

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

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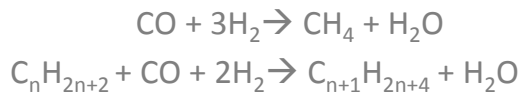
Outline

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

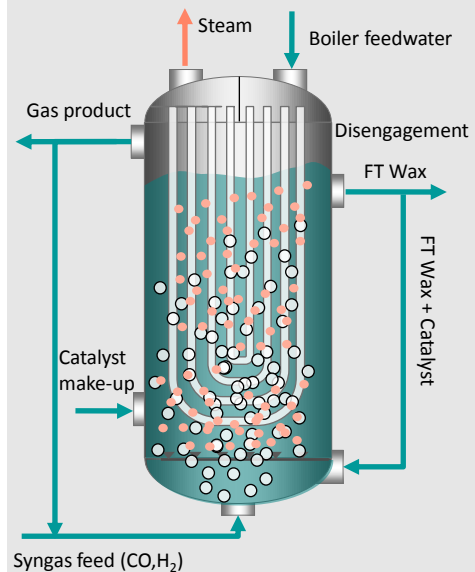
Model description and deployment requirements

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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

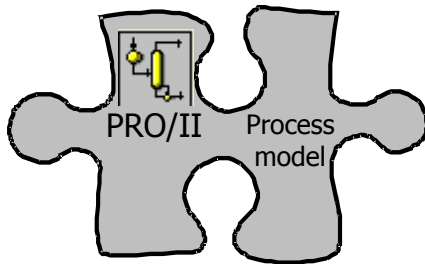


- Translate model from ACM to gPROMS
- Improve model performance:
 - Non-uniform grids
 - Smooth discontinuities in hydrodynamic model
 - Review of variable types and equation scaling
- Implement robust initialization procedure
 - Solves sequence of 5 problems of increasing complexity
 - No initial guesses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

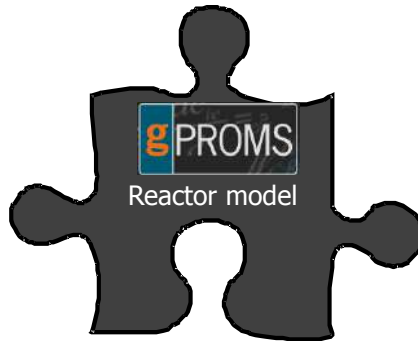
Close PSE/Invensys collaboration to address software issues

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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

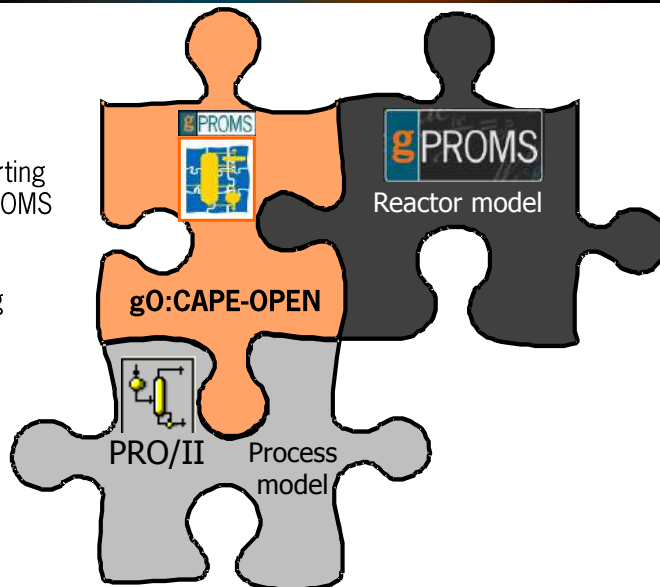
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1) gPROMS CO Unit plug allows model to be exported for use as a CAPE-OPEN unit operation within PRO/II



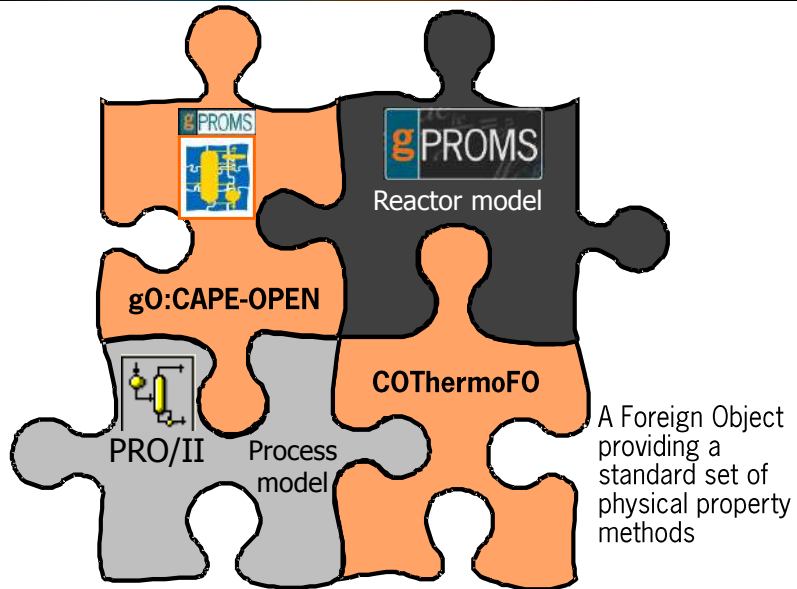
Wizard for exporting model from gPROMS ModelBuilder:

no programming required



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

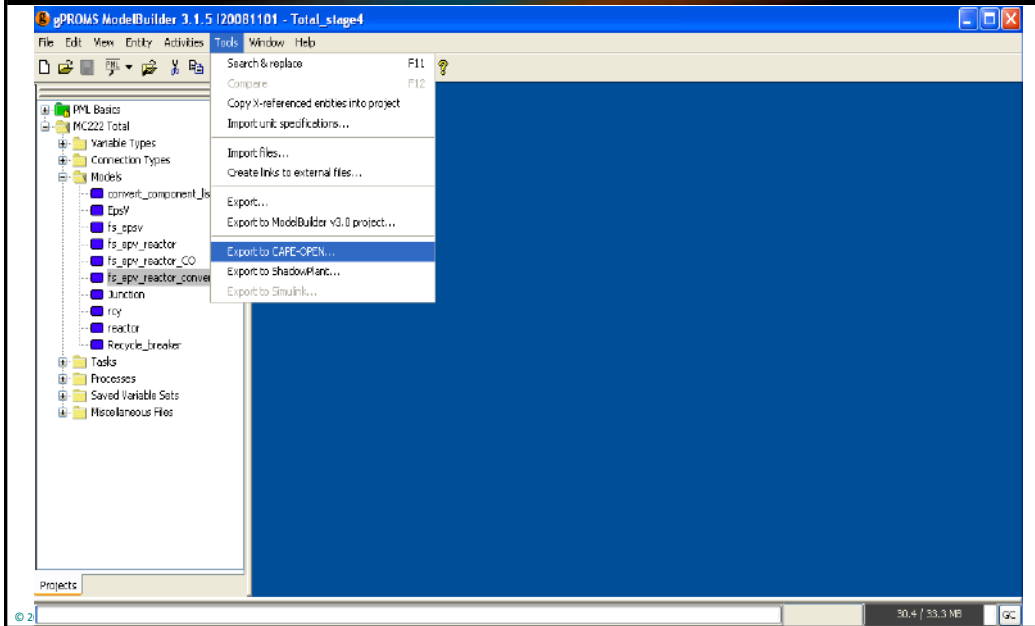


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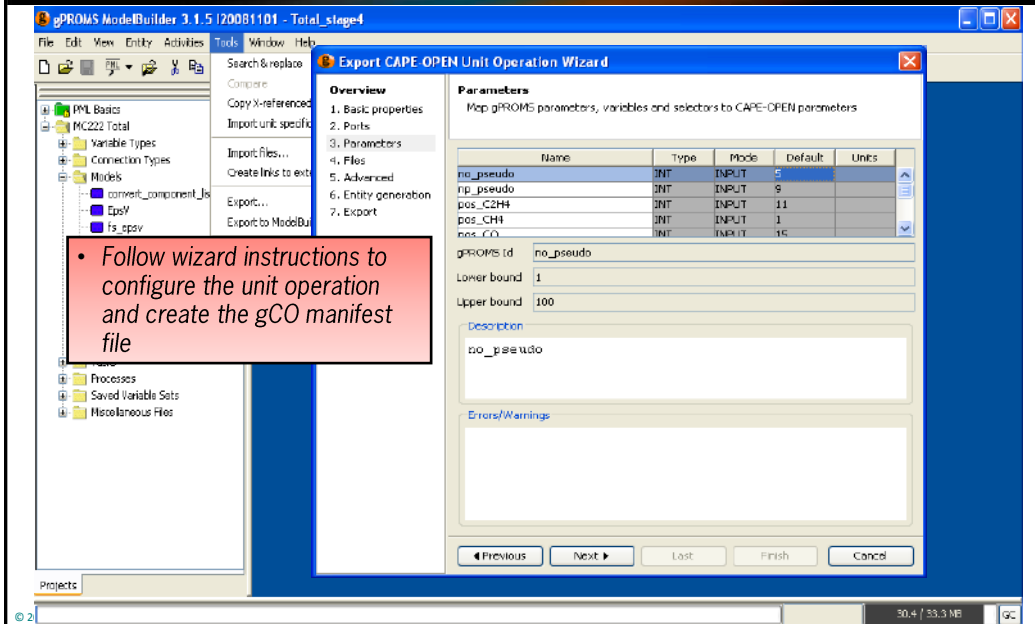
The work flow in detail

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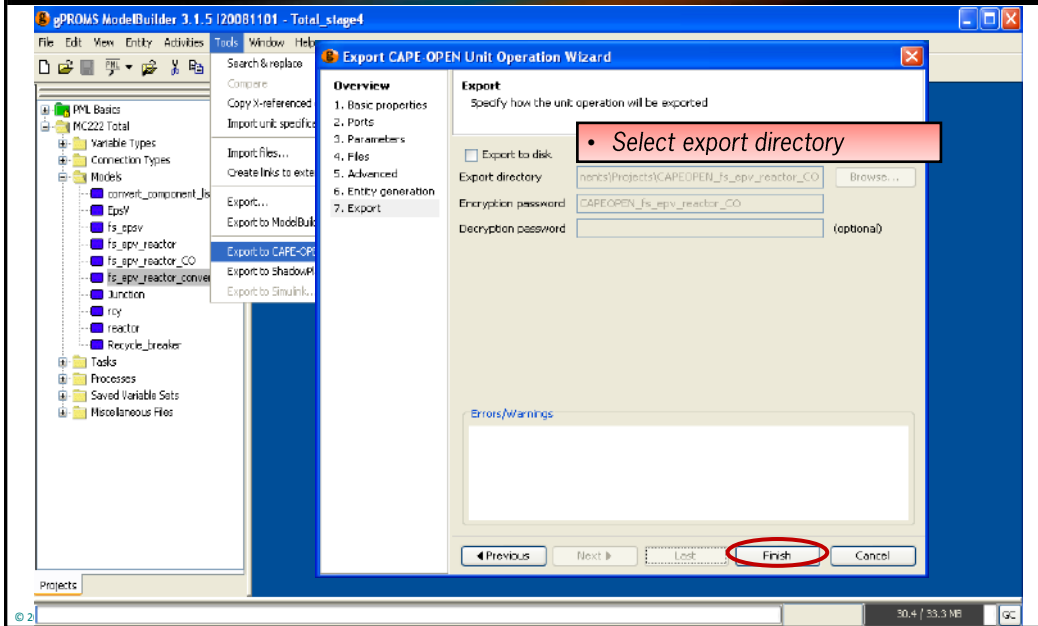
1. Export model to CAPE-OPEN



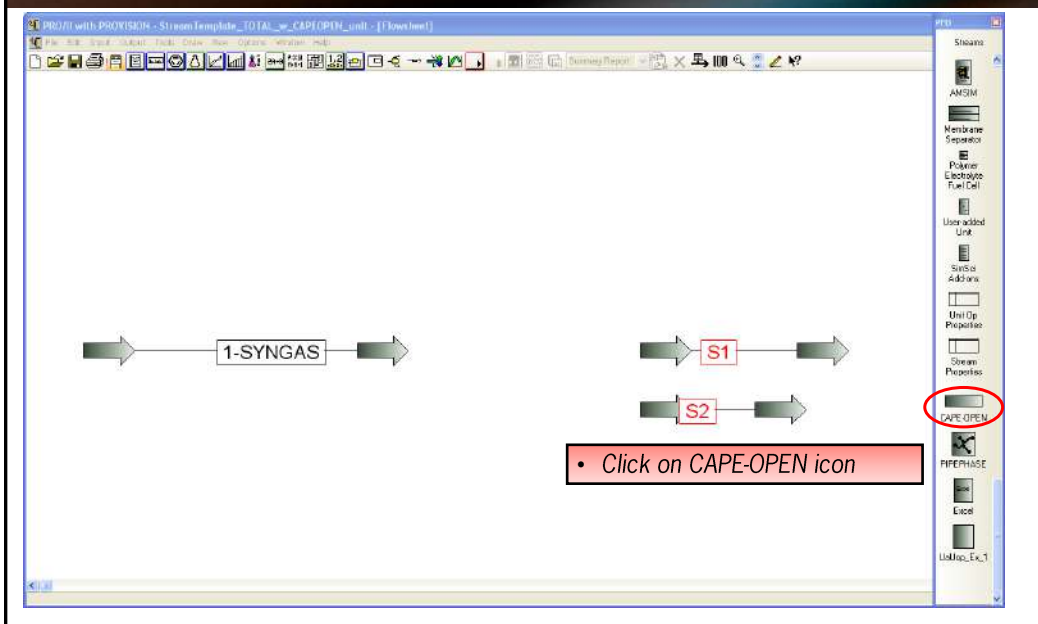
1. Export model to CAPE-OPEN



1. Export model to CAPE-OPEN



2. Insert exported CAPE-OPEN unit into flowsheet



2. Insert exported CAPE-OPEN unit into flowsheet

The screenshot shows the PRO/II interface with a flowsheet window. On the left, a 'PRO/II CAPE-OPEN' dialog box is open, displaying a list of available CAPE-OPEN unit operations. A red callout box points to the 'PSEUnitLibrary.gOCAPEOPEN.1' entry in the list. The flowsheet itself shows a rectangular unit being inserted into a process stream, with two output streams labeled 'S1' and 'S2'. The right-hand side of the interface shows a 'Streams' panel with various unit icons.

- Select "PSEUnitLibrary.gOCAPEOPEN.1" from the drop down options

2. Insert exported CAPE-OPEN unit into flowsheet

The screenshot shows the PRO/II interface with a flowsheet window. A red callout box points to the 'gO:CAPE-OPEN unit manifest file' (*gCO) option in the file selection dialog. The dialog box is open, showing the 'Total' folder containing a file named 'RS_esp_reactor_converter_CO.gco'. The file name and type are entered in the dialog's fields. The flowsheet shows a unit labeled '1-SYNGAS' with two output streams.

- Select the "gO:CAPE-OPEN unit manifest file" (*gCO), which was generated after exporting the gPROMS model to CAPE-OPEN

2. Insert exported CAPE-OPEN unit into flowsheet

The screenshot shows a software interface for creating a process flowsheet. The main window displays a process flow with an inlet stream labeled '1-SYNGAS' entering a unit labeled 'CO1'. Two outlet streams, 'S1' and 'S2', exit the unit. A red callout box contains the instruction: *• Connect the CO unit operation to the inlet and outlet streams*. On the right side, there is a 'Streams' palette with various unit icons, including 'CAPE-OPEN'. At the bottom, a status bar reads: 'Add new Units/Streams from PFD Palette. Double-click on Units/Streams for input. © 2009 Process Systems Enterprise Limited'.

3. Configure the unit through its dialog box

This screenshot is identical to the previous one, showing the process flowsheet with the 'CO1' unit and streams '1-SYNGAS', 'S1', and 'S2'. The red callout box now contains the instruction: *• Double-click on CAPE-OPEN unit icon to access model dialog box*. In the 'Streams' palette on the right, the 'CAPE-OPEN' icon is highlighted with a mouse cursor. The status bar at the bottom remains the same: 'Add new Units/Streams from PFD Palette. Double-click on Units/Streams for input. © 2009 Process Systems Enterprise Limited'.

3. Configure the unit through its dialog box

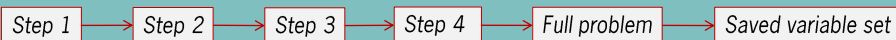
Parameters selected during "Export to CAPE OPEN" are accessible in PRO/II

Name	Units	Type	Mode	Value	Lower Bound	Upper Bound
BASIS		OPTION	INPUT	none	n/a	n/a
MO_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
reactor.n_k		INTEGER	INPUT	13	1	100
reactor.n_k_olef		INTEGER	INPUT	5	1	100
reactor.n_k_pure		INTEGER	INPUT	1	1	100
reactor.n_k_olef		INTEGER	INPUT	3	1	100
reactor.n_k_pure		INTEGER	INPUT	2	1	100
reactor.n_k_olef		INTEGER	INPUT	4	1	100
reactor.n_k_pure		INTEGER	INPUT	17	1	100
reactor.j_pseudo_olef		INTEGER	INPUT	1	0	100
reactor.j_pseudo_pure		INTEGER	INPUT	4	0	100
reactor.n_k_olef		INTEGER	INPUT	11	1	100
reactor.n_k_pure		INTEGER	INPUT	11	1	100
reactor.no_pure		INTEGER	INPUT	3	3	100
reactor.no_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

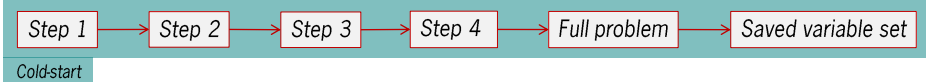
```

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_prop > 0.5 THEN
44 SWITCH
45 unitOp.reactor.phys_prop_source_ext := unitOp.reactor.external;
46 END
47 SWITCH
48 unitOp.reactor.n_simal := unitOp.reactor.complete_kin;
49 END
50 SWITCH
51 unitOp.reactor.thermo_model := unitOp.reactor.non_ideal;
52 unitOp.reactor.solution_mode := unitOp.reactor.normal;
53 unitOp.EPSV.carbon_number := unitOp.EPSV.calculated;
54 END
55 SWITCH
56 unitOp.EPSV.ig_mode := unitOp.epsv.normal;
57 unitOp.reactor.shol_closure := unitOp.reactor.close_shol;
58 END
59 SWITCH
60 unitOp.reactor.regime := unitOp.reactor.non_isotherm;
61 END
62 SAVE "reactor_init" #)
63 END #_sequence
64 END #_if
65
  
```

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

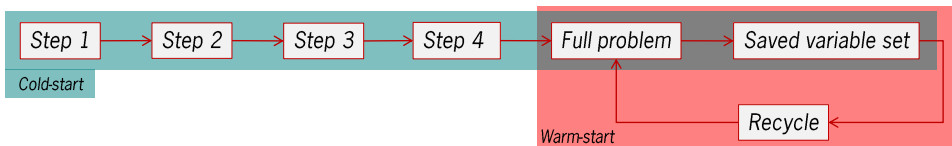


- Simple flowsheets (no recycles): **Cold-start** (~ 5 min.)

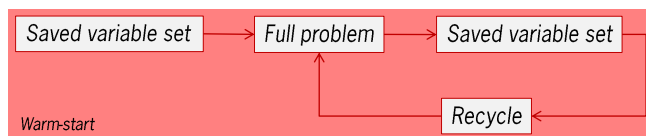


- Complex flowsheets

- 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)	513.840	528.671	528.878
Enthalpy (J/mol)	9757.23	120925	24899.8
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	1.0705	3753.76
(kg/s)	79.9886	0.198095	78.8088
Energy Flow (J/s)	5.58157E+007	129814	9.34343E+007

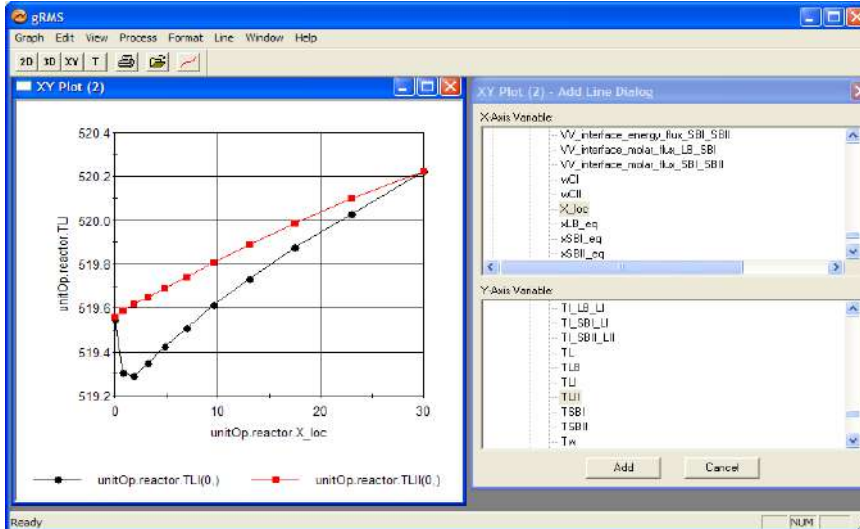
Overall Mole Fractions (mol/mol)	FeedStream	productStream	vap. Stream
CO	0.285989	0.00862365	0.143832
H2	0.572808	0.0144047	0.287641
CO2	0.0716857	0.0179257	0.139806
H2O	0.0739027	0.0876012	0.275852
HC1	0.0149957	0.00999777	0.0061287
HC2	0.008289088	0.008811946	0.00404667
HC3	0.008225583	0.00185939	0.00343769
HC4	0.001879938	0.00150881	0.00216394
HC10	0.008794876	0.0735401	0.0121134
HC11	0.39477E-005	0.294869	0.00127933
HC12	4.409508E-006	0.281102	0.05015E-005
HC13	4.408717E-008	0.0842224	0.0016E-007
HC54	3.24787E-010	0.0117782	4.94834E-009
DC2	1.2753E-005	3.29238E-005	0.000194348
DC3	0.000118302	0.000561247	0.00180283
DC4	9.240259E-005	0.00714792	0.00180238
DC10	0.00014776	0.0128459	0.00225179
H2	0.0259528	0.00214986	0.0395282

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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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- 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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- Diego Larrain, HT Ceramics (formerly at PSE)
- Michel Pons, CO-LaN

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