

Deployment of a gPROMS-based three-phase reactor model as a CAPE-OPEN unit operation within PRO/II

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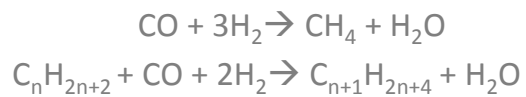
Outline

- Model description and deployment requirements
- Project approach
- Work flow
- Enhancements to PRO/II and gPROMS CAPE-OPEN components
- Conclusions

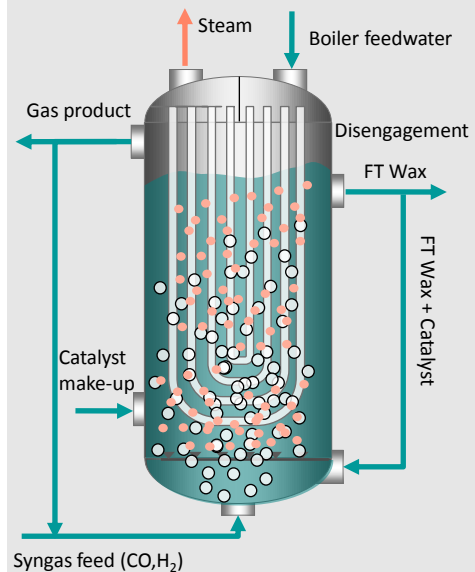
Model description and deployment requirements

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Model of slurry reactor for Fischer-Tropsch synthesis



- Multiphase slurry bubble column reactor model
- Objective: predict conversion, selectivity, product distribution
- Scope:
 - 2D momentum balance
 - 1D species and energy balances in each phase
 - Detailed FT kinetic mechanism
 - Transport of species and energy between phases



Original model implementation

- Developed by in collaboration by Laval University and TOTAL:
Iliuta I., F. Larachi, J. Anfray, N. Dromard, and D. Schweich,
“Multicomponent multicompartiment model for Fischer-Tropsch SCBR,” AIChE Journal, Vol. 53, No. 8, 2062-2083, 2007.
- Implemented using Aspen Custom Modeler
- Internally coded thermodynamic calculations
- 280,000 to 400,000 variables
- Solution time: ~ 35 minutes
- Manual intervention during initialization

TOTAL wished to deploy model within flowsheet of entire process developed in PRO/II

End user requirements:

- Modify model input parameters within PRO/II without recompilation
- Initialization without manual intervention
- Decrease memory use
- Increase speed
- Access to internal model variables at the converged solution
- Option to use PRO/II thermodynamic calculations

Achievable using **gPROMS** and its CAPE-OPEN components

Project approach



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Project approach

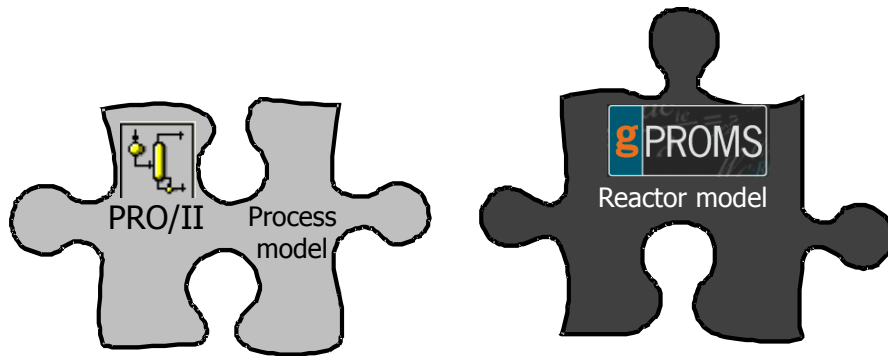


- Translate model from ACM to gPROMS
- Improve model performance:
 - Non-uniform grids
 - Smooth discontinuities in hydrodynamic model
 - Review of variable types and equation scaling
- Implement robust initialization procedure
 - Solves sequence of 5 problems of increasing complexity
 - No initial guesses required
- Add physical property calculations through calls to CAPE-OPEN compliant physical property packages.
- Test model within PRO/II.

Close PSE/Invensys collaboration to address software issues

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Implementation: bringing the pieces together



PRO/II flowsheet of any complexity
including recycle streams

gPROMS model of any complexity
including 1D, 2D, 3D+ IPDAEs

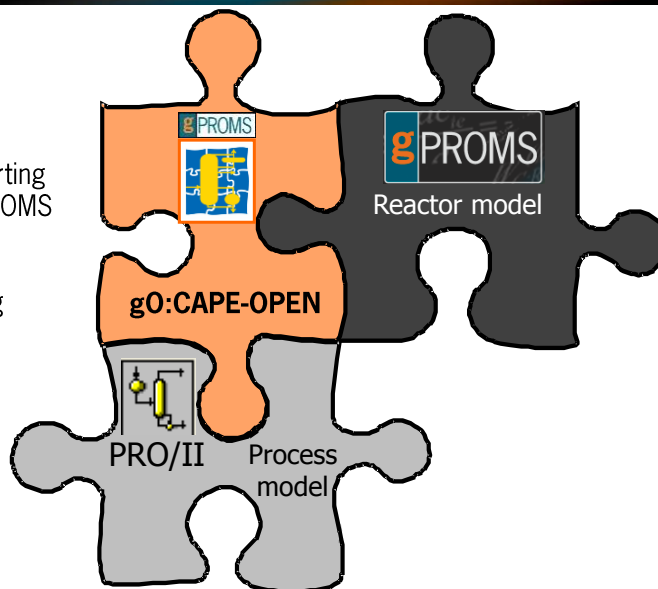
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1) gPROMS CO Unit plug allows model to be exported for use as a CAPE-OPEN unit operation within PRO/II



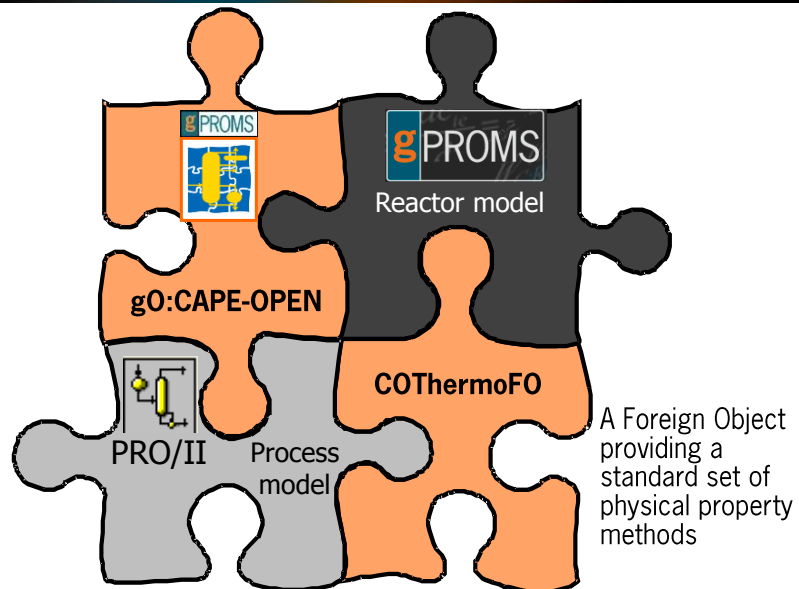
Wizard for exporting
model from gPROMS
ModelBuilder:

no programming
required



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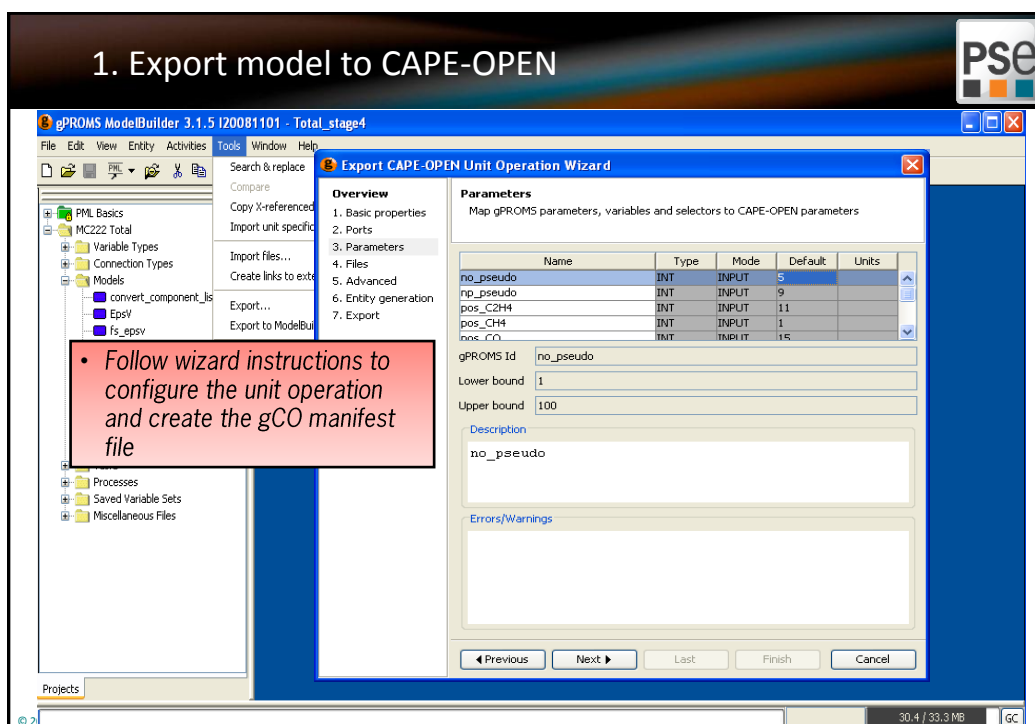
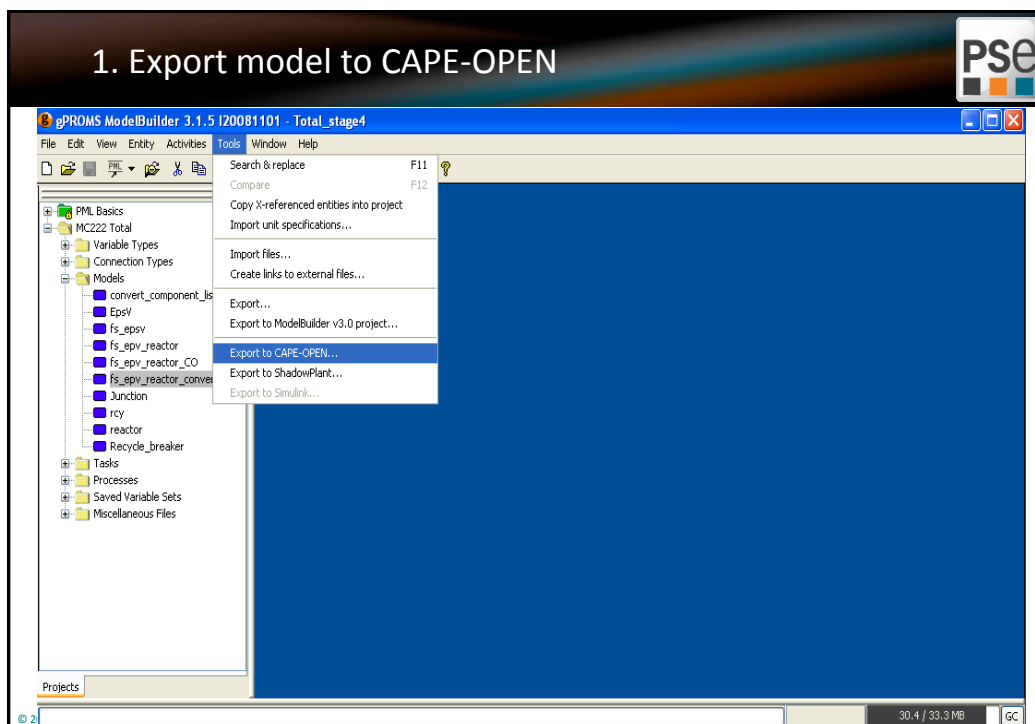
2) gPROMS CO thermo socket allows reactor model to use PRO/II physical properties in its calculations



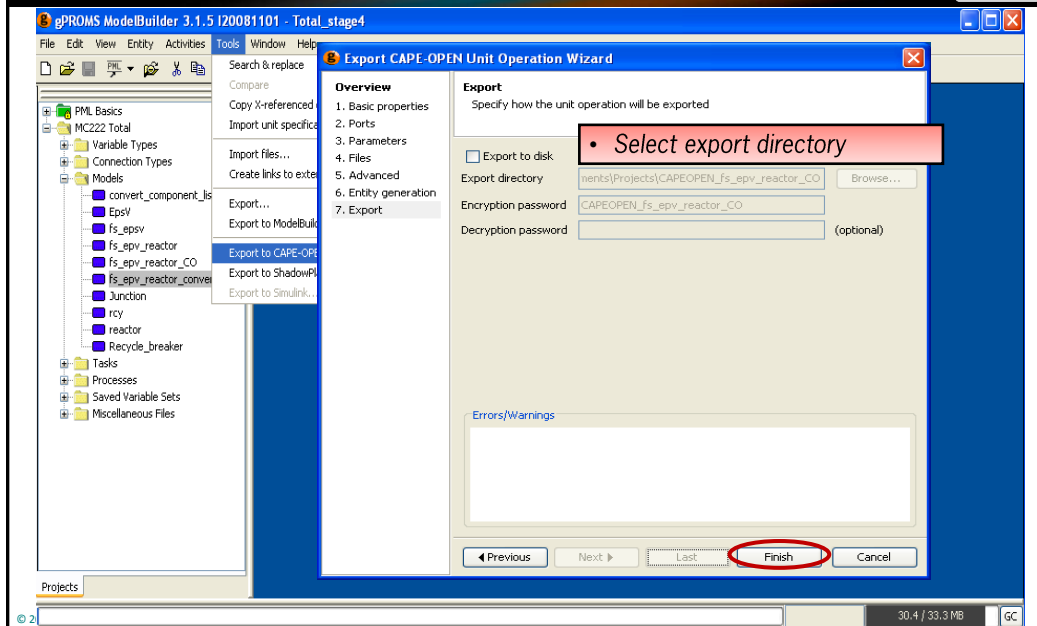
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The work flow in detail

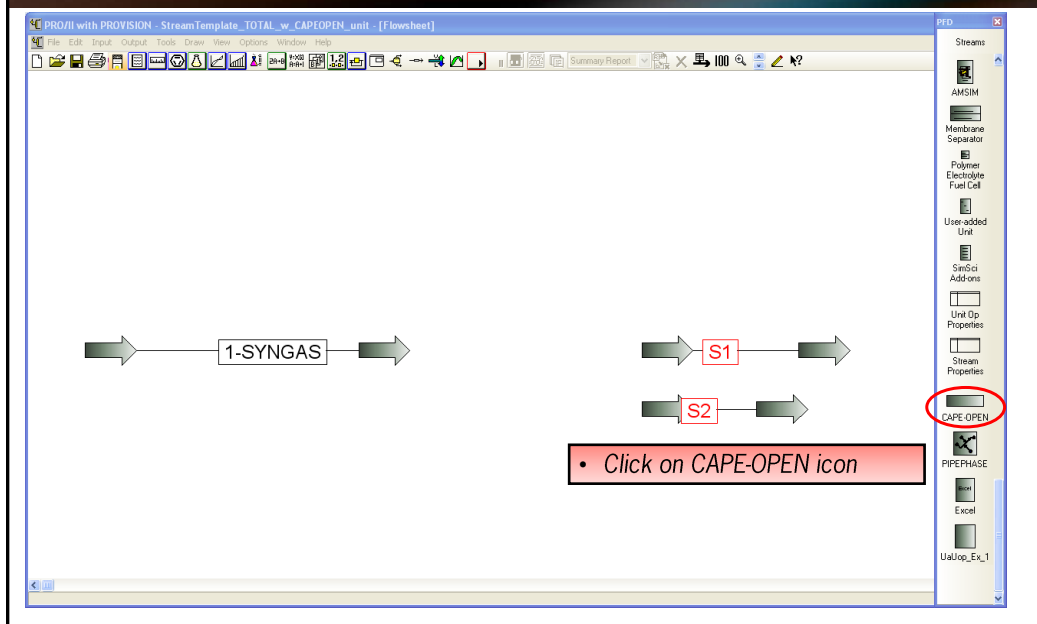
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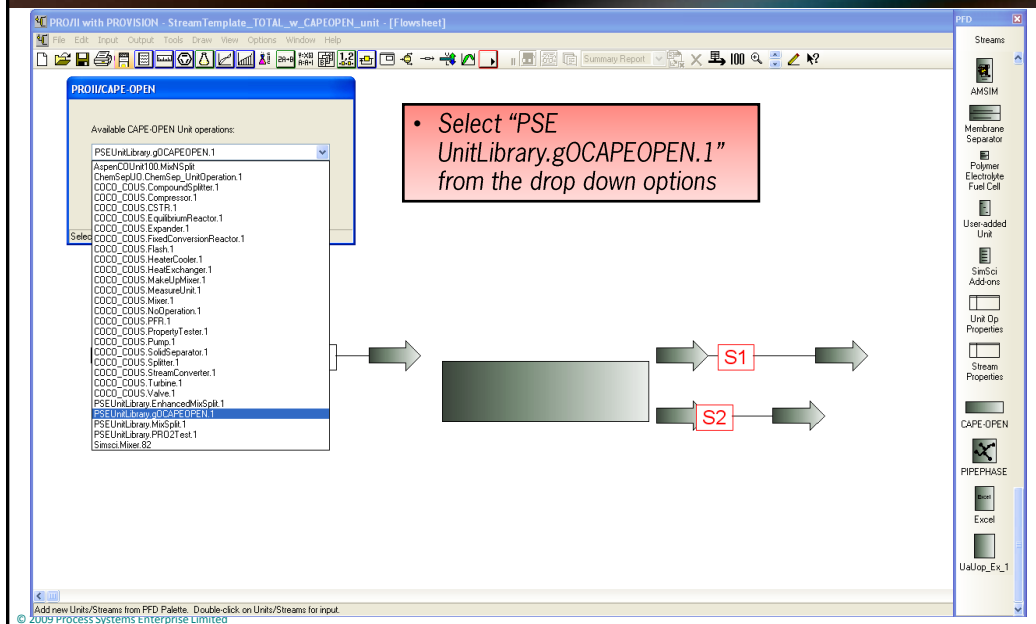
1. Export model to CAPE-OPEN



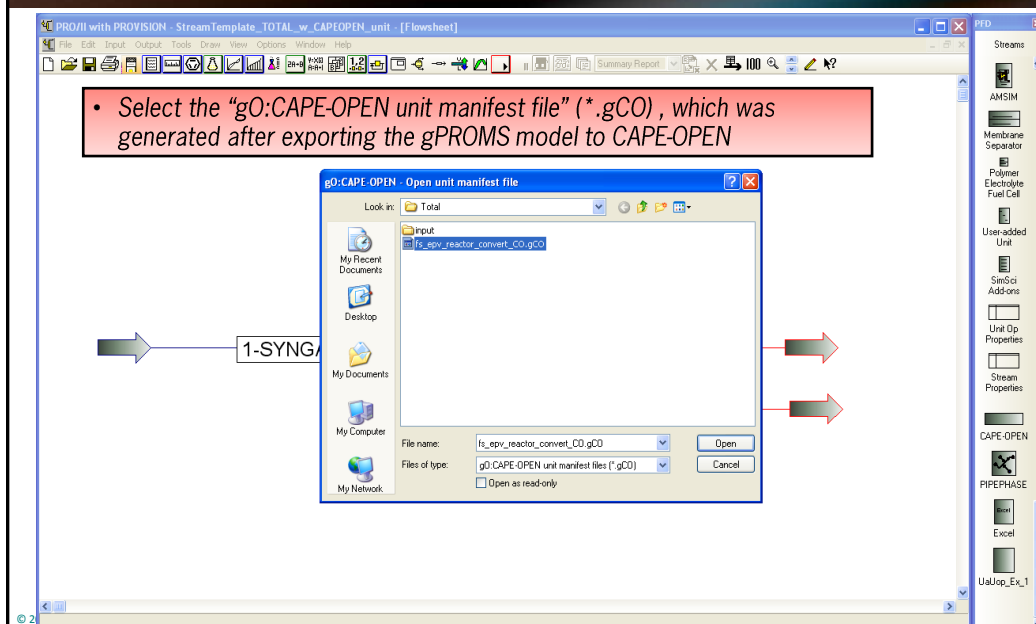
2. Insert exported CAPE-OPEN unit into flowsheet



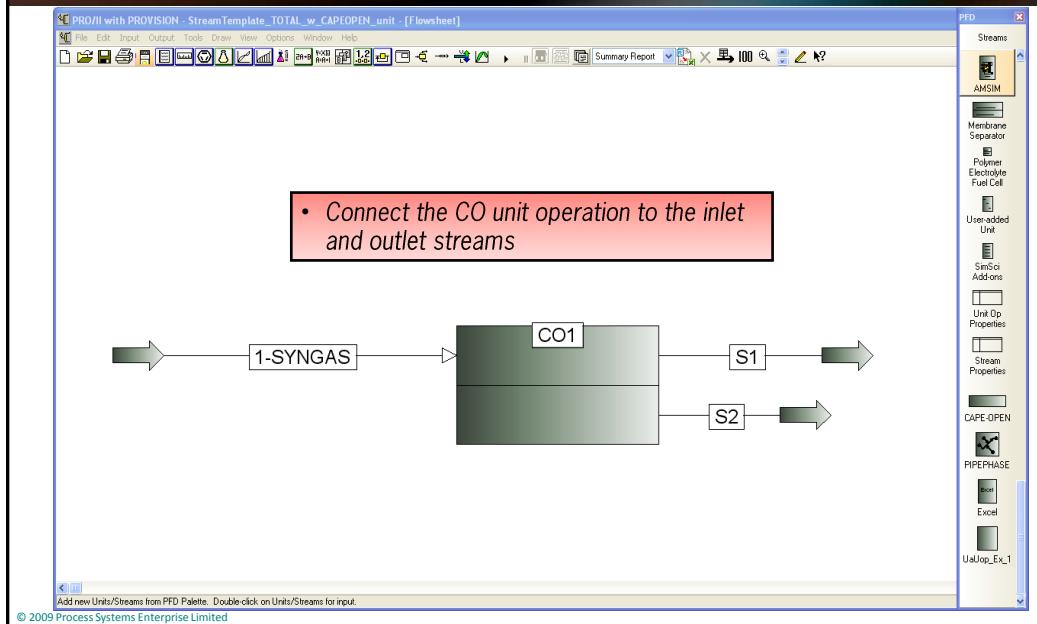
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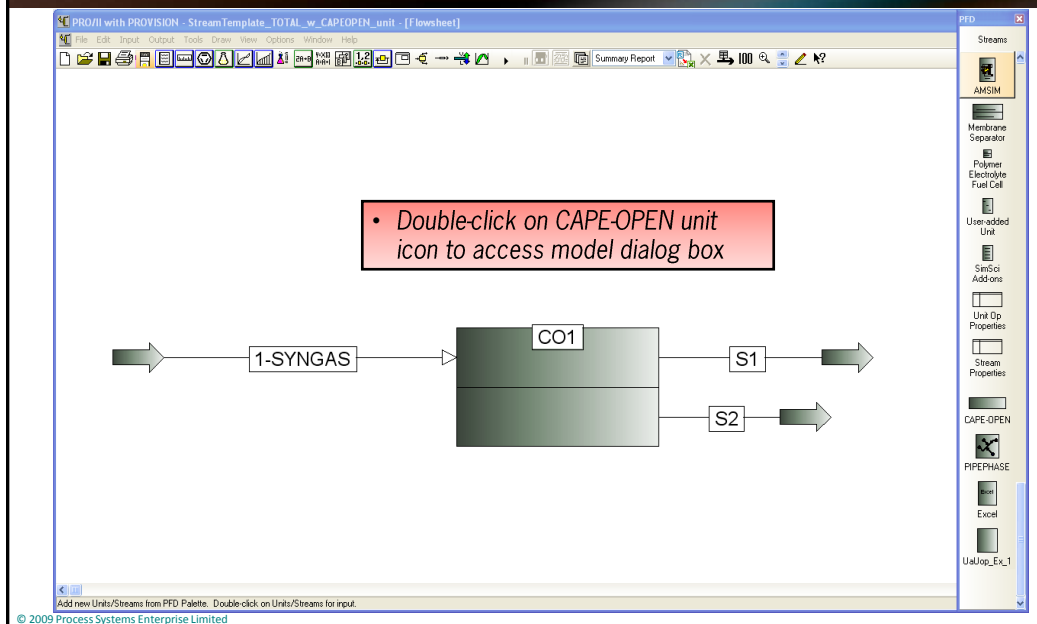
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2. Insert exported CAPE-OPEN unit into flowsheet



3. Configure the unit through its dialog box



3. Configure the unit through its dialog box

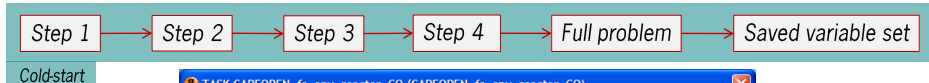
Parameters selected during "Export to CAPE OPEN" are accessible in PRO/II

Name	Units	Type	Mode	Value	Lower Bound	Upper Bound
BASIS		OPTION	INPUT	mole	n/a	n/a
NO_DIAGNOSTICS		BOOLEAN	INPUT	false	n/a	n/a
EPSV.Pres		REAL	INPUT	25	20	30
EPSV.Rmax	m	REAL	INPUT	3.5	0.2	10
eps_C2H4		INTEGER	INPUT	13	1	100
				5	1	100
				1	1	100
				3	1	100
				2	1	100
				4	1	100
				17	1	100
reactor.J_pseudo_olef		INTEGER	INPUT	1	0	100
reactor.J_pseudo_par		INTEGER	INPUT	4	0	100
reactor.n_k_olef		INTEGER	INPUT	11	1	100
reactor.n_k_par		INTEGER	INPUT	11	1	100
reactor.no_pure		INTEGER	INPUT	3	3	100
reactor.np_pure		INTEGER	INPUT	4	4	100
phys_prop_source		OPTION	INPUT	external	n/a	n/a
start_type		INTEGER	INPUT	0	0	100

4. Converge the flowsheet (automatic procedure executed by gPROMS unit operation)



- Simple flowsheets (no recycles): **Cold-start (~ 5 min.)**



Cold-start

```

TASK CAPEOPEN_fs_epv_reactor_CO (CAPEOPEN_fs_epv_reactor_CO)
41 IF start_type < unitOp.reactor.warm_start THEN
42 SEQUENCE
43 IF phys_props > 0.5 THEN
44 SWITCH
45 unitOp.reactor.phys_prop_source_ext := unitOp.reactor.external;
46 END
47 END
48 SWITCH
49 unitOp.reactor.n_simul := unitOp.reactor.complete_kin;
50 END
51 SWITCH
52 unitOp.reactor.thermo_model := unitOp.reactor.non_ideal;
53 unitOp.reactor.solution_mode := unitOp.reactor.normal;
54 unitOp.EPSV.carbon_number := unitOp.EPSV.calculated;
55 END
56 SWITCH
57 unitOp.EPSV.Ug_mode := unitOp.epsv.normal;
58 unitOp.reactor.rhoI_closure := unitOp.reactor.close_rhoI;
59 END
60 SWITCH
61 unitOp.reactor.regime := unitOp.reactor.non_isotherm;
62 END
63 SAVE "reactor_init" #)
64 END # sequence
65 END # if
  
```

4. Converge the flowsheet (automatic procedure executed by gPROMS unit operation)

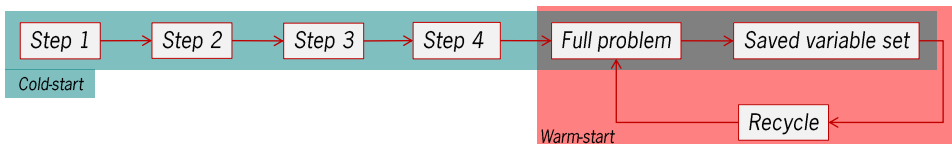


- Simple flowsheets (no recycles): **Cold-start** (~ 5 min.)

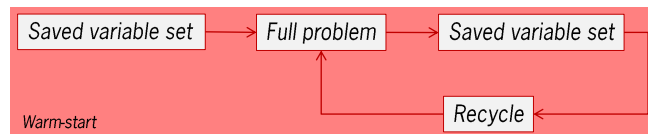


- Complex flowsheets

- Cold-start** followed by **warm-start** (~ 30 seconds per pass)



- Option to use a **warm-start** if a saved variable set is available



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5. Examine results

- Within unit's model report in PRO/II

	feedStream	productStream	vap_Stream
Pressure (Pa)	2.7E+006	2.38164E+006	2.38164E+006
Temperature (K)	513.849	523.871	523.878
Enthalpy (J/mol)	9757.23	120925	24890.8
Enthalpy (J/kg)	698564	655608	1.18558E+006
Vap. Frac. (mol/mol)	1	0	1
(kg/kg)	1	0	1
Flow (mol/s)	5720.44	1.0735	3753.76
(kg/s)	79.9006	0.198005	78.8088
Energy Flow (J/s)	5.58157E+007	129814	9.34343E+007

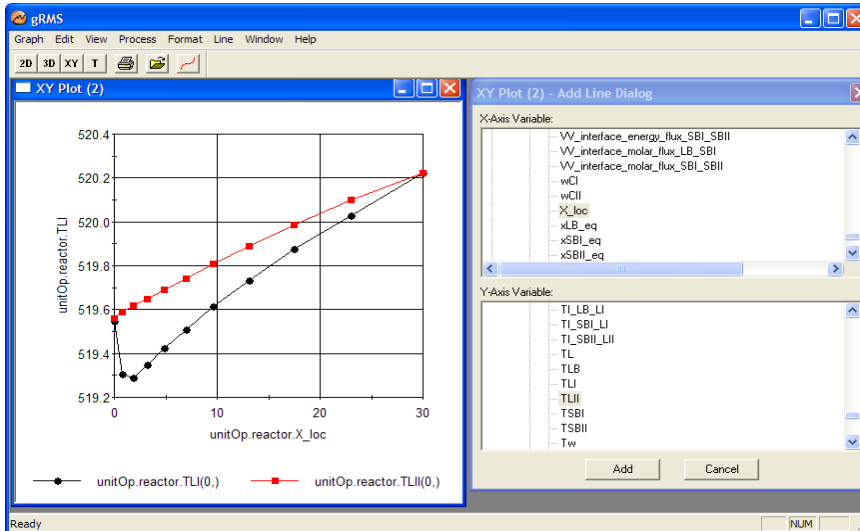
Overall Mole Fractions (mol/mol)			
CO	0.285989	0.00862365	0.143432
H2	0.572028	0.0144047	0.287641
CO2	0.0716857	0.0179257	0.138406
H2O	0.0273927	0.0876912	0.275852
NC1	0.0149957	0.00909777	0.0061287
NC2	0.000289038	0.000811946	0.00440467
NC3	0.000225583	0.00105939	0.00343769
NC4	0.000187933	0.00150881	0.00286394
NC10	0.000794876	0.0735401	0.0121134
NC11	0.39477E-005	0.294869	0.00127933
NC12	4.49508E-006	0.381132	6.85015E-005
NC13	4.48717E-008	0.0012224	6.83816E-007
NC54	3.24707E-010	0.0117782	4.94834E-009
OC2	1.2753E-005	3.29238E-005	0.000194348
OC3	0.000118302	0.000561247	0.00180283
OC4	9.28239E-005	0.000744742	0.00140238
OC10	0.00014776	0.0128459	0.00225179
N2	0.0259528	0.00214986	0.0095202

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5. Examine results



■ Within gPROMS visualization tool gRMS



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Recent enhancements to PRO/II and gPROMS
CAPE-OPEN components

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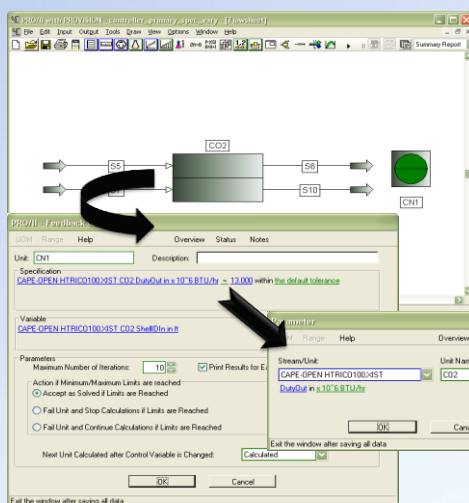
CAPE-OPEN Enhancements in PRO/II

- Reviewed and modified the CAPE-OPEN integration architecture to provide better lifetime management of CAPE-OPEN objects and eliminate memory leaks and errors.
- Improved interoperability by allowing seamless use of mass/mole basis and fixing calculation and access issues for thermodynamic properties.
- Added a logging capability to facilitate diagnosis and troubleshooting.
- Extended the controller and the “define” infrastructure to include support for “real” parameters of CAPE-OPEN unit operations¹.

¹ For additional information, refer to the PRO/II 8.3 Keyword Manual.

inven.s.s

Controlling a CAPE-OPEN Parameter through the GUI



- Parameters are taken from the CAPE-OPEN unit and filtered:

- A controller can SPEC “output” and “input/output” parameters
- A controller can VARY “input” and “input/output” parameters

inven.s.s

■ gPROMS 3.1.6:

- Added the ability to control whether the gPROMS components use mass or mole basis for calls to the PME physical property package.
- Ability to map gPROMS selectors to CAPE-OPEN option parameters
- Option to launch gRMS for visualization of internal variables

■ gPROMS 3.2.0:

- Option to permit the gPROMS model's execution diagnostics to be made visible to the end user.
- COThermoFO now has a COMPONENTS() method allowing a gPROMS component name lists to be initialized with the list of component names from the CAPE-OPEN thermo package.

■ gPROMS 3.2.1 (coming soon):

- Multiple instances of gO:CAPE-OPEN units can be used within a single flowsheet

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Conclusions

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Conclusions

- Interoperability of a complex gPROMS model within a PRO II flowsheet has been demonstrated.
 - Linear flowsheets
 - Flowsheets with recycles
- Key success factors in first-time CAPE-OPEN integration projects:
 - Clear articulation of requirements by end user
 - Strong dialog between software providers to identify and correct interoperability problems

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- Michel Pons, CO-LaN

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See me at the end of the session
if interested in a live demo