Exchanger Rating Using CAPE-OPEN in a Process Modeling Environment

Joseph W. Holmes, Heat Transfer Research, Inc., David L. Johnson, BP p.l.c., Sunday Ogundiran, BP p.l.c., and Mark Lichtenauer, Consultant

Introduction

A critical part of the everyday workflow for process engineers today is the increasing number of software tools. These programs perform such critical functions as generating fluid physical properties, modeling processes, rating unit operations, and estimating costs. In a perfect world, a single piece of software would perform all these functions and use information specified by the engineer for all calculations.

Unfortunately, we do not live in that perfect world, and process engineers have to rely on multiple software tools from different vendors. Each tool has a different interface, a different input format, a different set of output reports, etc. The impact is that process engineers may spend more time manually transferring input and output between formats than actually using the engineering tools. In addition to time lost, there are the issues of transcription errors and physical property consistency. Manually transferring data can result in transcription errors with resultant loss in the accuracy of the calculated results. Because many engineering calculations rely on fluid physical properties, many process engineering tools have their own property calculation systems. Of course, individual property systems mean potentially different results for the same fluids at the same conditions.

As soon as more than one engineering program became available, vendors started developing interfaces between the various tools. However, each pair of software tools required a separate interface, and each interface worked differently. Some interfaces required specific versions of the software on each end. Although these interfaces eased the problem, they did not provide a real solution.

CAPE-OPEN

In the early and mid 1990s, a group of end-users, software vendors, and academic institutions worked together in the CAPE-OPEN and Global CAPE-OPEN projects to develop a set of interface standards. These standards were designed to be process simulator centric (i.e., to allow interfacing of process simulators with various plug-in components). As this presentation will show, the interfaces turn out to be somewhat more flexible than originally planned.

Since the release of version 1.0 of the CAPE-OPEN standards, a number of the major engineering software providers, including Heat Transfer Research, Inc. (HTRI), have implemented these interfaces.

CAPE-OPEN defines a number of interface types to cover a wide range of usage scenarios, and HTRI has focused on two: Unit Operations and Thermodynamics and Physical Properties. As implemented in HTRI software, the Unit Operation interfaces allow embedding of an external unit operation in a process simulator, while the Thermodynamics and Physical

Properties interfaces allow an external program to use a process simulator or other property package as a property server to generate fluid physical properties.

CAPE-OPEN not only addresses the problematic issues defined in the introduction but also goes one step further. In addition to allowing transfer of data between separate programs, CAPE-OPEN allows these programs to interoperate. That is, separate programs with different capabilities can be run simultaneously, almost as a single program. In many cases, this interoperability provides the most effective process model.

In the case of heat exchangers, the subject of this presentation, the process model often depends upon detailed rating of the heat exchangers present in the flow sheet. For instance, the actual pressure drop present in an exchanger can determine the operating pressure of subsequent unit operations. This effect may significantly impact the predicted performance of these unit operations. In addition, if the unit operation models execute as a part of the process flow sheet, there is no need to iterate between the flow sheet and unit operation models.

Example Application

Although HTRI and our partner vendors extensively tested the CAPE-OPEN interfaces in the HTRI ***X****changer Suite*® software, it is desirable to document actual use in a production environment. BP p.l.c. is an HTRI member and also a member of CO-LaN, the organization that maintains the CAPE-OPEN standards. Because this technology may improve the efficiency of their process modeling efforts, BP agreed to test the CAPE-OPEN interfaces in their production environment.

BP uses HTRI ***X****changer Suite* for rating heat exchangers and AspenTech Aspen Plus™ for modeling some of their processes. For this test, BP selected a typical gas processing flow sheet, as illustrated in Figure 1.

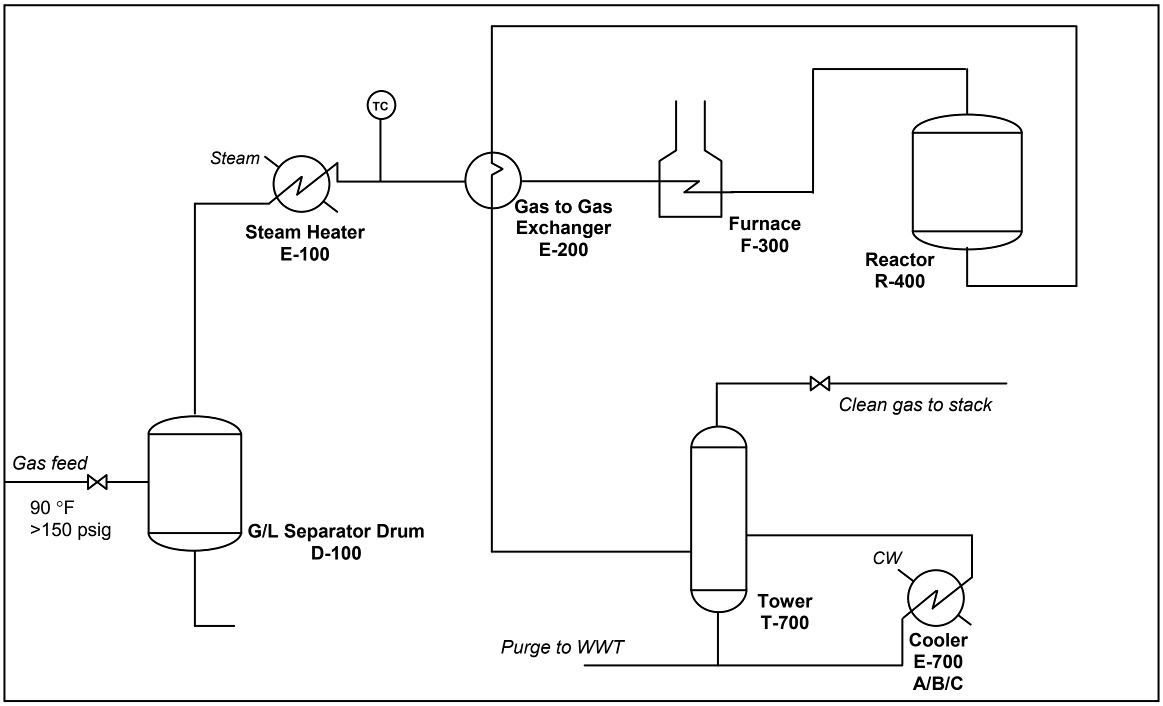

Figure 1. Gas processing flow sheet

BP had modeled this process previously and understood the system well. It contains several heat exchangers using both single-phase and two-phase fluids. In this case, BP modeled the flow sheet using Aspen Plus 12.1.9 and HTRI ***X****changer Suite* 5.0. This version of ***X****changer Suite* is the latest released version, but the version of Aspen Plus is several years old. It is important to note that the latest version of the process simulator is not required. Large organizations typically require an intensive validation before they accept new versions of process simulation software. The CAPE-OPEN technology available now uses widely distributed versions of the major process simulation software.

To implement the flow sheet in Figure 1, BP followed a simple procedure:

1) Run simulation using ASPEN generic heater blocks and obtain a converged solution.
2) Re-run simulation three times, converting the ASPEN heater blocks to CAPE-OPEN blocks one at a time until all three blocks are converted.
3) Adjust utility (e.g., steam and cooling water) flow rates to match process stream duties and re-run simulation. (This step allowed the HTRI software to rigorously rate the exchangers.)
4) Re-initialize the simulation to purge all prior results. Restart and run the simulation. The runtime for step 4 was approximately equal to that of step 3 and demonstrated that the flow sheet convergence was not impacted by use of the rigorous unit operation models.

The procedure outlined above demonstrates a few differences when CAPE-OPEN interfaces are used.

- Instead of a native simulator unit operation, you must select a generic CAPE-OPEN unit operation and then choose from a list of all registered CAPE-OPEN unit operations installed on your PC. For ***X****changer Suite*, this list includes operations for shell-and-tube exchangers, air-cooled exchangers, economizers, and plate-and-frame exchangers. Additional unit operations are available from other vendors.
- The input for a CAPE-OPEN unit operation is typically more complex than a native simulator unit operation, a consequence of a more rigorous calculation that allows the user much more control over the unit operation.
- Runtimes are generally longer than with native unit operations. Depending upon the flow sheet and the complexity of the unit operations, the simulator runtimes may actually be dominated by the CAPE-OPEN unit operation runtimes. However, the total runtime is still much less than the time required to iterate between simulator and unit operation calculations separately and transfer data between each iteration.

BP also tested fluid property generation. They were able to verify that the properties generated via the CAPE-OPEN interface were identical to those generated with their in-house interface that extracts properties from Aspen Plus.

As a final test, BP exported the CAPE-OPEN exchangers from Aspen Plus to native HTRI formats. These unit operations were then run in a standalone fashion independently of Aspen Plus. As expected, the results were identical to the exchangers embedded in the flow sheet.

Portability

One goal of the CAPE-OPEN interfaces is *portability*. Interfaces written to CAPE-OPEN specifications should work equally well in other environments. To test this portability, the same process as in the first example was generated in another simulator (UniSim Design) that contains CAPE-OPEN interfaces. The geometry of the exchangers from the Aspen Plus run were exported and then imported into the UniSim Design flow sheet. Similar (e.g., cubic equation of state) but not identical physical property models were selected in the UniSim Design flow sheet.

Table 1. Unit operation results

Exchanger	Overdesign,%	ΔP, kpa	
		Shell	Tube
E-100			
Aspen Plus	8.39	16.7	16.9
UniSim Design	8.73	16.9	16.9
E-200			
Aspen Plus	7.83	19.6	12.3
UniSim Design	-0.99	19.5	12.2
E-700			
Aspen Plus	6.99	54.6	47.0
UniSim Design	8.93	54.3	46.8

Overdesign is a measure of the amount of excess surface area present in the specified exchanger geometry. The greatest difference appeared in the E-200 exchanger, but even it exhibited less than a 10% difference in estimated performance due to different property predictions between the two simulators.

Workflows

Not surprisingly, any interface that requires a substantial change in workflow will face opposition prior to acceptance. Ideally, CAPE-OPEN interfaces should require no or few changes in workflow. This section will discuss various usage scenarios (in the context of exchanger rating) that CAPE-OPEN interfaces support.

Simultaneous process and unit operation modeling

The first workflow (the one BP employed in their test) appears in Figure 2.

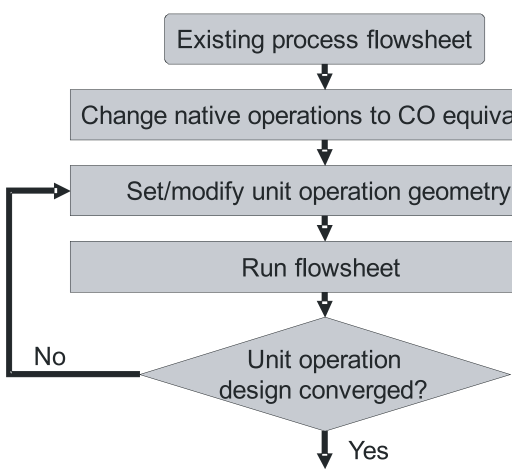

Figure 2. Embedded simulation

In this workflow, the process flow sheet is developed normally in the process simulation software except that the native exchanger unit operations are replaced with CAPE-OPEN equivalents. The flow sheet is executed, and changes are made to the exchanger geometry as necessary for proper process design.

This workflow is probably the most intuitive one for a user who typically works in the process simulation environment. It also has the advantage of simultaneously handling process and unit operation design. The tradeoffs are that the flow sheet may take longer to run with the rigorous unit operation models and that flow sheet convergence may be less robust.

When a flow sheet converges, the exchanger unit operations behave realistically with possible non-linear behavior as a function of process conditions (e.g., flow rates, pressures, and temperatures). Thus, engineers obtain a more realistic process model at the expense of convergence stability. If necessary to improve convergence stability, users may initially define exchanger duties. One at a time (or more as the flow sheet allows), users can let the exchanger duties be predicted and converge the exchangers individually if necessary.

Offline modeling of unit operations

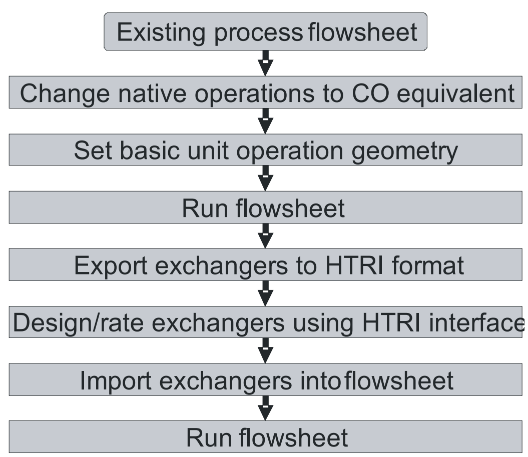

Figure 3. Offline modeling

In this workflow, the iteration of the exchanger designs occurs offline after the initial iteration through the flow sheet that causes the CAPE-OPEN units to generate the necessary fluid physical properties for performance prediction. The CAPE-OPEN exchangers are exported to native HTRI format, after which the ***X****changer Suite* interface handles the exchanger design. After the geometry is finalized, it can be imported back into the process flow sheet. The efficiency of this workflow depends mainly upon 1) the user's comfort level in ***X****changer Suite* versus the process simulator interface and 2) runtimes of the process flow sheet with the embedded CAPE-OPEN units.

Process simulator as unit operation interface

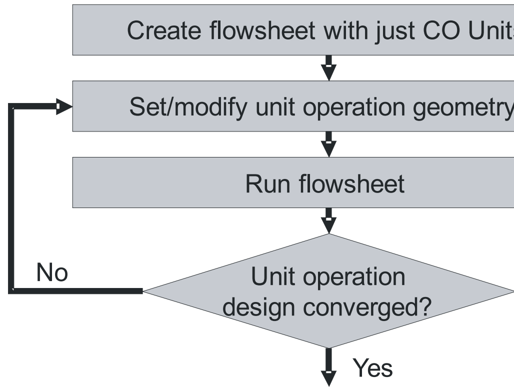

Figure 4. Simulator as interface

The workflow diagrammed in Figure 4 represents a scenario that HTRI did not deliberately set out to support but that the CAPE-OPEN interfaces enable; a number of users who are not very familiar with the ***X****changer Suite* interface but are very comfortable in the process simulator environment have used this workflow. It allows users to perform standalone exchanger design using the process simulator as a front end, bypassing the need to specify or generate fluid physical properties in ***X****changer Suite*. The user creates material streams with compositions, process specifications, and property models in the simulator environment and then connects them to a CAPE-OPEN unit operation. The ***X****changer Suite* interface is used only as a mechanism to specify exchanger geometry.

Process simulator as property generator

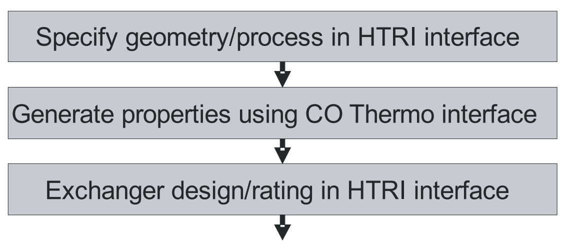

Figure 5.Simulator as property generator

In this final workflow, the exchanger design is specified in ***X****changer Suite*; the fluid properties are generated using the CAPE-OPEN Thermodynamic interface to drive a process simulator or other property package that supports these interfaces. The property generation happens transparently in ***X****changer Suite*. This workflow is most suited to experienced users of HTRI software who are very familiar with the ***X****changer Suite* interface.

Future Work

HTRI is planning to enhance our implementation of CAPE-OPEN interfaces to address some of the concerns outlined above.

Currently, if users want to switch between a rigorous unit operation model and one that simply provides heat and mass balances, they must delete the existing unit operation, replace it with a different type, and reconnect the material streams. HTRI plans to provide a switch in the rigorous model that allows it to behave as a native heat exchanger unit operation.

Users will then be able to switch easily between rigorous and simple unit operation models without modifying the flow sheet itself.

Along similar lines, we plan to implement an option that enables the user to run a rigorous model after the fact without having to rerun the flow sheet. In this scenario, users converge the flow sheet using CAPE-OPEN unit operations in the simple heat and energy balance mode and then rigorously rate individual exchangers on demand.

Summary

When implemented, CAPE-OPEN fulfills the promise of a single interface that connects multiple programs. These interfaces support a variety of workflows that offer users different ways to achieve their design goals without requiring substantial changes in their procedures.

The CAPE-OPEN interfaces offer a number of tangible benefits:

- Simultaneous process simulation and unit operation rating
- Inclusion of the effect of rigorous unit operation models in a process model
- Transparent transfer of process and property information

However, using these interfaces does involve a few trade-offs:

- At present, reporting is not well integrated. Reports must be generated in both the process simulator and unit operation interface to obtain complete results.
- Runtimes for process models can be significantly longer with embedded rigorous unit operation models. This increase is offset, however, by eliminating the need to run the unit operation models as a separate step.
- The potential exists for reduced flow sheet stability. The more realistic behavior of the rigorous unit operation models can affect flow sheet convergence.

CAPE-OPEN interfaces provide a cost effective way for vendors to develop standardized interfaces between various types of process engineering software. The end-users ultimately benefit from the availability of high quality interfaces between most (if not all) of their process software.