2.4 Current compliant components

Commercial PMCs and PMEs

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™ 2004, Aspen Properties 2004
  - Aspen Hysys 2004 COM Thermo, Distil
- SimSci-ESSCOR
  - PRO/II v7.0…7.1
- Process Systems Enterprise Ltd
  - gPROMS 2.4…3.0, go:CAPE-OPEN
- Infochem Computer Services Ltd
  - MultiFlash 3.4
- Heat Transfer Research Inc.
  - Xchanger Suite 4
- ProSim SA
  - SIMULIS 1.0
- Fluent Inc.
  - FLUENT 6.1.18

Available commercial CO-compliant software

- Belsim SA
  - VALI 4.0
- Réalisation en Systémique Industrielle (RSI)
  - INDISS 1.6
- TUV-NEL
  - PPDS
- Virtual Materials Group
  - VMGThermo

AspenTech / Hyprotech

- Key member of the CAPE-OPEN initiative
  - was the first simulation vendor having a prototype version of a CAPE-OPEN compliant simulator.
- AspenTech has a large experience in implementing and using CAPE-OPEN interfaces: see Andrew McGough presentation.
- Aspen Plus provides a number of CAPE-OPEN interfaces
  - UNIT Operation socket – sequential modular
    - Allows any CO compliant Unit to be used in an Aspen Plus simulation
  - Thermo socket
    - Allows CO Property Packages to provide property calculations in Aspen Plus simulations
  - Thermo plug
    - Use Aspen Plus to create CO Property Packages to be used in other software

AspenTech CAPE-OPEN

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

File View Help

Name: testprob

Description: CAPE-OPEN Property Package generated by the AspenTech Property Package Manager on 10: 00: 42, Friday, August 13,

About:
AspenTech Ltd
Titan House, Castle Park
Cambridge CB3 0AY
England Phone: +44/1223-819700
Fax: +44/1223-366980

Vendor: http://www.aspentech.com

CO Version: 1.0.0

Comp. Version: 12.1

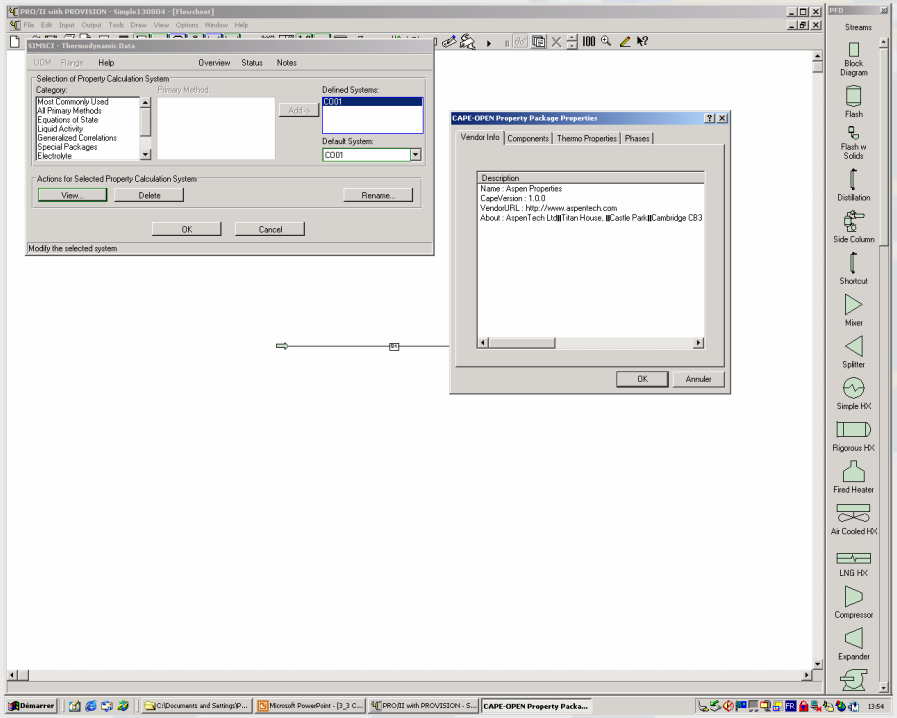
Comp. Help:

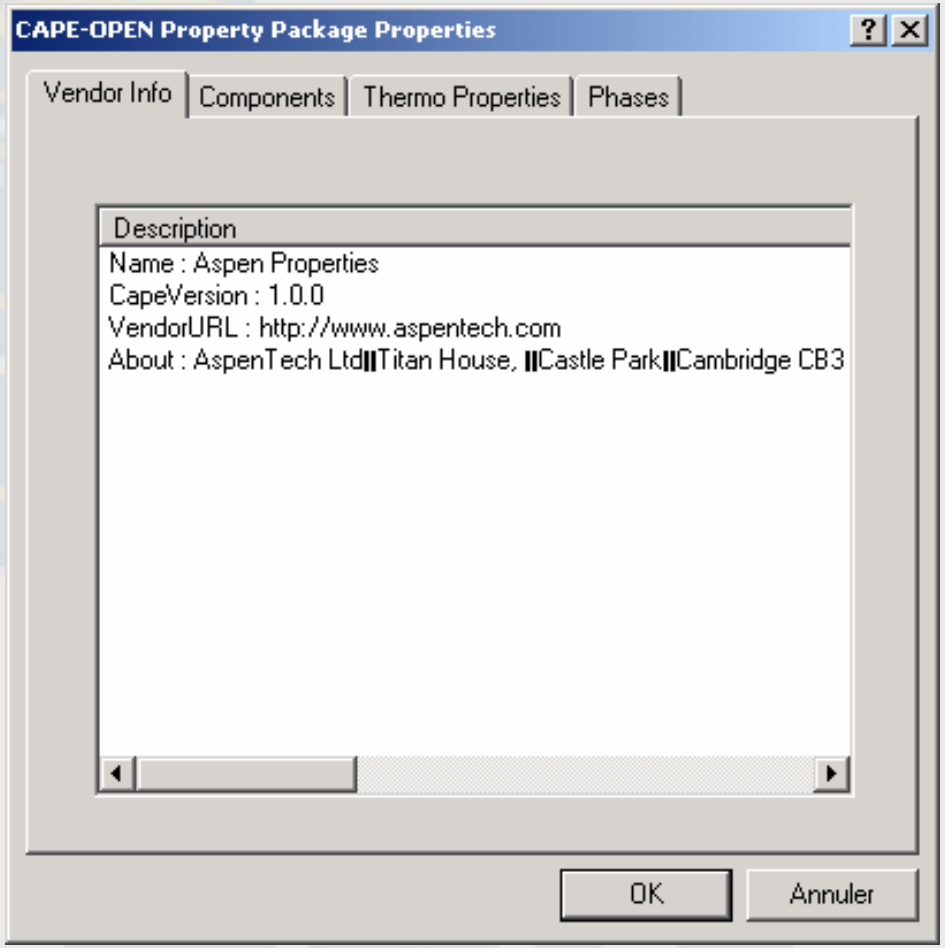
Advanced >

SimSci-ESSCOR

- SimSci participated in CAPE-OPEN project.
- PRO/II 7.0 and 7.1 provide:
  - CAPE-OPEN UNIT operation socket
    - Allows any CO compliant Unit to be used in a PRO/II simulation
  - CAPE-OPEN Thermo socket
    - Allows CO Property Packages to provide property calculations in PRO/II simulations
- A more detailed presentation will be made by David Jerome.

Aspen Plus PP within PRO/II



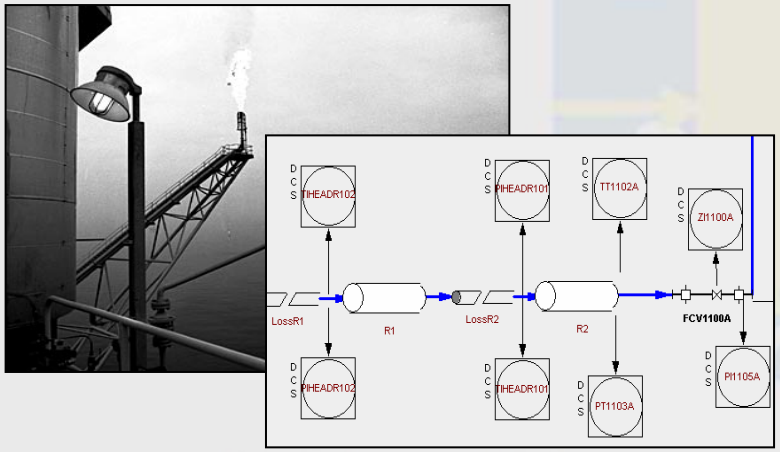


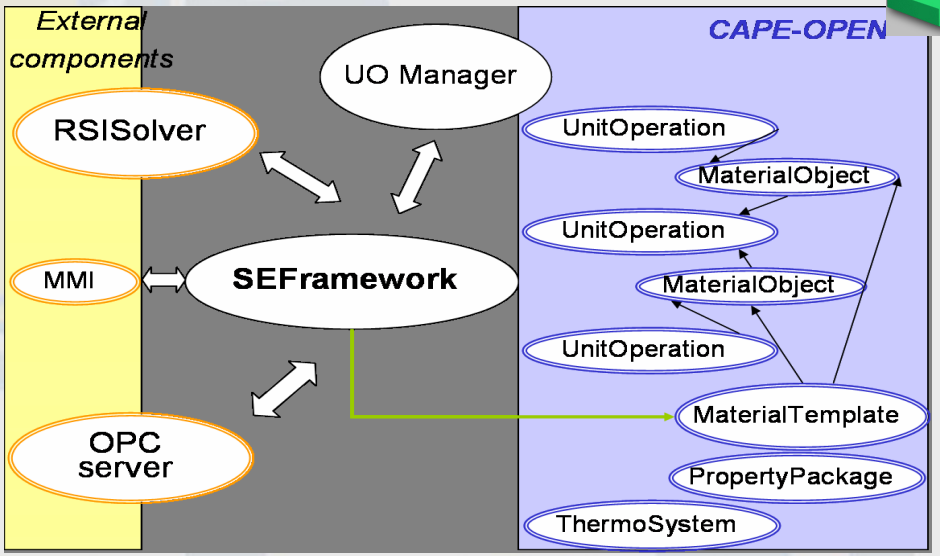
RSI (Réalisation en Systémique Industrielle)

- RSI (www.rsi-france.com), a subsidiary company of IFP, is a 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 products (WellComOn and INDISS) are implementing CAPE-OPEN interfaces for UNIT and THRM (sockets).
- Bertrand Braunschweig will demonstrate INDISS.

WellCoMon: Well Control & Monitoring System

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

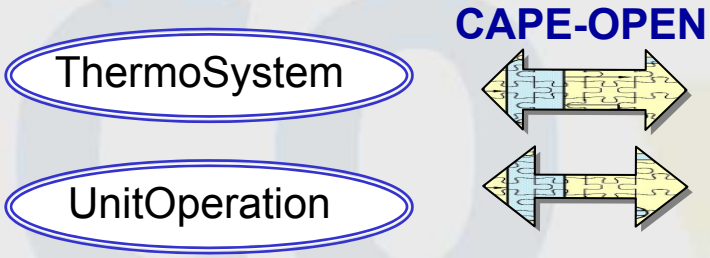


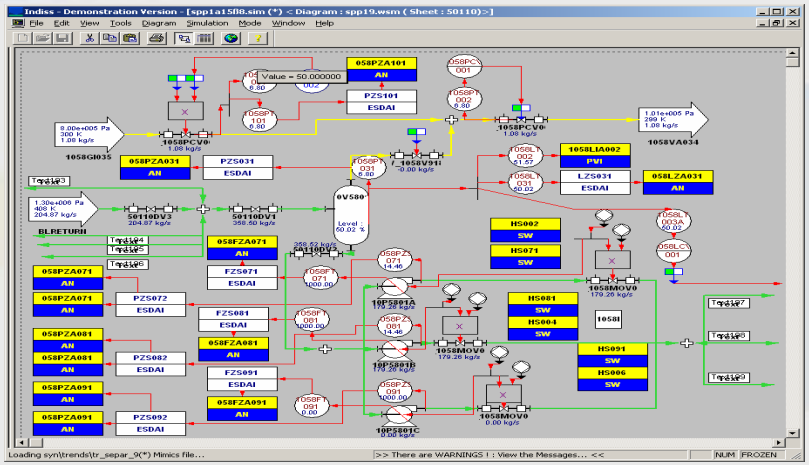


- WellCoMon complies with the CAPE-OPEN standard
  - Use of CAPE-OPEN Unit Operations
  - Use of CAPE-OPEN thermo server

INDISS: dynamic simulation

- **INDISS complies with CAPE-OPEN standard**
  - **Thermodynamic interfaces**
    - 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.
- gPROMS (general-purpose process modelling and optimisation environment) provides:
  - CAPE-OPEN THRM socket
  - CAPE-OPEN UNIT plug (gO:CAPE-OPEN)
- A more detailed presentation will be made by Ben Keeping

PSE

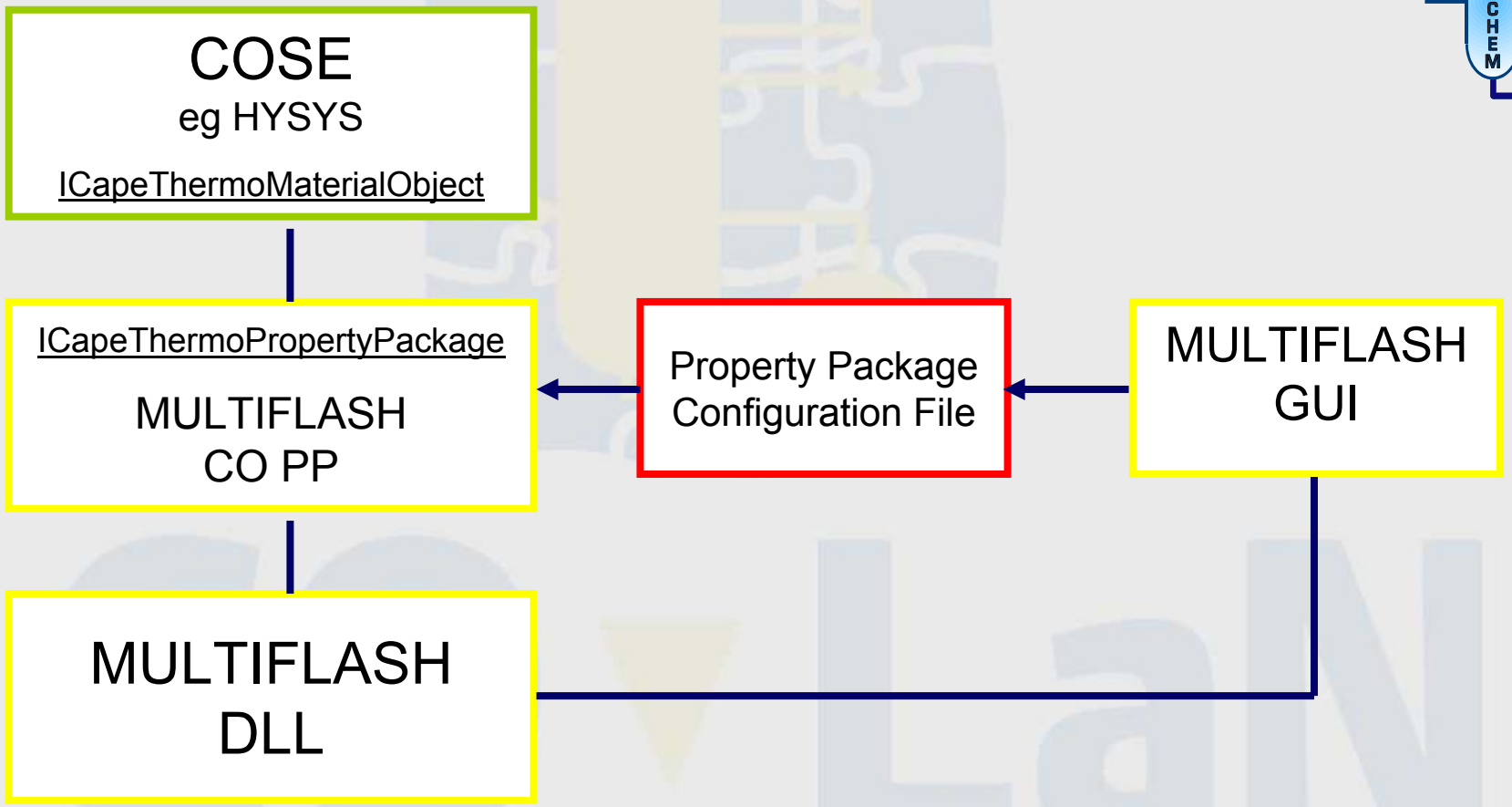
gO:CAPE-OPEN overview

- 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) is a leading independent supplier of thermodynamic software (MultiFlash) 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 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 [HD
    - Optimized HYP/SRK EOS HDA [H
  - Hyprotech COMThermo server [Hyprol
- Thermo Property Packages
  - HYP/SRK EOS HDA [HDAPPack.HD
  - HYP/SRK EOS 3 COMPS [COPropPa
  - Optimized HYP/SRK EOS HDA [HyHD
  - 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 modelling 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.
- A detailed presentation will be made by Fernando Aguirre.

CAPE-OPEN interfaces

- **Built into HTRI software suite:**
  - Shell and tube exchangers
  - Air-coolers
  - Plate and frame exchangers
- **HTRI software acts as a CAPE-OPEN UNIT plug**
  - Allows HTRI software to be used in Aspen Plus, PRO/II, HYSYS, etc… simulations
- **HTRI software implements CAPE-OPEN Thermo socket**
  - Allows 3rd party Property Packages to be plugged into HTRI stand-alone software

Flowsheet with HTRI UNIT

TestCO.hsc - HYSYS

File Edit Simulation Flowsheet PFD Tools Window Help

PFD - Case (Main)

Default Colour Scheme

Hydrocarbons

Cooling Water

CAPE OPEN

Condenser

Outlet Water

Condensed Hydrocarbons

Condenser

Feed, Product Streams and Material Ports

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

Unit Variables | General

Not Solved

Show Unit GUI

HTRI Xchanger Suite - untitled1

File Edit View Input Tools Window Help

Xist - [Input] - untitled1 - Condenser - Input Summary

- Input Summary
  - Geometry
  - Piping
  - Process
  - Hot Fluid Properties
  - Cold Fluid Properties
  - Design
  - Control

<< Previous | Next >>

Case Mode: Rating / Simulation / Design

Process Conditions

	Hot Shell		Cold Tube		
Flow rate	220.46		110.23		1000-lb/hr
Inlet/outlet Y		/		/ 0	Weight fraction vapor
Inlet/outlet T	391.98	/	58.98	/	F
Inlet P/allow dP	29.008	/	29.008	/	psia / psi

Shell Geometry

TEMA type	A E S	
ID	36	inch
Orientation	Horizontal	
Hot fluid	Shellside	

Baffle Geometry

Type	Single segmental	
Orientation	Program sets	
Cut		% ID
Spacing	20	inch

Tube Geometry

Type	Plain		Wall thickness	0.083	inch
Length	20	ft	Layout angle	30	degrees
Tube OD	1	inch	Tubepasses	1	
Pitch	1.33	inch	Tubecount		

Shell Type

Exchanger type	TEMA	Shell wall thickness		inch
Closure type		U-Bend type		

Input | Reports | Graphs | Drawings | Shells-in-series | Design | Xist 3.00

For Help, press F1 | Run Failed

ProSim SA (www.prosim.net)

- One of the few Eruopean independent and privately held companies to supply software and service solutions for
  - modelling, simulation and optimization to process industries.

- Range of products
  - ProSimPlus: process flowsheeting software
  - ProSimPlus HNO3: 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

New CAPE Components - developed by ProSim SA

ProSim

- **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)
  - Allows creation and deployment within an organization of *Simulis® Thermodynamics* Packages (CAPE-OPEN compliant)
  - Offers a CAPE OPEN compliant thermodynamic socket for external property packages

- **A detailed presentation will be made.**

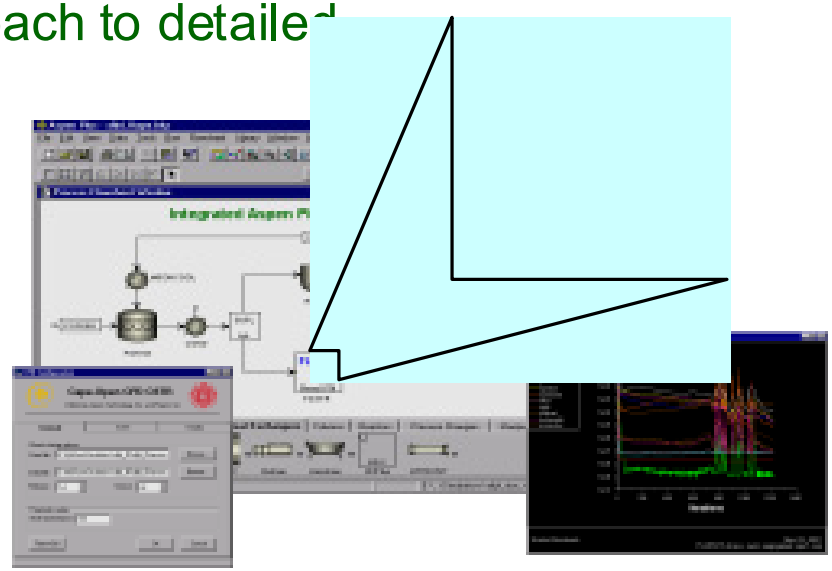
CO LaN

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 Maxwell Osawe.

Integration of Process Simulation and CFD
Improved Asset Optimization

- Configure, solve, analyze, and visualize CFD models from within a process simulator
- Evolutionary approach to detailed plant design
- Offers new capabilities to optimize CFD models in the context of an overall process simulation



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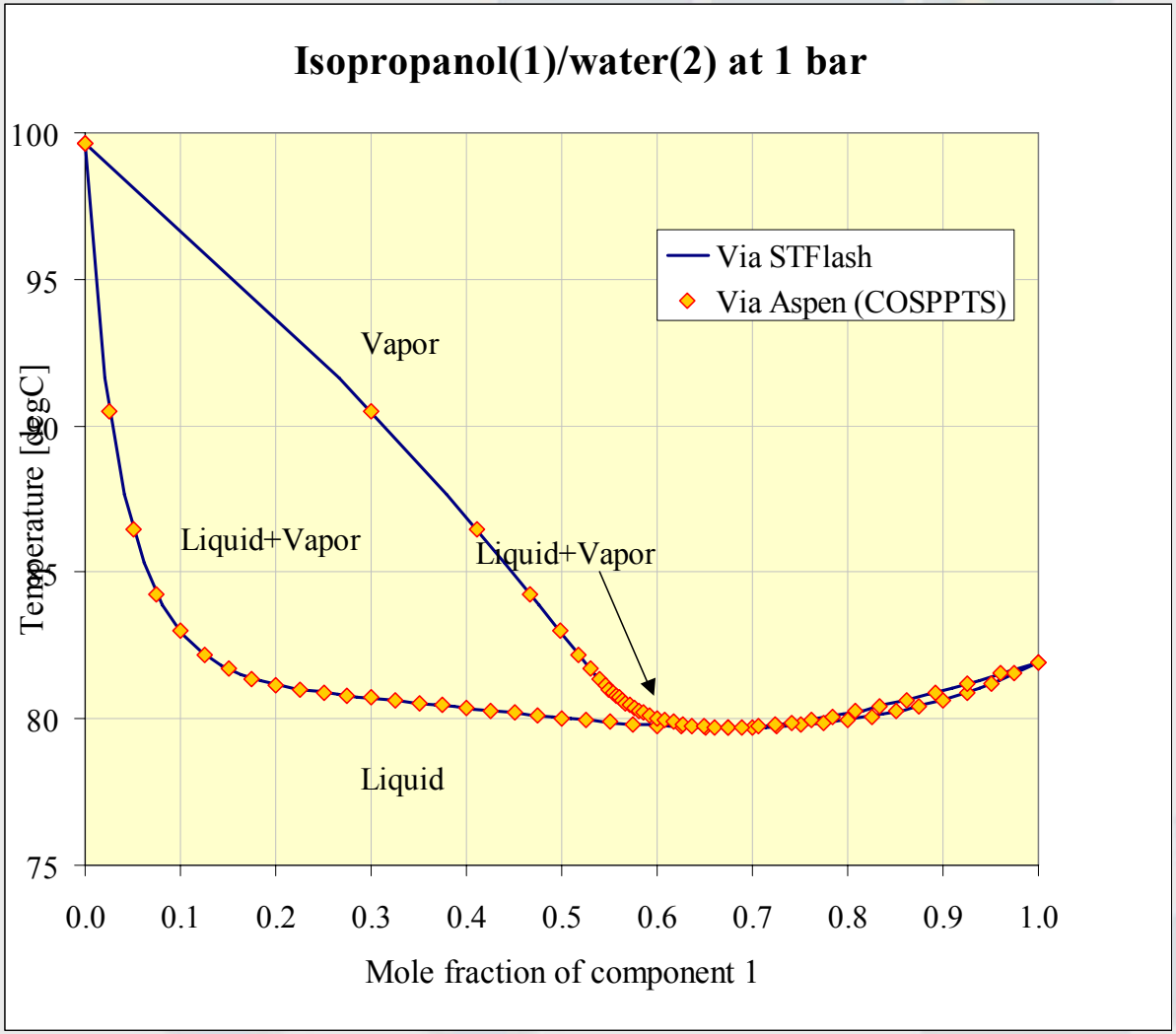
Proprietary Industrial PMCs

Bringing in-house software to CAPE-OPEN compliance

Shell thermo server

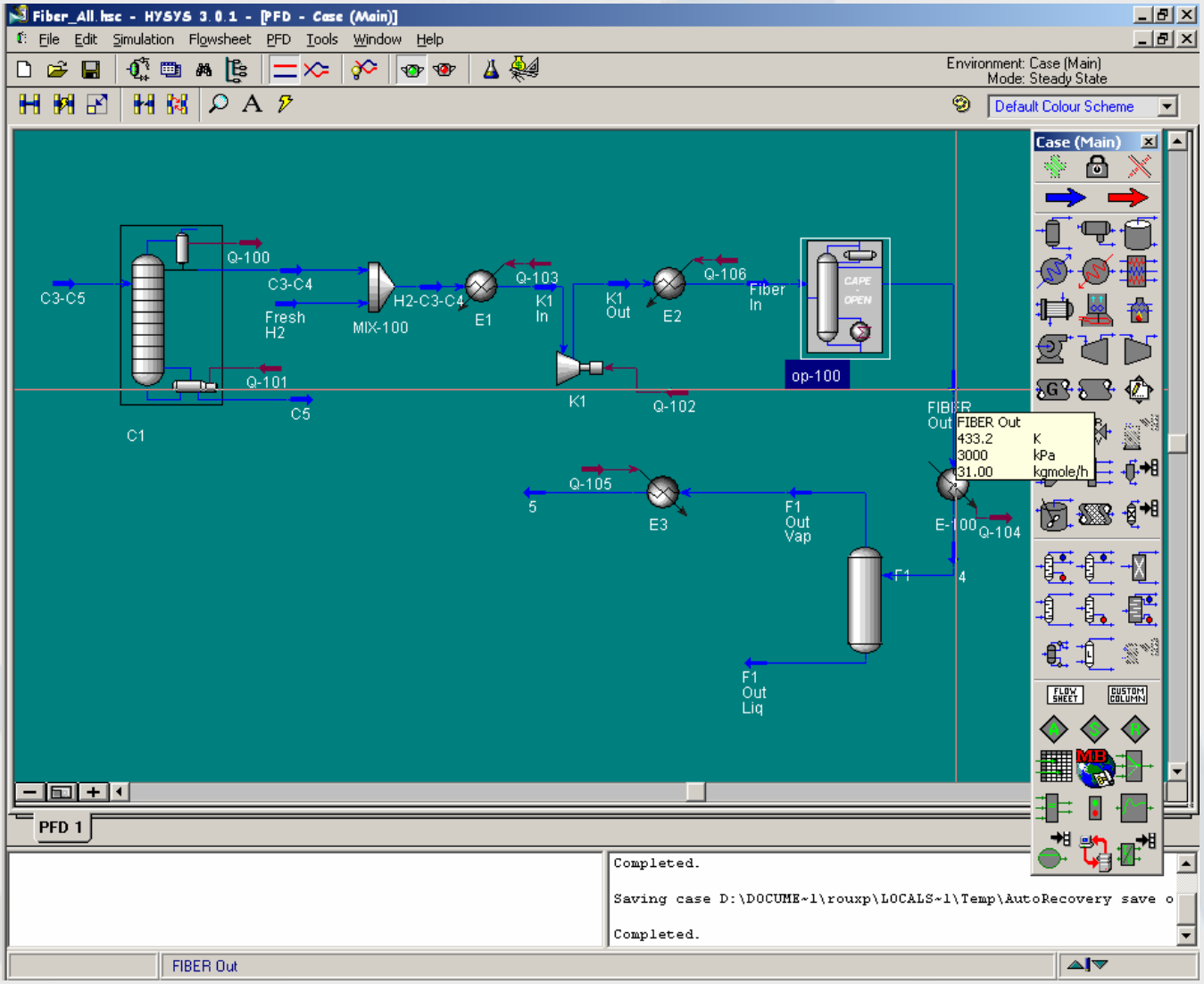
IFP unit operation

Shell COSPPTS

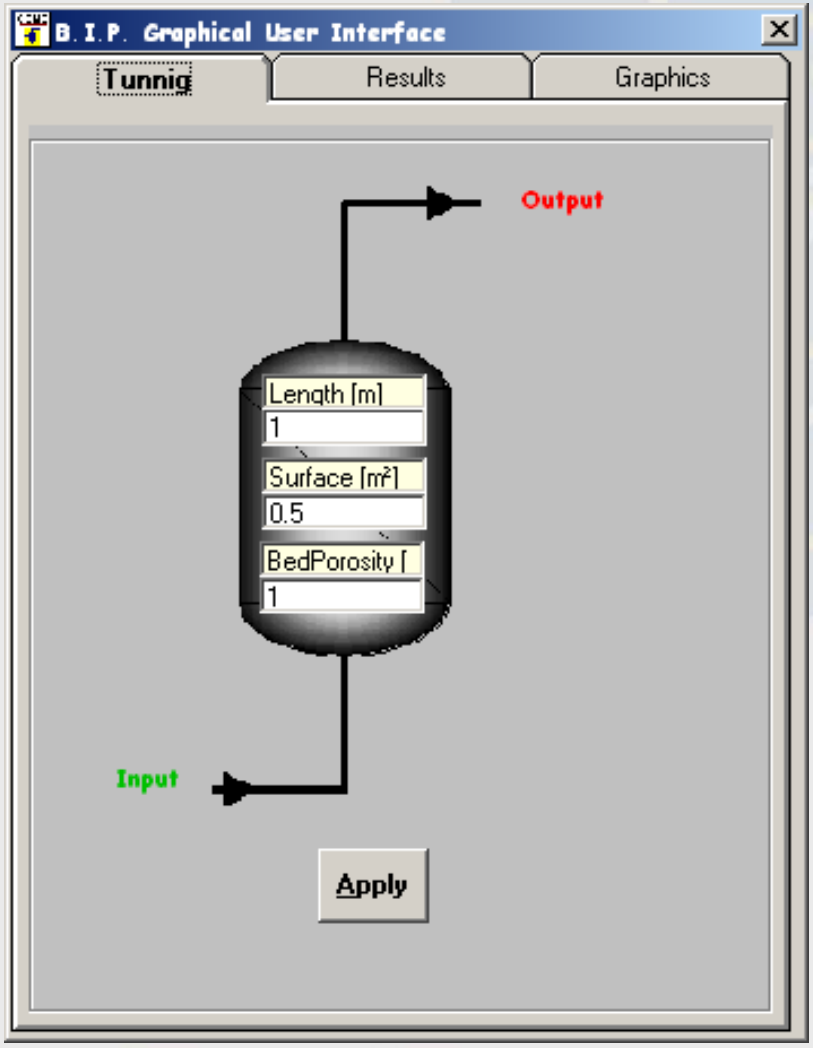


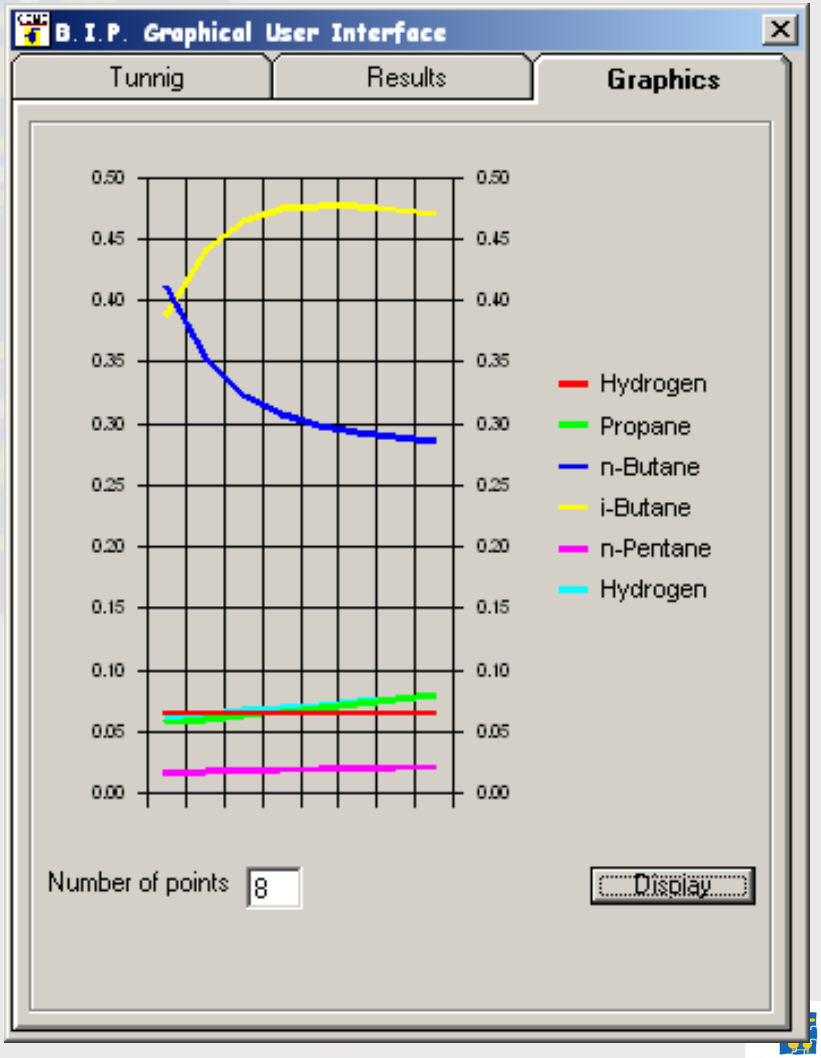
- Specific Thermodynamic model
- To be used within several Process Modeling Environments

IFP Butane Isomerisation Process Reactor



IFP Butane Isomerisation Process Reactor





Academic and research organizations PMCs

Making research results available through CAPE-OPEN

Thermo servers, Solvers, Unit operations, Simulators

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.
- CO Thermo System developed: Cubic-Plus-Association (CPA) equation of state + PC SAFT

IVC SEP
Center for Phase Equilibria and Separation Processes

CO LaN

Property Package plugged into Aspen Plus

Aspen Plus - Simulation 1 - [Setup - Data Browser]

File Edit View Data Tools Run Plot Library Window Help

Setup

- Setup
- Components
- Properti
- Flowshe
- Streams
- Utilities
- Blocks
- Reactior
- Converg
- Flowshe
- Model A
- EO Conf
- Results

METC | All

Global | Description | Accounting | Diagnostics

Available Property Packages

Property Packages

- IVC-SEP Thermo System
  - JulePack
  - PCSAFT_test
- HYP/SRK ThermoSystem
- Aspen Properties
- Standalone Property Packages

Name: IVCSEPThermoSystem.IVCSEPSystem.1

Description

About

Vendor

CAPE-OPEN version

Component version

Component help

OK | Cancel | Help | Package Details

Text to appear on each page of the report file. See Help.

Input Complete

For Help, press F1 | C:\AspenTech\Aspen Plus 12.1 | Flowsheet Not Complete

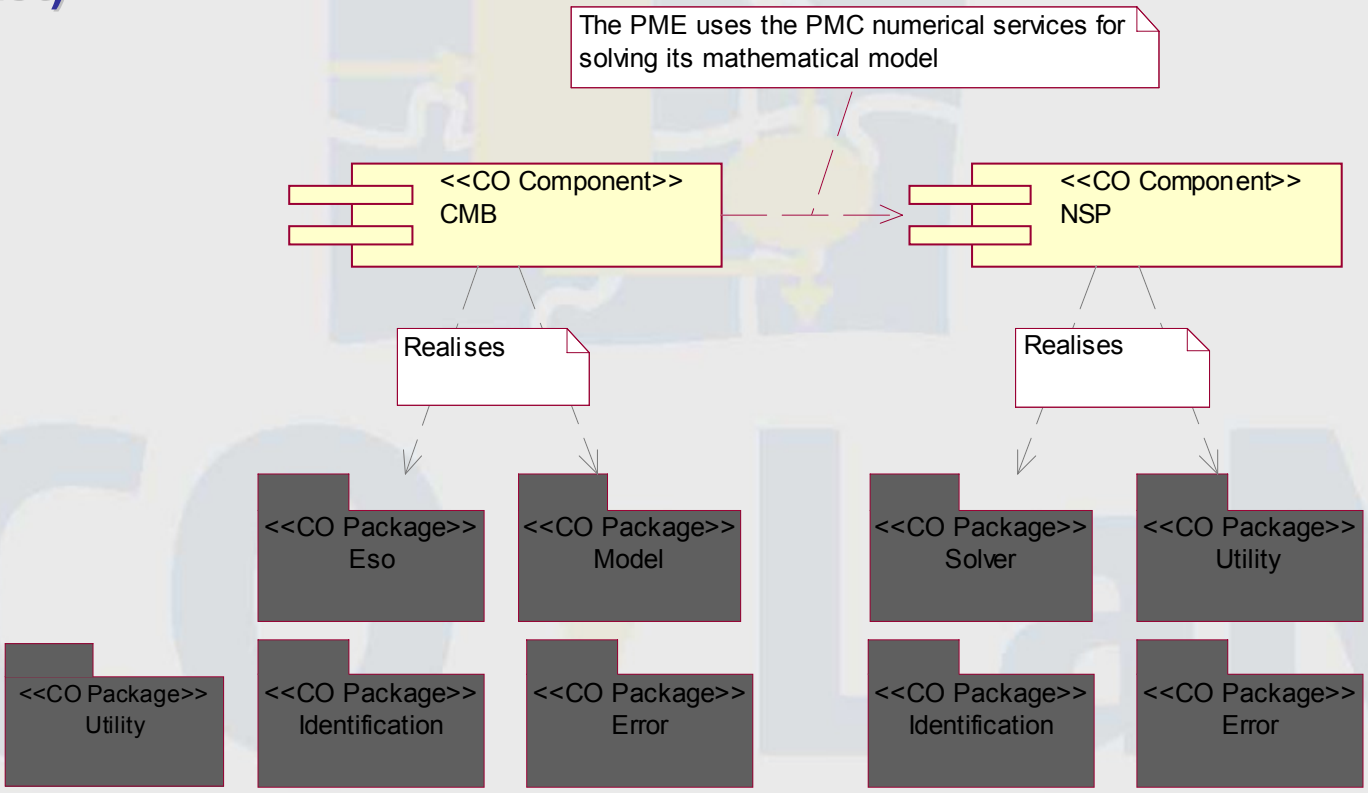
start | Document2 ... | IVCSEPTher... | Aspen Plus -... | DA | 12:18

INPT-ENSIACET

- French education and research center 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)**

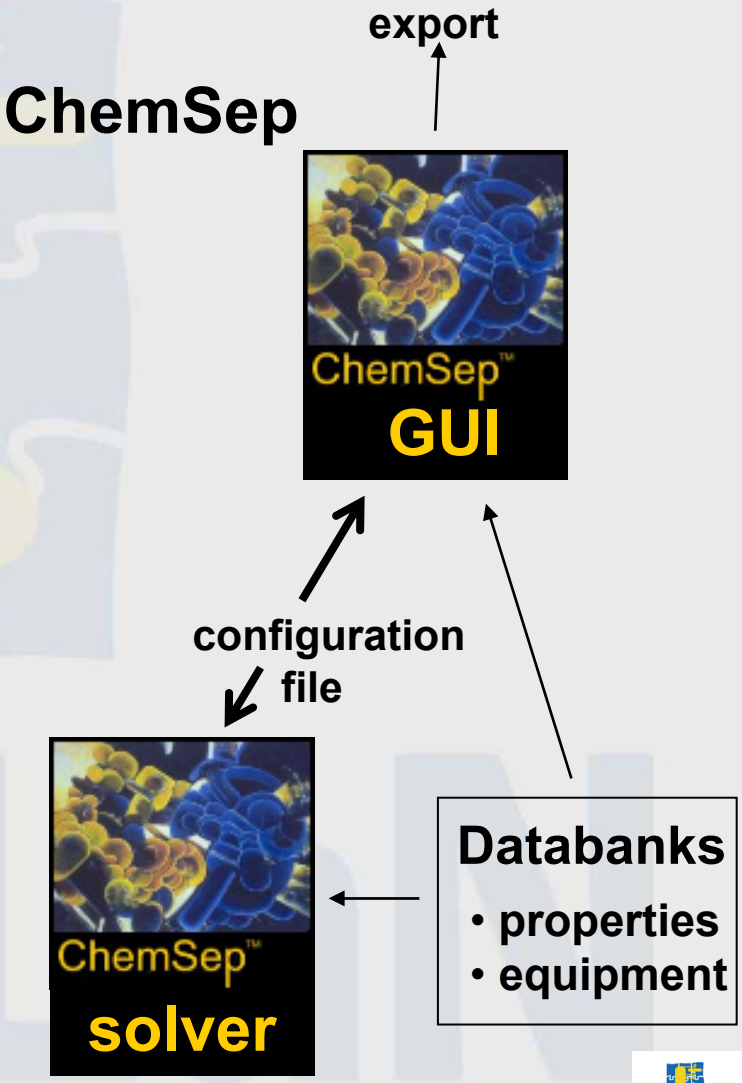


IPOPT from CMU

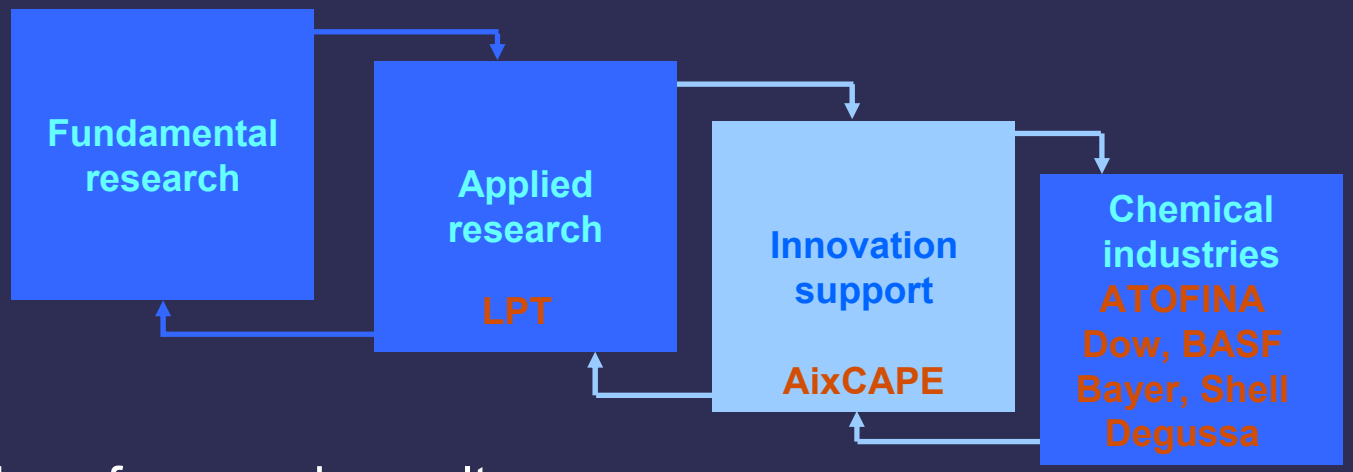
- NLP solver
- Able to solve large-scale NLP problems
- Delivered as open source software
- Made CAPE-OPEN compliant by wrapping it according to the MINLP interface specification
- Presentation by Larry Biegler and Yidong Lang

ChemSep.org

- Detailed rate-based model of distillation columns
- Made a CAPE-OPEN compliant Unit Operation
- Works in Aspen Plus, Aspen HYSYS and PRO/II
- To be demonstrated by Prof. Ross Taylor



AixCAPE: Innovation-oriented network



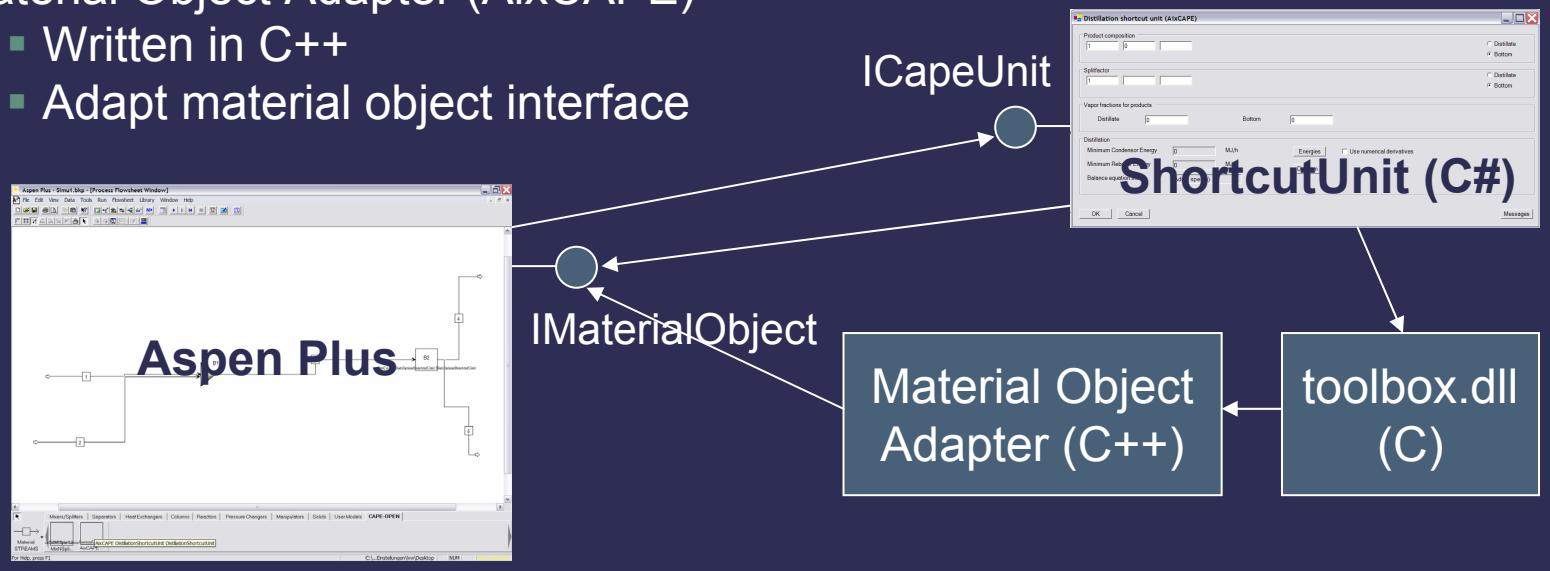
- Use of research results
  - Often difficult in practice
  - Not only a technical problem
  - AixCAPE supports the process of innovation
    - Screening of new methods and tools
    - Evaluation of novel developments in practical cases
    - Implement research results in pre-commercial products
    - Feedback of requirements and potential into research

AixCAPE

Implementation of Shortcut Unit

Shortcut Unit

- Dynamic library toolbox.dll
  - Realized in C at LPT
  - Thermodynamics, azeotrope search, rectification body method
- Shortcut Unit (AixCAPE)
  - Developed using Microsoft .net / C#
  - GUI (Parameterization)
  - Stream connections (ports)
- Material Object Adapter (AixCAPE)
  - Written in C++
  - Adapt material object interface



AixCAPE

US EPA MPPTS software tool

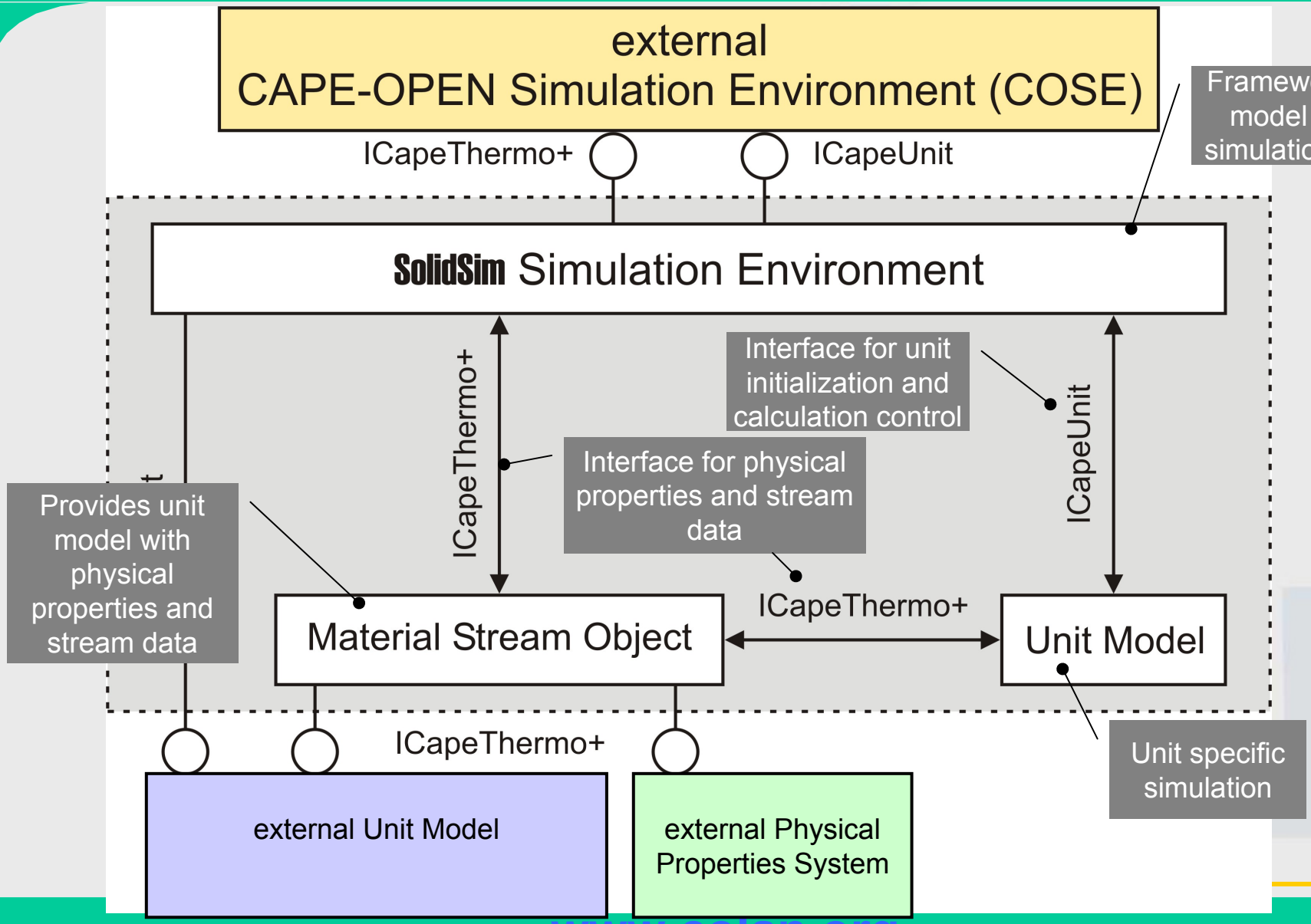
- Sequential modular process simulator
- Evaluate metal finishing processes for waste reduction
- Use of .NET framework
- Distributed as an open-source application
- Presentation by Bill Barrett

SolidSim

- Flowsheet simulator for solids processes allows
  - Development of flowsheets for complex processes
  - Design studies for process alternatives
  - Sensitivity analysis for process parameters
  - Fast and easy optimization of processes involving solids
- Establish a model library for solids processing equipment and unit operations
- Support education of chemical engineering students

TUHH
Technische Universität Hamburg-Harburg

SolidSim Simulation Framework



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 CO models

- Market is adopting CAPE-OPEN
  - Major commercial software tools are compliant
  - Proprietary material being moved to CO
  - Transfer from universities/research beginning