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

Alejandro Cano, Rodrigo Blanco, Thomas Williams
Process Systems Enterprise

David Jerome, Krishna Penukonda
Invensys Process Systems

Pierre Duchet-Suchaux and Sabine Savin
TOTAL, S.A.

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Outline

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

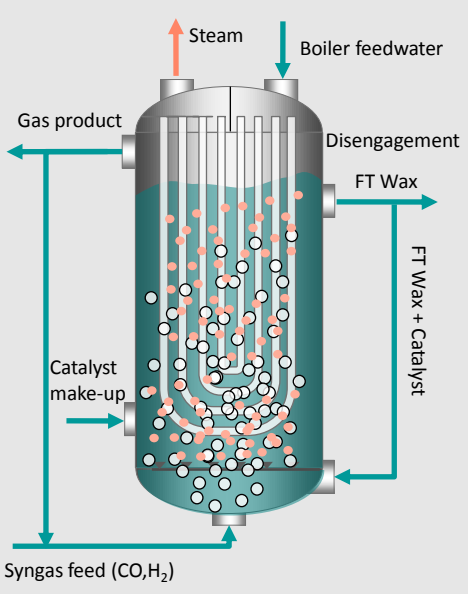
Model description and deployment requirements

Model of slurry reactor for Fischer-Tropsch synthesis

$$CO + 3H_2 \rightarrow CH_4 + H_2O$$

$$C_nH_{2n+2} + CO + 2H_2 \rightarrow C_{n+1}H_{2n+4} + H_2O$$

- 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 multicompartment 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

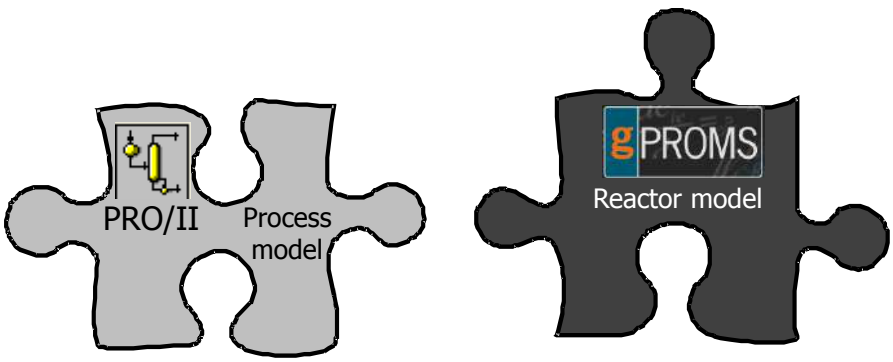
Project approach

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

Implementation: bringing the pieces together



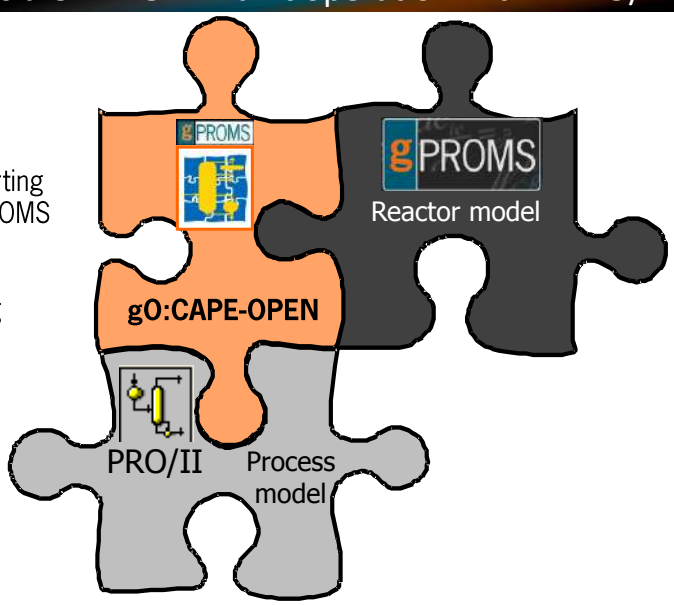
PRO/II flowsheet of any complexity including recycle streams

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

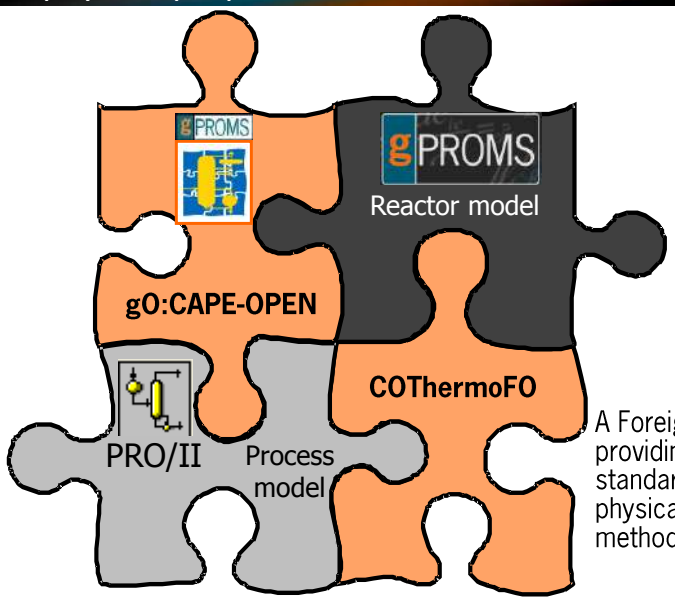
1) gPROMS CO Unit plug allows model to be exported for use as a CAPE-OPEN unit operation within PRO/II

Wizard for exporting model from gPROMS ModelBuilder:

no programming required

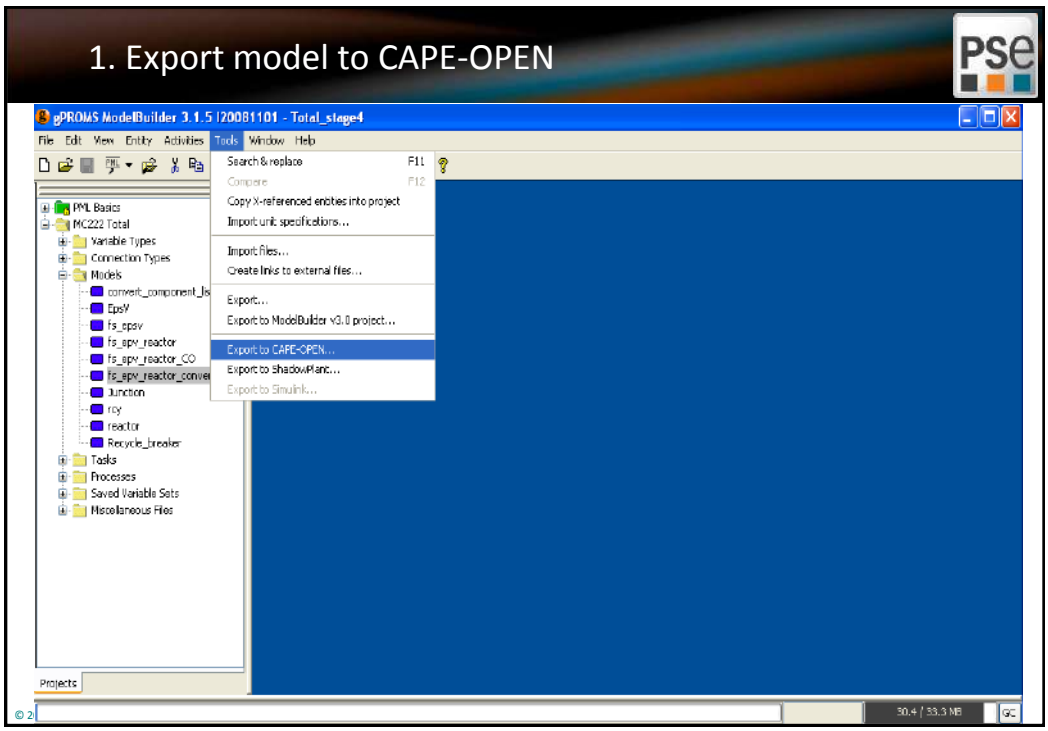


2) gPROMS CO thermo socket allows reactor model to use PRO/II physical properties in its calculations



The work flow in detail

1. Export model to CAPE-OPEN



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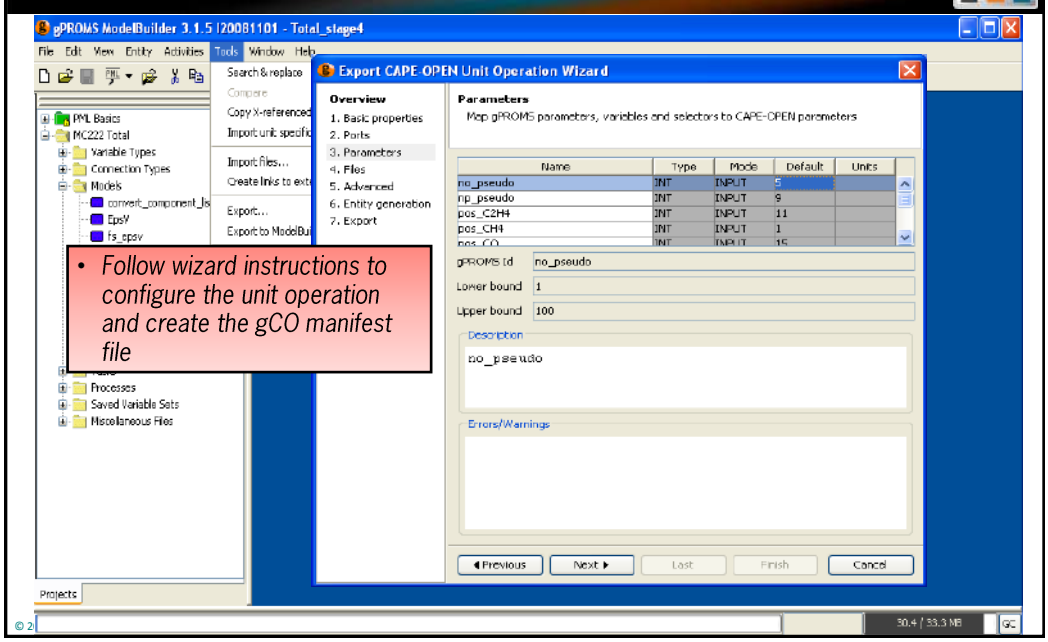

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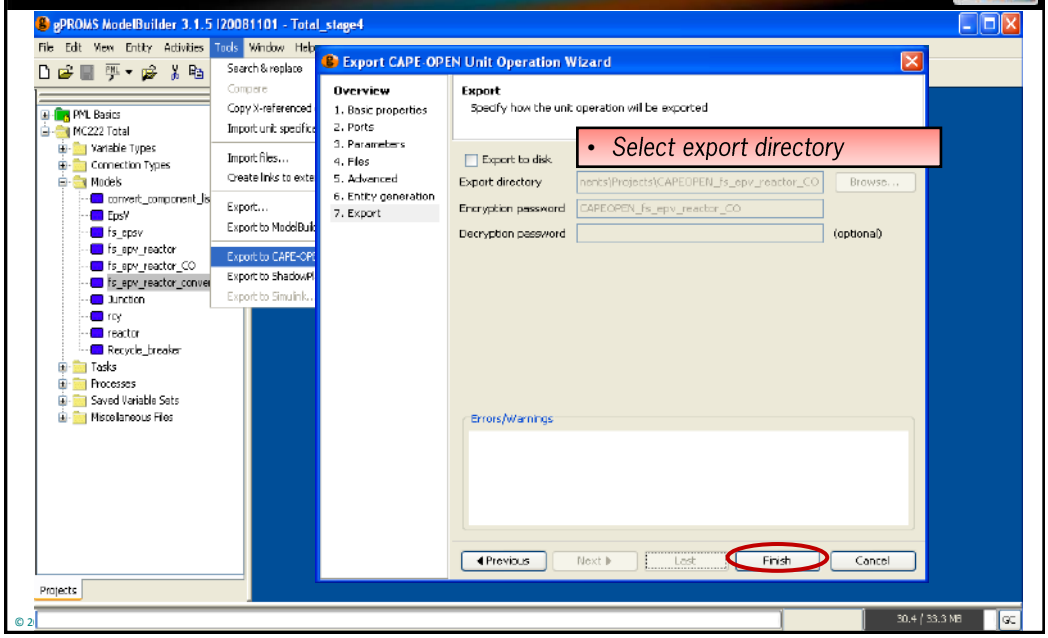
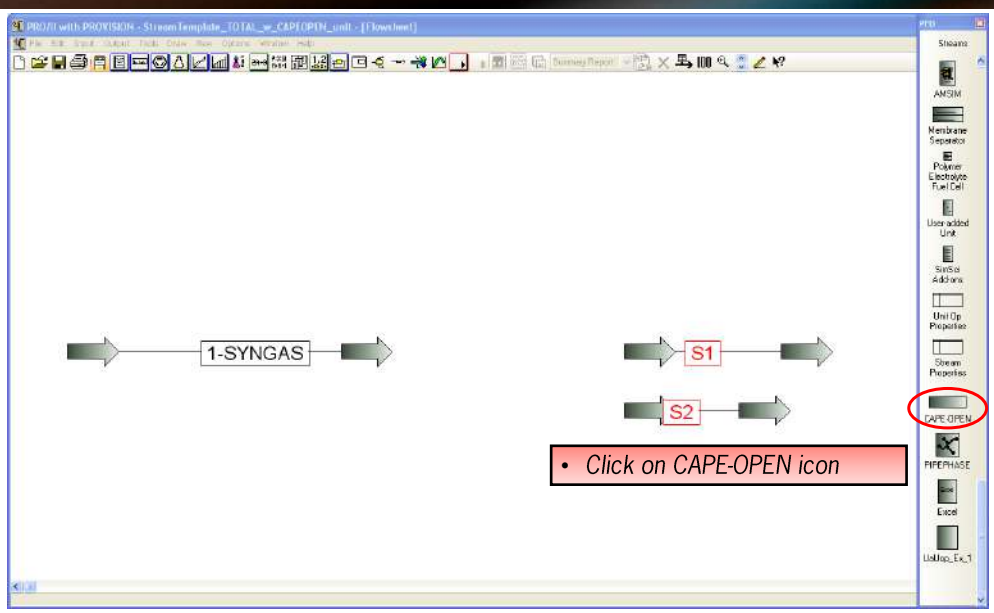


2. Insert exported CAPE-OPEN unit into flowsheet



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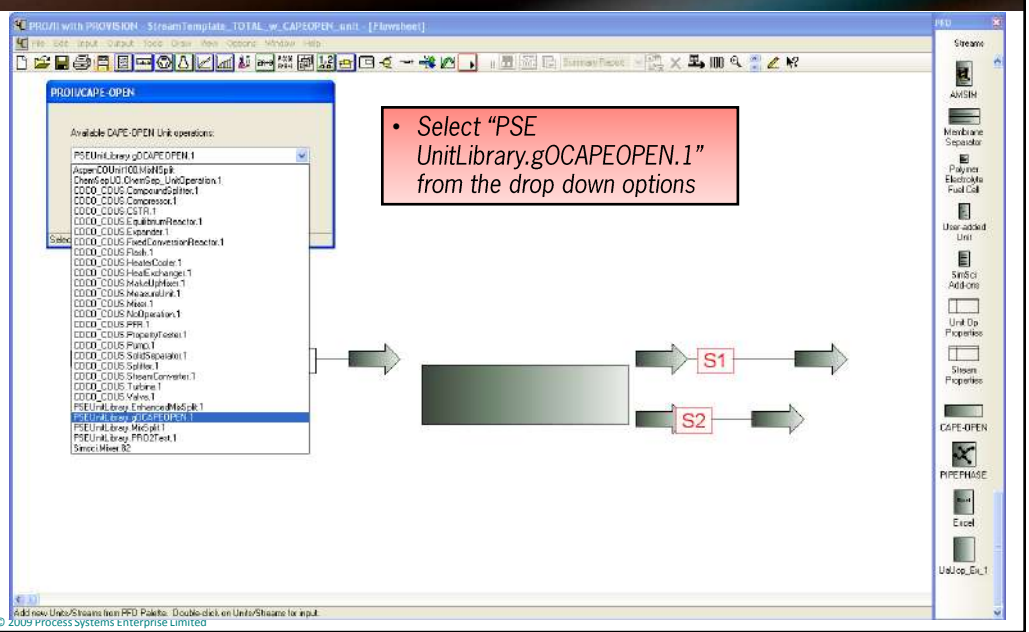

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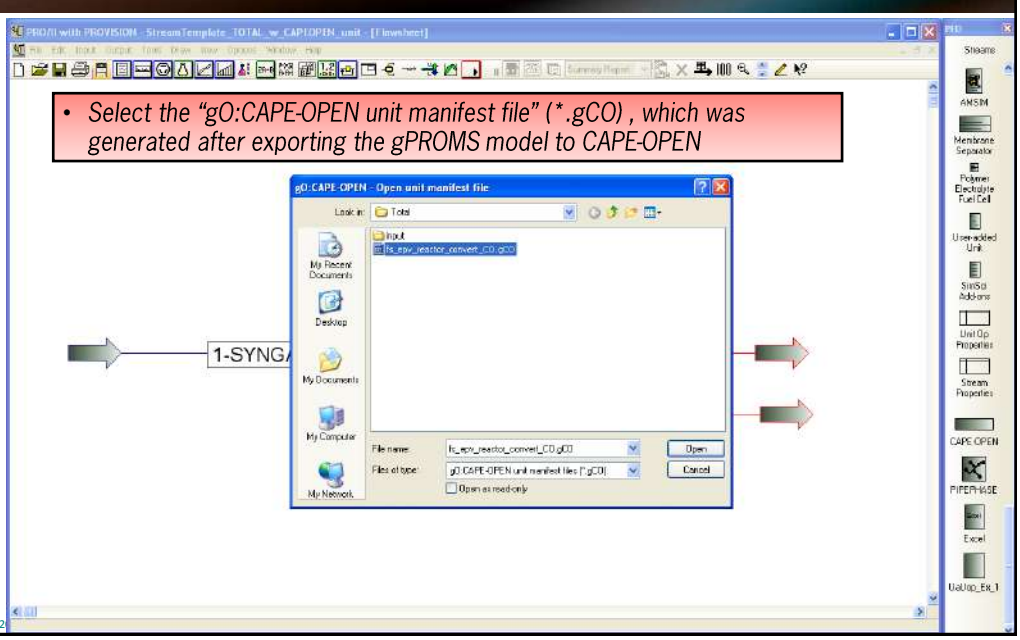

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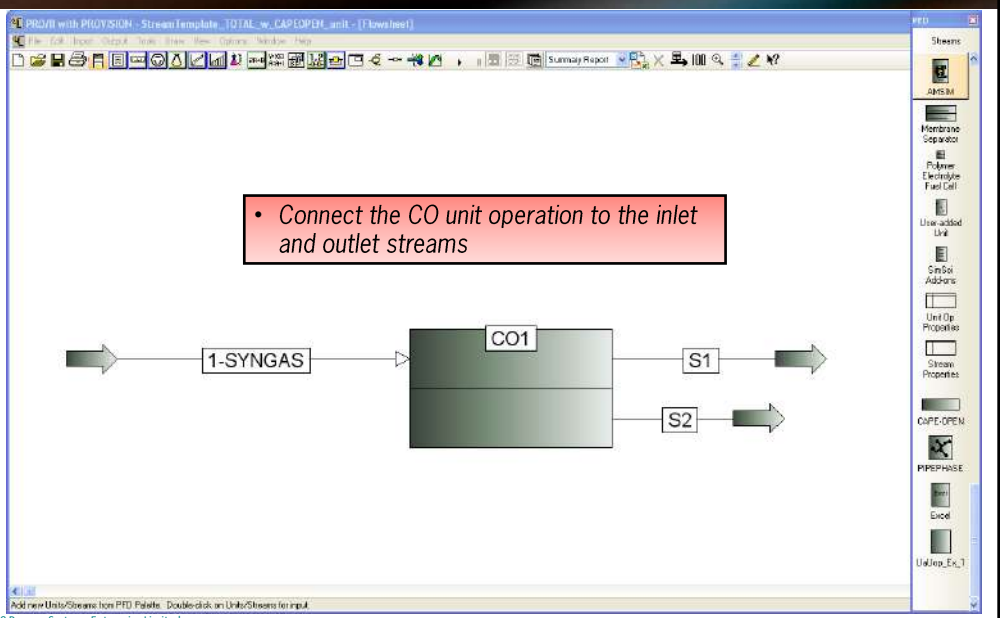
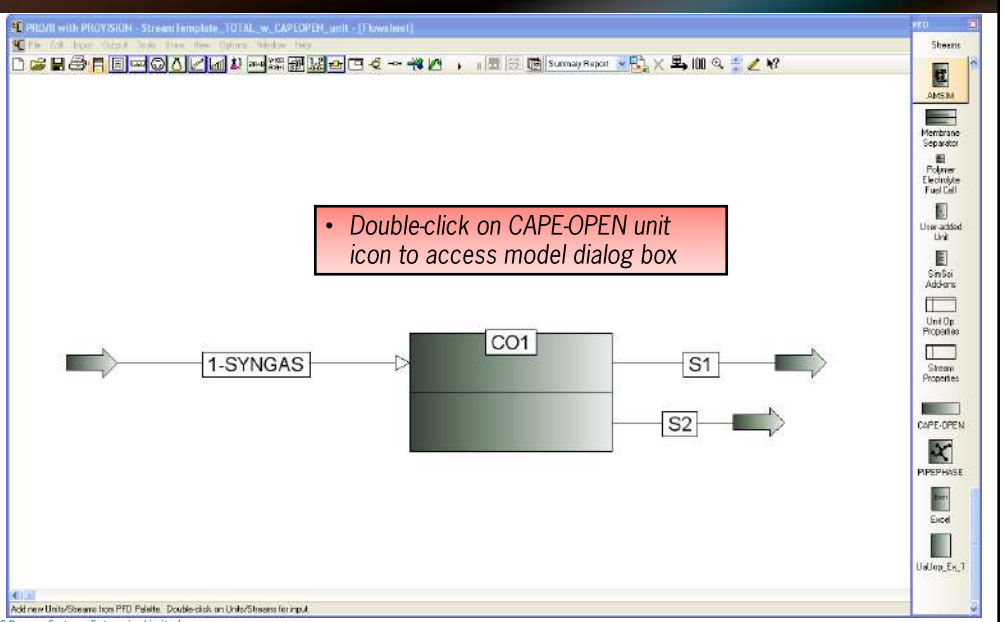


3. Configure the unit through its dialog box



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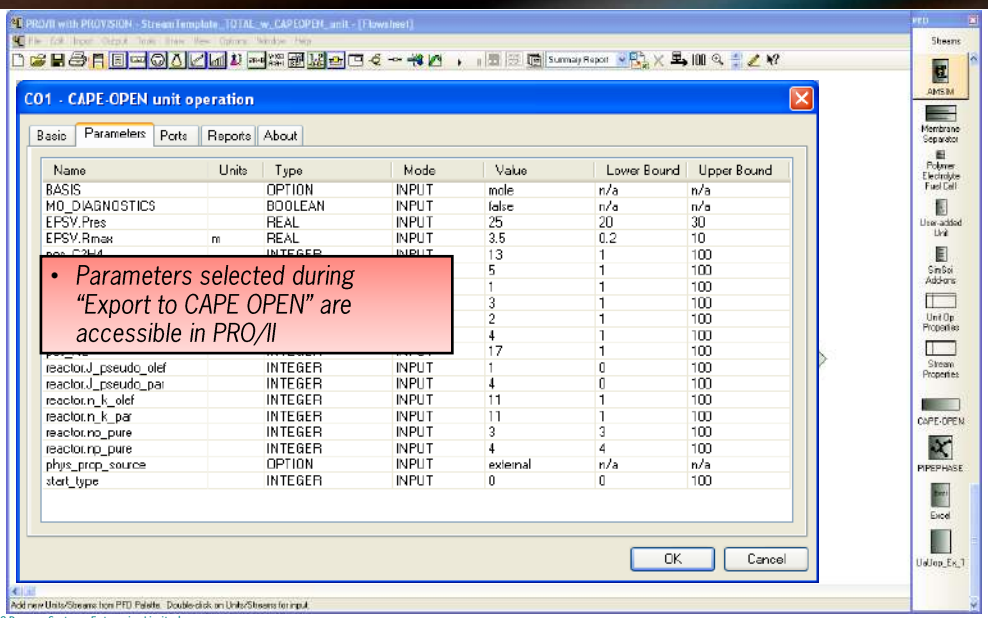
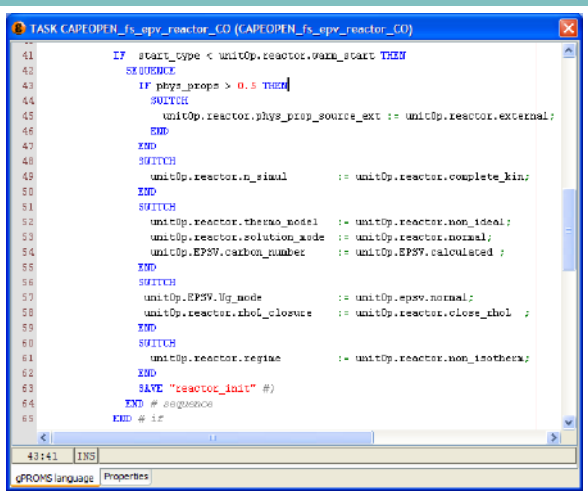


4. Converge the flowsheet (automatic procedure executed by gPROMS unit operation)

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

Step 1 → Step 2 → Step 3 → Step 4 → Full problem → Saved variable set

Cold-start



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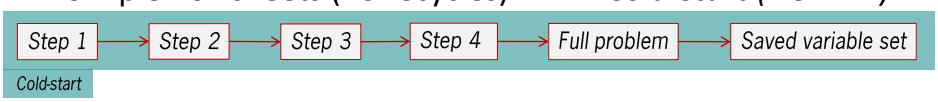
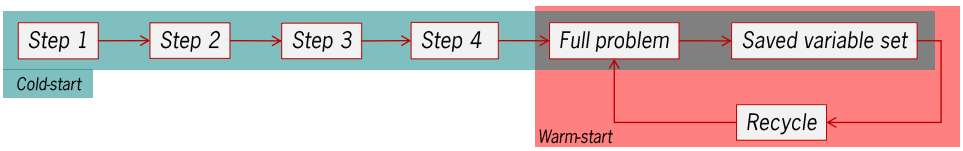
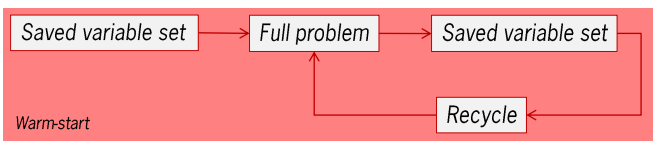


- Complex flowsheets
  1. ***Cold-start*** followed by ***warm-start*** *(~ 30 seconds per pass)*

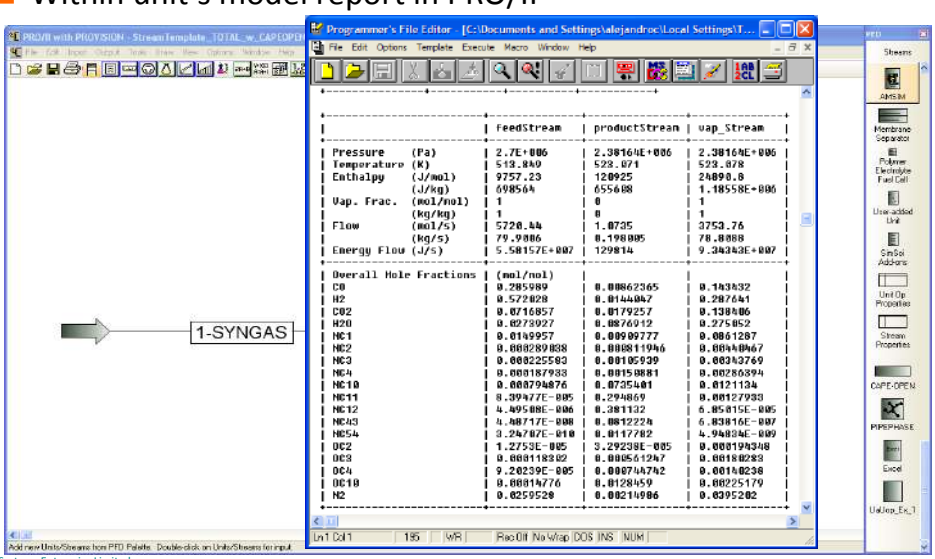


- Option to use a ***warm-start*** if a saved variable set is available



5. Examine results

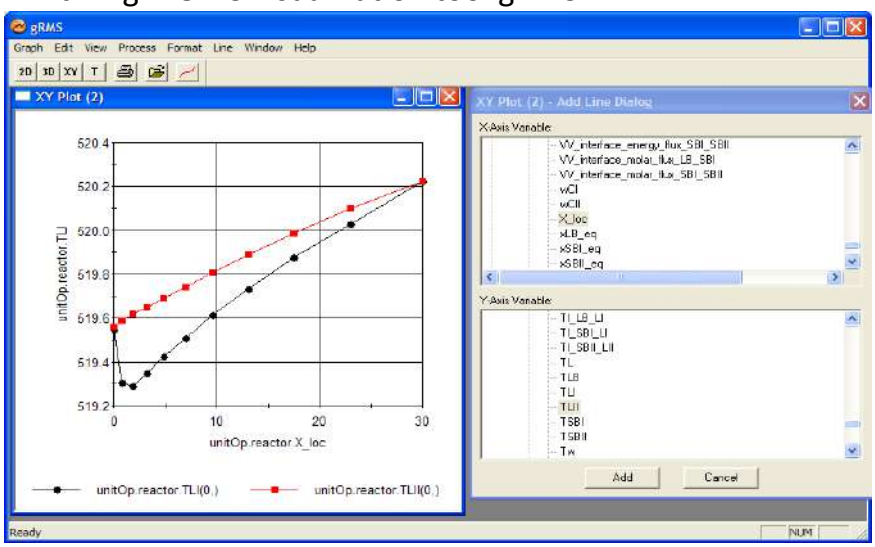
- Within unit's model report in PRO/II



	FeedStream	productStream	vap_Stream
Pressure (Pa)	2.7E+006	2.38164E+006	2.3816%E+006
Temperature (K)	513.849	523.071	523.078
Enthalpy (J/mol)	9757.23	120925	24890.8
(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)	79.9086	0.198005	78.8088
Energy Flow (J/s)	5.58157E+007	129814	9.34343E+007
Overall Mole Fractions	(mol/nol)		
C0	0.285989	0.00862365	0.143432
H2	0.572028	0.0144047	0.287641
C02	0.0716857	0.0179257	0.138406
H20	0.0273927	0.0876912	0.275852
HC1	0.0149957	0.00999777	0.0061287
HC2	0.000289038	0.00081194%	0.0044%467
HC3	0.000225583	0.00105939	0.00343769
HC4	0.000187933	0.00158881	0.00286394
HC10	0.000794876	0.0735401	0.0121134
HC11	8.39477E-005	0.294869	0.00127933
HC12	4.4958%E-006	0.381132	6.85815E-005
HC43	4.98717E-008	0.0012224	6.83816E-007
HC54	3.24787E-010	0.0117782	4.94834E-009
OC2	1.2753E-005	3.29238E-005	0.000194348
OC3	0.000118302	0.00056124%	0.00180283
OC4	9.20239E-005	0.00074%742	0.0014%238
OC10	0.00814776	0.0128459	0.00225179
N2	0.0259528	0.00214986	0.0395202

5. Examine results

- Within gPROMS visualization tool gRMS



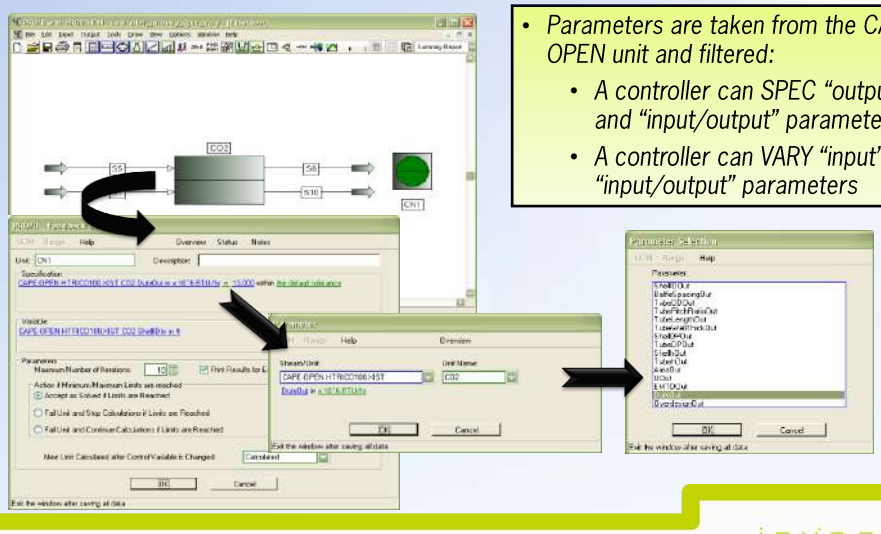
Recent enhancements to PRO/II and gPROMS CAPE-OPEN components

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 operations[1].

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

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*

CAPE-OPEN Enhancements in gPROMS

- 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

Conclusions

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

Acknowledgements

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