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.

6th CAPE-OPEN U.S. Conference
11 November 2009

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

\[
\begin{align*}
\text{CO} + 3\text{H}_2 & \rightarrow \text{CH}_4 + \text{H}_2\text{O} \\
\text{C}_n\text{H}_{2n+2} + \text{CO} + 2\text{H}_2 & \rightarrow \text{C}_{n+1}\text{H}_{2n+4} + \text{H}_2\text{O}
\end{align*}
\]

- 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-
- 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

- 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

A Foreign Object providing a standard set of physical property methods

The work flow in detail
1. Export model to CAPE-OPEN

- Follow wizard instructions to configure the unit operation and create the gCO manifest file
1. Export model to CAPE-OPEN

- Export model to CAPE-OPEN

- Insert exported CAPE-OPEN unit into flowsheet
  
  - Select export directory
  
  - Click on CAPE-OPEN icon
2. Insert exported CAPE-OPEN unit into flowsheet

- Select “PSE UnitLibrary.gOCAPEOPEN.1” from the drop down options

---

2. Insert exported CAPE-OPEN unit into flowsheet

- 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

- Connect the CO unit operation to the inlet and outlet streams

3. Configure the unit through its dialog box

- Double-click on CAPE-OPEN unit icon to access model dialog box
3. Configure the unit through its dialog box

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

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

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

- Complex flowsheets
  1. **Cold-start** followed by **warm-start (~ 30 seconds per pass)**
     - Step 1 → Step 2 → Step 3 → Step 4 → Full problem → Saved variable set

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

5. Examine results

- Within unit’s model report in PRO/II
5. Examine results

- **Within gPROMS visualization tool gRMS**

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

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
CAFE-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.
  - COTermoFO 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 g0: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

- Ion Iliuta, Laval University
- Jérôme Anfray, TOTAL
- Diego Larrain, HT Ceramics (formerly at PSE)
- Michel Pons, CO-LaN
Deployment of a gPROMS-based three-phase reactor model as a CAPE-OPEN unit operation within PRO/II

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