

Advances on CAPE-OPEN Unit Operation interfaces

The CAPE-OPEN Unit Operation Interface applied in industrial context

ECCE-8 on September 27, 2011 in Berlin, Germany

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This presentation, made by Richard Baur at the eighth European congress of chemical engineering in Berlin on September 27th 2011, will sketch the history and current state of the CAPE-OPEN Unit Operation Interface specification standard.

Presentation outline

- ❖ **Selected milestones of CAPE-OPEN**
- ❖ **CAPE-OPEN Unit Operation SIG**
- ❖ **Reasons to use CAPE-OPEN (with industrial background)**
- ❖ **Conclusion**

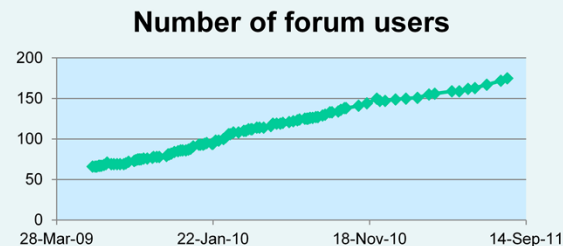
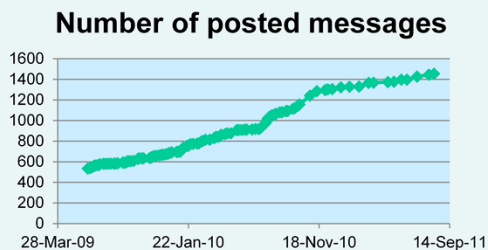
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First, a short overview will be presented of CAPE-OPEN, to illustrate where we are coming from. Next, the tasks of the Special Interest Group for the Unit Operation standard will be listed. The larger part of this presentation deals with showing why people in industry are choosing CAPE-OPEN based Unit Operation implementations. And we will finish with some conclusions.

Selected milestones of CAPE-OPEN

- ❖ 1994: first idea by BP
- ❖ 1997-1999: CAPE-OPEN project
 - ❖ Feasibility demo ESCAPE-9 May 1999
- ❖ January 2001: CO-LaN
- ❖ 2002
 - ❖ January: version 1.0 published
 - ❖ August: IFP FIBER Unit Operation
 - ❖ December : Unit SIG
- ❖ 2008: CAPE-OPEN forum



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CAPE-OPEN is an adventure and a development process that spans more than 10 years nowadays. The idea emerged from BP in 1994 with the concept of taking Unit Operation models from the shelf and plugging them into any process simulator. The idea was shaped into the form of the CAPE-OPEN project that ran from January 1997 till mid 1999: the feasibility of CAPE-OPEN interoperability was publicly demonstrated at ESCAPE-9 on June 1st, 1999 using the first ever-made CAPE-OPEN Unit Operations. Then the Global CAPE-OPEN project pushed successfully for the commercial availability of CAPE-OPEN interfaces and much work was done within the Interoperability Task Force to test and debug the first implementations of the Unit Operation interfaces.

CO-LaN, a deliverable of the Global CAPE-OPEN project, was founded in 2001 and its UNIT Special Interest Group started up in December 2002 with responsibilities on managing the UNIT specification. 2002 saw also the release of version 1.0 of the CAPE-OPEN standards where the UNIT interface specification was almost identical to the version released at the end of CAPE-OPEN.

The first industrial CAPE-OPEN Unit Operation to be publicly mentioned may have been the FIBER Unit Operation from IFP in August 2002 while others were developed in-house in several companies around the same period. Ever since, scores of CAPE-OPEN Unit Operations have been developed, distributed and used. Mention of a number of these developments may be found on the CAPE-OPEN forum which has been developed since 2008.

CAPE-OPEN Unit SIG

- ❖ **Unit Operation Special Interest Group (SIG) responsible for**
 - ⇒ **Maintaining and publishing the standard**
 - ⇒ **Responding to issues raised by developers and users**

- ❖ **2010 accomplishments:**
 - ⇒ **Revised standard specification ready for internal review**
 - ⇒ **Definition of energy and information streams**
 - ⇒ **Revision of parameter dimensionalities**
 - ⇒ **Dynamic Unit specification is converging**

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Each of the interface specifications within the CAPE-OPEN standard was developed within a work package of either the CAPE-OPEN or the Global CAPE-OPEN projects. Maintenance of these specifications is now the responsibility of Special Interest Groups created by CO-LaN in order to fulfill industrial needs.

The Unit Operation Special Interest Group is one of those. It has the responsibility to maintain, publish and promote the Unit Operation interface standard, and it solves issues that are raised by users and developers. Recently, a revision of the document describing the Unit Operation interface specification was formulated, with a number of corrections and clarifications, as well as a clear definition of energy and information streams. This document is under revision for publication. Also, work is underway on formulating an interface specification for Unit Operations in the context of dynamic simulations.

CAPE-OPEN Unit SIG

❖ Members:

- ⇒ Richard Baur (Shell Global Solutions), SIG leader
- ⇒ Jasper van Baten (AmsterCHEM)
- ⇒ Didier Paen (RSI)
- ⇒ Thomas Williams (PSE)
- ⇒ Alain Vacher (Prosim SA)

❖ Join? Contact Richard Baur

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The Unit Operation SIG currently has 5 members, all with different backgrounds. As with most Special Interest Group an end-user representative is leading the group. If you have a special interest in Unit Operations, and you feel your contribution can be useful, you can join. Please contact Richard Baur.

Reasons to use the CAPE-OPEN Unit Interface

- ❖ Write once, target multiple platforms
- ❖ Integrate software packages
- ❖ Achieve consistency across simulation platforms
- ❖ Use of existing in-house models
- ❖ Support joint development projects
- ❖ Use Unit Operations as numerical tools
- ❖ Deal with limited access to 3rd Party Software
- ❖ Target enhanced flexibility
 - ❖ quick prototyping using generic solvers
- ❖ Apply recognized worldwide industry standard

In the next section, we will look at a number of compelling reasons to use the CAPE-OPEN Unit Operation interface standard for integration of Unit Operations in simulation environments. All of these points are illustrated with examples taken from industry. Reasons are many and all make use of the underlying functionality provided by CAPE-OPEN: seamless interoperability.

Write once, target multiple platforms

HTRI *Xchanger Suite*®

Rigorous heat exchanger modeling

The HTRI logo consists of the letters "HTRI" in a white, serif font, with a registered trademark symbol (®) to the upper right. The logo is set against a dark blue rectangular background.

- ▶ Thermodynamic and Physical Properties
Generate fluid properties within *Xchanger Suite* interface
- ▶ Unit Operations
Embed rigorous heat exchanger models in process flowsheet
 - Shell-and-tube heat exchangers in *Xist*®
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Write once, target multiple platforms is of course one of the main arguments to use CAPE-OPEN. The unit operations of the Heat Transfer Research Institute HTRI are a good example of this. Their heat exchangers use thermodynamics consistent with the flowsheet they are running in to generate the properties of the fluids. They do this in the form of a CAPE-OPEN Unit Operation. The Xchanger Suite contains rigorous models for shell-and-tube exchangers, air coolers and economizers, and plate-and-frame exchangers.

Write once, target multiple platforms

HTRI Xchanger Suite®

Same interface with multiple packages

HTRI®

Tested with most major packages

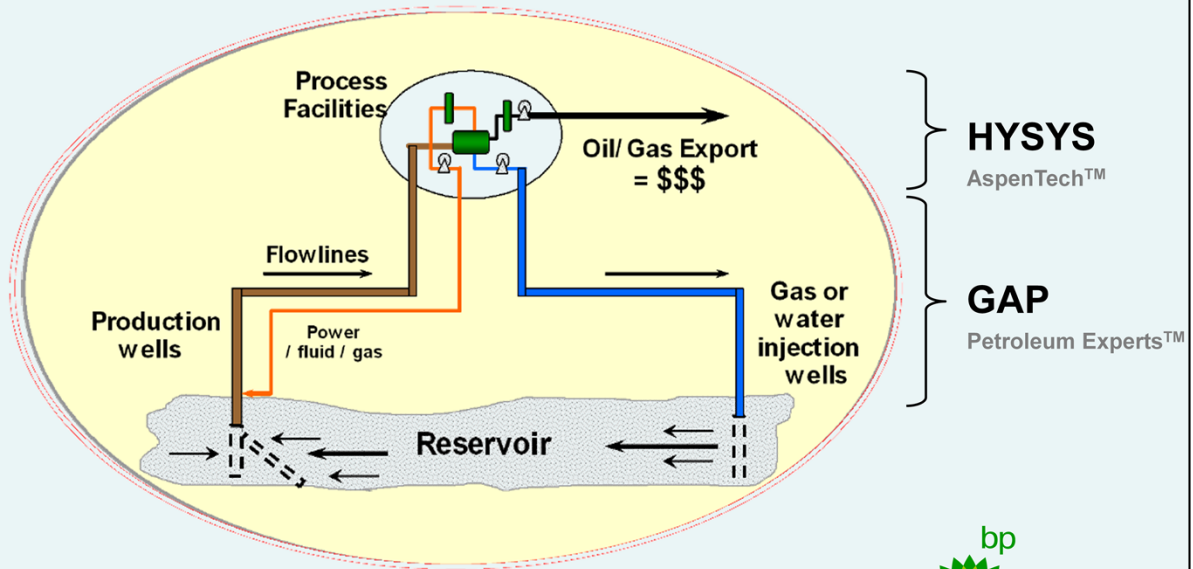
- ▶ Honeywell UniSim® Design
- ▶ KBC Petro-SIM™
- ▶ Invensys PRO/II™
- ▶ AspenTech Aspen Plus®
- ▶ AspenTech Aspen HYSYS®
- ▶ ProSim®
 - ProSimPlus
 - Simulis® Thermodynamics
Thermo only
- ▶ TÜV SÜD NEL
Physical Property Data
Service (PPDS)
Thermo only

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HTRI received the CAPE-OPEN award in 2005 for “successful commercial implementation of the CAPE-OPEN Unit interface in a specialized engineering software suite with a global user base”. In this context, their unit operations have been tested to function with Honeywell Unisim Design, KBC Petro-SIM, Invensys Pro/II, AspenTech’s AspenPlus and Aspen HYSYS and ProSim, and tested in conjunction with thermodynamic servers as well, including PPDS of TUV-NEL. And more. All of this using a single CAPE-OPEN plug.

Integrating software packages



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For steady state simulations of well and pipeline networks, BP, and many other companies active in the oil and gas, uses the GAP software package from Petroleum Experts. BP upstream uses Aspen HYSYS for simulation of the process facilities. From this picture it is clear that the downstream and upstream processing are part of the same process, yet they are simulated in separate software applications.

Integrating software packages

Benefits of integration include:

- Maximizing production whilst ensuring the asset remains within the safe operating envelope
- Underpin a common understanding of the asset across disciplines

Existing integrated simulation environments:

- Drivers are required for each client application
- End-user needs to learn yet another application
- Closing recycles requires dedicated optimizers

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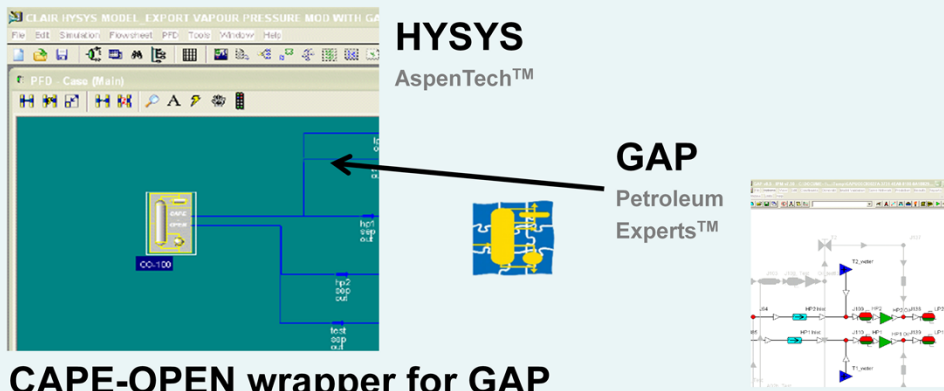
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Integrated simulation environments that combine the two packages are available, but require specific drivers for each of the programs to be included in the integration. The end-user needs to learn to work with additional software tools, and user mapping between the two approaches may be required. Closing recycles in such an approach is not an easy task.

However integrating the two approaches into a single simulation allows for system optimization within safe operation limits, and underpins cross-discipline understanding.

Integrating software packages



CAPE-OPEN wrapper for GAP

- Uses “OpenServer”
- Can be used in any CAPE-OPEN process simulator
- Development took approximately 2 weeks
- Required no modifications to GAP

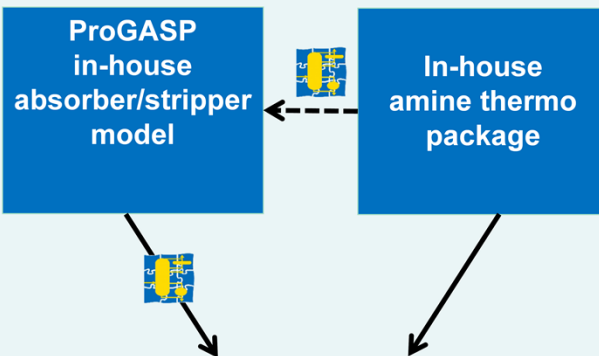
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The solution that was chosen was to simply wrap a GAP simulation as a CAPE-OPEN Unit Operation using GAP's OpenServer facilities. The GAP unit operation runs in any CAPE-OPEN compliant flowsheet simulator, including Aspen HYSYS. The development of GAP as a CAPE-OPEN Unit Operation was funded by CO-LaN, and is in use by BP. It is available to all CO-LaN full members. The development of the GAP Unit Operation took approximately two weeks, and required no modification to the GAP application.

Consistency across simulation platforms



“CAPE-OPEN enables us to use our in-house unit in two commercial simulation platforms without customization and so ensures consistency across the simulation platforms.”

Peter Nellen
Shell Global Solutions, Netherlands

Used in UniSim and PRO/II for down & upstream applications.

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Some companies use more than one process simulator. Shell Global Solutions for example uses both Unisim Design by Honeywell, and Pro/II by Invensys. It is important however that certain equipments in the two simulation scenarios give consistent simulation results. So the same model should be integrated in both environments. This example shows the GASP in-house absorber / stripper model. This model deals with amine based systems, and is best operated using the in-house amine thermo system SADIP. Both the Unit Operation and the thermodynamics can run in either of the simulation platforms, as their integration is CAPE-OPEN based.

Joint development projects

- ⇒ Wax deposition model (TUWAX)
 - ⇒ A pipe model (written in FORTRAN) simulating wax deposition over time and using advanced thermodynamics



- ⇒ HYSIFLO: Hydrate Flow Module Unit Operation in C++
 - ⇒ Evaluate flow properties and predict risk of blockage



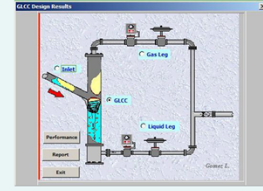
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Adopting CAPE-OPEN in joint development projects ensures that the resulting deliverable, if it is a Unit Operation model, will be usable by all partners whatever the process simulator to be used in each company. It is the case for TUWAX where TOTAL wanted to use a model of wax deposition in pipes within a process simulator model rather than just as a stand-alone tool. TUWAX is common to many companies within the PUPDP project at the University of Tulsa. Around IFP New Energy, HYSIFLO gathered partners using different process simulators and CAPE-OPEN was the common denominator for the unit operation model delivered.

Joint development projects

- ⇒ **Gas-Liquid Cylindrical Cyclone (GLCC®)**
 - ⇒ An original design and rating program written in Visual Basic 6



- ⇒ **Simulation tool for flow assurance studies (TINA)**
 - ⇒ IFPEN Pipe modules (steady-state and dynamic modes)



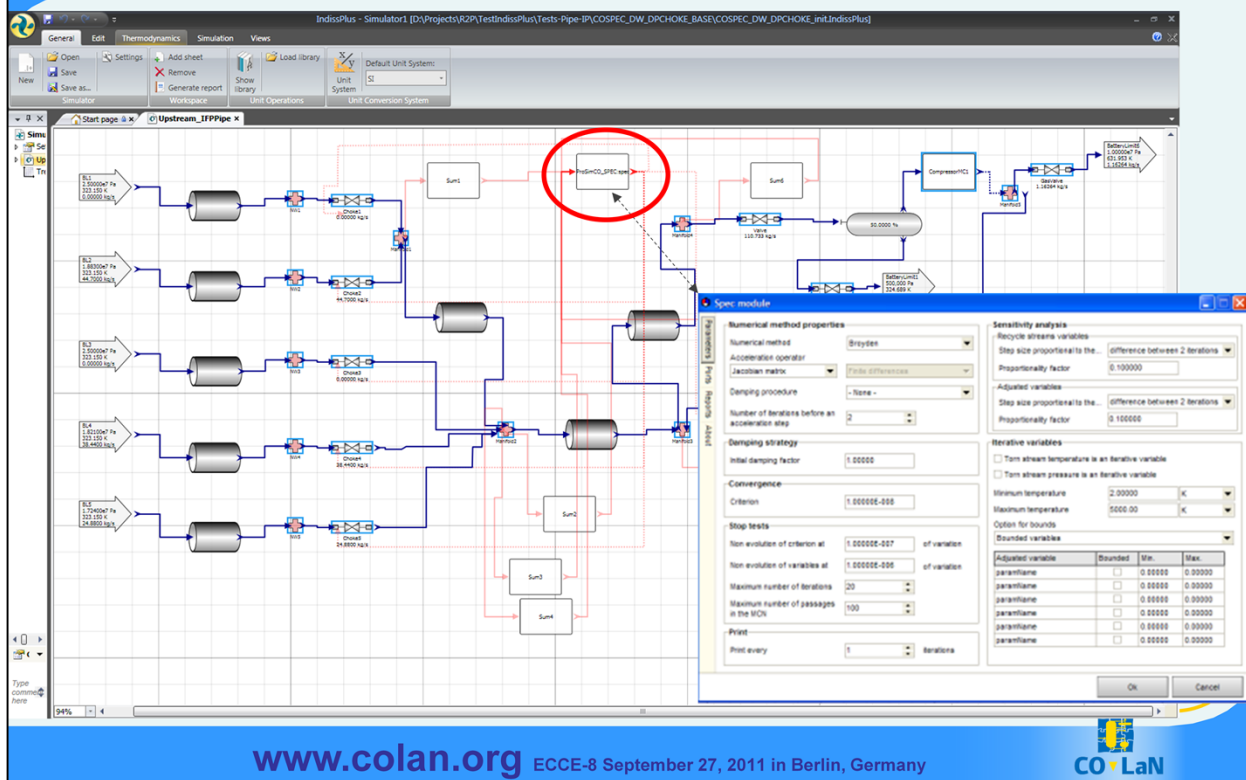
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GLCC is a software tool originally developed as a stand-alone design and verification model for a specific piece of equipment. Making this model a CAPE-OPEN Unit Operation enables one to use it in the same way one is using a heat exchanger design and verification software.

The R&D TINA project between IFP New Energy and TOTAL, apart from paving the road to a new process simulator at RSI for both steady-state and transient simulations, developed a number of unit operations, mostly representing oil and gas multiphase flow in pipes.

ProSim SPEC UO / IFPEN Pipes in INDISS+



In this slide we see the TINA project in action. Several pipe units of IFP New Energy are shown here in the INDISS Plus simulation environment, representing an oil and gas production field. Circled in red is another interesting feature of this particular simulation: this CAPE-OPEN based Unit Operation is not actually representing equipment, but rather a calculation of a convergence specification. The specification is passed on to the simulation environment's solver via a CAPE-OPEN information port. Which brings us to our next point..

Unit Operations as numerical tools

- ⇒ Simulation tool for flow assurance studies (TINA)
 - ⇒ Prosim solvers used as UOs (CO-SPEC / CO-OPTI)



- ⇒ Stochastic simulation functionality (STOSIM)
 - ⇒ To take into account variability of parameters and inputs (UO in Visual Basic 6)

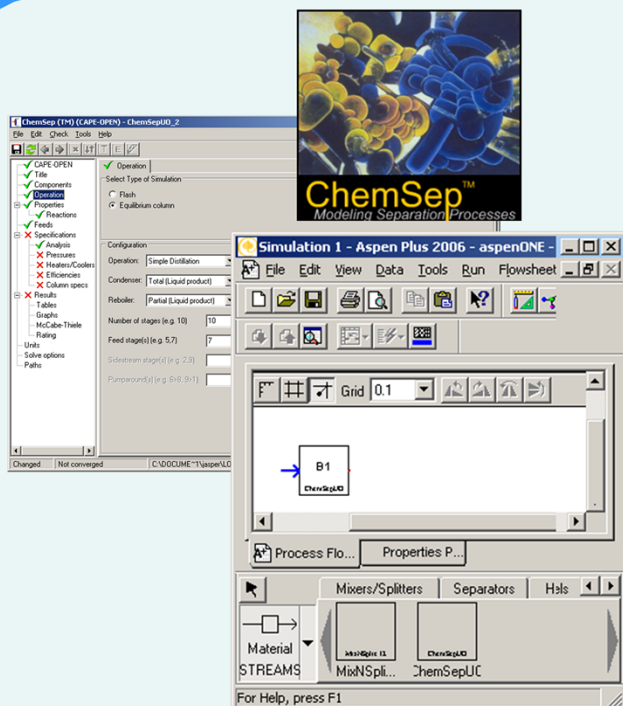


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You can use Unit Operations in a flowsheet for other purposes than just simulation of pieces of equipment. A unit operation has access to the streams it is connected to, and can therefore be used to provide meta information about the simulation; the Prosim solver specification unit shown in the previous slide exemplifies this. Similarly an optimizer has been wrapped as a CAPE-OPEN Unit Operation within the same TINA project. Or you can just use a unit operation to gather information about the process model and to define new simulations to be run, as STOSIM does. The stochastic variability of the inputs and of the results at solution is used in a post-processing step to analyze the process robustness.

Dealing with limited access to 3rd Party Software



“Using CAPE-OPEN we were able to develop a unit operation just once, and clients can run it in simulation environments to which we do not have access...”

Prof. Ross Taylor
ChemSep

The ChemSep Unit Operation has been used industrially by BP for simulations in AspenPlus.

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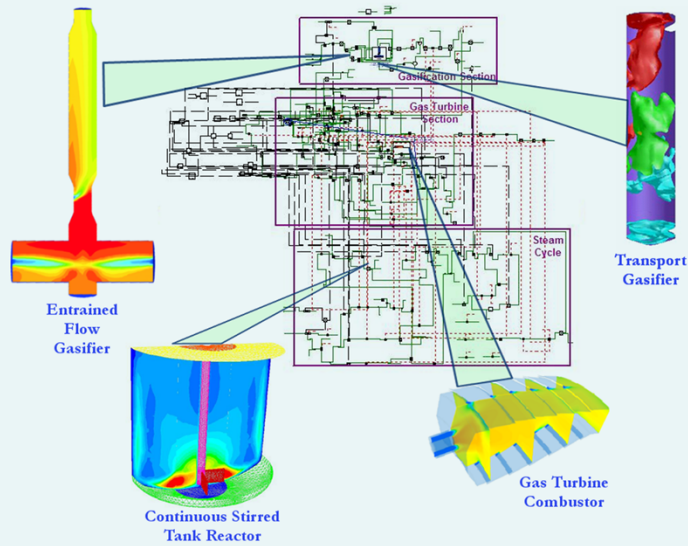
Not all companies have access to all simulation environments. Still you may want a unit operation to run in a simulation environment that is used by clients. CAPE-OPEN offers the way out, because if you can get the CAPE-OPEN compliant Unit Operation to work in one simulator, its compliancy can be tested and evaluated. It should then also run in other compliant simulators.

ChemSep is a separation column simulation package by Ross Taylor and Harry Kooijman. ChemSep is widely used in the academic and industrial world. A light version is available free-of-charge featuring an equilibrium distillation model, while a state of the art rate-based separation model is available commercially via the ChemSep consortium. The developers of ChemSep required a method of integration into process environments, with a wide support for different platforms, but did not have access to each of these platforms to allow platform specific couplings. Hence, CAPE-OPEN was chosen. The ChemSep CAPE-OPEN Unit Operation has been tested in many simulation environments. The ChemSep Unit Operation has been used industrially by BP for simulations in Aspen Plus.

Flexibility

ANSYS

- ❖ Co-simulation of process flowsheet models with ANSYS FLUENT CFD models
- ❖ Robust model database for local or remote storage of CFD equipment models
- ❖ Archival of a tailored, reusable library of high-fidelity and reduced-order equipment models
- ❖ Serial or parallel execution of CFD models on distributed Windows or Linux hardware
- ❖ ALSTOM Power has been a partner with ANSYS in demonstrating and validating the technology



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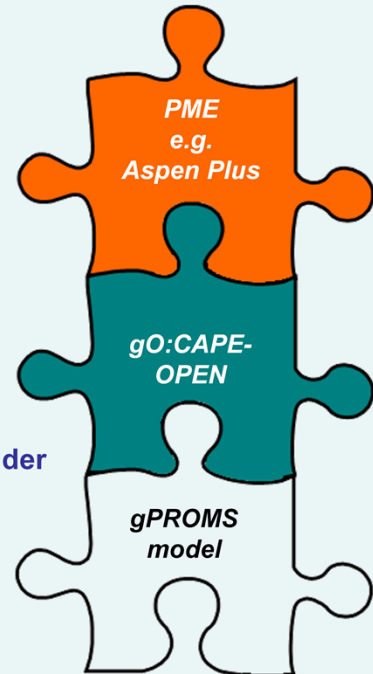
CO₂ LaN

The APECS Unit Operation of ANSYS enables the replacement of specific unit operation blocks in a flowsheet with Fluent CFD models (or custom in-house models) to provide a greater level of internal equipment detail, including profiles of temperature, pressure, chemical species fraction, velocity and more. As the interfacing is done via CAPE-OPEN, the APECS Unit Operation will run in any CAPE-OPEN compliant simulation environment, and the COM infrastructure allows for solving the CFD models in a distributed manner on remote computers. ALSTOM Power has demonstrated the technology with Alstom equipment/applications.

Flexibility

gPROMS CO Unit Plug

- Also known as “gO:CAPE-OPEN”
- Allows a gPROMS model to be embedded within a CAPE-OPEN PME, e.g.
 - Aspen Plus®, HYSYS®, UniSim®
 - PRO/II®, ProSim Plus®
 - COCO®/COFE®
- gPROMS model of any complexity
 - including 1D, 2D, 3D+ IPDAEs
- Wizard for exporting model from gPROMS ModelBuilder
 - no programming required
- Used by SASOL and TOTAL



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The gPROMS CO Unit Plug is another example of improved flexibility through CAPE-OPEN Unit Operations. One can set up a custom unit operation as a gPROMS model. Via the gPROMS ModelBuilder, a wizard is available to expose the model as CAPE-OPEN Unit Operation. At this point it can be run in a variety of simulation environments. The gPROMS CO Unit Plus is used by SASOL, TOTAL and others.

Flexibility

More Unit Operation implementations based on generic modeling tools:

- ❖ **ICAS/MoT based (DTU-CAPEC with ProSim SA)**
(ChERD, vol. 86 (2008) pp. 823–833)
- ❖ **Excel/Matlab/Scilab based (AmsterCHEM)**
<http://www.amsterchem.com/>
- ❖ **GAMS (CONICET)**
(ChERD, vol. 88 (2010), pp. 421-429)
- ❖ **Python (DWSIM)**
<http://sourceforge.net/projects/dwsim/>

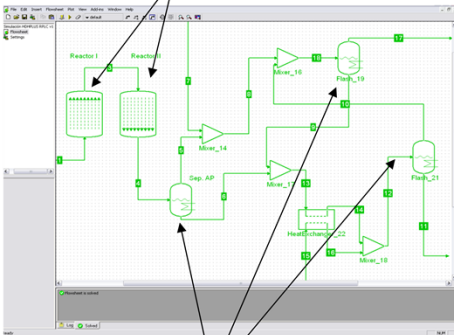
The list presented here of additional modeling techniques that can be applied to create CAPE-OPEN Unit Operations show the versatility and the flexibility of the current interface design. It emphasizes once more that CAPE-OPEN provides a reliable solution for developing and distributing models of unit operations.

World-wide CAPE-OPEN usage

Refinery processing



In-house Residue Vacuum Cracker Model



In-house Equilibrium Calculators



PDVSA
INTEVEP

“ We use CAPE-OPEN because it allows us to run our refinery reactor technology models and our in house equilibrium calculation models in different process modeling environments”

CÉSAR PERNALETE
Process Modeling group at PDVSA, Venezuela

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CAPE-OPEN was initiated by European and US end-user companies and already the Global CAPE-OPEN project was labeled as an Intelligent Manufacturing Systems project. IMS is an industry-led, international business innovation and research and development (R&D) program established to develop the next generation of manufacturing and processing technologies. As shown before

many European and US based companies are already applying the CAPE-OPEN standard. It is also the case in many other world regions including South America and China.

Here we see an example at PDSVA, the state oil company of Venezuela. César Pernaletе's group at PDVSA is quite active in CAPE-OPEN; recently they have developed and presented new equilibrium calculators and adapted an in-house vacuum cracking model as a CAPE-OPEN Unit Operation. Their motivation, common to many practitioners, is write once, run in multiple simulation applications.

World-wide CAPE-OPEN usage

SASOL

sasol
reaching new frontiers



- ❖ Using Delphi CAPE-OPEN Wizard
- ❖ Using gO:CAPE-OPEN (gProms)

- ❖ Most actively used during research and design

- ❖ Unit operations:
 - ❖ Glycol Ethers reactor
 - ❖ CatPoly reactor
 - ❖ Platformer reactor
 - ❖ Hydrocracker reactor
 - ❖ Three phase slurry models
 - ❖ PFR and CSTR models (Delphi Modeling Framework)

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SASOL, the South African coal and oil company, uses in addition to the gPROMS CAPE-OPEN plug, the Delphi CAPE-OPEN wizard. The Delphi CAPE-OPEN wizard is written by Christo Crause of SASOL and available as open source from SourceForge. SASOL uses CAPE-OPEN Unit Operation mostly in research and design. The group of Christo Crause uses a variety of reactor unit operation models via CAPE-OPEN.

Conclusion

- ❖ **From concept to applications in 10 years**
- ❖ **Wide support in simulation applications**
- ❖ **Wide variety of industrial CAPE-OPEN Unit Operations**
- ❖ **Interoperability**
- ❖ **Proven Technology**

Some words of conclusion. We have shown that in the slightly over 10 years of history of CAPE-OPEN, a concept has become something that is being applied on a fairly large scale. It must have been clear from the contexts shown in this presentation that the support for CAPE-OPEN is not present in one or two simulation environments, but in all major flowsheeting applications and quite a few specialty applications. Not only is there a large momentum for using the standard: the standard is also being applied to a large variety of actual Unit Operation implementations, throughout industry and all over the world. The reasons for using CAPE-OPEN always boil down to: interoperability. Whether it is computer programs, companies, or people interoperating. CAPE-OPEN can now be seen as a proven technology.

Use CAPE-OPEN Unit Operations!

- ❖ Thank you for your attention
- ❖ Questions?



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Thank you for your attention. We do hope that you will just jump in and develop and use CAPE-OPEN Unit Operations just like the pictured people did a short while ago!.