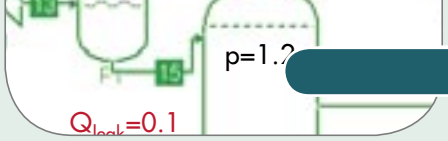

Cross Platform Chemical Processes

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CAPE-OPEN (CO) is an industry standard that allows the Plug-and-Play interoperability of simulation components, such as unit operations and thermodynamic models, inside chemical process model simulators like Aspen Plus and PRO/II (for a description of CAPE-OPEN see NPT Procestechnologie, February, 2005, pp. 11-13). At the annual CO meeting in Cannes in March 2006 market leaders such as Aspentech, Honeywell Process Solutions, Simulation Sciences, and Process Systems Enterprise Ltd. showed their commitment for the CO standard (see http://www.colan.org/News/Y05/news-0524.htm). At that same meeting end-users discussed their use of CO to model special unit operations or to obtain highly accurate thermodynamic properties:

Dow have used Aspen Plus for simulating chemical processes. However, the Aspen Plus model library does not include models for special unit operations, like e.g. membrane separators or trickle bed reactors. Dow explored modeling such units in the equation oriented simulators Aspen Customer Modeler and gPROMS, and linking these models to Aspen Plus using the CAPE-OPEN protocols. (http://www.colan.org/CO@Work2006/3-04-DOW.pdf)

Heat Transfer Research Inc. (HTRI) provides software for the detailed design of a wide variety of heat exchangers including shell and tube, air coolers/economizers, and plate and frame devices. HTRI already had integrated their design software with several major commercial flowsheet simulators. However, this integration came at a significant cost; each software system required a unique solution. HTRI could see that there would be significant long-term benefits if they could maintain just one code that could be interfaced with many other software tools. Their solution: CAPE OPEN.

ChemSep is a program for solving distillation, absorption, and extraction operations that features a non-equilibrium or rate-based model that has inspired the development of many other similar models (e.g. RATEFRAC). Though ChemSep has been around for 15 years the fact that it was not integrated with standard flowsheet simulators limited industrial usage. To change this it was deemed necessary to find a way to integrate the program with any flowsheeter. The solution once again, was CAPE OPEN.

Other industrial and governmental use of CAPE-OPEN includes:

- *Air Liquide:* uses Simulis Thermodynamics + DIPPR database of pure substances as R&D thermodynamic standard allowing the cohabitation of four simulators: HYSYS, Belsim, Prosim, and AspenPlus. They aim at using in-house CO reactor and membrane models to reduce development and maintenance cost,
- *BASF:* uses MultiFlash (InfoChem) as external thermodynamics server for the in-house CHEMASIM simulator,
- *BP:* uses the ChemSep rate-based column simulator,
- *IFP & Total:* integrated approach of dynamic fluid flow modeling from the reservoir to the topside process,
- *Sasol:* used CO interfaces to make reactor models independent from the process simulator,
- *Shell:* in-house thermodynamics server to re-use code in different simulators,
- *US Department of Energy/Alstrom:* combination of a Fluent CFD model and a process model for a power plants description,
- *US Environmental Protection Agency:* integration of unit operations in their Pollution Prevention Tool

At the meeting it also became apparent that small companies have started to fill the niches in the simulation market, such as *AmsterChem, BelSim, ChemSep, HTRI, ProSim*, etc. Free test- and logging software as

Modeling of with CAPE-OPEN

well as wizards for unit operation development were made available which will further enhance the growing adhesion between software vendors, end-users as well as academics users. Such tools will also reduce the ambiguity in the interpretations of the CO-standard. Here we want to highlight the practical benefits of CAPE-OPEN in industry.

Dow – Custom Process Unit Models in Flowsheet Simulator

Models for special unit operations like trickle bed reactors or membrane separators are not available in the model libraries of commercially available process simulators. For processes which include such unit operations two approaches are used:

- The special unit is mimicked by using a combination of unit operation models from the library. This may result in a correct representation of the (overall) mass and energy balance for a certain (small) range of conditions, but is usually not robust enough for exploring different process flowsheet schemes, process optimization or equipment design.
- A custom model of the special unit operation is incorporated in the flowsheet simulator. This approach is more robust and accurate, but the model development, interfacing and initialization procedures require (much) more development and maintenance efforts.

Dow explored the utilization of generic custom models – developed in Aspen Custom Modeler (ACM) or gPROMS – inside Aspen Plus. A trickle bed reactor and a generic membrane model were used in this study. Both unit models used a distributed parameter, rate based approach. The design of the membrane model allows for different configurations, like co- and counter-current flow, feed at the shell or the membrane side, using symmetric or asymmetric membrane types (see Figure 1). The conclusion of the Dow study is that this approach works, but that special measure need to be taken for the custom model initialization.

ChemSep – Simulating Interlinked / Rate-Based Columns

The CO implementation of ChemSep adds an extra layer between the simulator and the user interface allowing the selection of internal (1) or external property (2) calculations.
In the first case only inlet and outlet stream compositions and conditions are exchanged and internal properties routines and component data libraries are used. In the second case properties and component data are obtained from the flowsheeting package in a CAPE-OPEN manner. With the provision of this extra layer and logging of CO communications it was possible to resolve problems with the existing implementations in the flowsheet packages AspenPlus and PRO/II. Full compliance was obtained with AspenPlus and COCO (AmsterChem). In PRO/II version 7.1 only allowed simulation with internal properties and did not allow any change in the number of feed- and product-streams. PRO/II 8.0 will include an improved CO-implementation. HYSYS and UniSim Design also only allow column simulations with internal properties. To aid vendors in properly implementing the CO-standard, ChemSep made a LITE version available as a free download. The new multi-column simulation capabilities are illustrated with the simulation of a cryogenic Air Separation Unit (ASU) using a side stripper to produce crude Argon, see figure 2. Note that this ASU was completely simulated with CO unit operations and CO thermodynamics models. Since 2005 the ChemSep CO compliant rate-based column simulator is used within BP.

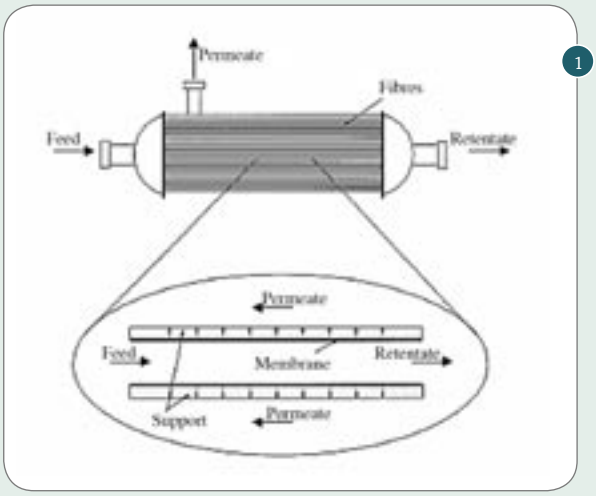

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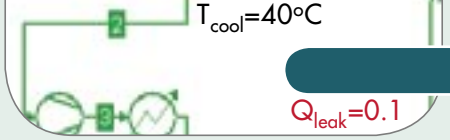
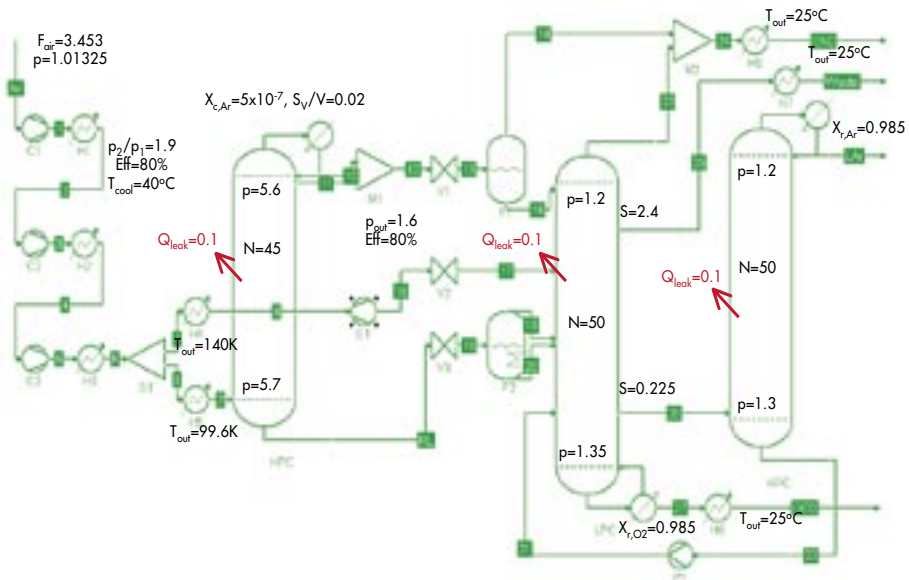
Fig. 1
Membrane unit operations containing distributed parameter systems

BASF – CHEMASIM Simulator with Thermo Interface

BASF has a large CAPE-User community using a vast variety of sophisticated CAPE tools. The in-house simulator CHEMASIM is used together with supporting programs for data supply, regression and visualization. CHEMASIM was developed over the past 30 years and



Air Separation Unit: Specifications



O_2 and Ar purities specified at 98.5%; Recoveries ≈75%, respectively ≈85%.
Better recoveries and purities can be obtained with more stages!

Air Separation Unit: Low Pressure Column

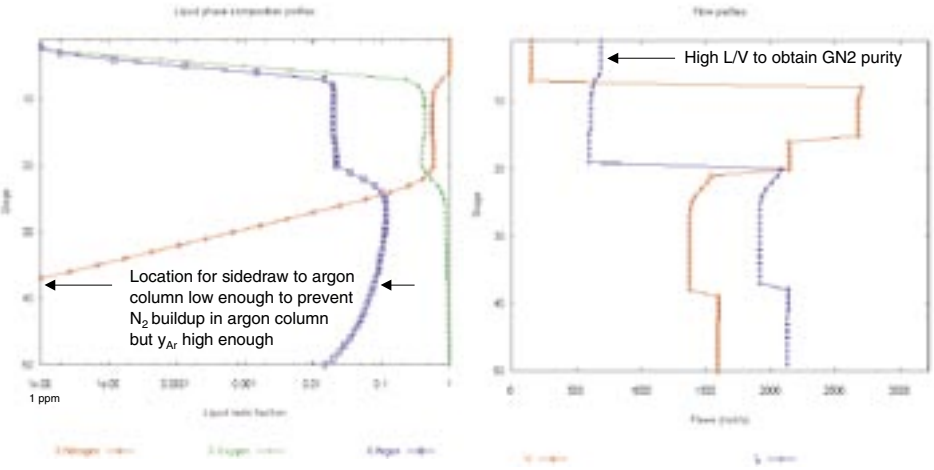


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Fig. 2
Air separation flowsheet solved in COCO/COFE flowsheeter using the ChemSep equilibrium column models. Note that the side stripper and the low pressure column are tightly connected as exemplified by the compositions and flow profiles of the low pressure column

is fitted to the special needs of BASF with a focus on low pressure calculations. Therefore, some of the newer thermodynamic models, especially equations of state, were missing. Multiflash was chosen as the external thermodynamics package, as it is easy to use and contains nearly all the missing models. The implementation of the CO thermo-interface (v1.0) turned out to be less easy than first anticipated. Extra time was spent on implementing the CO Material Object, on error handling (when properties are requested that Multiflash did not implement), and composition derivatives (which had to be obtained numerically). Despite these problems, the CO-interface now works. The use of external thermodynamic models via CO only slows down the calculation speed of CHEMASIM by a factor of two or less. Given the benefits this is quite acceptable.

Conclusion and Outlook

CAPE-OPEN has become an industry endorsed standard backed up by process simulation market leaders. It can reduce the overhead for implementing in-house unit operations and thermodynamic models. At the annual 2006 CO-meeting, vendors showed seamless integrations in a Plug-and-Play manner of different tools and versions in commercial process simulation environments, running at acceptable speeds. Thus, CAPE-OPEN allows industry to use the right mix of commercial and in-house proprietary software, speeds up model development, reduces maintenance costs, improves the model validation process, and allows niche software vendors to provide the market with CO-compliant components. New test- and logging software as well as development wizards are available that will accelerate the development of models and enhance the interoperability of simulation software. Use of CO-technology in academic and Joint Industry Projects can provide solutions that can directly be used by end-users, reducing the time to market. As the standard is transparent, the user does not need to change the way he works, but just plugs in a new thermodynamics model or new unit operation when needed. Such a new tool can be tested separately from the main simulator. This reduces risks and requires no strategic planning. As tools can be acquired in different numbers as our flowsheeting software, software-licensing costs can be reduced. New developments, such as petroleum properties and the enhanced handling of phase equilibria (3+ phases) will also stimulate the introduction of new simulation technology into the market. ●