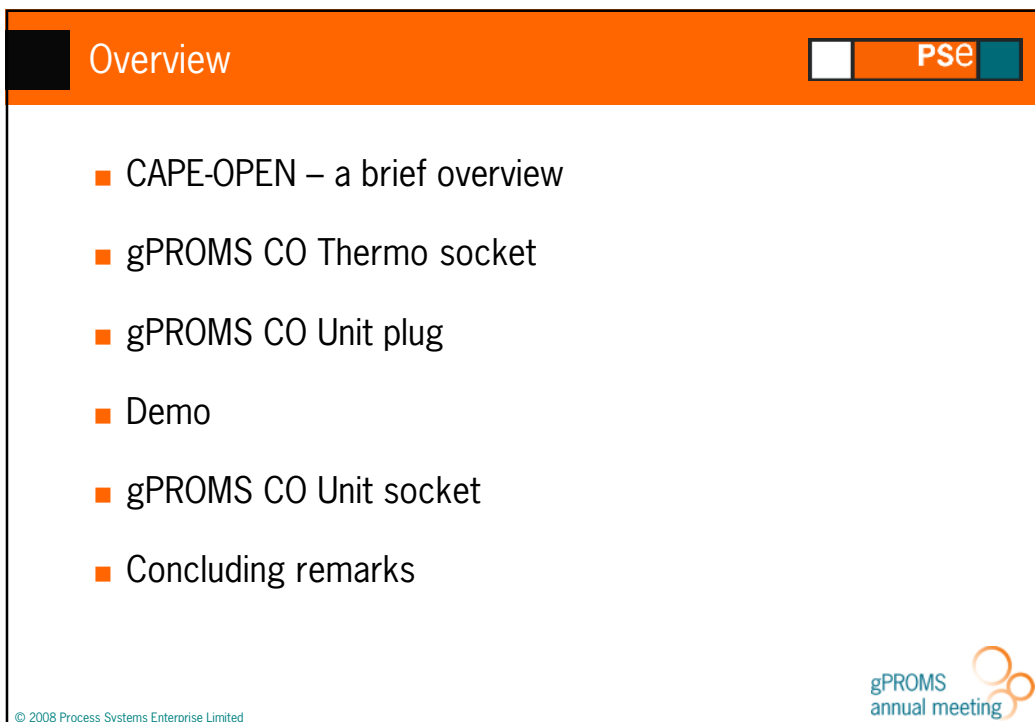


PSE

gPROMS v3.1+: CAPE-OPEN integration

Tom Williams – Principal Software Consultant

gPROMS
annual meeting



Overview

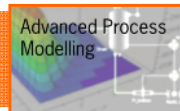
PSE

- CAPE-OPEN – a brief overview
- gPROMS CO Thermo socket
- gPROMS CO Unit plug
- Demo
- gPROMS CO Unit socket
- Concluding remarks

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CAPE-OPEN – a brief overview



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What is CAPE-OPEN?

- A freely available industry standard for interfaces between software components making up process simulation tools
- A successful collaboration between software vendors, end-users and academics
- A proven IT technology implemented in most process simulation tools
 - growing adherence by market leaders
- Maintained through CAPE-OPEN Laboratories Network (CO-LaN)
 - Michel Pons, Chief Technology Officer



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- Process Modelling Component (PMC)
 - well defined piece of software with a relatively narrow function
 - wide range of applications
 - physical/thermodynamic properties
 - unit operation modules
 - numerical solvers
 -
- Process Modelling Environment (PME)
 - allows construction of process model
 - from first-principles and/or library of unit operation models
 - supports a number of model-based applications
 - simulation, optimization, ...
 - may make use of one or more PMCs

- PSE has had a strong involvement from the beginning of the CAPE-OPEN initiative
 - initially via Imperial College London
 - helped define fundamental CO concepts & terminology
 - led design of numerical solvers interfaces
 - demonstrated use of CORBA middleware
- gPROMS was first **equation-oriented** PME to implement CAPE-OPEN sockets and plugs
 - thermo socket since gPROMS 2.1
 - unit plug since gPROMS 2.3
 - unit socket (prototype) since April 2007
 - kernel based on CAPE-OPEN numerical solvers

COThermoFO

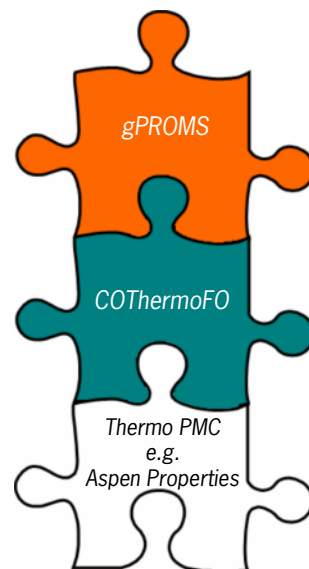
gPROMS CO Thermo socket




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gPROMS CO Thermo socket

- **COThermoFO** allows CO Thermo PMCs to be used within gPROMS, e.g.
 - Aspen Properties®, COMThermo (HYSYS®/UniSim®)
 - Multiflash® [CO interface]
 - Simulis® Thermodynamics, PPDS®, COCO®/TEA®
- A Foreign Object providing standard set of thermodynamic property methods
 - used by gPROMS PML and AMLs
 - alternative to native gPROMS interface to Multiflash®
- New since gPROMS 3.0.4
 - replaced earlier **CapeOpenThermo**
 - improved stability and diagnostics
 - improved PML compatibility
 - uniform treatment of thermo across all gPROMS' CAPE-OPEN components



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gO:CAPE-OPEN

gO:CAPE-OPEN
gPROMS CO Unit plug

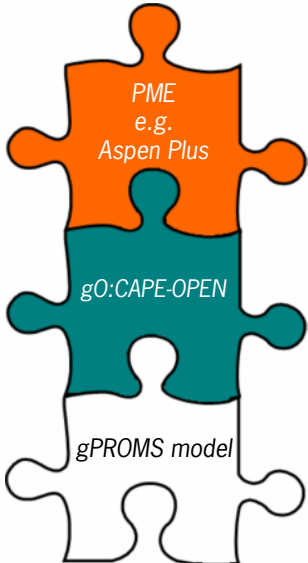
Advanced Process Modelling

Model-Based Innovation

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gPROMS CO Unit plug

- **gO:CAPE-OPEN** allows a gPROMS model to be embedded within a CAPE-OPEN PME, e.g.
 - Aspen Plus®, HYSYS®, UniSim®
 - PRO/II®, ProSim Plus®
 - COCO®/COFE®
- gPROMS model of any complexity
 - including 1D, 2D, 3D+ IPDAEs
- Wizard for exporting model from gPROMS ModelBuilder
 - no programming required
- New implementation for gPROMS 3.1
 - improved stability and diagnostics
 - improved compatibility with PML
 - uses same thermo implementation as **COThermoFO**
 - expose gPROMS PARAMETERS, SELECTORS and VARIABLES
 - allows use of TASK language for
 - model initialisation
 - dynamic models (e.g. batch distillation units) operating in "pseudo-steady" mode within steady-state PMEs



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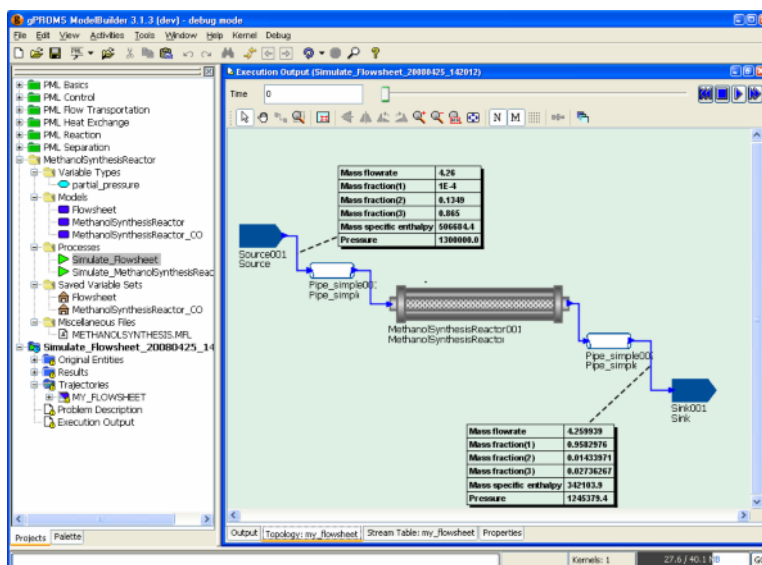
Demo

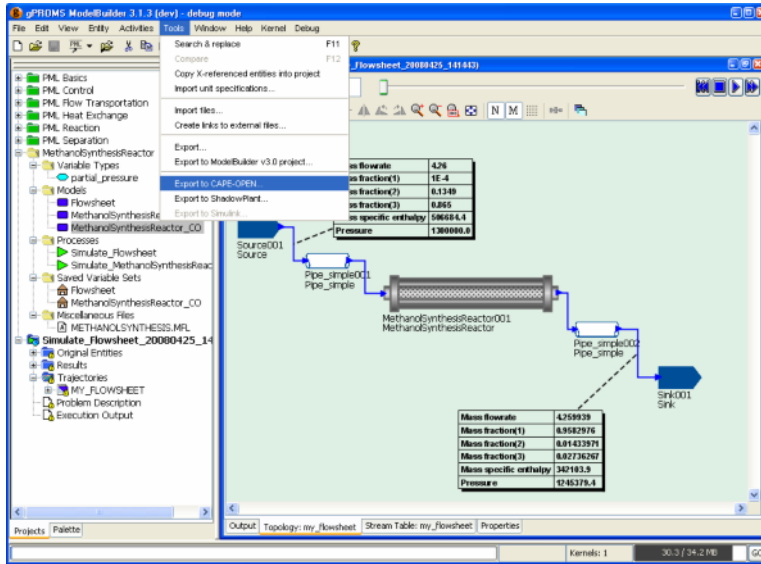
Exporting a gPROMS model as a CAPE-OPEN Unit Object

Advanced Process
Modelling

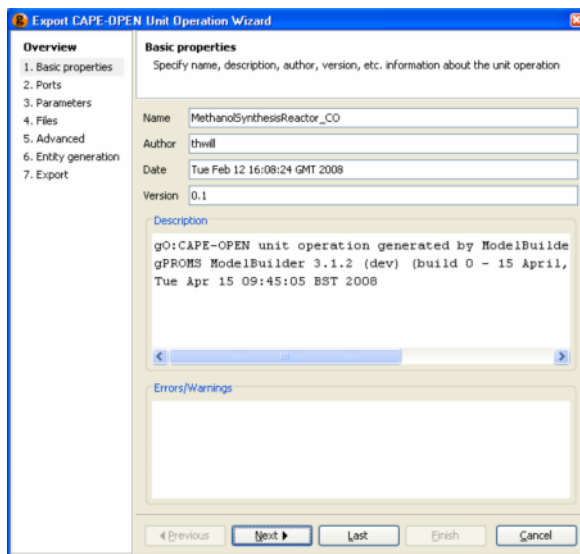
Model-Based
Innovation

Methanol reactor in gPROMS ModelBuilder





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Specifying...

- General information on model being exported

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Name	Type	Direction	Optional
feedStream	MATERIAL	INLET	<input type="checkbox"/>
productStream	MATERIAL	OUTLET	<input type="checkbox"/>

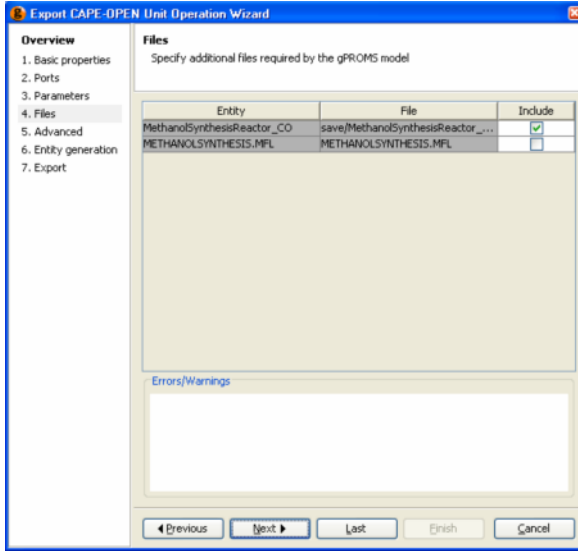
Specifying...

- General information on model being exported
- Connectivity information

Name	Type	Mode	Default	Units
Bed porosity	REAL	INPUT	0.48	
Catalyst density	REAL	INPUT	1700.0	
HTC	REAL	INPUT	1000.0	W/m2K
Heat input rate	REAL	INPUT	-1.1E7	J/s
Inner diameter	REAL	INPUT	1.2	m

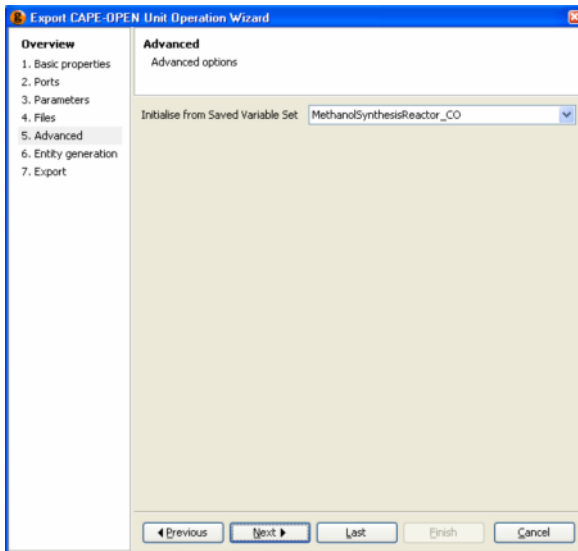
Specifying...

- General information on model being exported
- Connectivity information
- CAPE-OPEN parameters



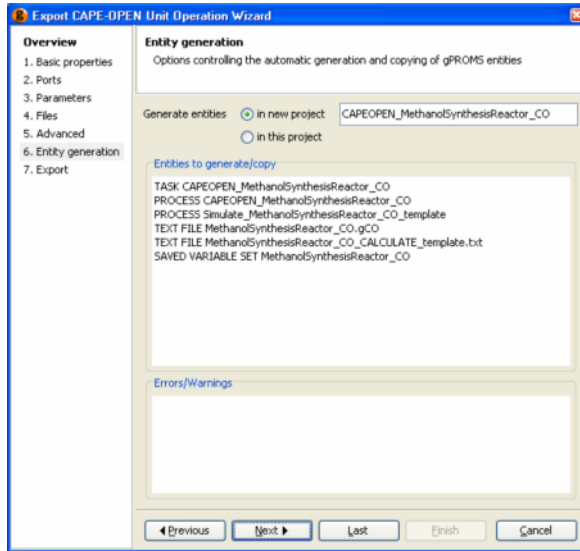
Specifying...

- General information on model being exported
- Connectivity information
- CAPE-OPEN parameters
- Additional files to be exported



Specifying...

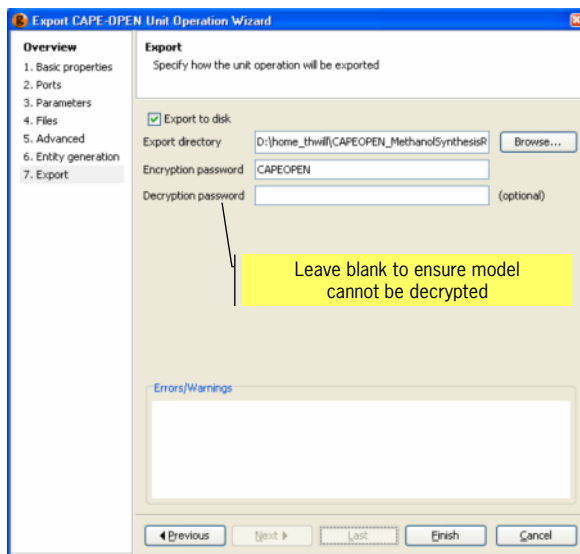
- General information on model being exported
- Connectivity information
- CAPE-OPEN parameters
- Additional files to be exported
- Other information



Specifying...

- General information on model being exported
- Connectivity information
- CAPE-OPEN parameters
- Additional files to be exported
- Other information

Wizard automatically generates all gPROMS entities and files required for communication between gPROMS Engine and CAPE-OPEN Unit



Specifying...

- General information on model being exported
- Connectivity information
- CAPE-OPEN parameters
- Additional files to be exported
- Other information

Wizard automatically generates all gPROMS entities and files required for communication between gPROMS Engine and CAPE-OPEN Unit

Export all necessary information to specified disk location



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Demo
Using a gPROMS CAPE-OPEN Unit Object
within a CAPE-OPEN compliant PME

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COCO from AmsterCHEM

PSE

amsterCHEM
tailor-made engineering software solutions



COCO

COCO (CAPE-OPEN to CAPE-OPEN) is a free-of-charge CAPE-OPEN compliant steady-state (sequential-modular) simulation environment

<http://www.cocosimulator.org/>

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Inserting missing reactor unit in COCO flowsheet

PSE

The screenshot shows the gPROMS interface with a COCO flowsheet. A dialog box titled "Insert stream" is open, with the "Insert unit operation" button highlighted. The flowsheet includes a Mixer, Compressor, reactorProduct, Cooler, and Splitter 1. Below the flowsheet is a table with process parameters and stream data.

Unit	parameter	value	unit
Compressor	Pressure increase	14830.0	Pa
Cooler	Pressure drop	0	Pa
Cooler	Heat duty	-0.2	MW
Splitter 1	Pressure drop	0	Pa
Splitter 1	Split fraction(D)	0.046	
Splitter 1	Split fraction(U)	0.95	

Stream	carbonMonoxideFeed	hydrogenFeed	reactorFeed	reactorProduct	cooledProduct	methanolProduct	purge	recycle	recycle2	Unit
Pressure	1.3e+006	1.3e+006	N/A	N/A	N/A	N/A	N/A	N/A	N/A	Pa
Temperature	475	475	N/A	N/A	N/A	N/A	N/A	N/A	N/A	K
Flow rate	2.865	0.576	N/A	N/A	N/A	N/A	N/A	N/A	N/A	kg/s
Mass frac Methanol	0	0	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
Mass frac Hydrogen	0	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
Mass frac Carbon monoxide	1	0	N/A	N/A	N/A	N/A	N/A	N/A	N/A	

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Selecting a gO:CAPE-OPEN unit

PSE

The screenshot shows the same gPROMS interface with the COCO flowsheet. A dialog box titled "Select Unit Operation" is open, displaying a tree view of available units. The "FLUENT" folder is expanded, showing sub-folders like "Generic", "PSE COLegacyUnit", "PSE COUnAFIPRProc", "PSE COUnAFIPRProc", and "SteamConverter". The "Heaters, Coolers & Heat exchangers" folder is also visible.

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Selecting the methanol reactor to be used under gO:CAPE-OPEN



The screenshot shows a gPROMS flowsheet with a dialog box titled 'gO:CAPE-OPEN - Open unit manifest file'. The dialog box contains a file explorer view showing 'MethanolSynthesisReactor_CO.gCO' selected. Below the dialog box, there are two tables: a parameter table and a stream table.

ID	parameter	value	unit
Compressor	Pressure increase	44820.8	Pa
Coiler	Pressure drop	0	Pa
Coiler	Heat duty	0.2	MW
Splitter 1	Pressure drop	0	Pa
Splitter 1	Split fraction[0]	0.046	
Splitter 1	Split fraction[1]	0.95	

Stream	carbonMonoxide	hydrogen	hydrogenFeed	reactorFeed	reactorProduct	lockedProduct	methanolProduct	purge	recycle	recycle2	Unit
Pressure	1.3e+006	1.3e+006	1.3e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	Pa
Temperature	475	475	474.874	502.478	481.123	481.123	481.123	481.123	481.123	484.846	K
Flow rate	3.658	0.575	4.46073	4.46076	4.46076	4.23773	0.0223038	0.200734	0.200734	0.200734	kg/s
Mass frac Methanol	0	0	0.0430044	0.05938	0.05938	0.05938	0.05938	0.05938	0.05938	0.05938	
Mass frac Hydrogen	0	1	0.125658	0.0146013	0.0146013	0.0146013	0.0146013	0.0146013	0.0146013	0.0146013	
Mass frac Carbon monoxide	1	0	0.827378	0.0284991	0.0284991	0.0284991	0.0284991	0.0284991	0.0284991	0.0284991	

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COCO flowsheet with gPROMS methanol reactor



The screenshot shows a gPROMS flowsheet with a 'gPROMS Reactor' unit highlighted in green. Below the flowsheet, there are two tables: a parameter table and a stream table.

ID	parameter	value	unit
Compressor	Pressure increase	44820.8	Pa
Coiler	Pressure drop	0	Pa
Coiler	Heat duty	0.2	MW
Splitter 1	Pressure drop	0	Pa
Splitter 1	Split fraction[0]	0.046	
Splitter 1	Split fraction[1]	0.95	

Stream	carbonMonoxideFeed	hydrogenFeed	reactorFeed	reactorProduct	lockedProduct	methanolProduct	purge	recycle	recycle2	Unit
Pressure	1.3e+006	1.3e+006	1.3e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	1.28517e+006	Pa
Temperature	475	475	474.874	502.478	481.123	481.123	481.123	481.123	484.846	K
Flow rate	3.658	0.575	4.46073	4.46076	4.46076	4.23773	0.0223038	0.200734	0.200734	kg/s
Mass frac Methanol	0	0	0.0430044	0.05938	0.05938	0.05938	0.05938	0.05938	0.05938	
Mass frac Hydrogen	0	1	0.125658	0.0146013	0.0146013	0.0146013	0.0146013	0.0146013	0.0146013	
Mass frac Carbon monoxide	1	0	0.827378	0.0284991	0.0284991	0.0284991	0.0284991	0.0284991	0.0284991	

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gO:CAPE-OPEN "edit dialog"

PSE

gPROMS Reactor - CAPE-OPEN unit operation

Basic | Parameters | Plots | Reports | About

gPROMS
gO:CAPE-OPEN 3.1.4
Built Apr 25 2008

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gO:CAPE-OPEN allows gPROMS models to be used within CAPE-OPEN compliant steady-state modular equation-oriented software. It conforms to CAPE-OPEN Unit Object 1.0.0 as described in document [CO-LaV \[CO_standards\]](#)

Support, bug reports and suggestions to:
support.gproms@pseenterprise.com

Visit our website for more information:
<http://www.pseenterprise.com>

OK Cancel

UID	parameter	value	unit
Compressor	Pressure increase	4830.5	Pa
Cooler	Pressure drop	0	Pa
Cooler	Heat duty	0.2	MW
Splitter 1	Pressure drop	0	Pa
Splitter 1	Split fraction[0]	0.046	
Splitter 1	Split fraction[1]	0.95	

Stream	carbonMonoxideFeed	hydrogenFeed	reactorFeed	reactorProduct	CO
Pressure	1.5e+006	1.5e+006	1.5e+006	1.25517e+008	1
Temperature	475	475	474.874	452.478	481
Flow rate	3.655	0.575	4.46073	14.46076	4
Mass fraction Methanol	0	0	0.0430044	0.05698	0
Mass fraction Hydrogen	0	1	0.123658	0.0445613	0
Mass fraction Carbon monoxide	1	0	0.827378	0.6284691	0

Starting solve
Solve finished

Ready

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gO:CAPE-OPEN "edit dialog" Basic information for methanol reactor

PSE

gPROMS Reactor - CAPE-OPEN unit operation

Basic | Parameters | Plots | Reports | About

gPROMS
gPROMS Reactor

Author: thvill
Date: Tue Feb 12 16:08:24 GMT 2008
Project: PSEUnitLibrary.gO:CAPE-OPEN.1
CLSID: EC90E93C-02D5-4402-9A09-E8E5E038CE52

gO:CAPE-OPEN
gO:CAPE-OPEN unit operation generated by ModelBuilder 'Export to CAPE-OPEN' wizard
gPROMS ModelBuilder 3.1.3 (dev) (build 0 - 21 April, 2008), running with Java 1.6.0_02
Mon Apr 21 11:30:43 EST 2008

OK Cancel

UID	parameter	value	unit
Compressor	Pressure increase	4830.5	Pa
Cooler	Pressure drop	0	Pa
Cooler	Heat duty	0.2	MW
Splitter 1	Pressure drop	0	Pa
Splitter 1	Split fraction[0]	0.046	
Splitter 1	Split fraction[1]	0.95	

Stream	carbonMonoxideFeed	hydrogenFeed	reactorFeed	reactorProduct	CO
Pressure	1.5e+006	1.5e+006	1.5e+006	1.25517e+008	1
Temperature	475	475	474.874	452.478	481
Flow rate	3.655	0.575	4.46073	14.46076	4
Mass fraction Methanol	0	0	0.0430044	0.05698	0
Mass fraction Hydrogen	0	1	0.123658	0.0445613	0
Mass fraction Carbon monoxide	1	0	0.827378	0.6284691	0

Starting solve
Solve finished

Ready

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gO:CAPE-OPEN "edit dialog"
CAPE-OPEN parameters for methanol reactor



The screenshot shows the gPROMS software interface with a process flow diagram and an open dialog box titled "gPROMS Reactor - CAPE-OPEN unit operation". The dialog box has tabs for "Basic", "Parameters", "Ports", "Reports", and "About". The "Parameters" tab is active, showing a table of parameters:

Name	Units	Type	Mode	Value	Lower Bound	Upper Bound
BASIS	OPTION	INPUT	mass	n/a	n/a	n/a
MD_DIAGNOSTICS	BOOLEAN	INPUT		<input checked="" type="checkbox"/>	n/a	n/a
Bld density	REAL	INPUT		0.45	0.4	0.5
Catalyst density	REAL	INPUT		1700	1500	2000
HTC	W/m ² K	REAL	INPUT	1000	100	2000
Heat input rate	J/s	REAL	INPUT	-11020000	-1e+010	1e+010
Inner diameter	m	REAL	INPUT	1.2	1	2
Outer diameter	m	REAL	INPUT	1.3	1	2
Length	m	REAL	INPUT	10	5	15

Below the table, there is a "Starting solve" button and a "Solve finished" status indicator. The background shows a process flow diagram with a central reactor unit and various feed and product streams.

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gO:CAPE-OPEN "edit dialog"
CAPE-OPEN ports for methanol reactor



The screenshot shows the gPROMS software interface with a process flow diagram and an open dialog box titled "gPROMS Reactor - CAPE-OPEN unit operation". The dialog box has tabs for "Basic", "Parameters", "Ports", "Reports", and "About". The "Ports" tab is active, showing a table of ports:

Name	Type	Direction	Optional
productStream	MATERIAL	OUTLET	false
feedStream	MATERIAL	INLET	false

Below the table, there is a "Starting solve" button and a "Solve finished" status indicator. The background shows a process flow diagram with a central reactor unit and various feed and product streams.

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gO:CAPE-OPEN "edit dialog" Execution diagnostics

PSE

gPROMS Reactor - CAPE-OPEN unit operation

Report: execution output

```

License granted by server(s) pseed1887.
Performing initialisation calculation at time: 0
Attempting solution with the currently active IF and CASE branches
Initialisation calculation completed.
Initialising Foreign Process Interface: eventFPI::CAPEOPEN_MethanolSynthesisReu
Loaded 'eventFPI.dll'.
Initialising Foreign Process Interface for process CAPEOPEN_MethanolSynthesisRe
Initialisation of Foreign Process Interface completed successfully.
Performing reinitialisation calculation at time: 0
Attempting solution with the currently active IF and CASE branches
Reinitialisation calculation completed.
Performing reinitialisation calculation at time: 0
Attempting solution with the currently active IF and CASE branches
Reinitialisation calculation completed.
Performing reinitialisation calculation at time: 0
Attempting solution with the currently active IF and CASE branches
Reinitialisation calculation completed.
Reinitialisation calculation completed.
    
```

Stream	carbonMonoxideFeed	hydrogenFeed	reactorFeed	reactorProduct	CO
Pressure	1.3e+006	1.3e+006	1.3e+006	1.25517e+008	1
Temperature	475	475	474.874	472.478	481
Flowrate	2.655	0.575	4.46073	14.46076	1
Mass Frae Methanol	0	0	0.0400544	0.05698	1
Mass Frae Hydrogen	0	1	0.126558	0.0445613	1
Mass Frae Carbon monoxide	1	0	0.827378	0.6224591	1

Starting solve
Solve finished
Ready

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gPROMS annual meeting

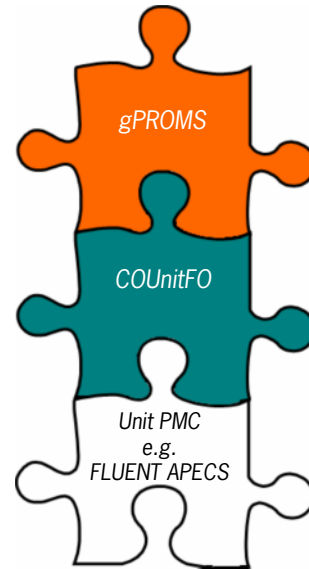
COUnitFO gPROMS CO Unit socket

PSE

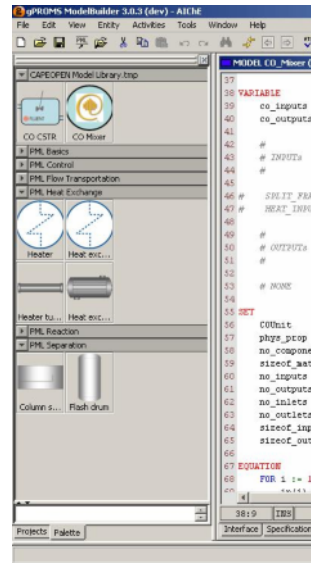
Advanced Process
Modelling

Model-Based
Innovation

- **COUnitFO** allows CO Unit operation PMCs to be used within gPROMS, e.g.
 - FLUENT®/APECS®
 - HTRI® (Heat Exchangers)
 - ChemSep® (Distillation Columns)
 - COLegacyUnit
 - A Foreign Object providing a Calculate() method
 - “given the unit’s inputs, calculate its outputs”
 - ... but there is more to a CO Unit than an input/output calculation, e.g.
 - inlet/outlet structure
 - physical property calculations
 - own user interface
 -
- ⇒ **CO Units are wrapped within native gPROMS MODELS**
- a CAPE-OPEN MODEL library in gPROMS
 - compatible with PML and AMLs



- Wrapping CO Units within gPROMS MODELS allows advanced customisation, e.g.
 - addition of further equations in symbolic form
 - unit specification dialogs
 - custom reports
 - specification of icon
- Wrapping quite simple
 - currently a semi-automatic command-line utility
 - to be replaced by an import wizard within ModelBuilder
- Prototype version compatible with gPROMS 3.1 available to interested parties

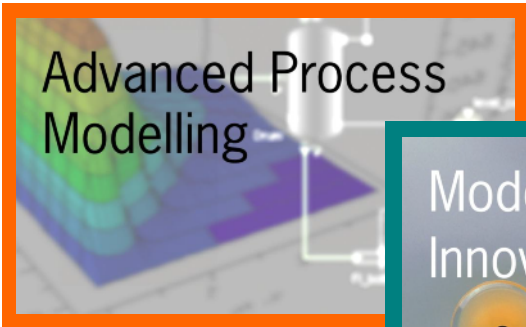


Concluding remarks

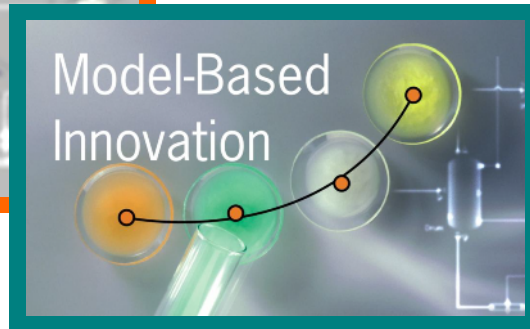


Concluding remarks

- PSE strongly committed to CAPE-OPEN ideas & standards
 - significant benefits to process engineering software and its users
- gPROMS 3.1 comes with
 - CO Thermo socket (COThermoFO)
 - CO Unit plug (gO:CAPE-OPEN)
- Future developments
 - lots more interoperability testing
 - consolidate CO Unit socket prototype
 - enhance CO Unit plug
 - more initialisation options
 - customizable “Edit Dialog”
 - CO Thermo 1.1 support
 - development of “Extended Sequential Modular” Unit plug/socket



Thank you !



www.psenetprise.com