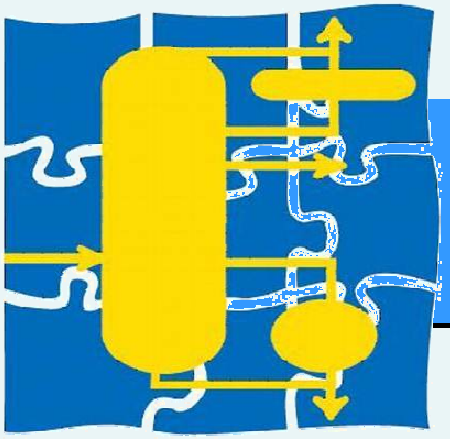


CAPE-OPEN applications in Shell

Lunch & Learn, February 7th, Amsterdam

General introduction on CAPE OPEN

Demo of the amine absorption model

Demo of the hydrotreating model

Demo of model prototyping toolboxes in Excel & MatLab

Richard Baur, Anja Olijve, Peter Nellen, Jasper van Baten

What is CAPE-OPEN?

CAPE: Computer-Aided Process Engineering

OPEN: Freely available standard specification

Expanding Process Modeling Capability through Software Interoperability Standards

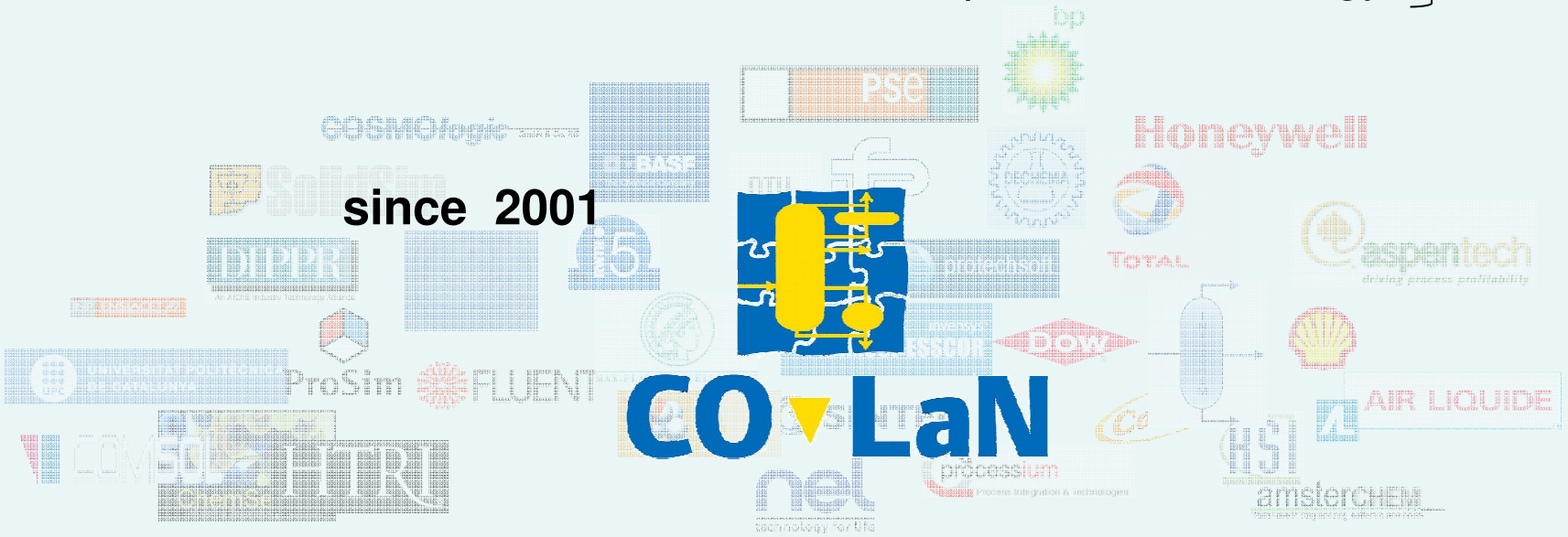
What is CAPE-OPEN?

1994 first idea by BP

1997-1999 CAPE-OPEN project: concept proven

1999- 2001 GLOBAL CAPE-OPEN: implement technology

EU funded initiative

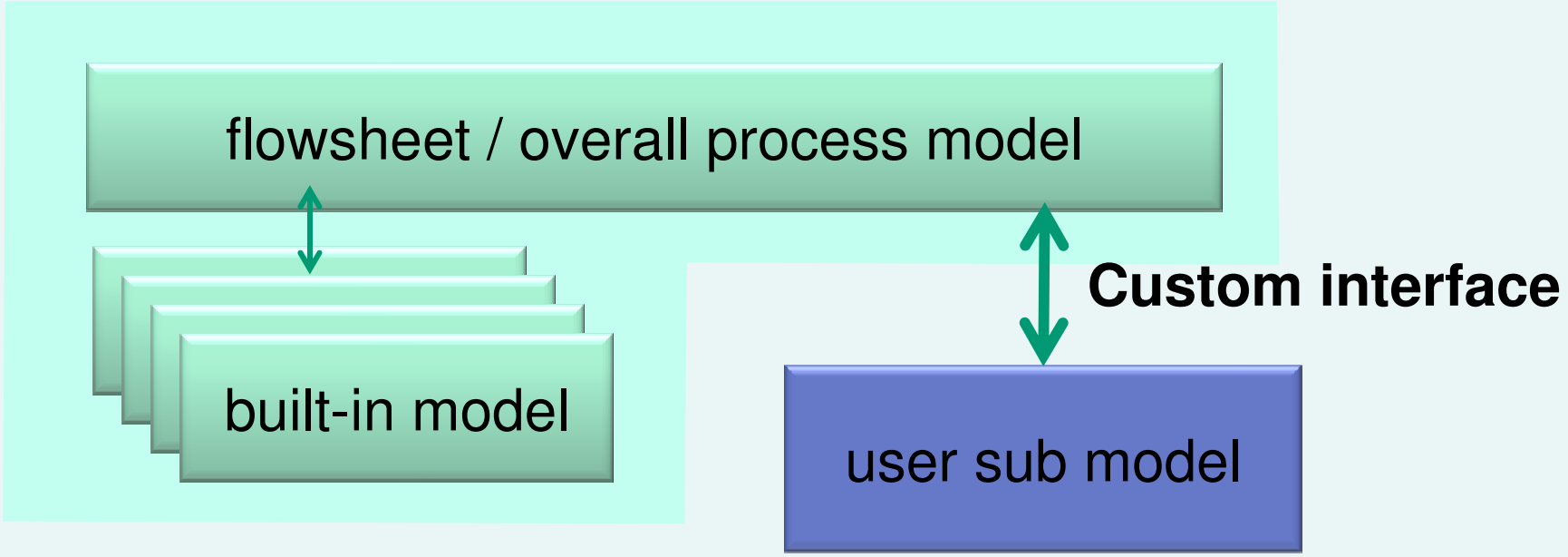


48 Software vendors (nearly all major players) & 24 Academic institutions
many more operating companies & individuals

What is CAPE-OPEN?

PME: process modeling environment

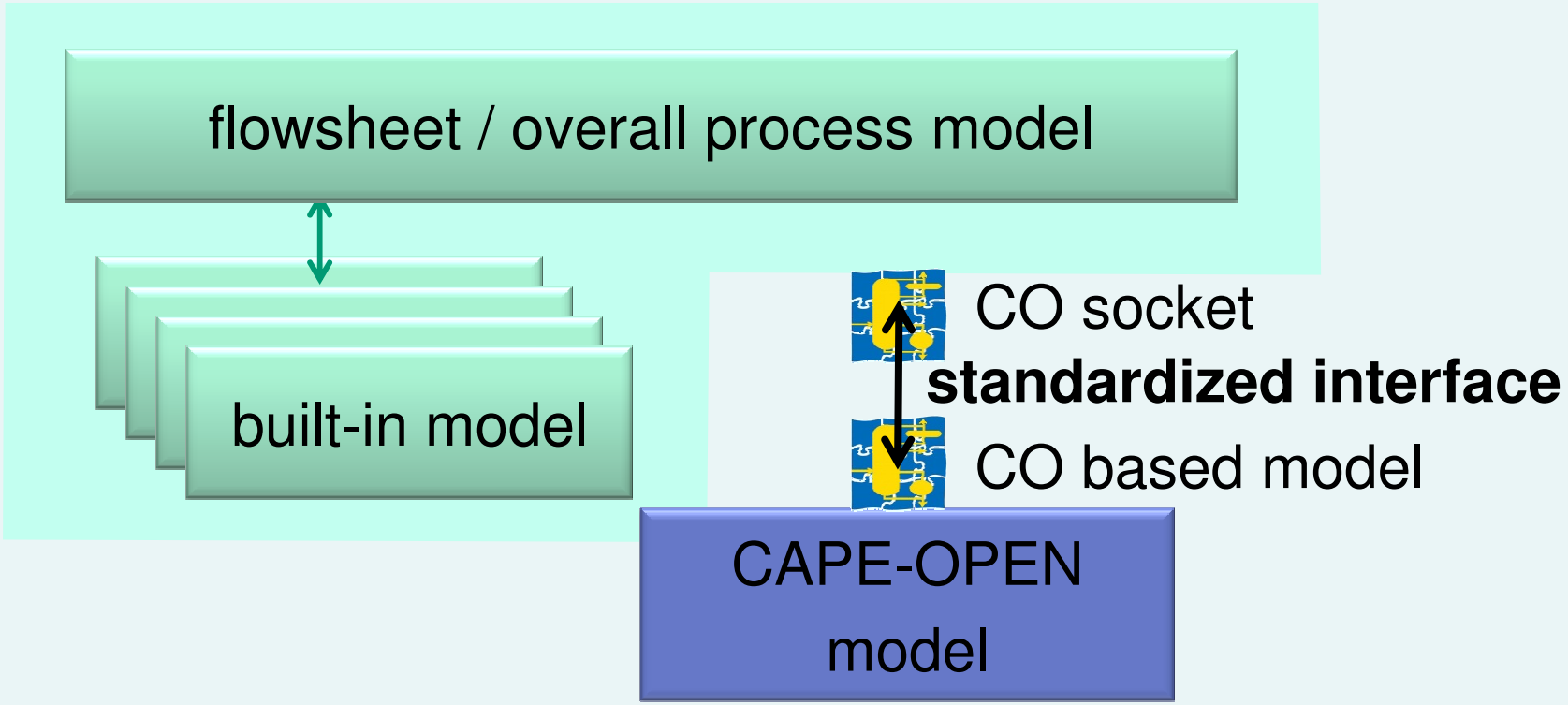
any model-based applications, optimizer, flowsheeting environment, excel, matlab, etc…



PMC: process modeling components

Physical properties, Unit operation modules,
Numerical solvers, flowsheet,
Excel spreadsheet calculation etc…

What is CAPE-OPEN?



Current implementations use COM as Middleware
Therefore: currently limited to Windows

DRIVERS FOR CAPE-OPEN

CAPE-OPEN interfaces are built once & reused many times. Their maturity increase continuously with time.

Software vendors

- Reduce expenditures for connectivity when targeting multiple platforms
- Increase license sale by integrating applications / combining software packages

DRIVERS FOR CAPE – OPEN

End users:

- Flexibility on the choice of software to be used.
- No cost for creating and upgrading custom interfaces through operating system or device vendor changes
- Consistency across simulation platforms
- Facilitates work in joint development projects

CO sockets

	Aspen	PROII	USD	PROSIM	HYSYS
Thermo v1.0	✓	✓	✓	✓	✓
Thermo v1.1		✓		✓	✓
Petro properties		✓			
Unit Operations	✓	✓	✓	✓	✓

Dynamic unit operations: prototype implementation in INDISS
Hydrodynamic specification: prototype under development (IFP)

CO plugs

- **Thermo servers:** AspenProps, COM Thermo, Honeywell Thermo, Infochem, VMG, ProSim Simulis, TUV/NEL, AIX, TEA, (and more …)

  Shell in-house: SPPTS(?)

- **Unit operations:** ANSYS, PSE, Chemsep, HTRI, COUSCOUS, (many more …)

  Shell in-house: LNG heat exchanger model, amine absorption model, hydrotreating model, etc...

Subsequent slides are copied from a presentation at the ECCE-8, 2011 in Berlin, Germany

Write once, target multiple platforms

HTRI *Xchanger Suite*®

Rigorous heat exchanger modeling

- Thermodynamic and Physical Properties

  Generate fluid properties within ***X****changer Suite* interface

- Unit Operations

  Embed rigorous heat exchanger models in process flowsheet

  - Shell-and-tube heat exchangers in ***X****ist*®
  - Air coolers and economizers in ***X****ace*®
  - Plate-and-frame heat exchangers in ***X****phe*®

Write once, target multiple platforms

HTRI *Xchanger Suite*®

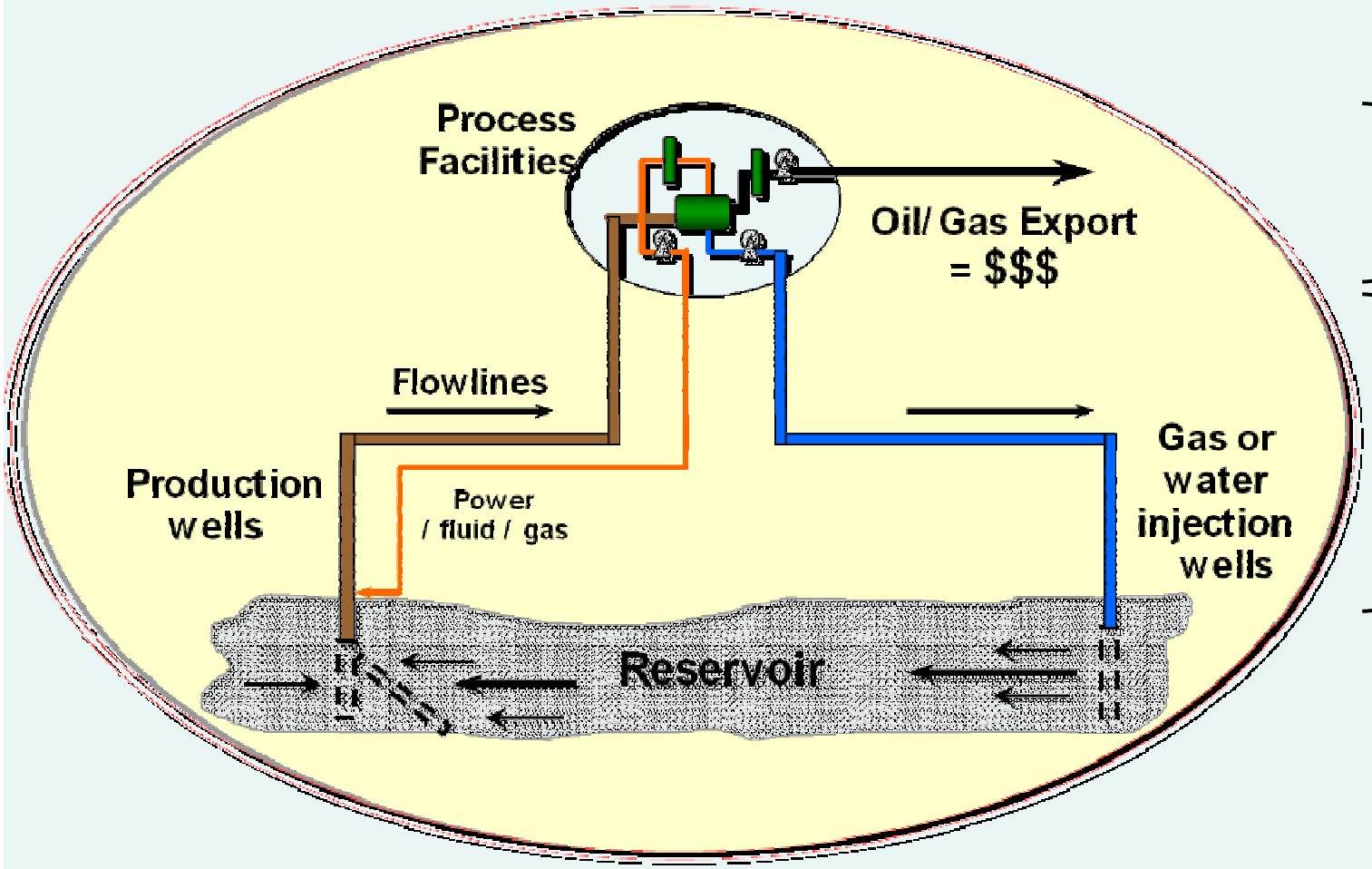
Same interface with multiple packages

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

Integrating software packages



HYSYS
AspenTech™

GAP
Petroleum Experts™

Reproduced with permission from BP: presentation made at Optimize 2011, May 2011

Integrating software packages

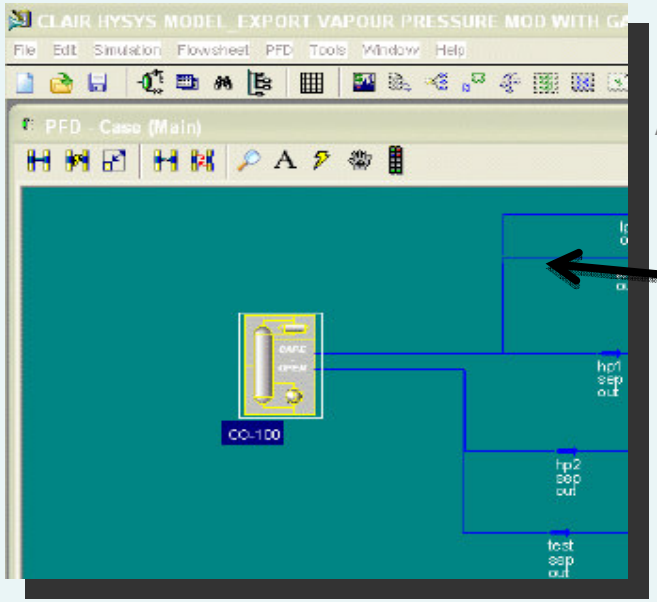
Benefits of integration include:

- **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**

Integrating software packages

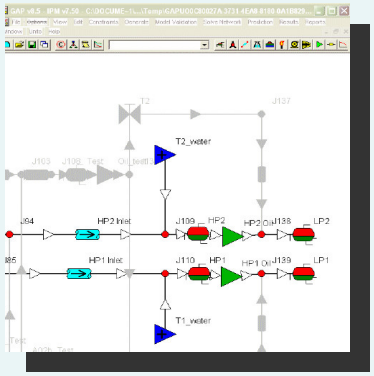


HYSYS

AspenTech™

GAP

Petroleum Experts™

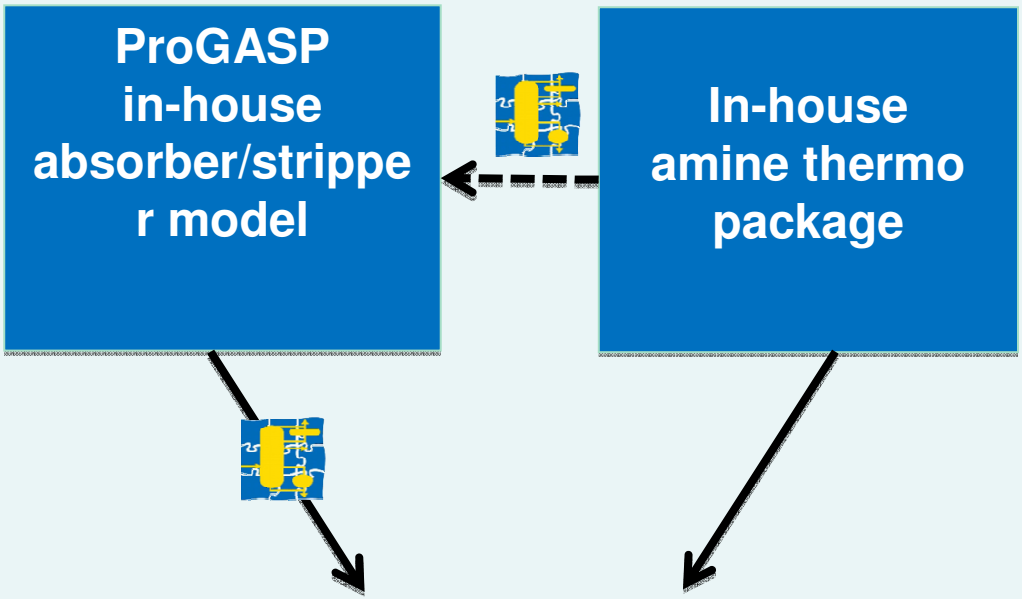


CAPE-OPEN wrapper for GAP

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

Reproduced with permission from BP from presentation at Optimize 2011, May 2011

Consistency across simulation platforms



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

"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

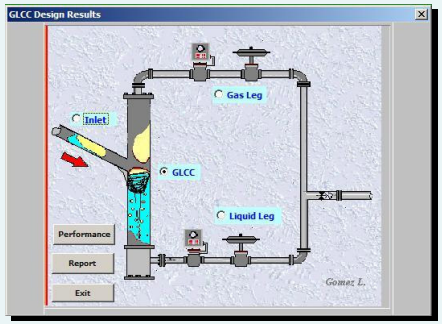
Joint development projects

- 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

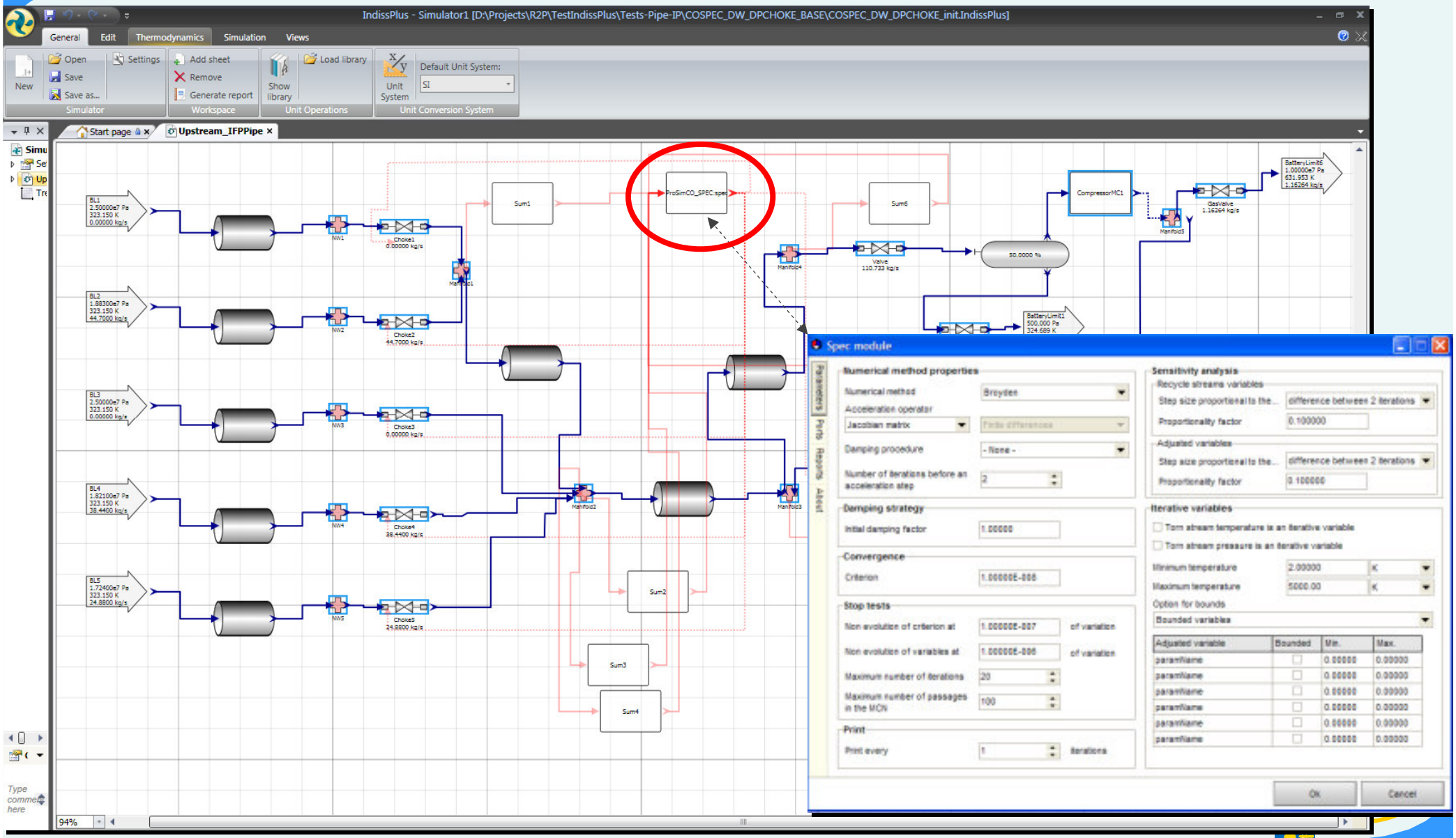
Joint development projects

- 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)

ProSim SPEC UO / IFPEN Pipes in INDISS+

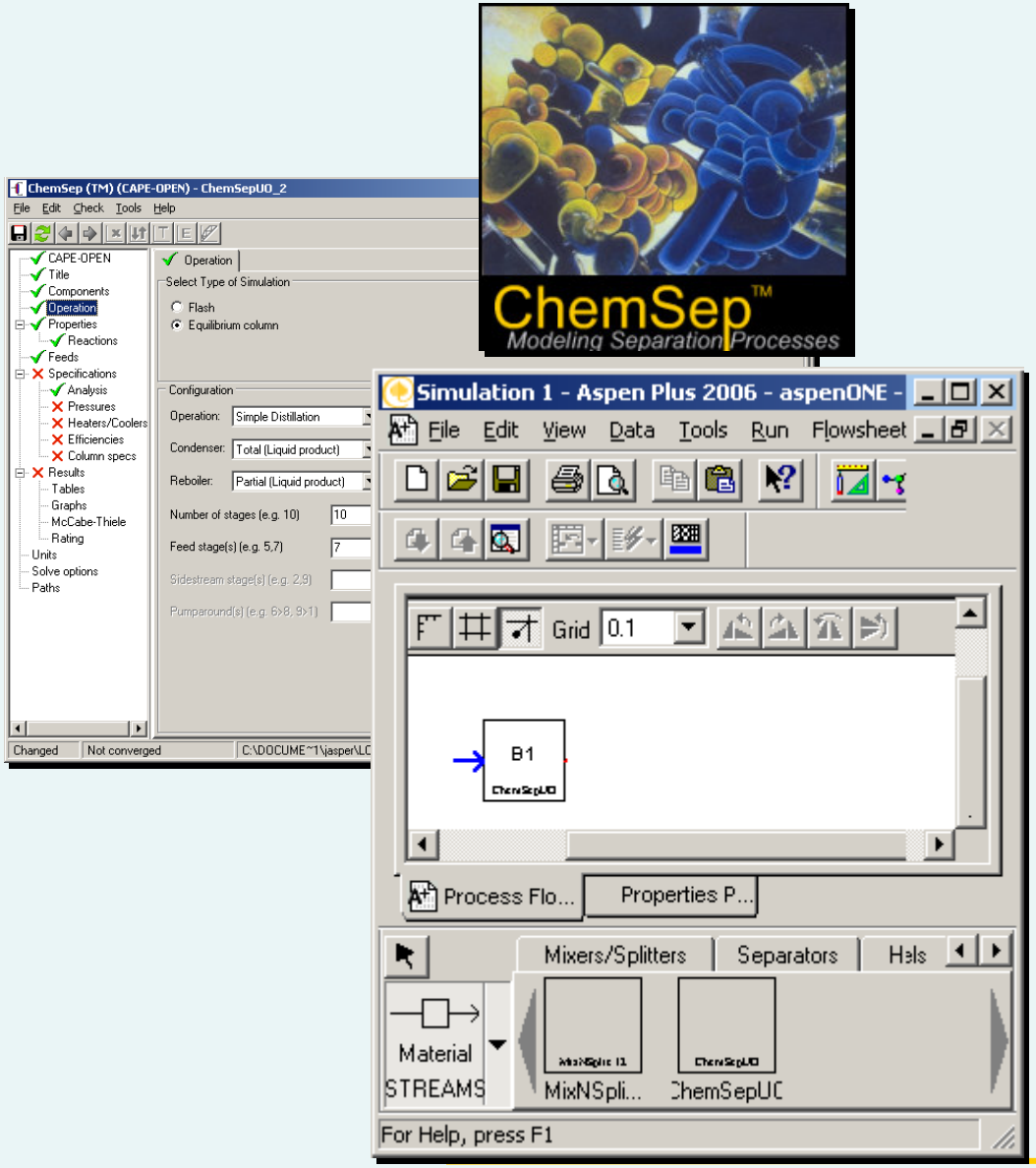


Unit Operations as numerical tools

- 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)

Dealing with limited access to 3rd Party Software



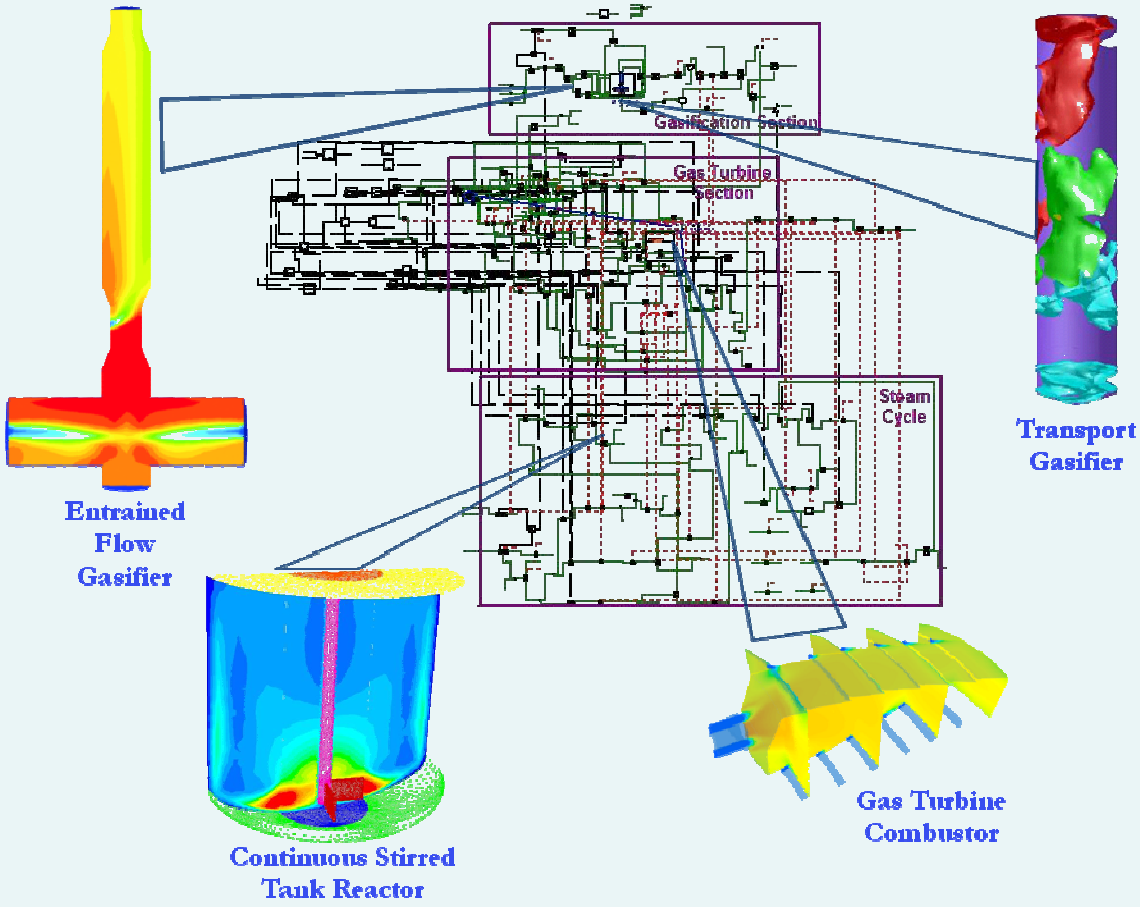
"Using CAPE-OPEN we were able to develop a unit operation just once, and clients can run it in simulation environments to which we do not have access..."

Prof. Ross Taylor
ChemSep

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

Flexibility

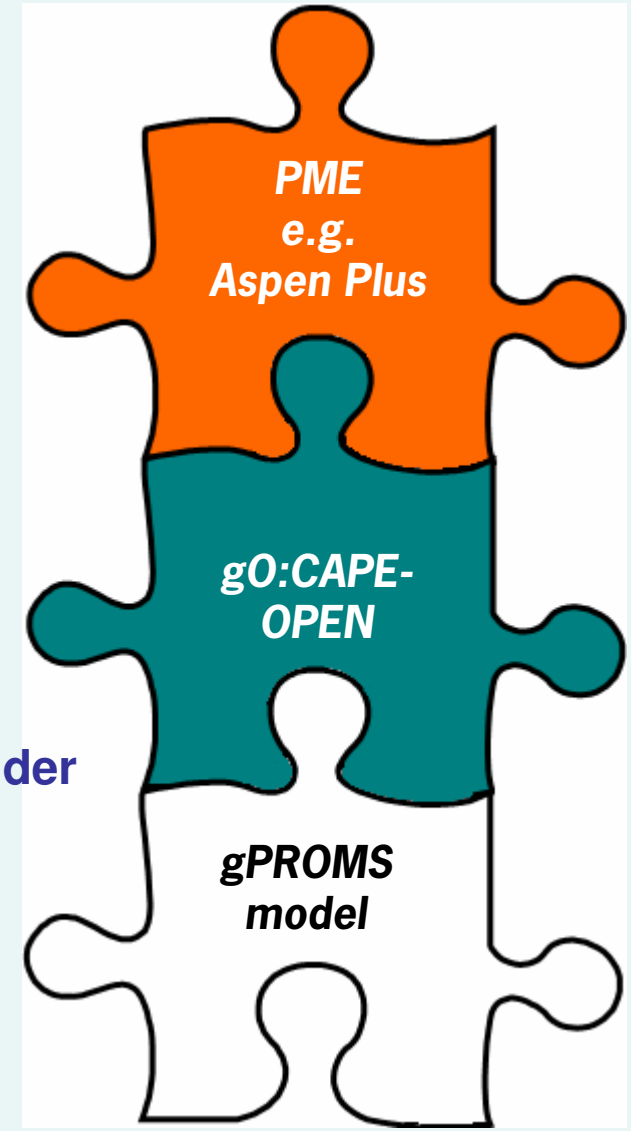
- Co-simulation of process flowsheet models with ANSYS FLUENT CFD models
- Robust model database for local or remote storage of CFD equipment models
- Archival of a tailored, reusable library of high-fidelity and reduced-order equipment models
- Serial or parallel execution of CFD models on distributed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



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**



PSE

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/

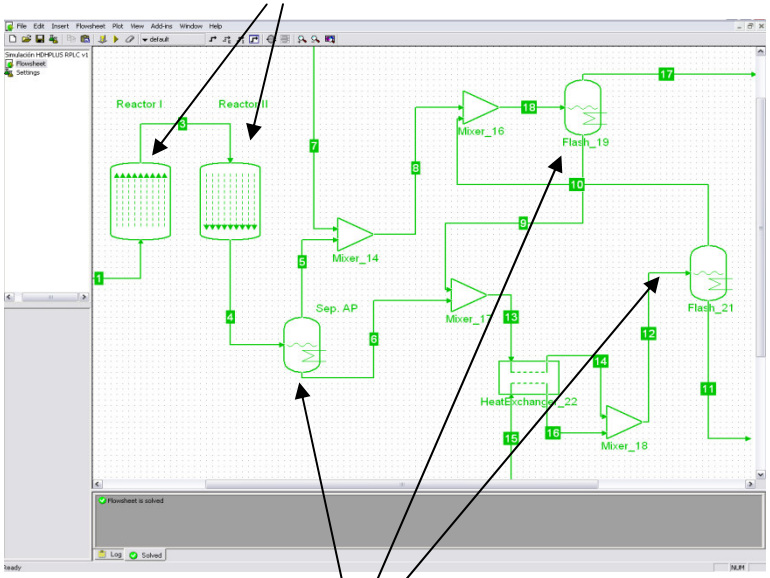
- GAMS (CONICET)
  (ChERD. vol. 88 (2010), pp. 421-429)

- Python (DWSIM)
  http://sourceforge.net/projects/dwsim/

World-wide CAPE-OPEN usage

Refinery processing

In-house Residue Vacuum Cracker Model



In-house Equilibrium Calculators

PDVSA INTEVEP

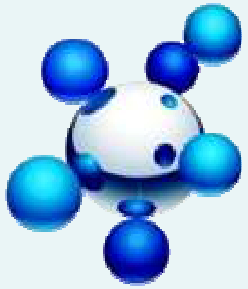
" We use CAPE-OPEN because it allows us to run our refinery reactor technology models and our in house equilibrium calculation models in different process modeling environments"

CÉSAR PERNALETE
Process Modeling group at PDVSA, Venezuela

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)

Conclusion

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

Use CAPE-OPEN Unit Operations!

- Thank you for your attention
- Questions?