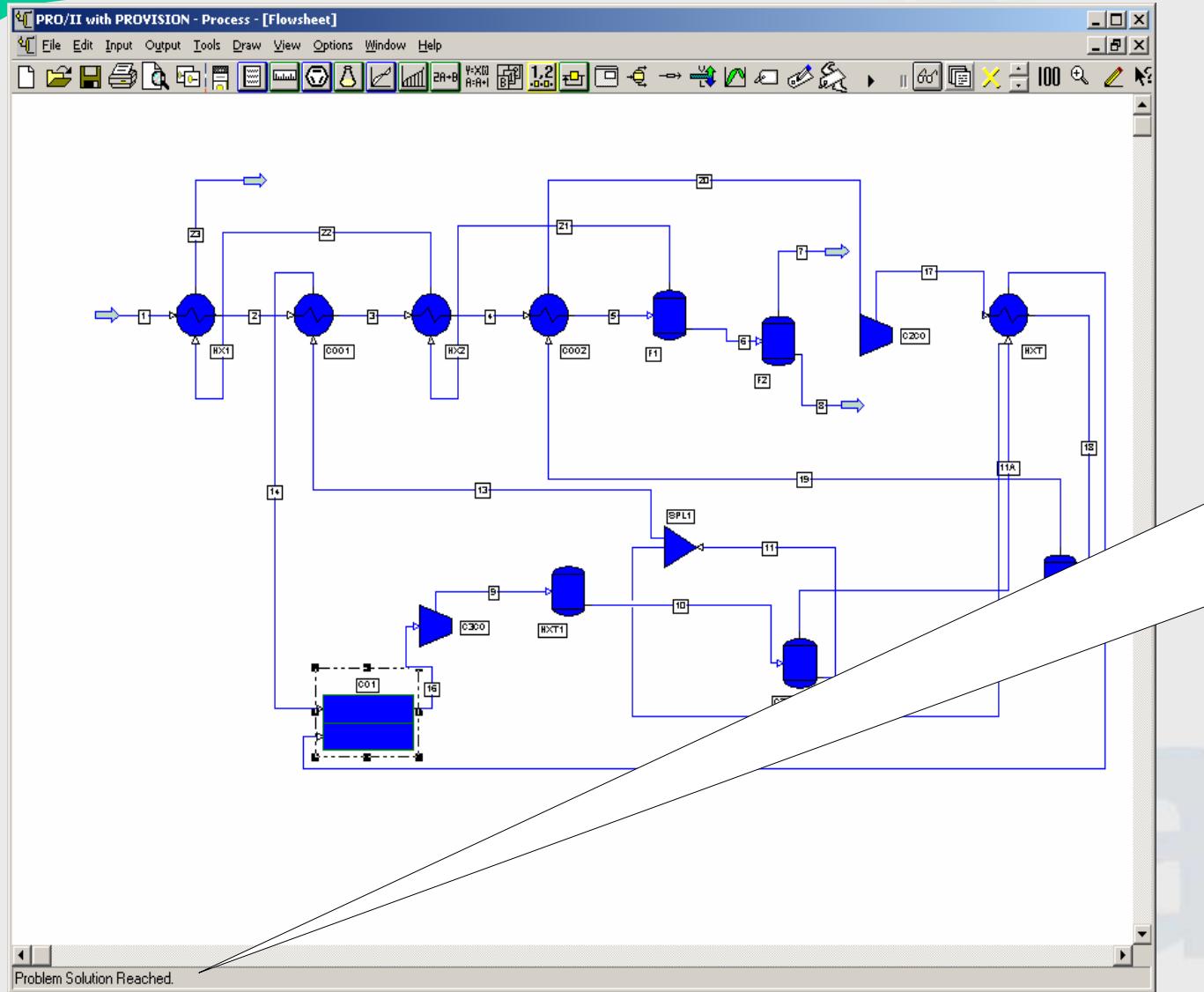
In order to access parameters, gO:CAPE-OPEN GUI is automatically displayed by PRO/II



# Set energy input / pressure drop to zero



# Run simulation and reach convergence



After a few iterations,  
convergence  
is achieved



# Mixer output results

## gProms Mixer

**Programmer's File Editor**

File Edit Options Template Execute Macro Window Help

C:\Documents and Settings\POONS\Local Settings\TEMP\VW4A.tmp

THERMODYNAMIC SYSTEM PR

STREAM '16'

	TOTAL	VAPOR
RATE, LB-MOL/HR	50.0000	50.0000
TEMPERATURE, F	252.95	252.95
PRESSURE, PSIA	11.14	11.14
MOLECULAR WEIGHT	44.0970	44.0970
FRACTION		1.0000
ENTHALPY, BTU/LB-MOL	11690.6858	11690.6858
CP, BTU/LB-F	0.5089	0.5089

MOLAR FLOWRATES, LB-MOL/HR

1 - C1	0.0000	0.0000
2 - C2	0.0000	0.0000
3 - C3	50.0000	50.0000
4 - IC4	0.0000	0.0000
5 - NC4	0.0000	0.0000
6 - IC5	0.0000	0.0000
7 - NC5	0.0000	0.0000
8 - NC6	0.0000	0.0000

MOLAR COMPOSITIONS

1 - C1	0.0000	0.0000
2 - C2	0.0000	0.0000
3 - C3	1.0000	1.0000
4 - IC4	0.0000	0.0000
5 - NC4	0.0000	0.0000
6 - IC5	0.0000	0.0000
7 - NC5	0.0000	0.0000
8 - NC6	0.0000	0.0000

Ln 1 Col 1 33 WR Rec Off No Wrap DOS INS

## Pro/II native Mixer

**Programmer's File Editor**

File Edit Options Template Execute Macro Window Help

C:\Documents and Settings\POONS\Local Settings\TEMP\VW3F.tmp

THERMODYNAMIC SYSTEM PR

STREAM '16'

	TOTAL	VAPOR
RATE, LB-MOL/HR	50.0000	50.0000
TEMPERATURE, F	252.95	252.95
PRESSURE, PSIA	11.14	11.14
MOLECULAR WEIGHT	44.0970	44.0970
FRACTION		1.0000
ENTHALPY, BTU/LB-MOL	11690.6862	11690.6862
CP, BTU/LB-F	0.5089	0.5089

MOLAR FLOWRATES, LB-MOL/HR

1 - C1	0.0000	0.0000
2 - C2	0.0000	0.0000
3 - C3	50.0000	50.0000
4 - IC4	0.0000	0.0000
5 - NC4	0.0000	0.0000
6 - IC5	0.0000	0.0000
7 - NC5	0.0000	0.0000
8 - NC6	0.0000	0.0000

MOLAR COMPOSITIONS

1 - C1	0.0000	0.0000
2 - C2	0.0000	0.0000
3 - C3	1.0000	1.0000
4 - IC4	0.0000	0.0000
5 - NC4	0.0000	0.0000
6 - IC5	0.0000	0.0000
7 - NC5	0.0000	0.0000
8 - NC6	0.0000	0.0000

Ln 1 Col 1 33 WR Rec Off No Wrap DOS INS



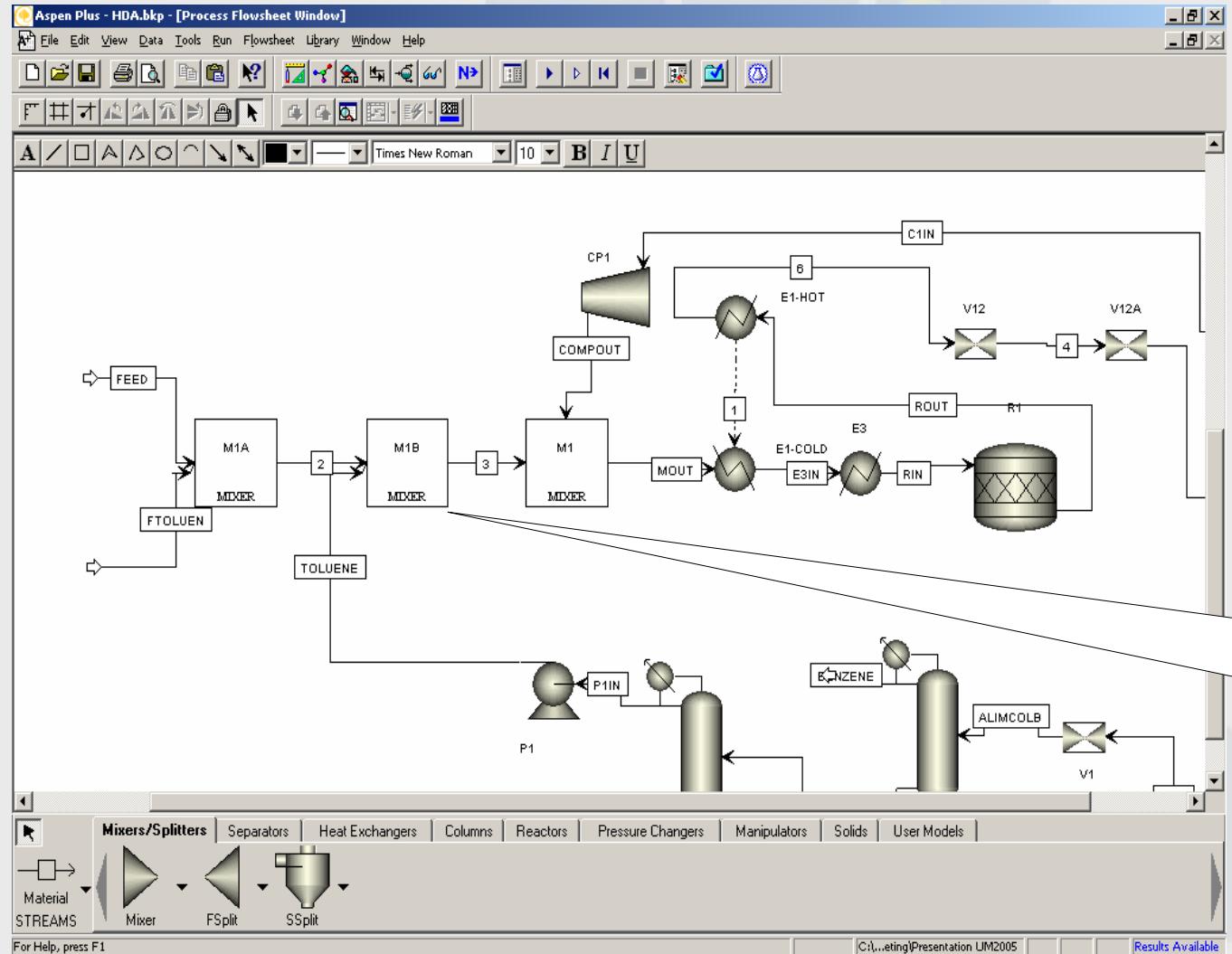


## Running gPROMS model in Aspen Plus

CO<sub>2</sub>LaN



# HDA Process model in Aspen Plus 12.1



# Native Aspen Plus Mixer output results

The screenshot shows the Aspen Plus software interface. The title bar reads "Aspen Plus - HDA.bkp - [Stream 3 (MATERIAL) Results - Data Browser]". The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Window, Help. The toolbar has various icons for file operations and analysis. The left sidebar has a tree view under "Results" showing streams 1 through 6, and other components like ALIMCOLB, BENZENE, COMPOUT, DIPHENYL, E3IN, FEED, FIN, FTOLIEN, H2-CH4, LIQOUT, MOUT, P1IN, PURGE, RIN, ROUT, TOLWENE, V1IN, VAPOUT, and Blocks. The main area is titled "Material" and displays Stream Table results for Stream 3. The table includes:

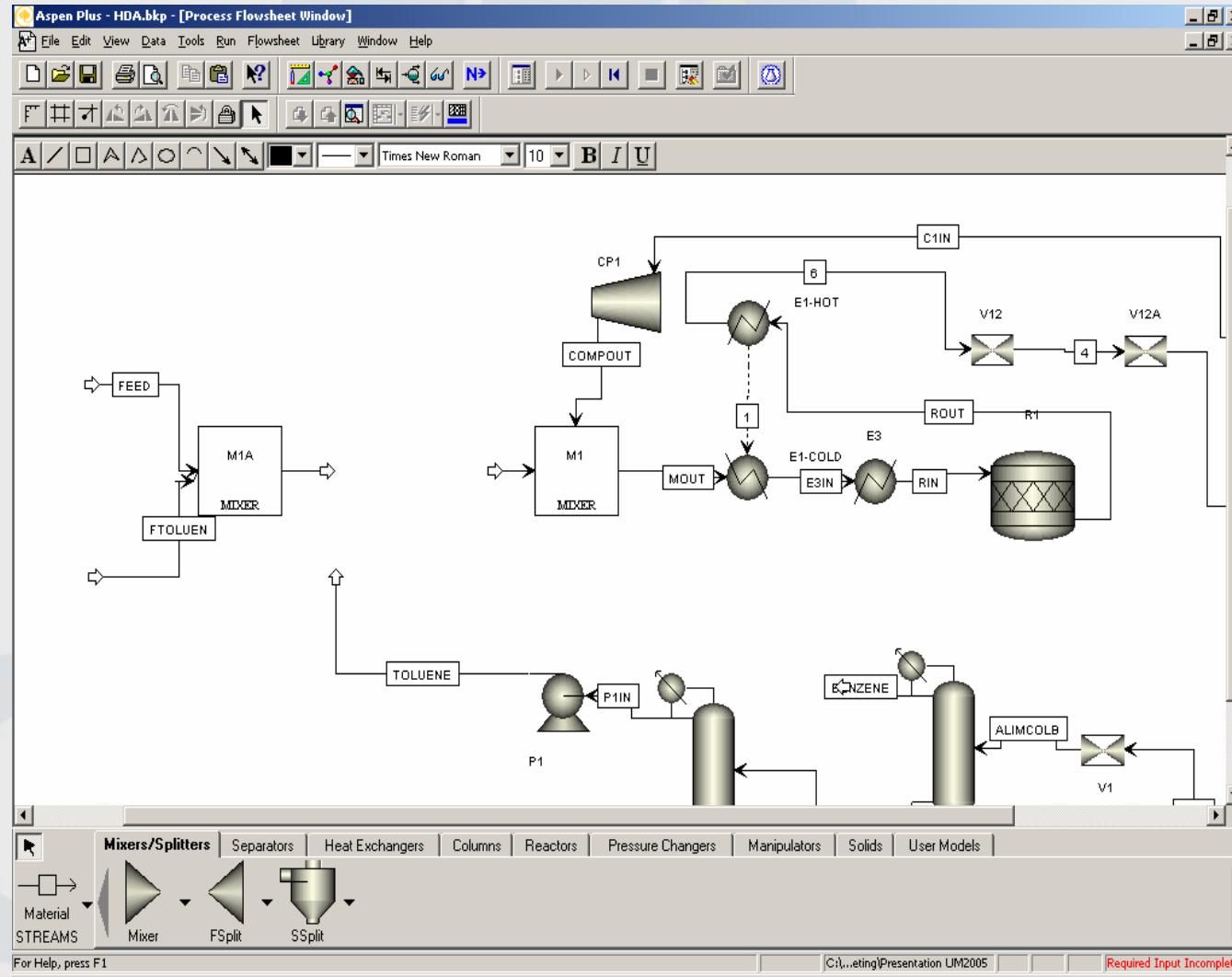
Substream: MIXED	3
Mole Flow lbmol/hr	
H2	467,4000
CH4	24,60000
BENZENE	1,78642E-3
TOLUENE	290,9473
DIPHENYL	,5756150
Total Flow lbmol/hr	783,5247
Total Flow lb/hr	28233.82
Total Flow cwt/hr	6189,717
Temperature F	101,2617
Pressure psi	535,0000
Manor.Frac.	6237596

At the bottom, there are tabs for Mixers/Splitters, Separators, Heat Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, and User Models. Icons for Material STREAMS, Mixer, FSPLIT, and SSPLIT are also present. A status bar at the bottom indicates "Results Available, Unreconciled." and "C:\...eting\Presentation UM2005".

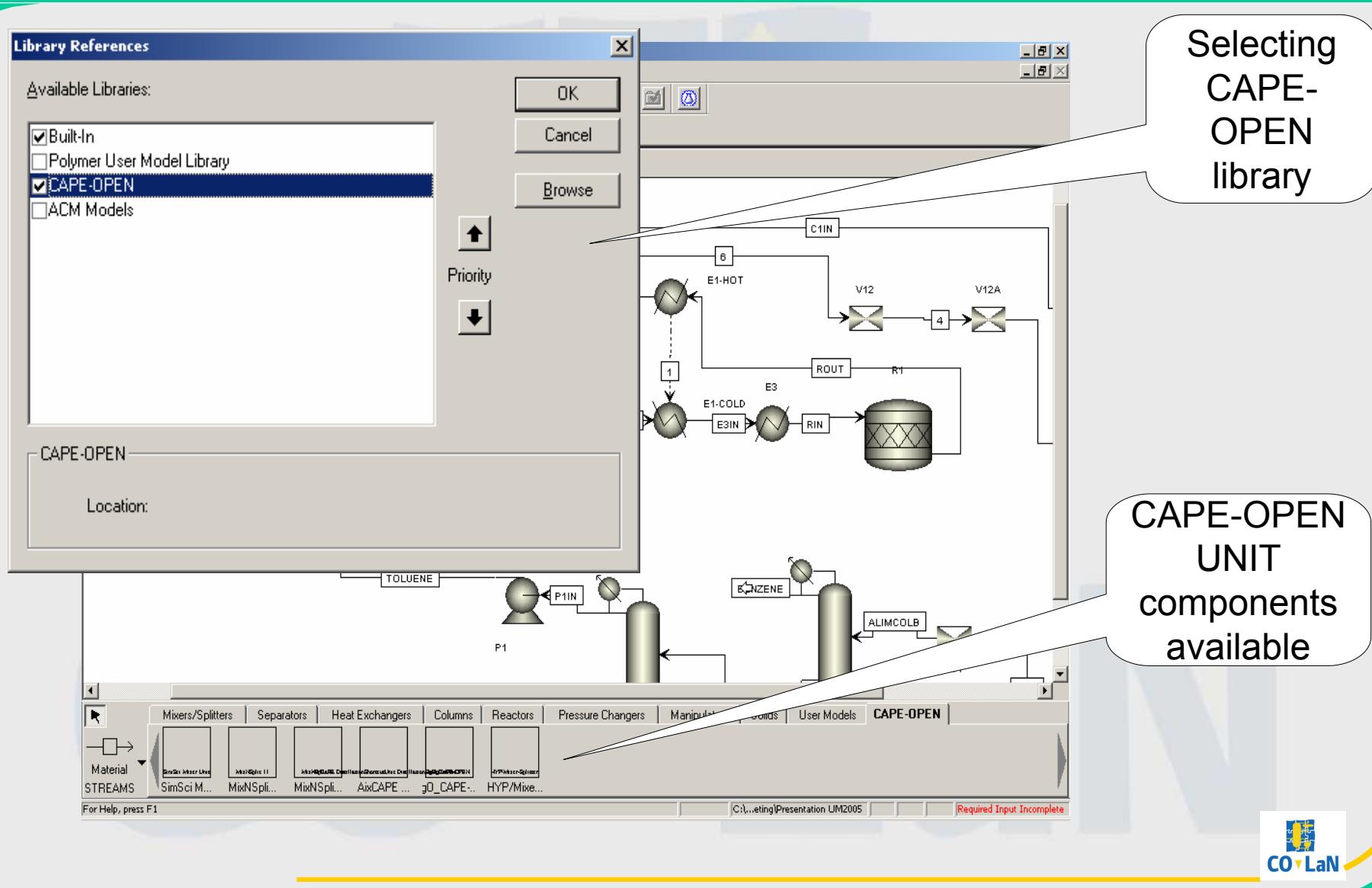
Since gPROMS mixer model involves basic material and energy balances, results with Aspen Plus native mixer and gPROMS mixer should be strictly the same



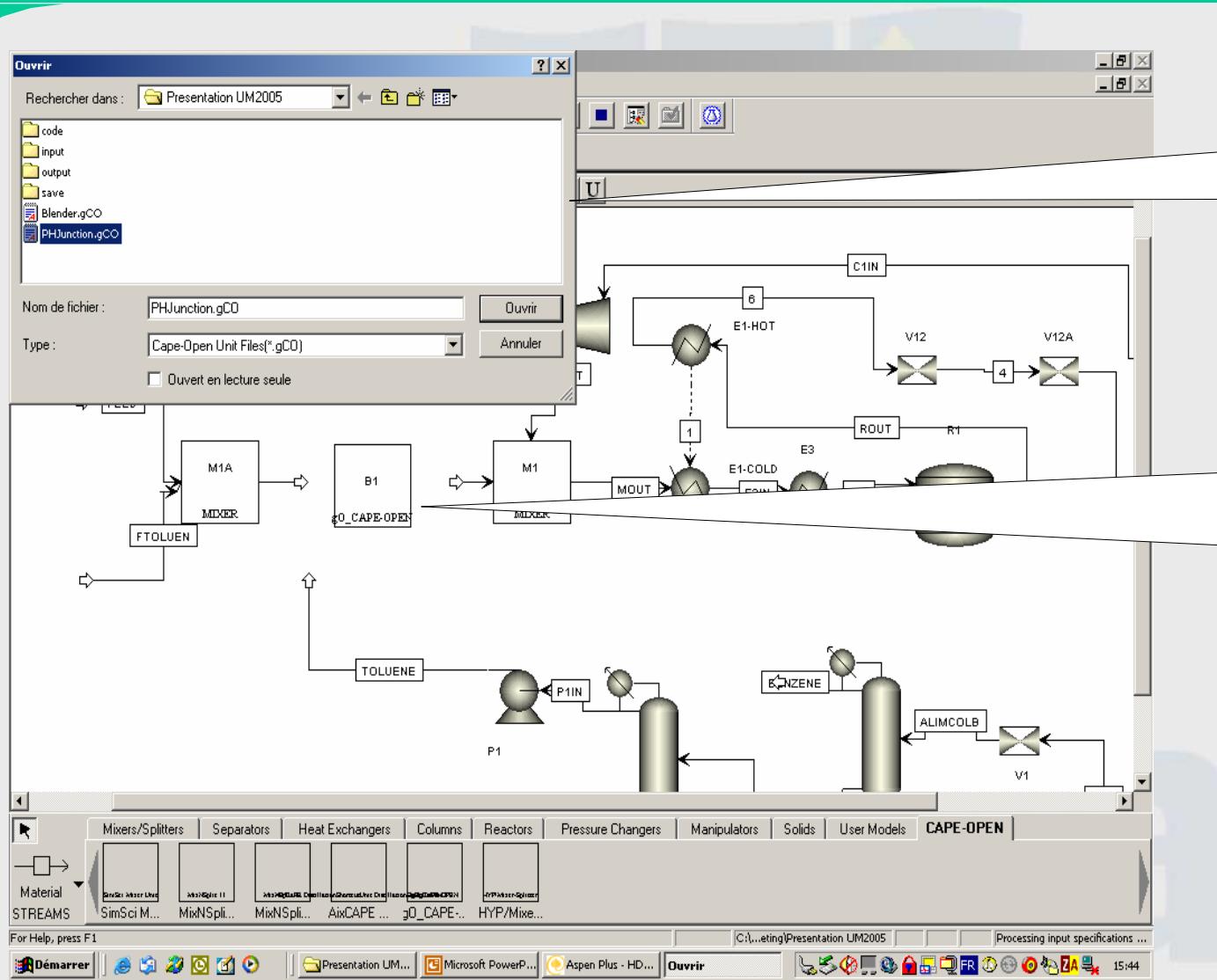
# Delete native Aspen Plus Mixer



# Display CAPE-OPEN UNIT Ops library



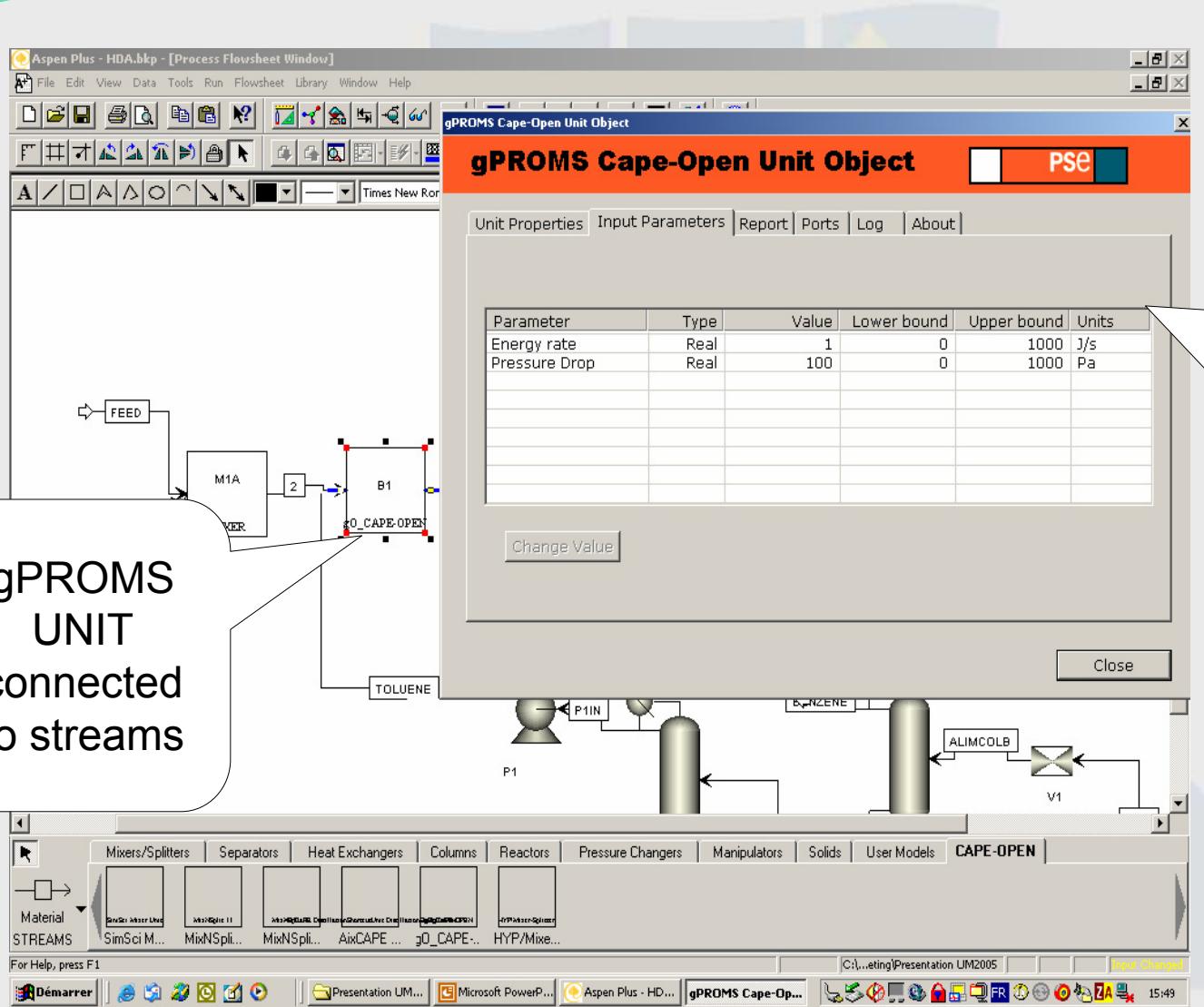
# Plug in gPROMS model



Selecting the  
gCO file to  
be used

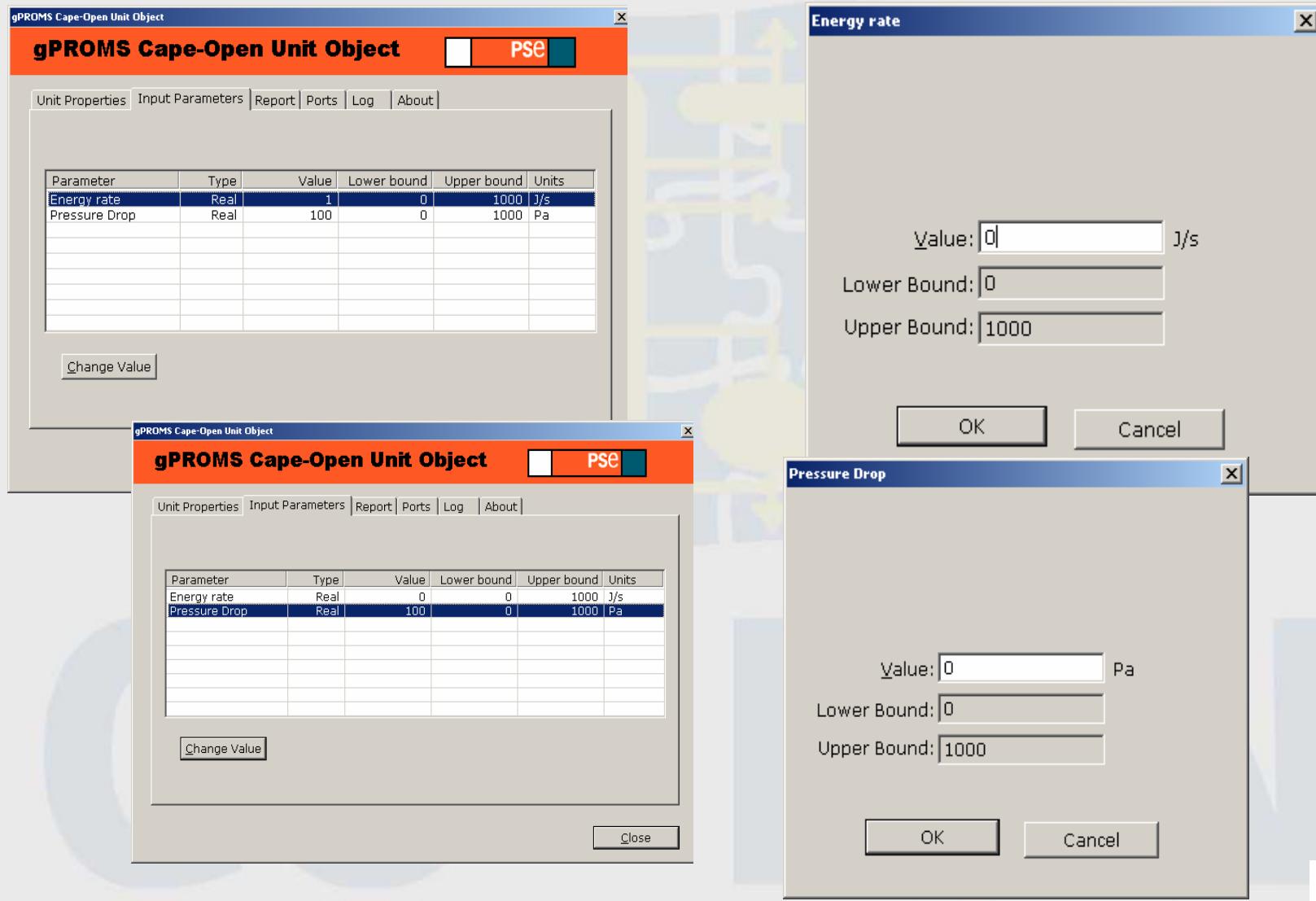
g0:CAPE-  
OPEN UNIT  
placed within  
the PFD  
(not yet  
connected)

# Open gProms UNIT GUI

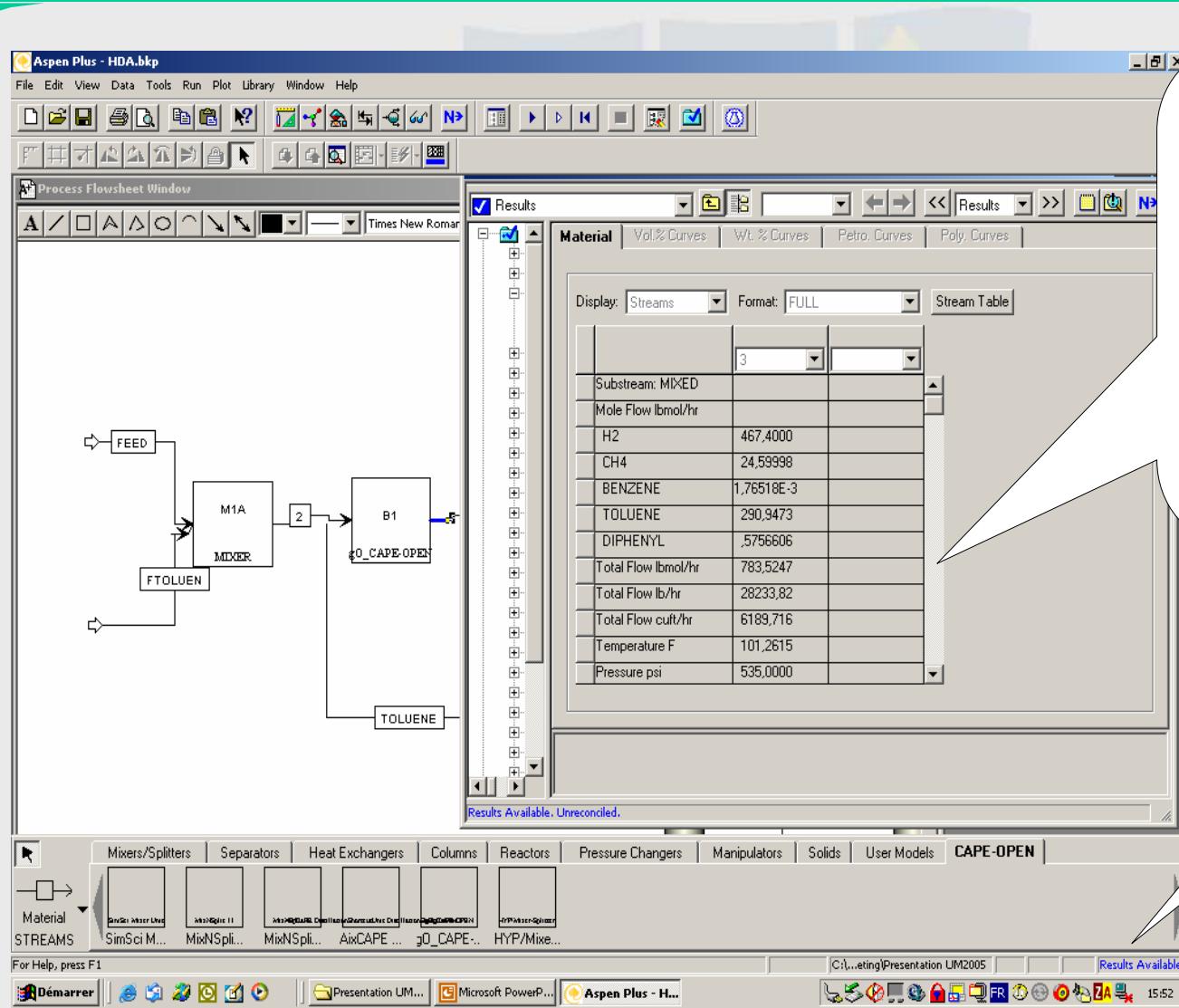


Same GUI  
as in PRO/II.  
Gives  
access to  
public unit  
parameters.

# Set energy input / pressure drop to zero



# gProms Mixer output results



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

Simulation  
converged.



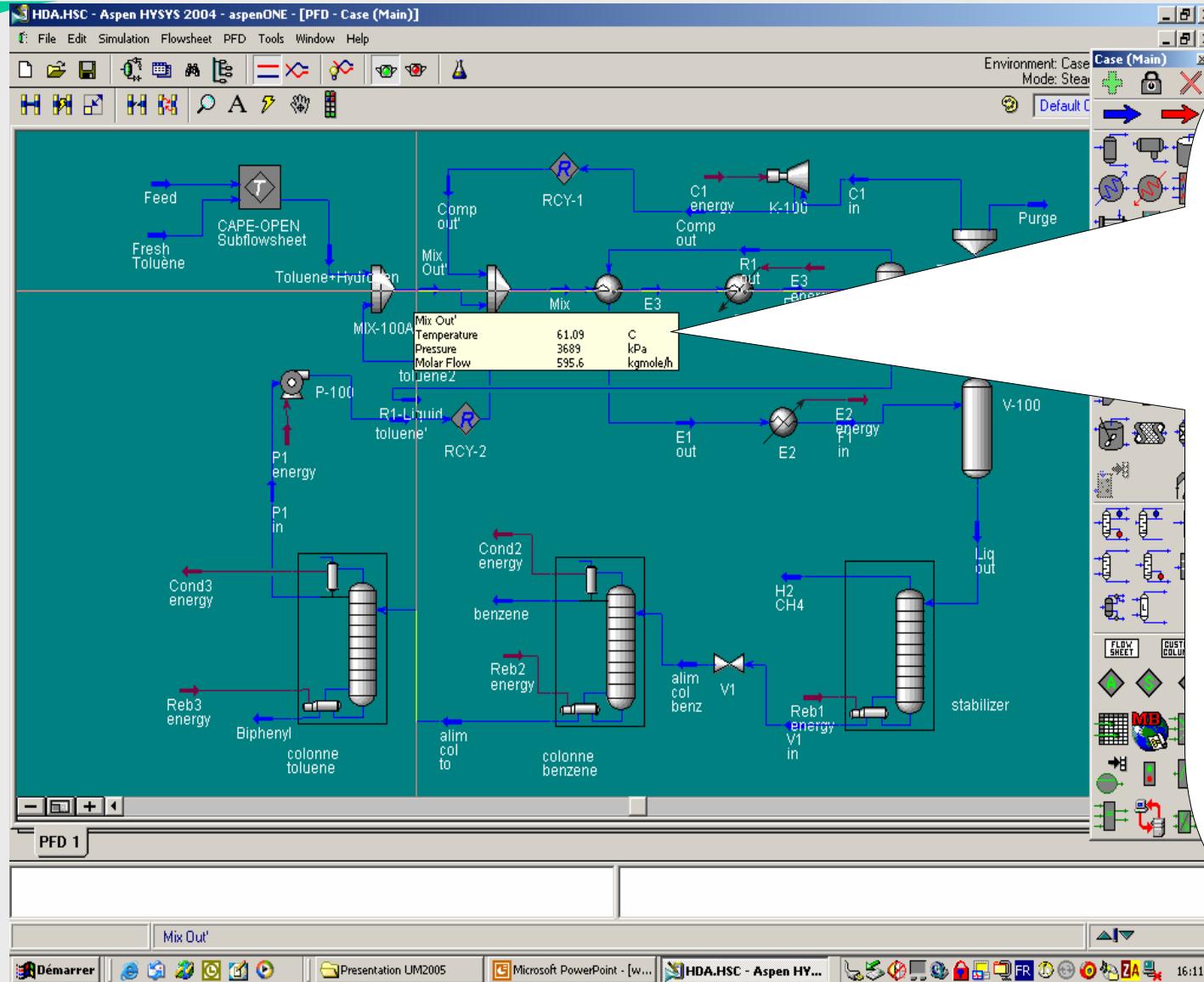


## Running gPROMS model in HYSYS.Process

CO<sub>2</sub>LaN



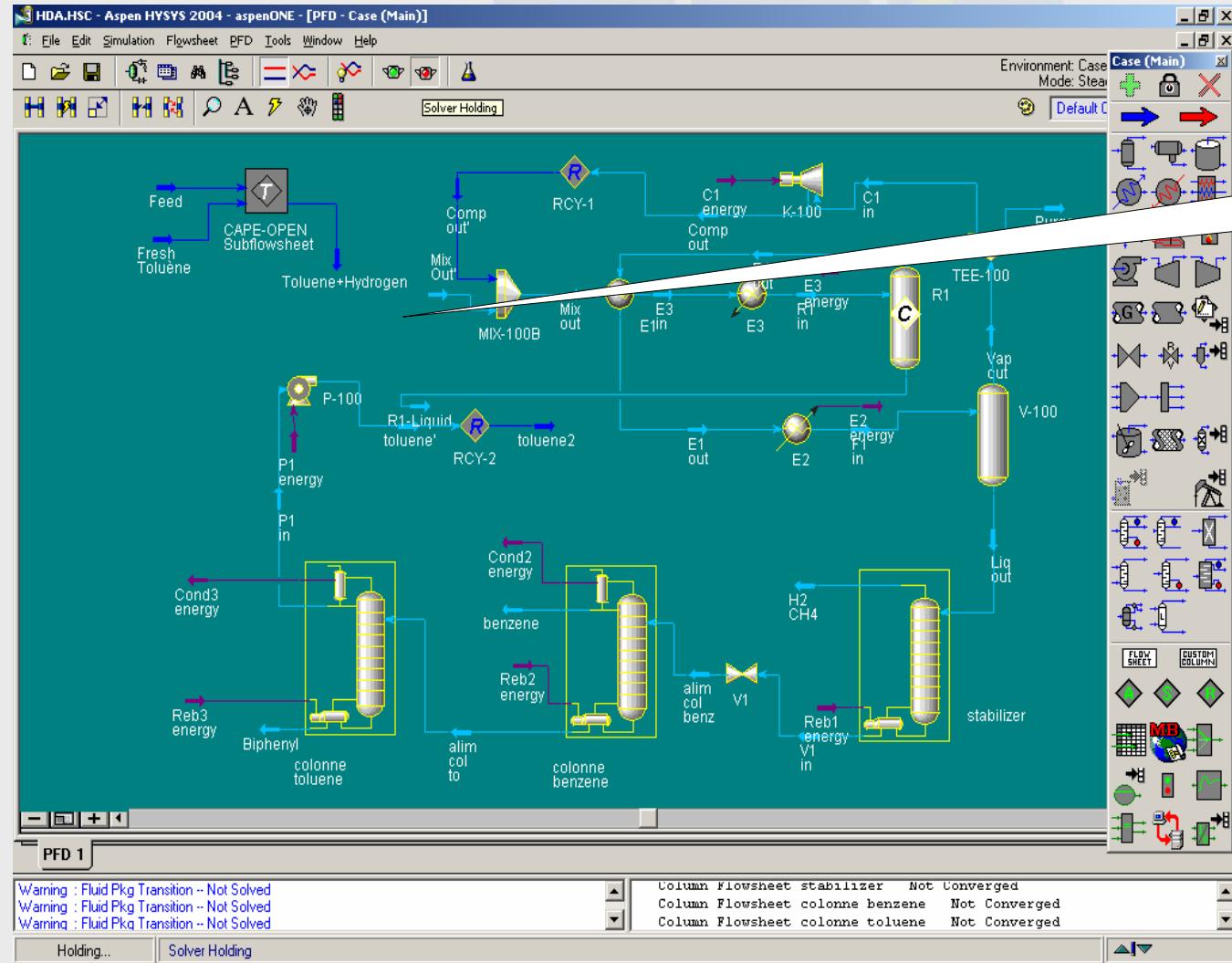
# HDA process model in Aspen HYSYS 2004



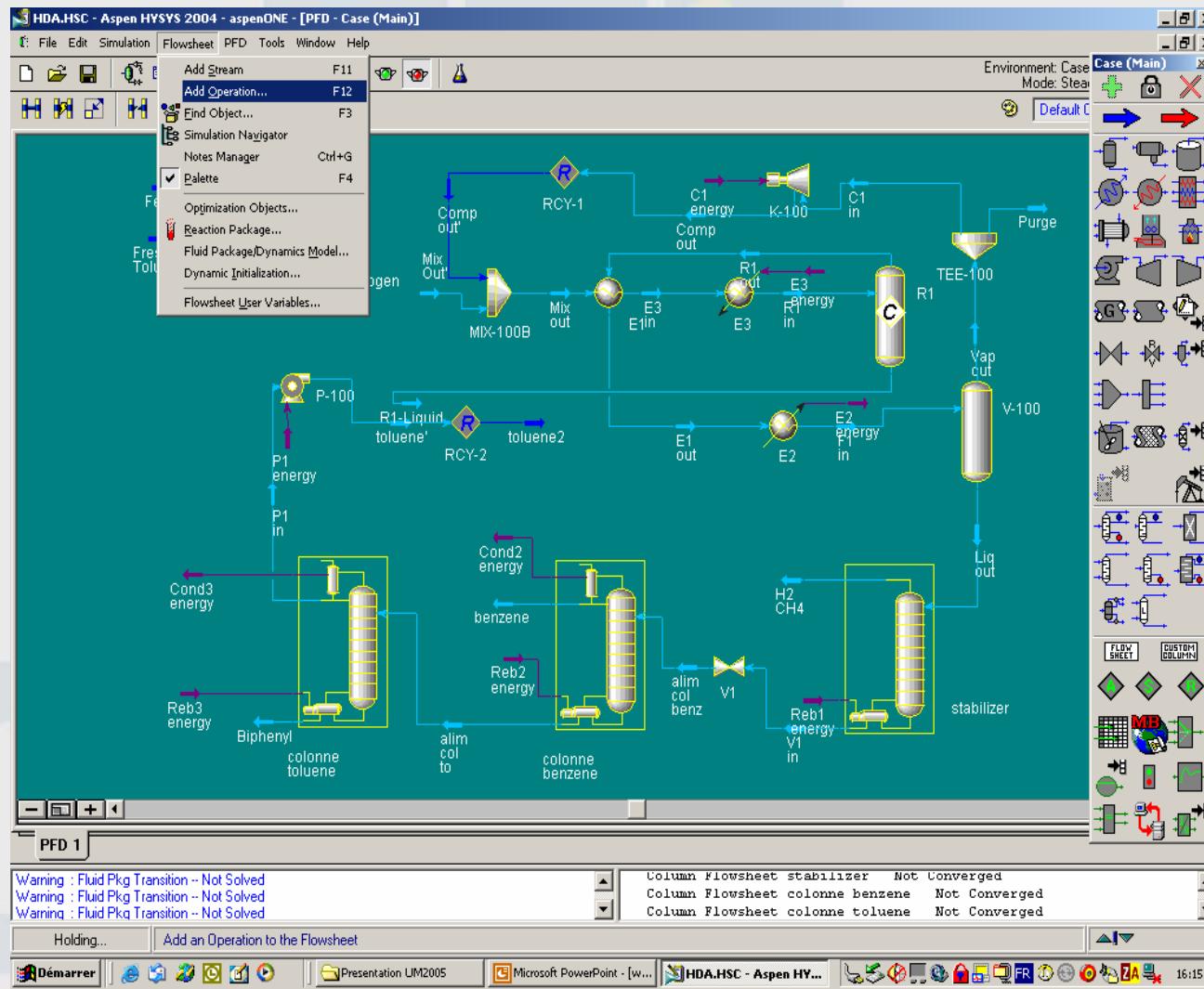
Since gPROMS mixer model involves basic material and energy balances, results with Aspen HYSYS 2004 native mixer and gPROMS mixer should be strictly the same.



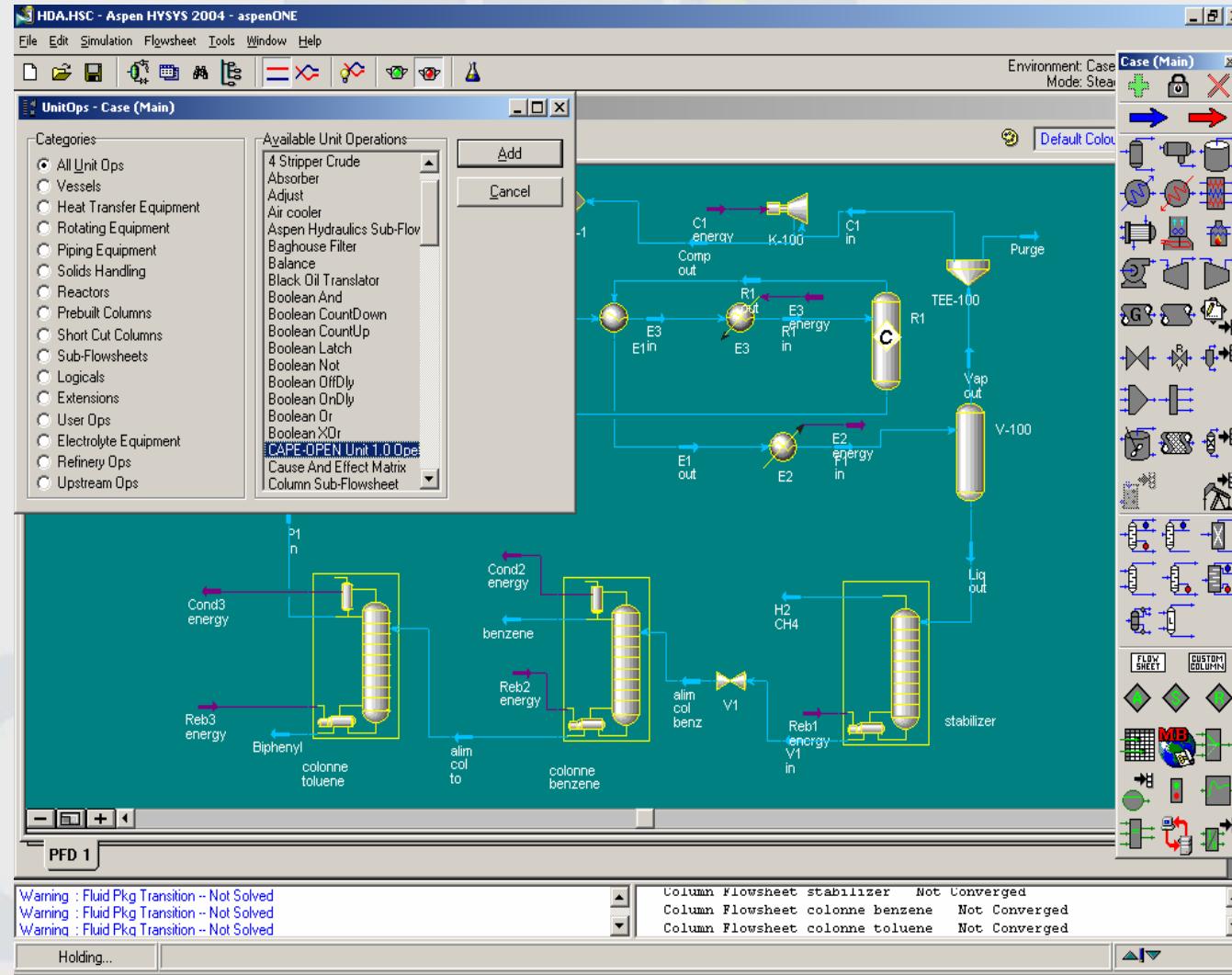
# Native mixer deleted and solver on hold



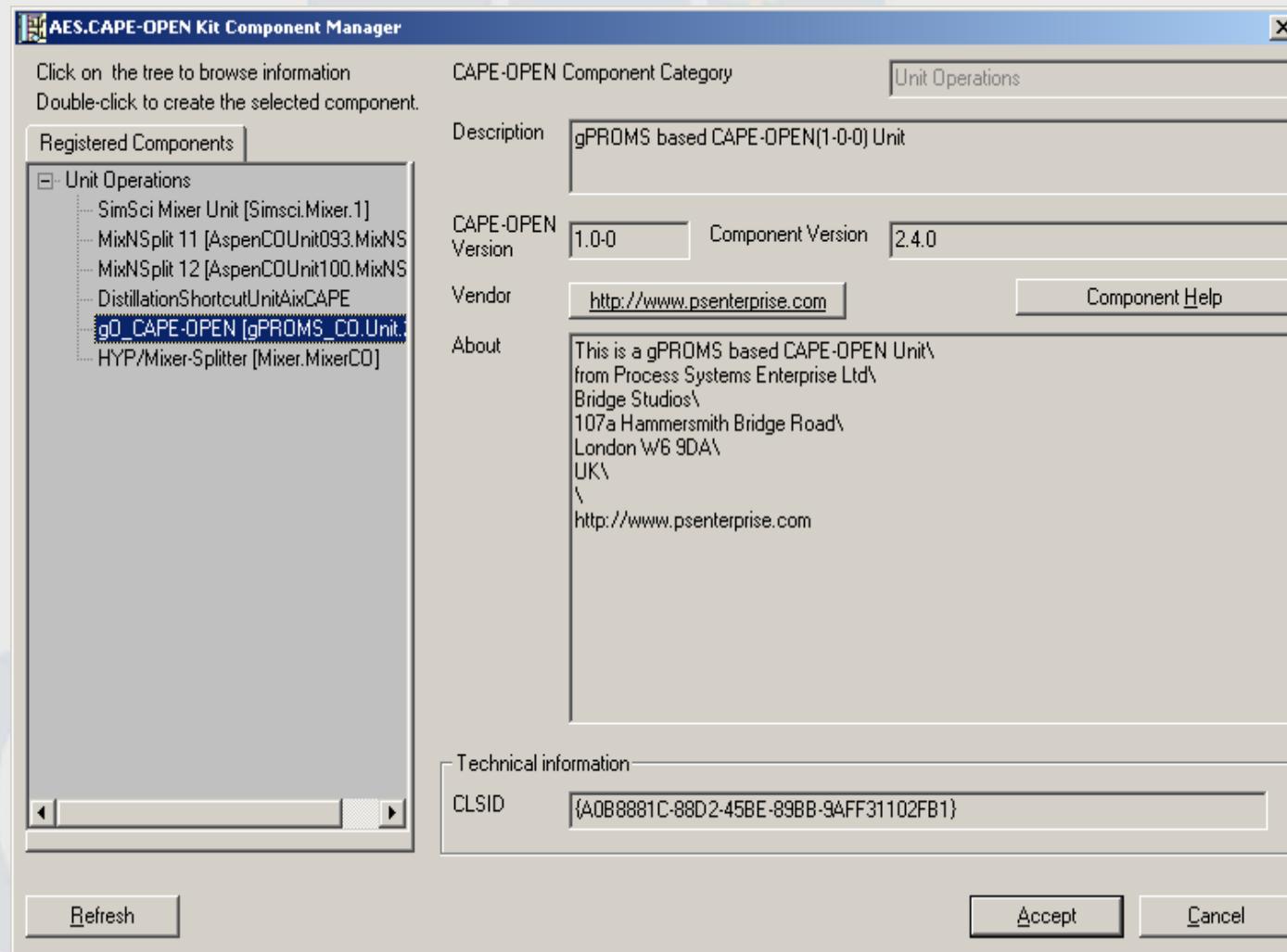
## Replace native Mixer



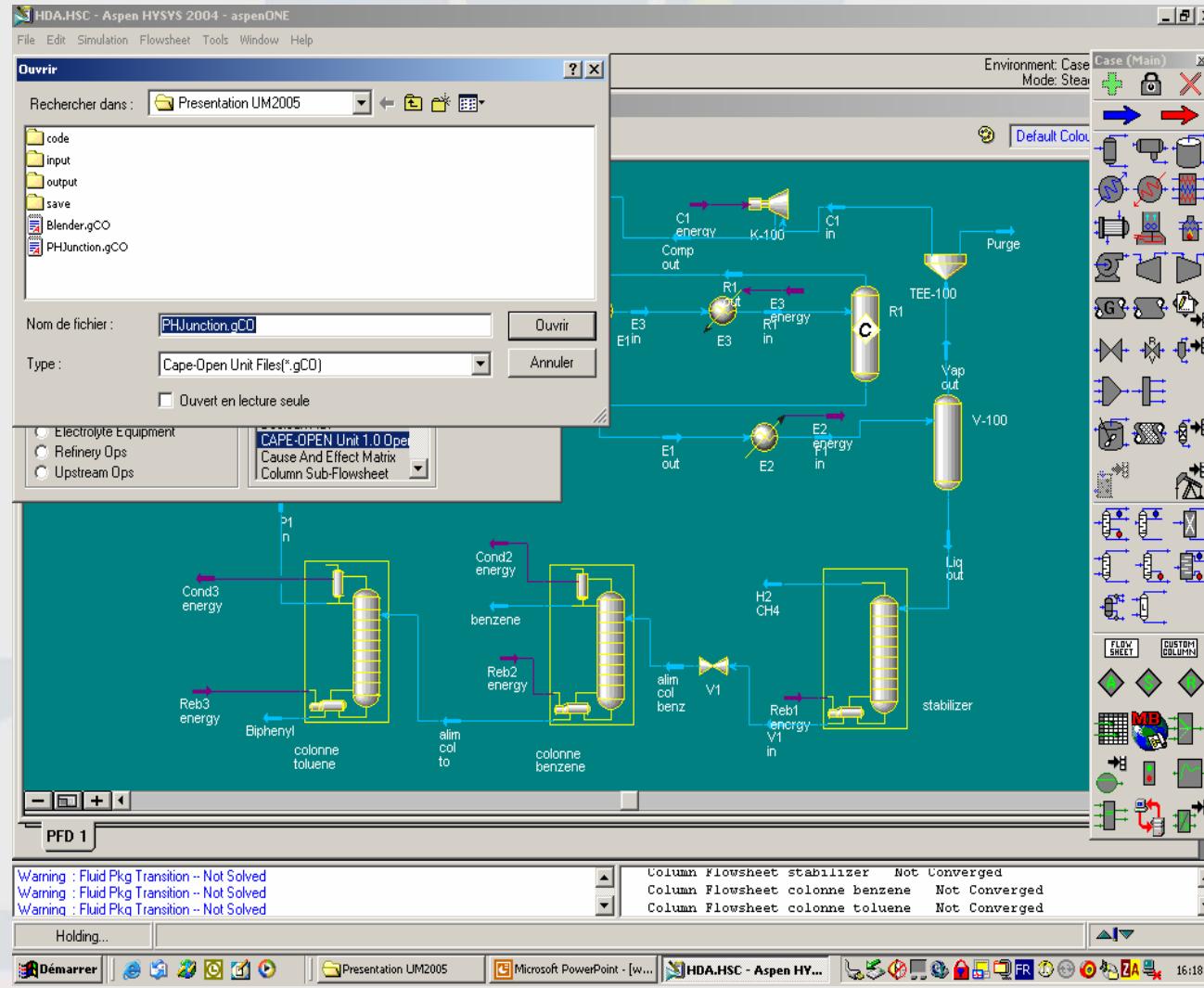
# Select CAPE-OPEN 1.0 UNIT Ops



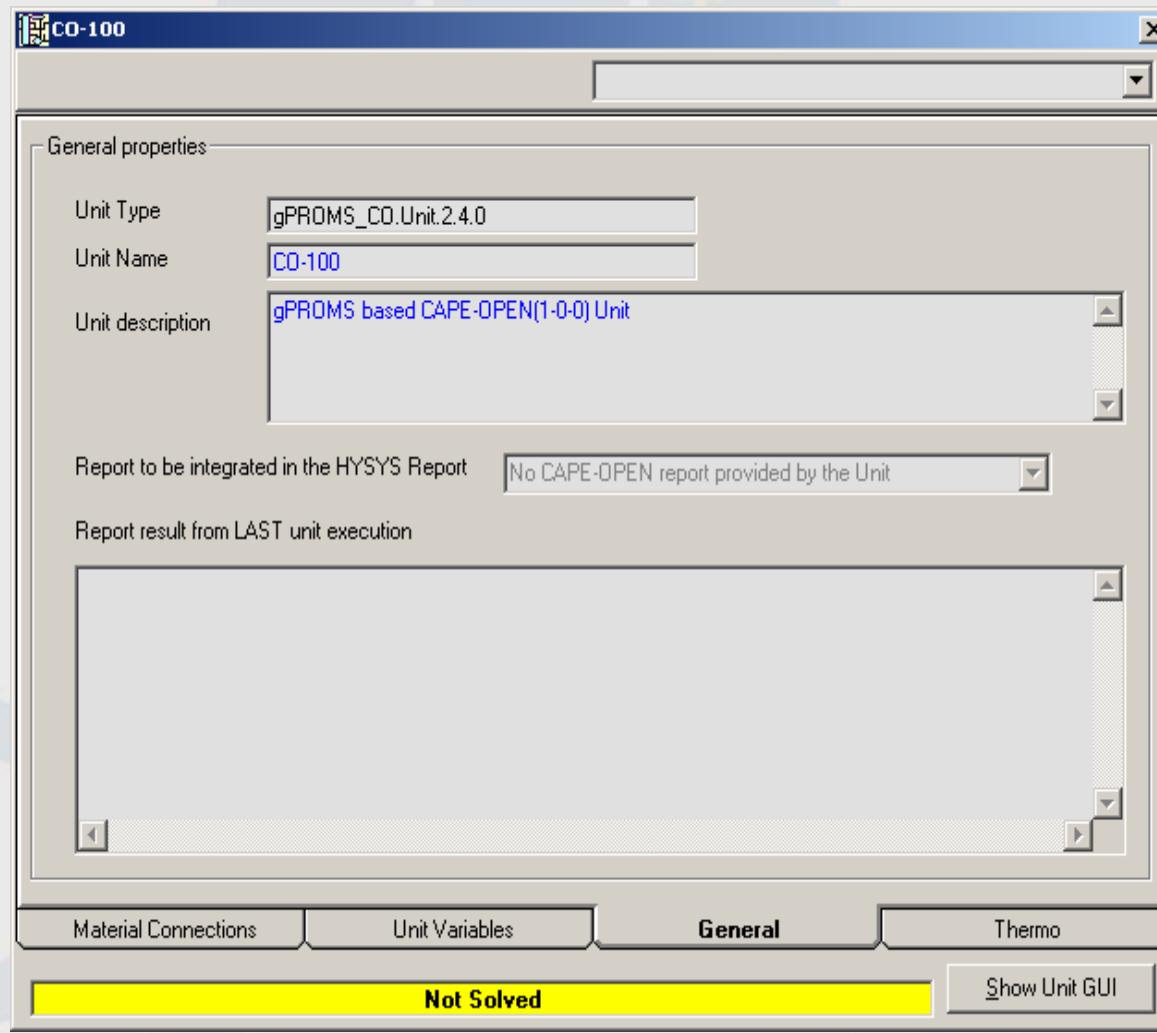
# Select gO:CAPE-OPEN wrapper



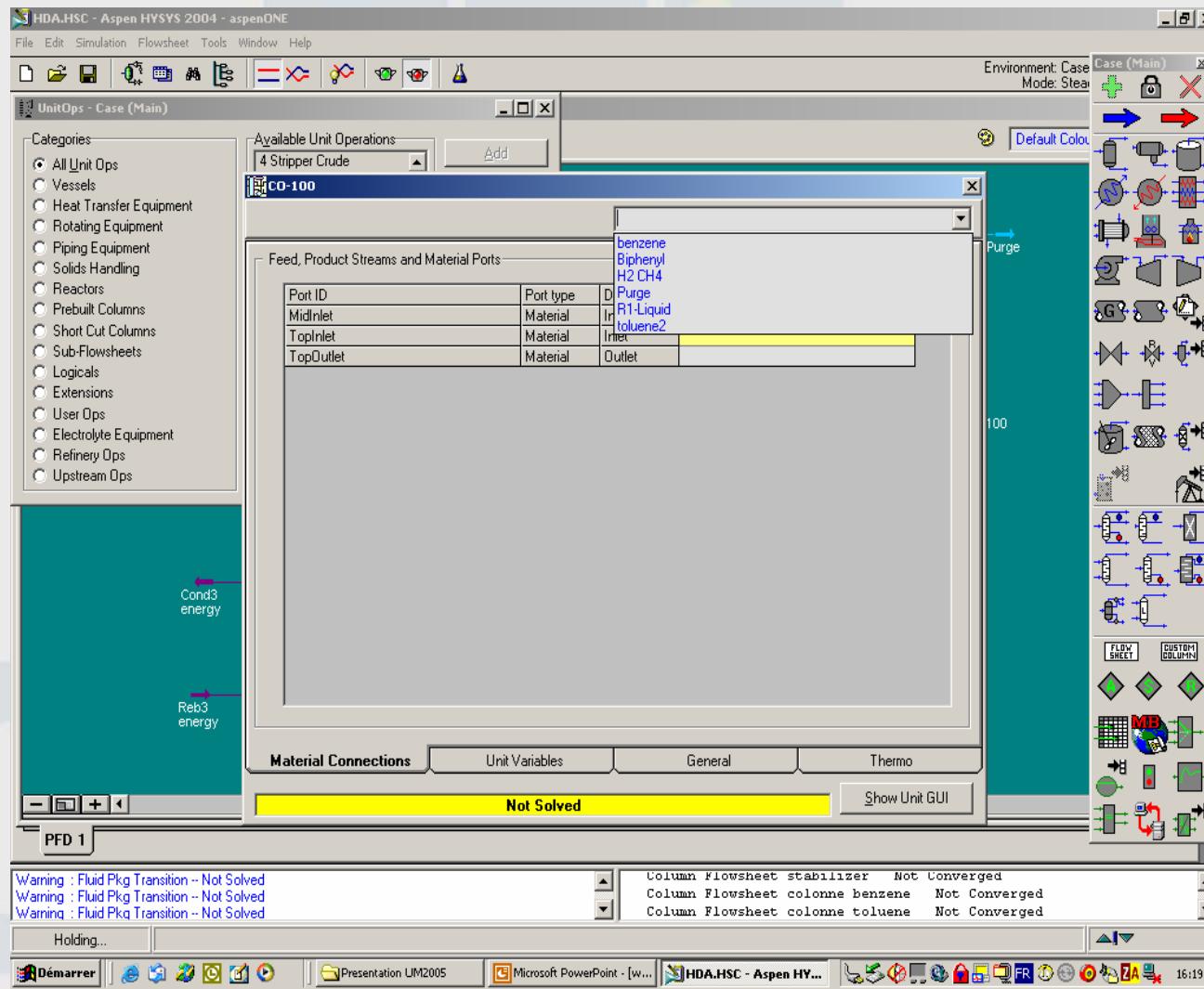
# Select the gCO file to be used



# Enter generic GUI provided by HYSYS



# Connect inlet and outlet ports to streams



# Set up the gPROMS model

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

**Left Window (Material Ports):**

- Title Bar:** CO-100
- Panel:** Mix Out'
- Section:** Feed, Product Streams and Material Ports
- Table:** Shows material ports with the following data:

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

**Bottom Buttons:**

- Material Connections
- Unit Variables
- General
- Not Solved
- Show Unit GUI

**Right Window (Unit Specific Data and Public Variables):**

- Title Bar:** CO-100
- Section:** Unit Specific Data and Public Variables
- Table:** Shows unit specific data and public variables with the following data:

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

**Bottom Buttons:**

- Material Connections
- Unit Variables
- General
- Not Solved
- Show Unit GUI
- Reset Parameters
- Thermo

**Annotations:**

- A callout bubble points to the bottom bar of the left window with the text: "All ports connected".
- A callout bubble points to the bottom bar of the right window with the text: "Initial parameter settings".



# Set energy input / pressure drop to zero

The screenshot shows two instances of the gPROMS Cape-Open Unit Object interface and two associated parameter modification dialog boxes.

**Top Left Window:** A standard gPROMS window titled "gPROMS Cape-Open Unit Object". It has tabs for "Unit Properties", "Input Parameters" (which is selected), "Report", "Ports", "Log", and "About". Below the tabs is a table of parameters:

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

A "Change Value" button is located at the bottom left of the window. A "Close" button is at the bottom right.

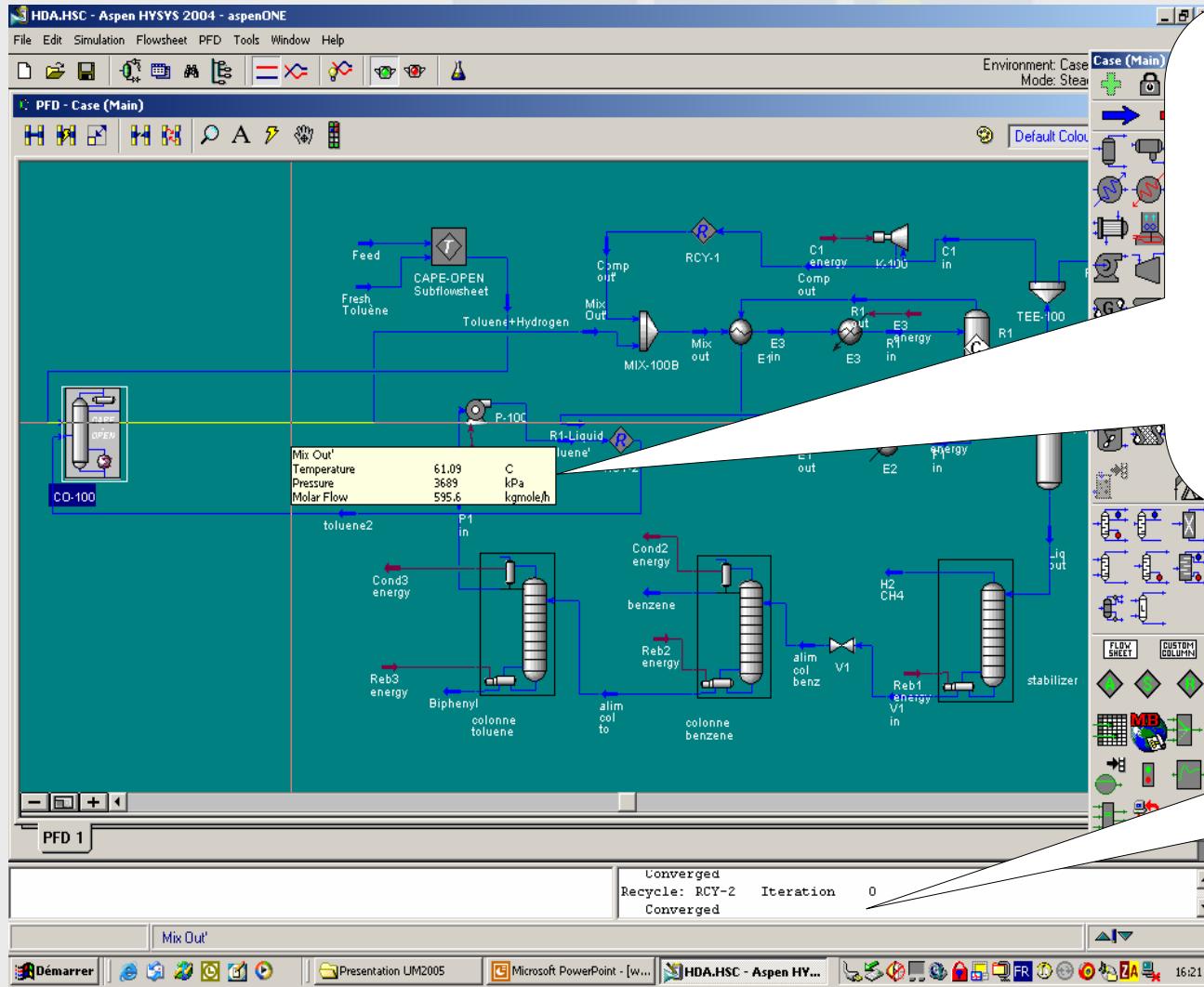
**Top Right Dialog:** A modal dialog titled "Energy rate" with fields for "Value" (0 J/s), "Lower Bound" (0), and "Upper Bound" (1000). It includes "OK" and "Cancel" buttons.

**Bottom Left Window:** A second instance of the gPROMS window, identical in structure to the top one, showing the same parameter values after modification.

**Bottom Right Dialog:** A modal dialog titled "Pressure Drop" with fields for "Value" (0 Pa), "Lower Bound" (0), and "Upper Bound" (1000). It includes "OK" and "Cancel" buttons.



# gPROMS Mixer output results



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

Simulation converged.



# Conclusion on interoperability

- ▼ Same gPROMS model usable in PRO/II (7.1), Aspen Plus 12.1, Aspen HYSYS 2004.
- ▼ No recoding necessary.
- ▼ gCO file easily deployable through an organization.
  - ⇒ Requests gO:CAPE-OPEN and gServer on target machine

