

## 2.3 Current compliant components

**Commercial PMCs and PME**  
**Proprietary industrial PMCs**  
**Academic PMCs**



## Commercial PMCs and PMEs

Meeting industrial needs through adoption  
of CAPE-OPEN standards



# Available commercial CO-compliant software

- **AspenTech - Hyprotech**
  - ⇒ Aspen Plus™ 12.1, Aspen Properties 12.1
  - ⇒ HYSYS.Process 3.2, COM Thermo, Distil
- **Other Software providers**
  - ⇒ **SimSci-ESSCOR**
    - **PRO/II v7.0**
  - ⇒ **Process Systems Enterprise**
    - **gPROMS 2.3.1, go:CAPE-OPEN**
  - ⇒ **Infochem**
    - **MultiFlash 3.3**
  - ⇒ **HTRI**
    - **Xist 3.0**
  - ⇒ **ProSim SA**
    - **SIMULIS 1.0**
  - ⇒ **Fluent Inc.**
    - **FLUENT 6.1.18**

# AspenTech / Hyprotech

- ❑ AspenTech is a key member of the CAPE-OPEN initiative, being the first simulation vendor having a prototype version of a CAPE-OPEN compliant simulator.
- ❑ During the CAPE-OPEN project, HYSYS was used as the validation platform to ensure correctness of the developed interfaces. This has allowed AspenTech to have a deep knowledge in implementing and using CAPE-OPEN interfaces.
- ❑ HYSYS's open architecture, particularly existing solutions for integrating external simulation models (HYSYS extensions), have facilitated supporting the CAPE-OPEN interfaces.
- ❑ HYSYS.CAPE-OPEN consists on HYSYS (v2.2 or later) and the HYSYS CAPE-OPEN sockets.
- ❑ All HYSYS users may download the required software to enable the HYSYS interfaces to CAPE-OPEN Unit Operations and Property packages.
- ❑ A more detailed presentation by Andrew McGough



# AspenTech CAPE-OPEN

**CAPE-OPEN Property Package --- AspenTech Property Package Manager**

File View Help

Name:

Description:

About:

Vendor:

CO Version:

Comp. Version:

Comp. Help:

# CAPE-OPEN Property Package

Package: Simple in ATCOProperties.COPropertySystem.1

Components		Available Properties and Phases			
iupacName	Component	casRegistryNumber	chemicalFormula	normalBoilingPoint	molecularWeight
BENZENE	BENZENE	71-43-2	C6H6	353.240	78.114
ETHANOL	ETHANOL	64-17-5	C2H6O-2	351.440	46.069
TOLUENE	TOLUENE	108-88-3	C7H8	383.780	92.141
WATER	WATER	7732-18-5	H2O	373.150	18.015

OK

# More details

Package: Simple in ATCOProperties.COPropertySystem.1

Components Available Properties and Phases

This package can calculate these 49 properties for these 4 phases.

Properties	Phases
activityCoefficient	Vapor
density	Liquid
diffusionCoefficient	Overall
diffusionCoefficient.Dmoles	L2
diffusionCoefficient.Dmolfraction	
diffusionCoefficient.Dtemperature	
enthalpy	
enthalpy.Dmoles	
enthalpy.Dmolfraction	
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enthalpy.Dtemperature	
entropy	
entropy.Dmoles	
entropy.Dmolfraction	
entropy.Dpressure	
entropy.Dtemperature	

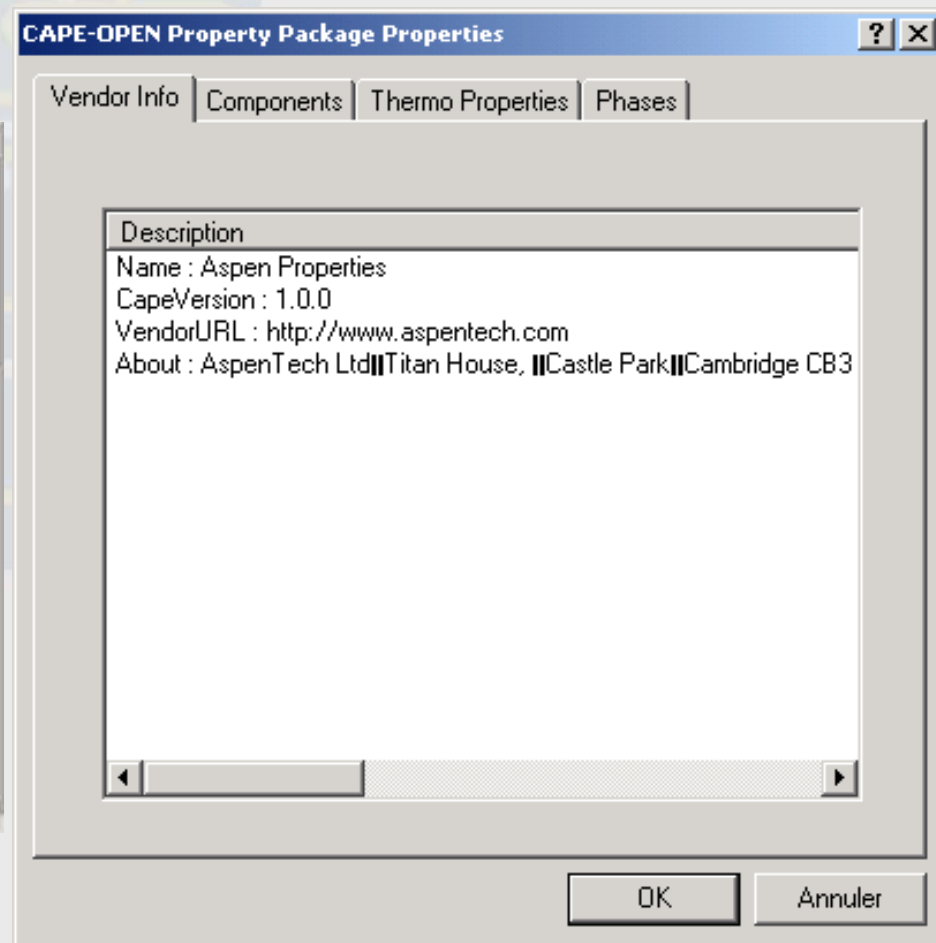
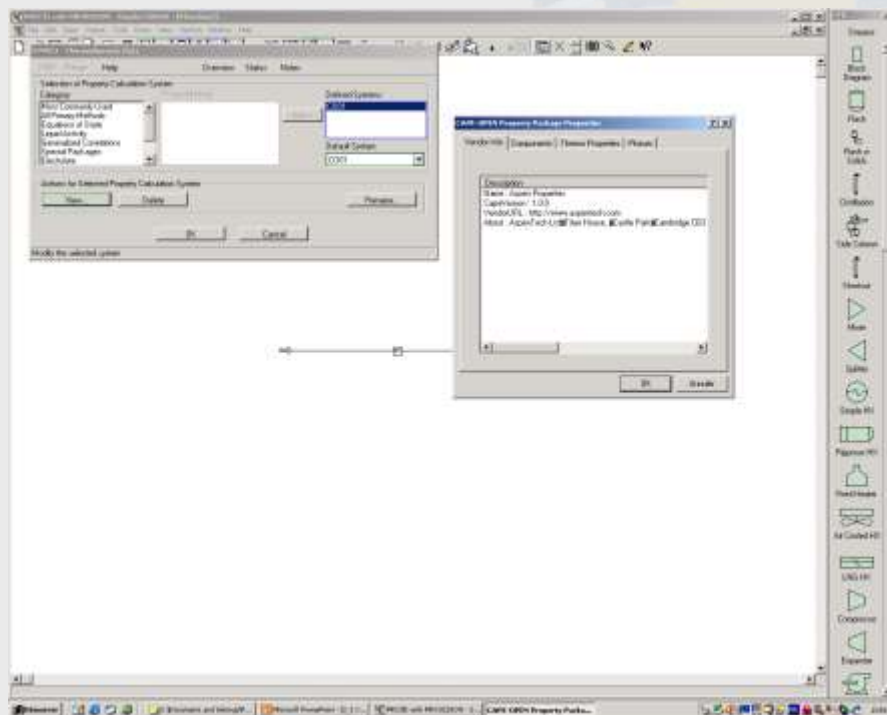
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# SimSci-ESSCOR

- SimSci-Esscor ([www.sims-ci-esscor.com](http://www.sims-ci-esscor.com)) is a leader in the development and deployment of industrial process simulation software and systems for a variety of industries.
- SimSci was a member of the CAPE-OPEN project. PRO/II 6.0 showed some CAPE-OPEN features while PRO/II 7.0 is targeted as being CAPE-OPEN compliant for UNIT operation and thermodynamics.
- A more detailed presentation will be made by SimSci-ESSCOR representative



# Aspen Plus PP within PRO/II

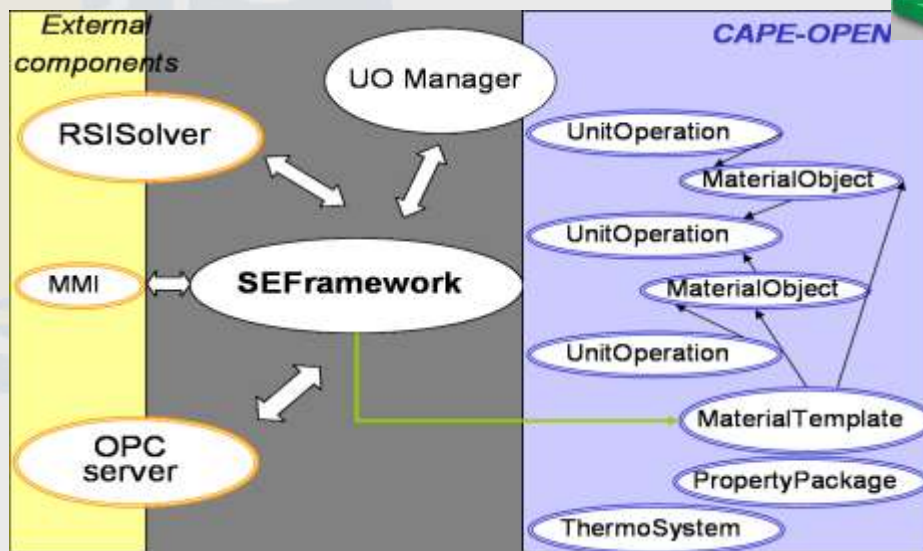
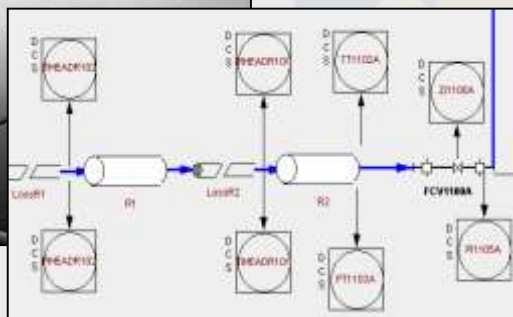
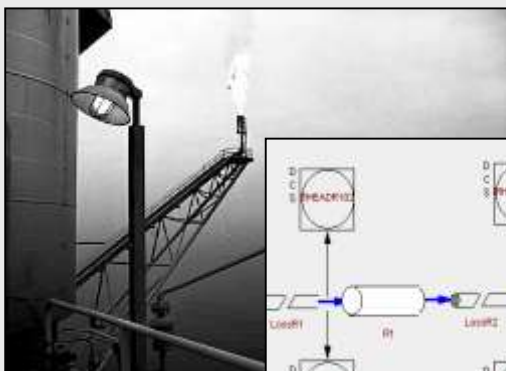


# RSI (Réalisation en Systémique Industrielle)

- RSI ([www.rsi-france.com](http://www.rsi-france.com)), a subsidiary company of IFP, is a leading supplier of training systems and simulation software for:
  - ⇒ Oil and Gas, Gas Reinjection, Pipelines, Gas Plants, LNG, Refineries, Ethylene, Aromatics, Polymers, Other Petrochemicals and Chemicals, Fossil Power Plants, Integrated Gasification & Combined Cycle Power Plants.
- RSI (started in 1980) develops and markets software tools and services, which provide consistent modelling solutions throughout the life cycle of process plants:
  - ⇒ design, start-up and operation.
- RSI's business (Sales 2002: 3.7 M€) is to provide the latest computer-based high technology for:
  - ⇒ Engineering Study Simulator, Operator Training Simulator, Process Operation Simulator, Advanced Process Control, Optimisation.

# WellCoMon: Well Control & Monitoring System

- Offshore field monitoring: estimation of oil production, GOR & Water Cut
- Given measured pressures and temperatures, WellCoMon simulates the whole production network, from reservoir to process facilities



- WellCoMon complies with the CAPE-OPEN standard
  - Integration of customer expertise is carried out with minimum effort
  - Use of CAPE-OPEN Unit Operations
  - Use of CAPE-OPEN thermo server



# INDISS: dynamic simulation



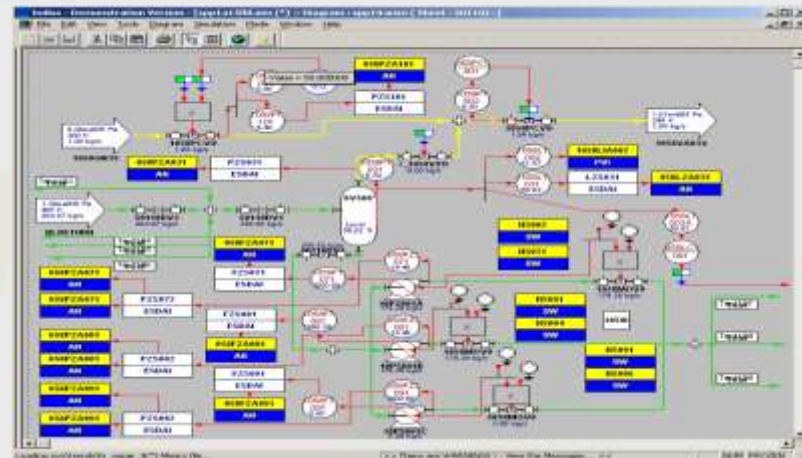
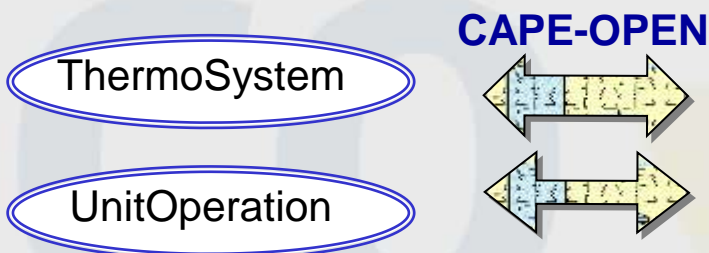
## INDISS complies with CAPE-OPEN standard

### Thermodynamic interfaces

- Full implementation: all thermodynamic requests are forwarded to the thermodynamic package through CAPE-OPEN interfaces

### RSI is involved in ICapeDynamicUnit Interface definition

- Natural extension of the existing Unit specification
- Specific calculation sequence for each time step

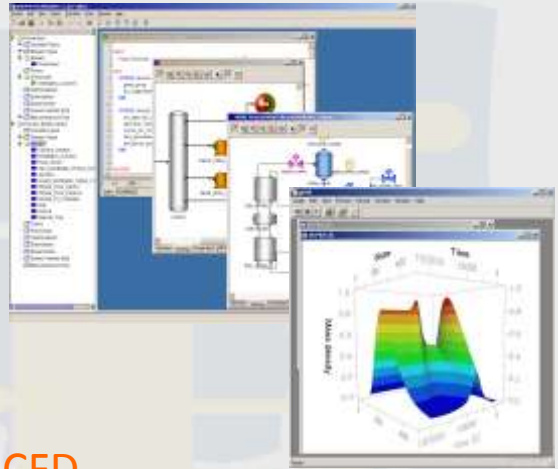


# Process Systems Enterprise Ltd (PSE)

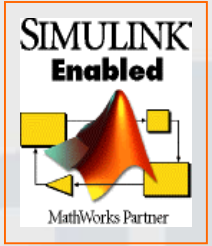
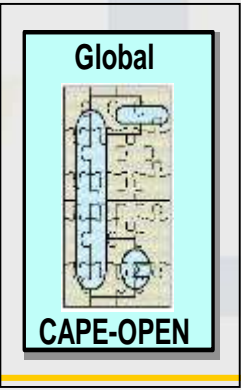
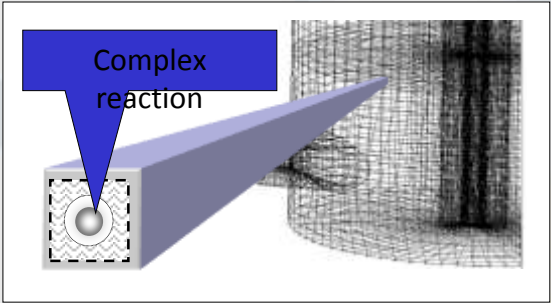
- Provider of advanced model-based technology and services to the process industries.
- PSE was launched in 1997 as a spin-off from the Centre for Process Systems Engineering at Imperial College, London.
- Products
  - ⇒ gPROMS: general-purpose process modelling and optimisation environment
  - ⇒ ModelEnterprise: integrated software framework for modelling process enterprises
- A more detailed presentation is made by Ben Keeping



gPROMS  
ModelBuilder



gO:CAPE-OPEN



## gO:CAPE-OPEN overview

- Introduce advanced gPROMS models within CAPE-OPEN compliant steady-state flowsheeting packages e.g.
  - ASPEN PLUS™
  - HYSYS™
- Use consistent physical properties throughout
- No programming required
  - retain advantages of gPROMS-based modelling

# Infochem Computer Services Ltd

- **Infochem Computer Services ([www.infochemuk.com](http://www.infochemuk.com)) is the leading independent supplier of thermodynamic software and consultancy services to the oil, gas and chemical industries.**
- **Expertise:**
  - ⇒ **Early assessment of potential problems such as solid deposition which may lead to formation damage or pipeline blockage**
  - ⇒ **Choice of the best remediation strategy or most efficient maintenance schedule**
  - ⇒ **Optimisation of production**
  - ⇒ **Avoidance of hazards to personnel or equipment due to fluid properties**
  - ⇒ **High fidelity modelling of processes for design, simulation or operator training**
  - ⇒ **Efficient implementation of thermodynamic software in a range of applications.**

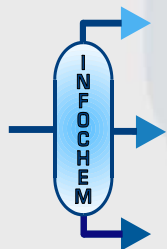




# Multiflash

## □ Comprehensive phase behaviour package

- ⇒ Main applications in the upstream oil & gas industry
- ⇒ Characterisation (compositional modelling) of petroleum fluids
- ⇒ Flow assurance studies (hydrates, waxes, asphaltenes)
- ⇒ Production optimisation
- ⇒ Multi-phase fluid/solid capability



## □ Enhanced industry-standard fluid models

- ⇒ Cubic EOS, density correction, GE mixing rules, chemical association
- ⇒ LKP, BWRS....
- ⇒ Activity models (NRTL, UNIQUAC, UNIFAC,...)

## □ PC-SAFT for polymers

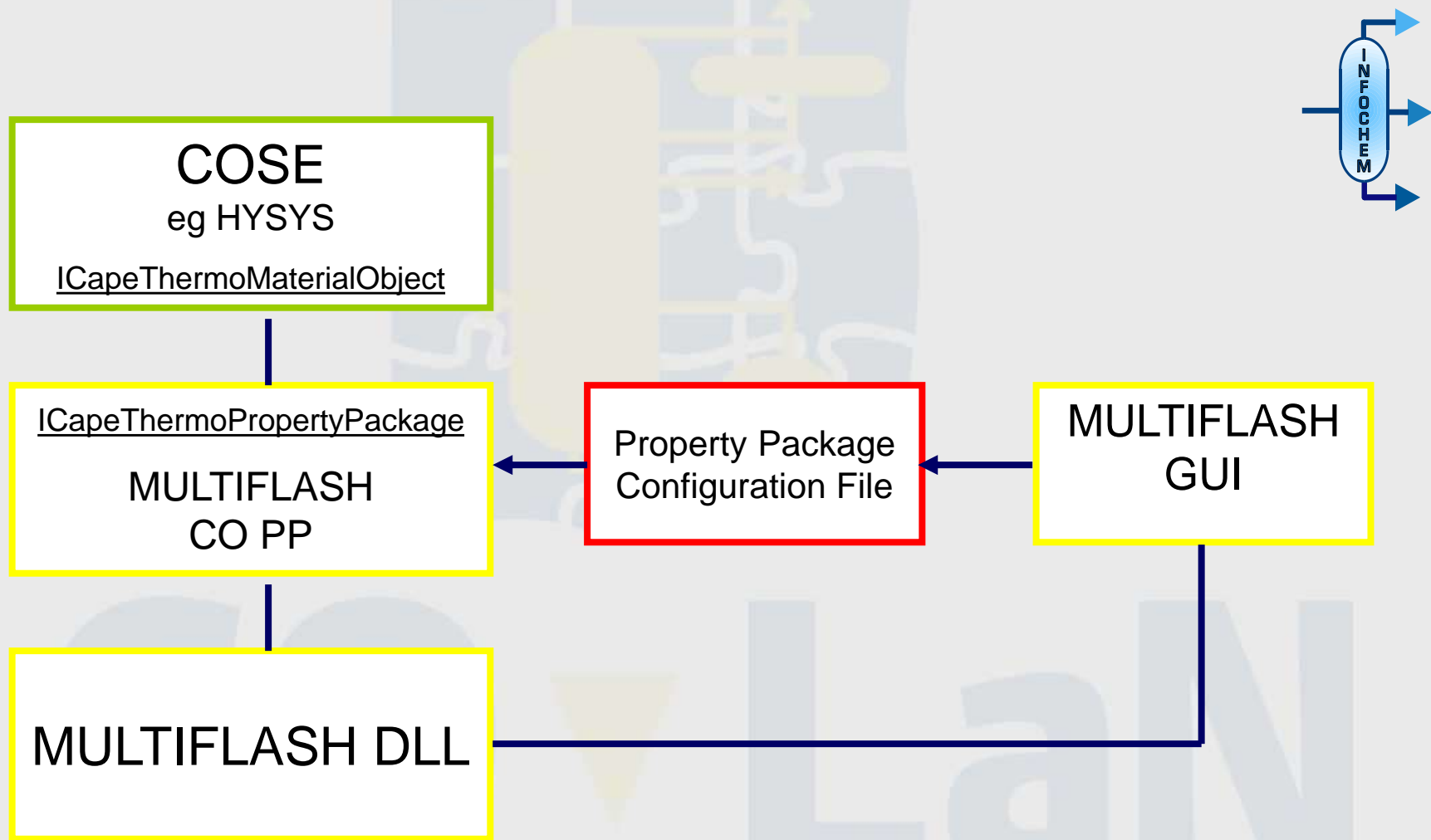
## □ Infochem models for solid phases

- ⇒ Hydrates, waxes, asphaltenes, mercury

## □ Analytical derivatives of calculated properties w.r.t. p, T and composition



# Multiflash CAPE-OPEN



# Multiflash PP in HYSYS

**HYP/CAPE-OPEN Kit Component Manager**

Click on the tree to browse information  
Double-click to create the selected component.

Registered Components

- Thermo Property Systems
  - Multiflash CO Thermo System [MFCOT]**
    - BENZETH.MFL
    - C3C5.MFL
    - C4C5.MFL
    - DICHLORO.MFL
    - EXH.MFL
    - HDA.MFL
  - HYP/SRK ThermoSystem [HyCOProp:
    - HYP/SRK EOS PropSys.3 COMP:
    - HYP/SRK EOS PropSys.HDA [HC
    - Optimized HYP/SRK EOS HDA [H
  - Hyprotech COMThermo server [Hypro
- Thermo Property Packages
  - HYP/SRK EOS HDA [HDAPPack.HD
  - HYP/SRK EOS 3 COMPS [COPropPa
  - Optimized HYP/SRK EOS HDA [HyHC
  - Multiflash CO Package [MFCOPPack.

CAPE-OPEN Component Category: Thermo Property Systems

Description: Multiflash CAPE-OPEN Thermo System

CAPE-OPEN Version: 0.93    Component Version: 0.93.3.1

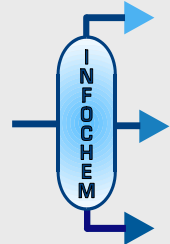
Vendor: <http://www.infochemuk.com>    Component Help

About: Infochem Computer Services Ltd  
13 Swan Court, 9 Tanner St  
London SE1 3LE  
UK  
Phone: +44 (0)20 7357 0800  
Fax: +44 (0)20 7407 3927

Technical information

CLSID: {653CE81C-DAD9-434B-B878-D5947CB16AD4}

Refresh    Accept    Cancel



# Heat Transfer Research, Inc (HTRI)

- **International consortium founded in 1962**
  - ⇒ **conducts research on industrial-scale heat transfer equipment**
  - ⇒ **develops software modeling and simulation tools based on this proprietary research data**
  - ⇒ **provides its customers with other complementary products, technical services, and training**
- **HTRI products, in use at more than 500 corporate sites worldwide**



# HTRI CAPE-OPEN Xist Interface

- Built into HTRI Xchanger Suite interface
- Currently functional with HYSYS simulator
- Initial release will be shell and tube exchangers
- Later releases extended to air-coolers, economizers, and plate and frame exchangers.
- Initial release scheduled mid 2004

# Demo Flowsheet with HTRI Interface

The screenshot displays the HTRI software interface with three main windows:

- PFD - Case (Main):** A process flow diagram showing a central red box labeled "CAPE Condenser". It has four ports: "Hydrocarbons" (inlet), "Cooling Water" (inlet), "Outlet Water" (outlet), and "Condensed Hydrocarbons" (outlet).
- Condenser:** A window titled "Feed, Product Streams and Material Ports" containing a table with the following data:

Port ID	Port type	Direction	Material name
HotInlet	Material	Inlet	Hydrocarbons
ColdInlet	Material	Inlet	Cooling Water
HotOutlet	Material	Outlet	Condensed Hydrocarbons
ColdOutlet	Material	Outlet	Outlet Water
- Xlist - [Input] - untitled1 - Condenser - Input Summary:** A configuration window for the condenser. It includes sections for:
  - Case Mode:** Simulation (selected)
  - Process Conditions:** Flow rate (Hot Shell: 200.41, Cold Tube: 110.23), Inlet/outlet T, Inlet P/allow dP.
  - Shell Geometry:** TEMA type (A-E-S), ID (36 inch), Orientation (Horizontal), Hot fluid (Shellside).
  - Baffle Geometry:** Type (Single segmental), Orientation (Program sets), Spacing (20 inch).
  - Tube Geometry:** Type (Plan), Length (20 ft), Tube OD (1 inch), Pitch (1.33 inch), Wall thickness (0.063 inch), Layout angle (30 degrees), Tubespaces (1), Tubecount.
  - Shell Type:** Exchanger type (TEMA), Shell wall thickness, Closure type, U-Bend type.

# ProSim SA ([www.prosim.net](http://www.prosim.net))

- One of the few independent and privately held companies to supply innovative software and service solutions for
  - ⇒ modelling, simulation and optimization to process industries.
  
- Range of products
  - ⇒ ProSimPlus: process flowsheeting software
  - ⇒ ProSimPlus HNO<sub>3</sub>: specific nitric acid plant simulator
  - ⇒ BatchColumn: dynamic behaviour of batch distillation process
  - ⇒ BatchReactor: kinetic parameter identification and simulation
  - ⇒ ProPhy Plus: user friendly fluid phase equilibrium tool
  - ⇒ BibPhy Add-In: making ProPhy Plus usable within Excel
  - ⇒ Component Plus: management of pure component databases



# SIMULIS® COMPONENTS SUITE

## New CAPE Components - developed by ProSim SA



### □ Simulis® Compounds

- ⇒ Server of pure substance properties
- ⇒ Includes a service for fitting temperature dependent properties
- ⇒ Allows access to different data sources: CAPE-OPEN Property Packages, Component Plus databases, *Simulis® Compounds* packages,...

### □ Simulis® Thermodynamics

- ⇒ Includes *Simulis® Compounds*
- ⇒ Mixture properties and phase equilibria calculation server (as powerful as the widely validated standard thermodynamic library of ProSim SA)
- ⇒ Includes an estimation service of binary interaction parameters from experimental data
- ⇒ Allows creation and deployment on a network of *Simulis® Thermodynamics* Packages (CAPE-OPEN compliant)
- ⇒ Offers a CAPE OPEN compliant thermodynamic socket for external property packages





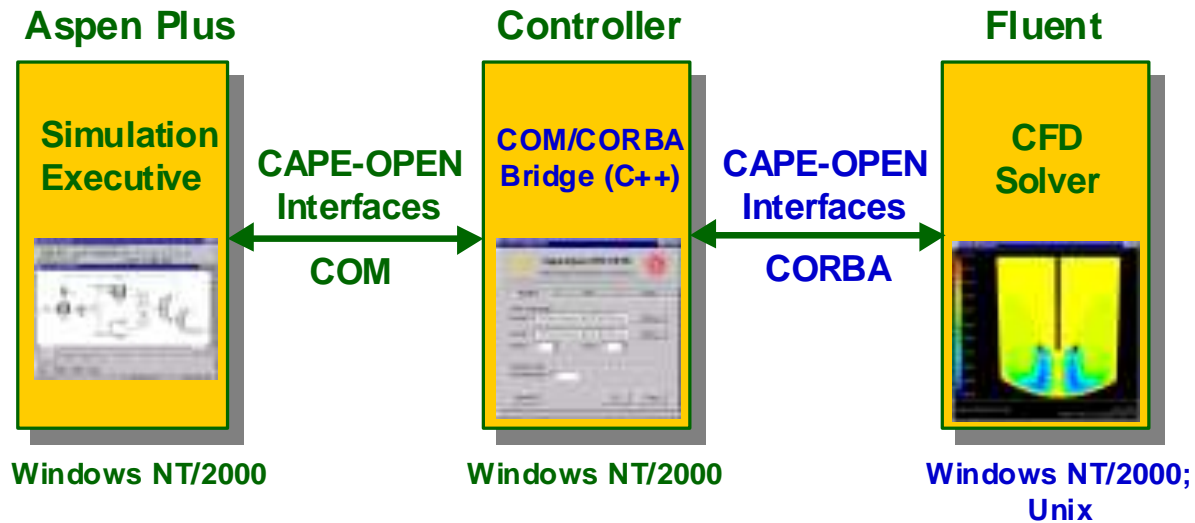
# Fluent

- Provider of commercial Computational Fluid Dynamics (CFD) software and services.
- Offers general-purpose CFD software for a wide range of industrial applications
- Within DOE sponsored project, AspenTech and Fluent have worked together to integrate CFD-fidelity equipment models in the context of the AspenTech's overall process models
- A more detailed presentation and demo will be made by Steve ZITNEY from DOE.

# Fluent Inc. – Aspen Technology Inc.



## COM/CORBA Bridge



### Advantages

- Fast bi-directional data exchange using inter-process communication
- Fluent process starts up and remains active
- Fluent runs on Windows and Unix systems

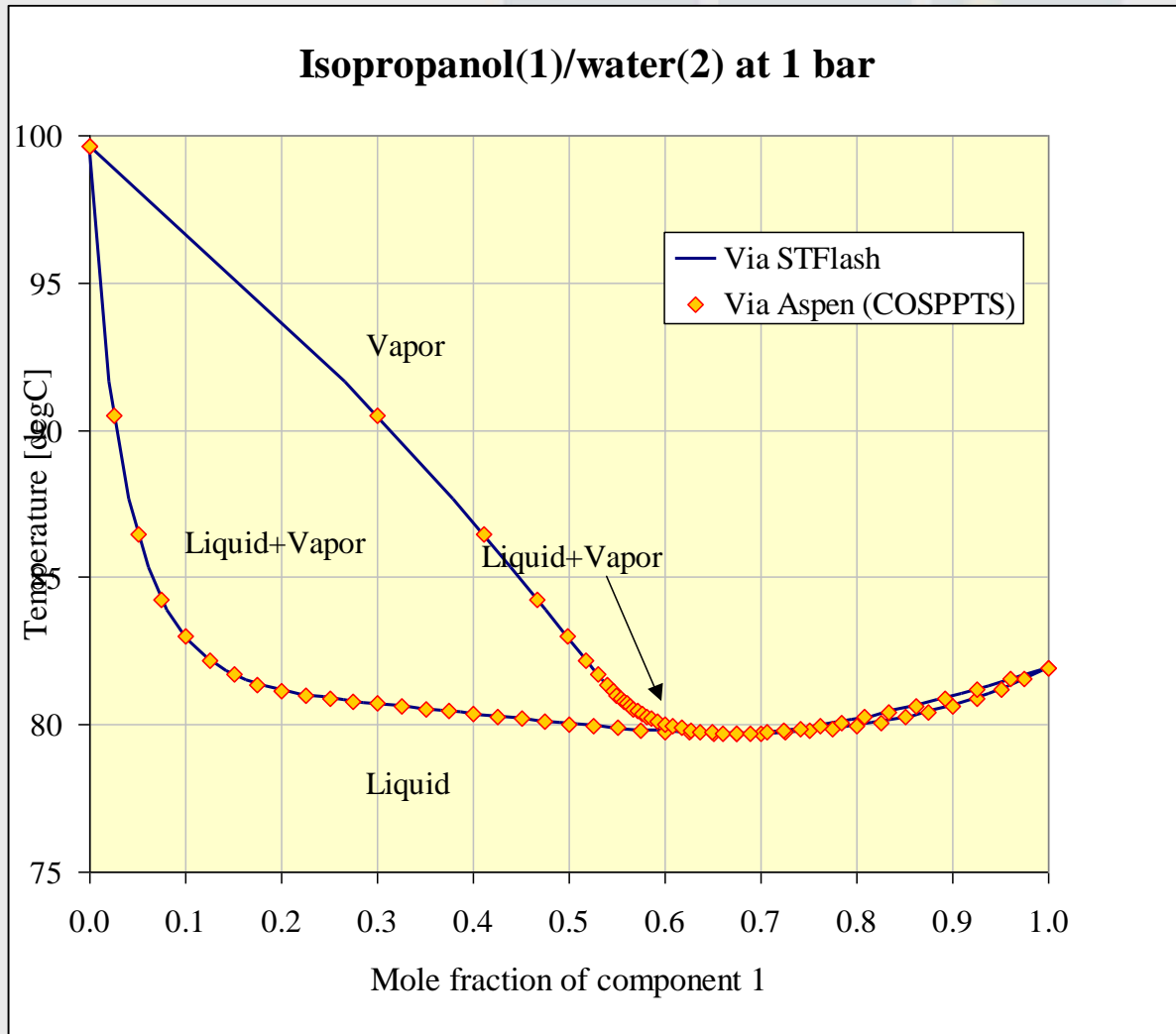


# Proprietary Industrial PMCs

**Bringing in-house software to CAPE-OPEN  
compliance**



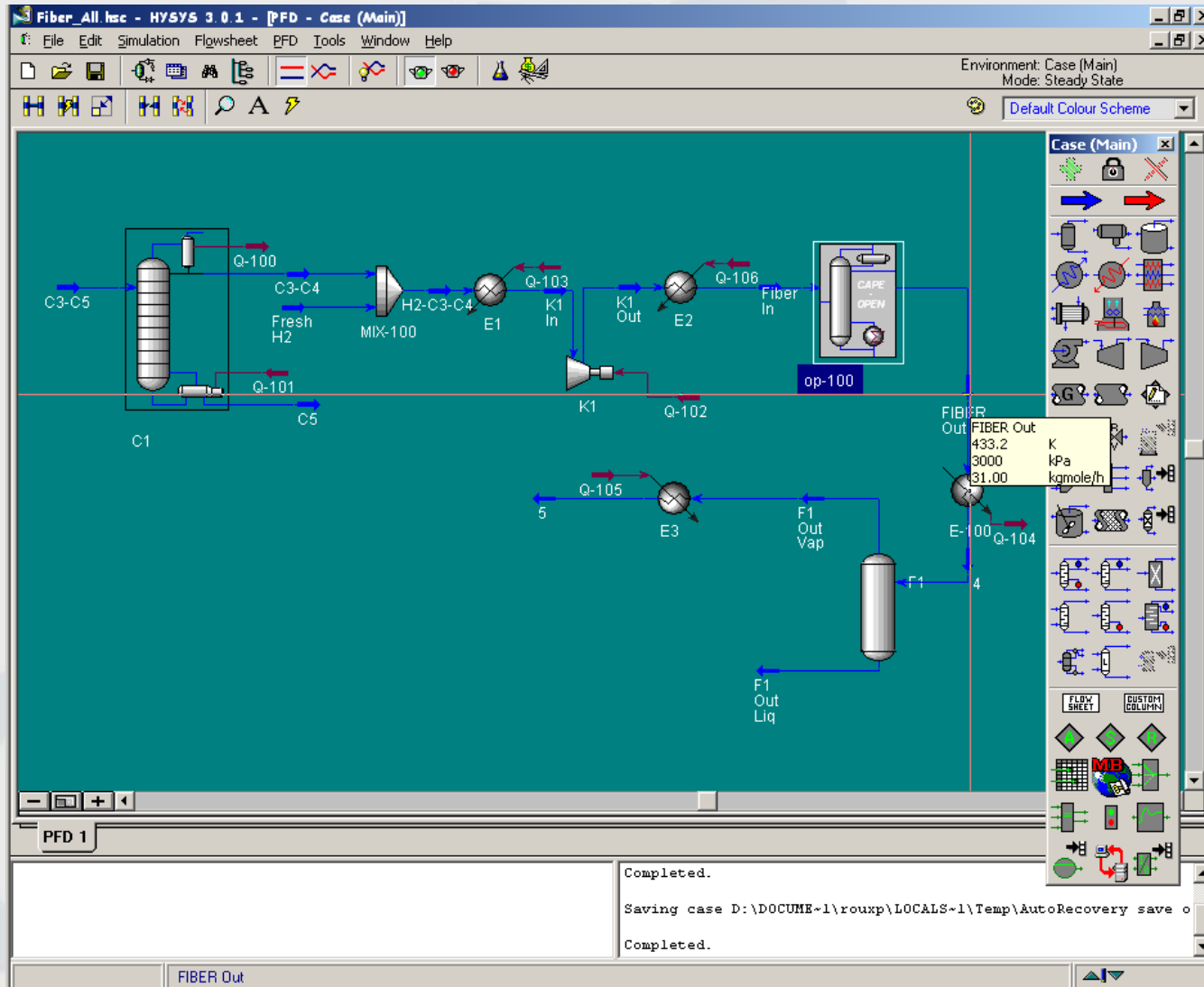
# Shell COSPPTS



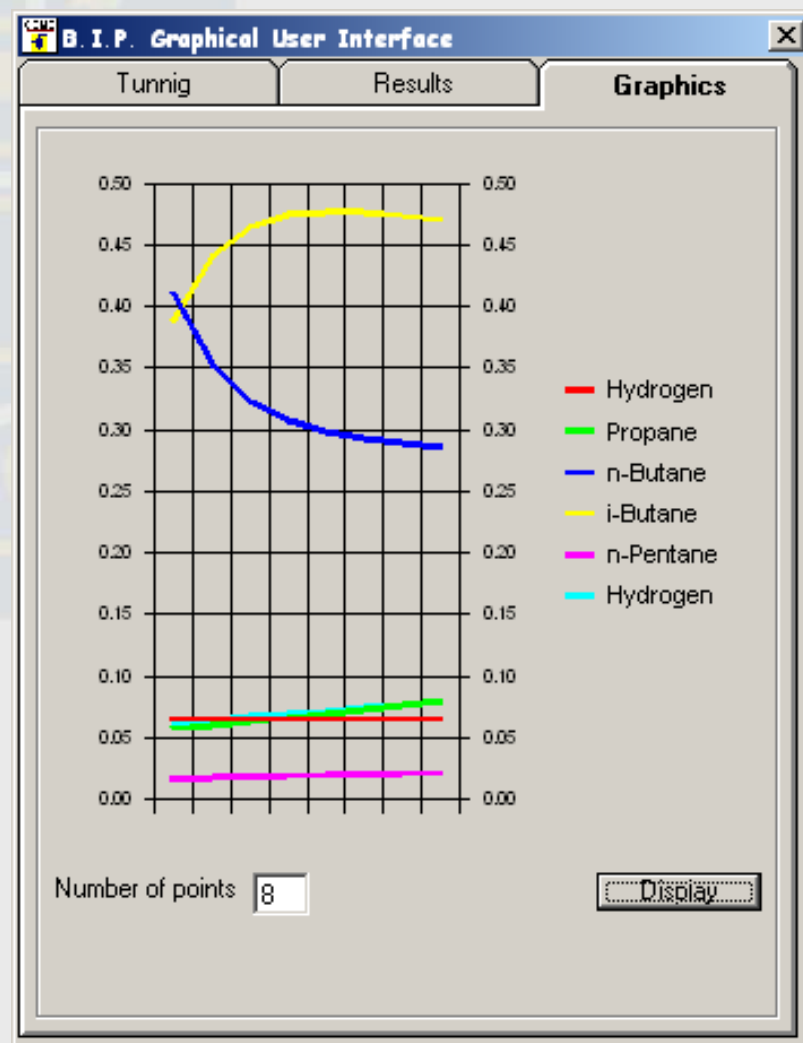
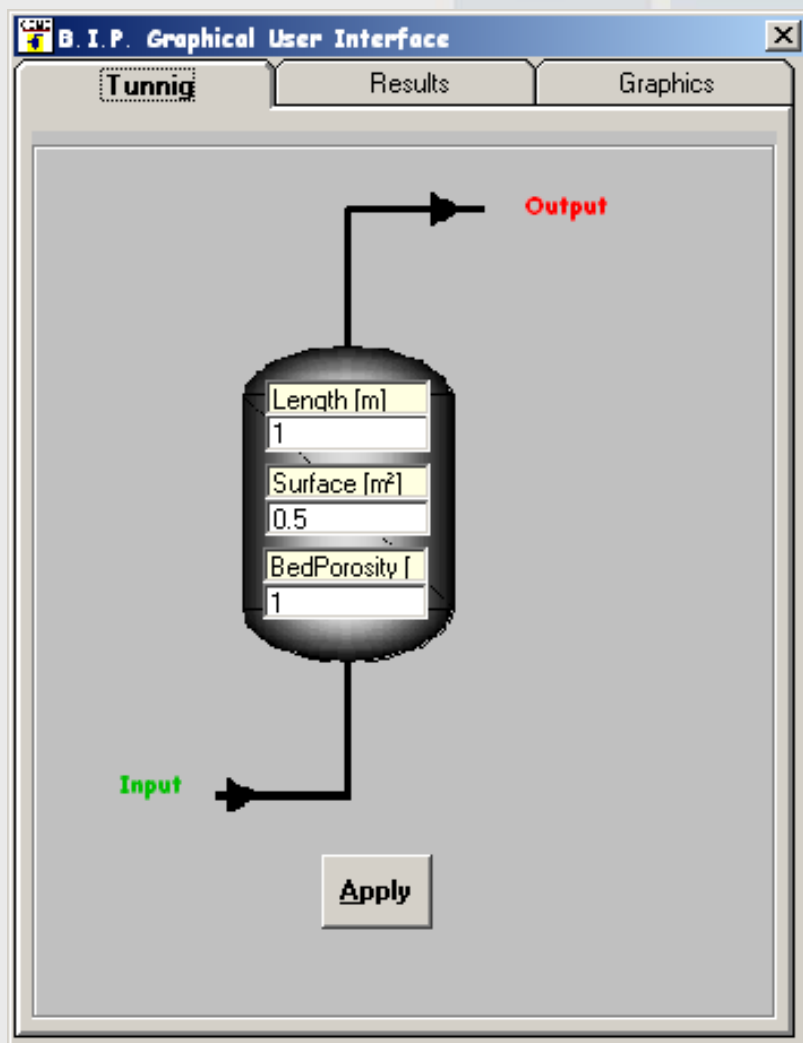
⇒ Specific  
Thermodynamic  
model

⇒ To be used  
within several  
Process  
Modeling  
Environments

# IFP Butane Isomerisation Process Reactor



# IFP Butane Isomerisation Process Reactor





## Academic PMCs

**Making research results available through  
CAPE-OPEN**



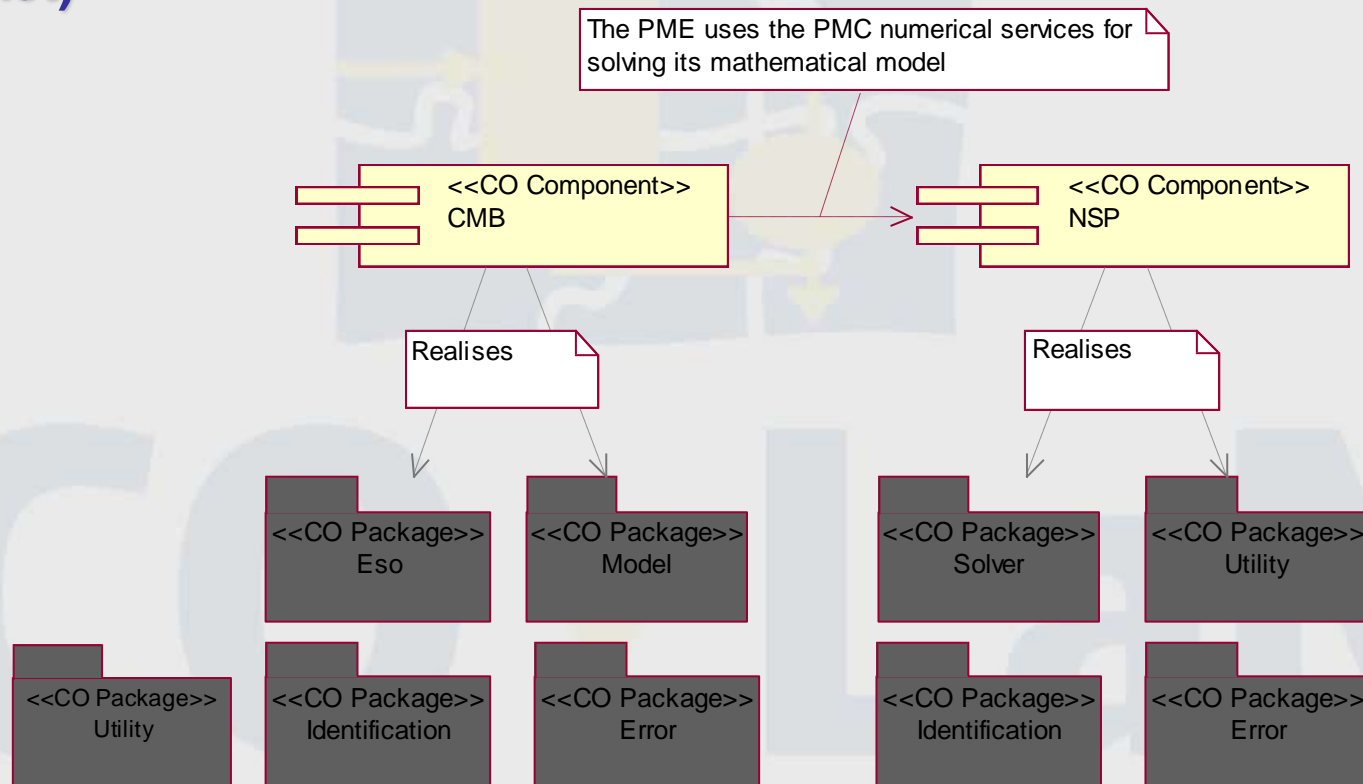
# INPT-ENSIACET

- French leading education and research center (<http://lgc.inp-toulouse.fr/>) in computer-aided process engineering
- Active in CAPE-OPEN since the start
- Focused their contribution on numerical interfaces and on common interfaces



# INPT Numerical Components

- Numerical Services Provider (NSP): a CO compliant software (plug)
- Continuous Model Builder (CMB): a CO compliant software (socket)



# IVC-SEP Thermo System

- One of Denmark first engineering research centres
- Research activities:
  - ⇒ Both experimental and theoretical work
  - ⇒ Emphasis on chemical and physical phase equilibrium, transport properties, multi-phase flow in porous materials and separation processes
  - ⇒ An industrial consortium of Danish and foreign member companies support IVC-SEP's research.
- A more detailed presentation by Nicolas Von Solms



# IVC-SEP Thermo System



**Scope:**  
**Cubic-Plus-Association**  
**PC SAFT**

**Project objective:**  
**Use them in CO compliant**  
**COSEs**

IVC-SEP.CAPE-OPEN Thermo System

Select Database

Standard  PC-SAFT

Select compounds from Database

Add --> << Remove

Available compounds		Selected compounds	
n-propylbenzene	103-65-1	ethylbenzene	100-41-4
octadecane	593-45-3	1-pentanol	71-41-0
o-xylene	95-47-6	1-propanol	71-23-8
pentadecane	629-62-9	water	7732-18-5
Poly(methylAcrylate)	9003-21-8		
Poly(vinylAcetate)	9003-20-7		
Polybutene	9003-29-6		
Polyisobutene	9003-27-4		
Polypropylene	9003-07-0		
Polystyrene	9003-53-6		
propane	74-98-6		
propylene	115-07-1		
p-xylene	106-42-3		
sulfur dioxide	7446-09-5		
tetradecane	629-59-4		
tetralin	119-64-2		
toluene	108-88-3		
tridecane	629-50-5		

NEXT ->>>>

start Document2... IVCSEPTher... IVC-SEP.CA... IVC-SEP.CA... DA 12:10

# Property Package plugged into Aspen Plus

The screenshot displays the Aspen Plus interface during a simulation setup. The main window is titled "Aspen Plus - Simulation 1 - [Setup - Data Browser]". A dialog box titled "Available Property Packages" is open, showing a list of property packages. The "IVC-SEP Thermo System" package is selected, with "PCSAFT\_test" highlighted. The "Name" field contains "IVCSEPThermoSystem.IVCSEPSystem.1". Other fields for "Description", "About", "Vendor", "CAPE-OPEN version", "Component version", and "Component help" are present but empty. The background window shows a tree view on the left with "Setup" expanded, and a menu bar at the top with options like "File", "Edit", "View", "Data", "Tools", "Run", "Plot", "Library", "Window", and "Help". The Windows taskbar at the bottom shows the "start" button, several open documents, and the system clock at 12:18.

# Conclusion

- **Read the Success stories on CO-LaN website for other examples**
  
- **More components need to be made available**
  - ⊗ **Multiple choices still lacking**
  - ⊗ **Equipment suppliers should offer models**
  
- **Market is adopting CAPE-OPEN**
  - ⊗ **Major commercial software tools are compliant**
  - ⊗ **Proprietary material being moved to CO**
  - ⊗ **Transfer from universities beginning**