

Interoperability demonstrations



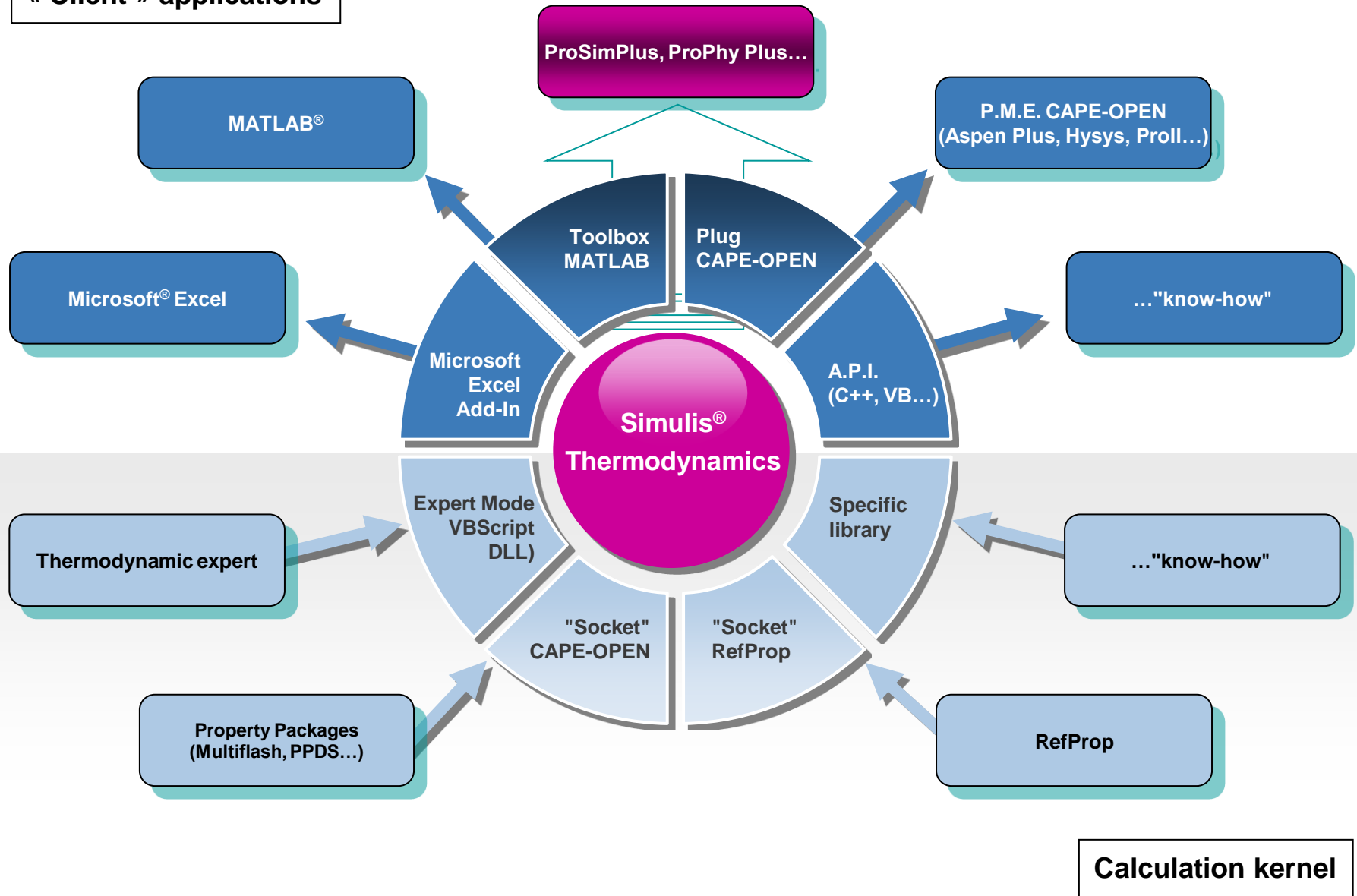
CO-LaN

CAPE-OPEN European Annual Conference
CO-LaN Annual General Meeting – Lyon 2012



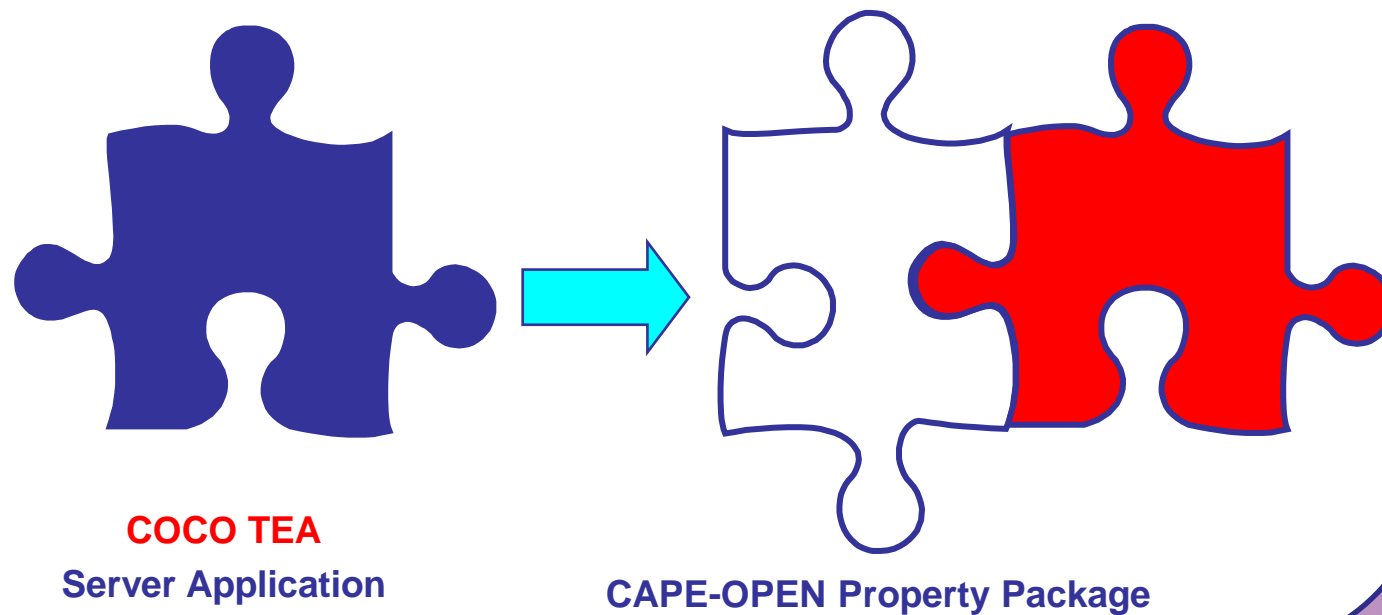
ProSim

« Client » applications



« Thermodynamic socket »

Demo



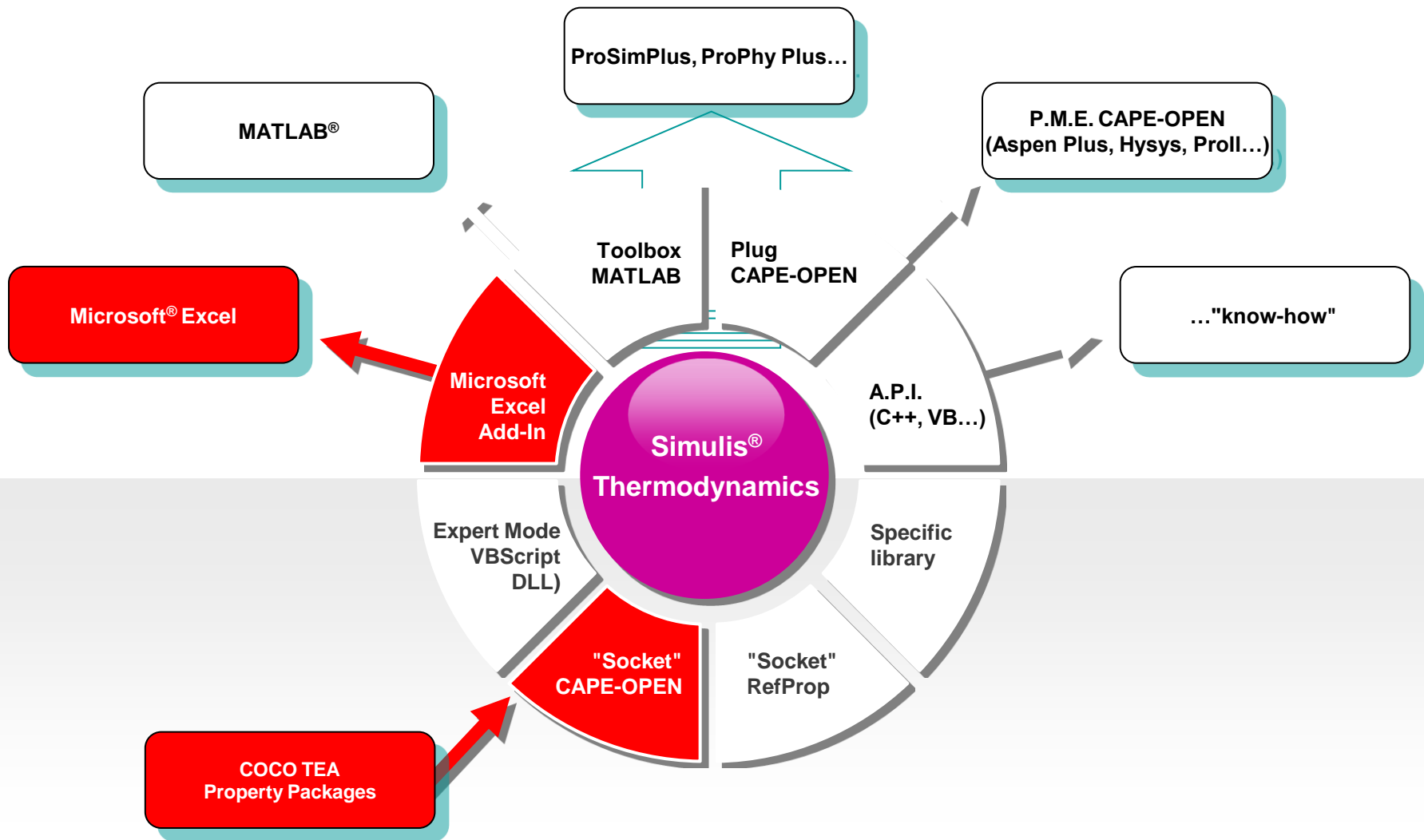
Simulis Thermodynamics
Client Application

COCO TEA

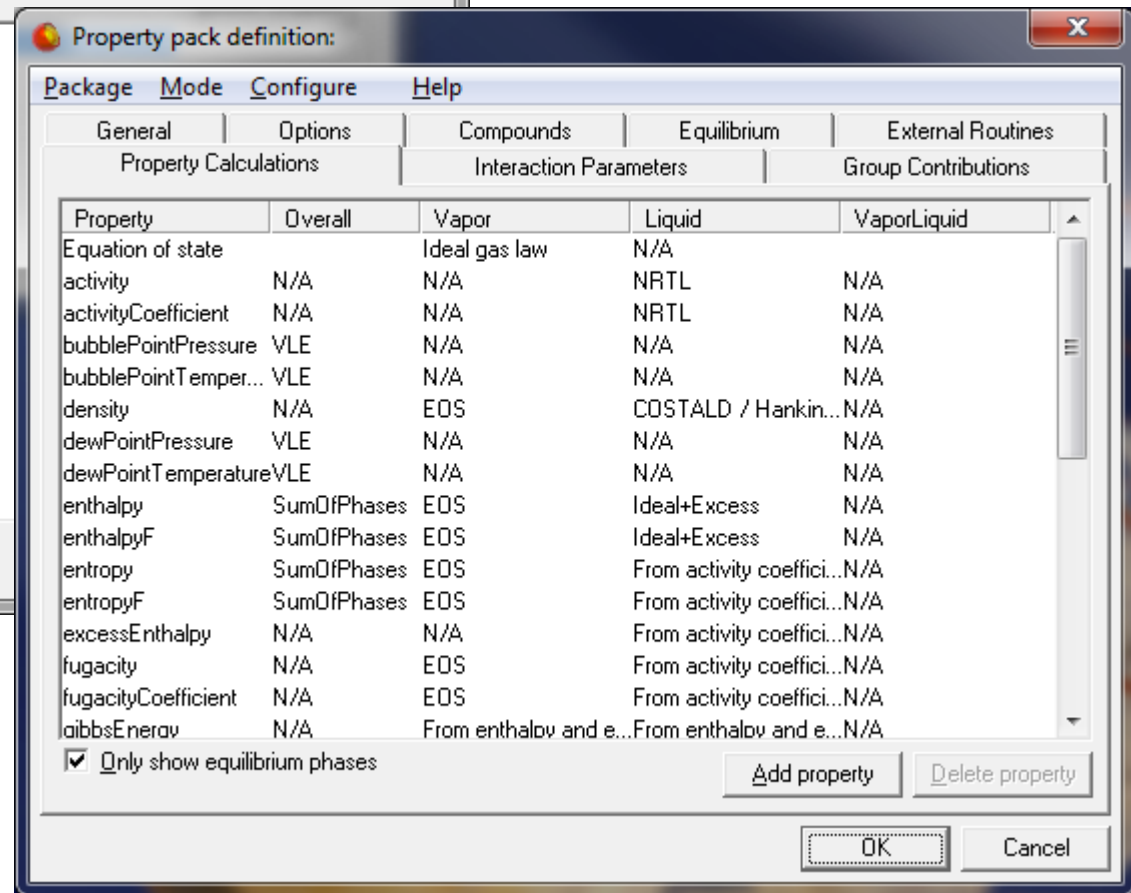
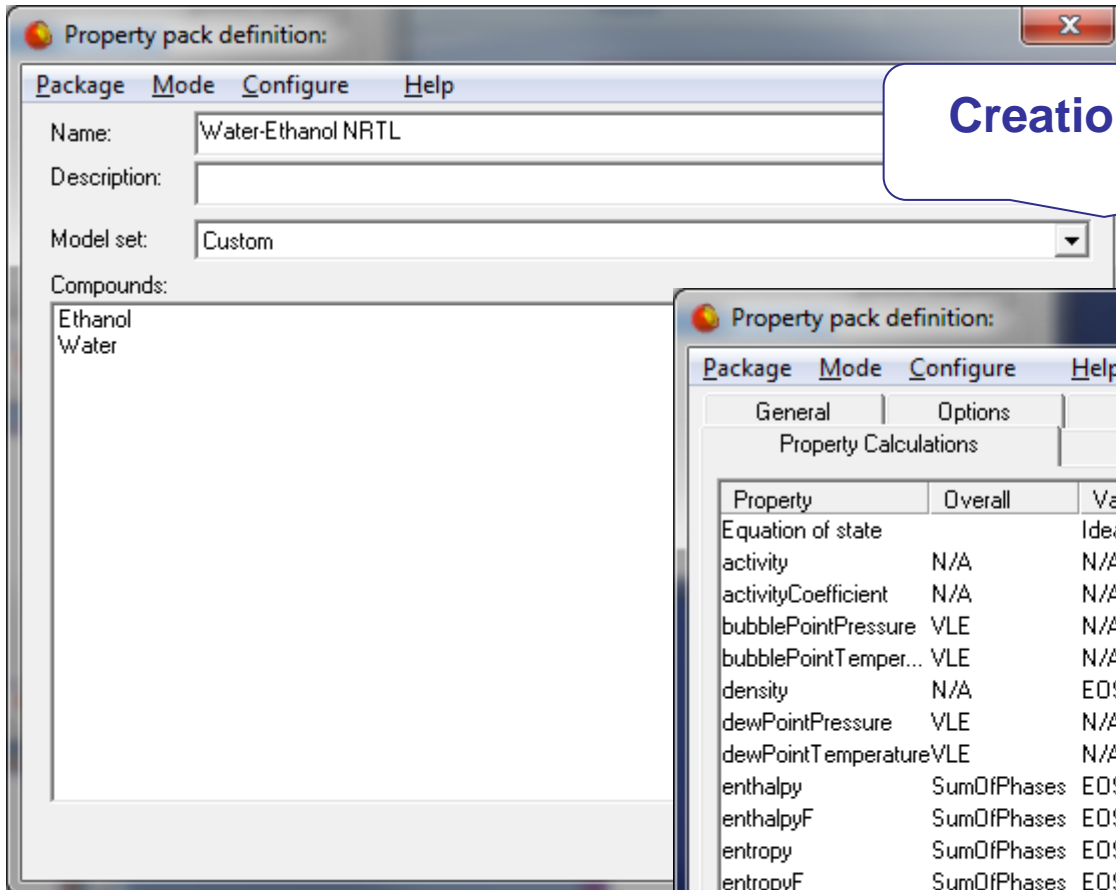
Server Application

CAPE-OPEN Property Package





Creation of a P.P using TEA



Selection of the TEA P.P. (version 1.0 or 1.1) using Simulis Thermodynamics

The image shows two windows from the Simulis Thermodynamics software. The background window is the 'CO Property Package Manager' with the following details:

- Source type: CO Property Package Manager
- Class ID: {B6AC41D3-7755-4ED5-B307-B58841E05C74}
- Container: TEA (CAPE-OPEN 1.1)
- Name: Water-Ethanol NRTL

The 'Configuration' section of the background window shows the 'Calculator type' set to 'CAPE-OPEN 1.1', which is circled in red.

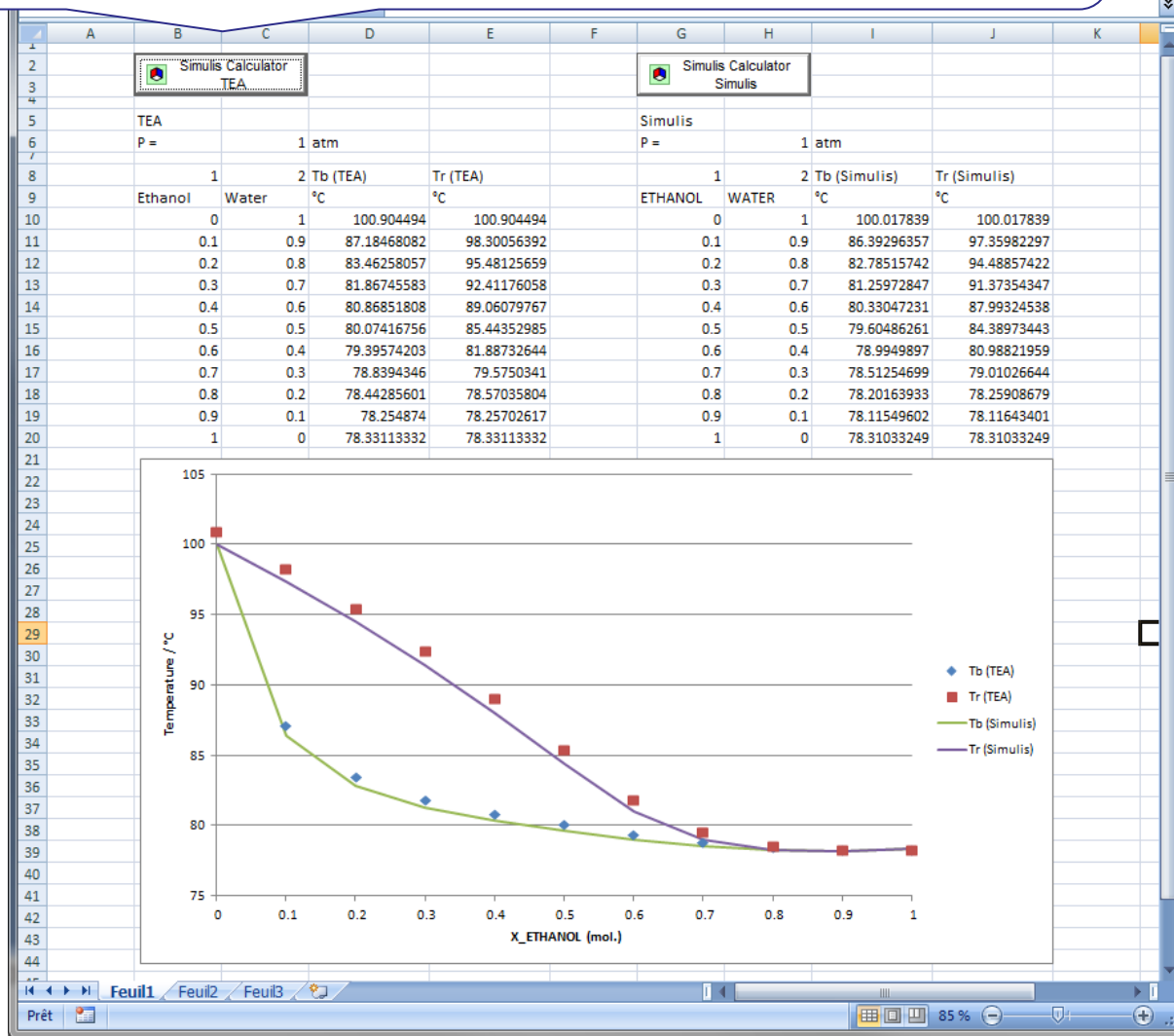
The foreground window is titled 'Selection of a CAPE-OPEN Thermodynamic Property ...' and displays a tree view of available packages:

- Standalone CAPE-OPEN® Thermo Property Packages (1.1)
 - Demo CAPE-OPEN 2011
 - Package Bender Kiwi (Simulis)
 - Water
 - Water-Ethanol (REFPROP)
 - Water-Ethanol NRTL (Simulis)
- Simulis CAPE-OPEN® Thermo System (1.0) / P.P.M. (1.1)
 - TEA (CAPE-OPEN 1.1)
 - C1_C2
 - C1_C2 (EOS)
 - COLan0
 - HDA
 - Water-Ethanol NRTL** (highlighted)
 - Water-UDHE
 - alkanes
 - n-depropanizer

At the bottom of the foreground window, there is a note: '(*) Simulis packages are in italic.' and buttons for 'Select' and 'Cancel'.

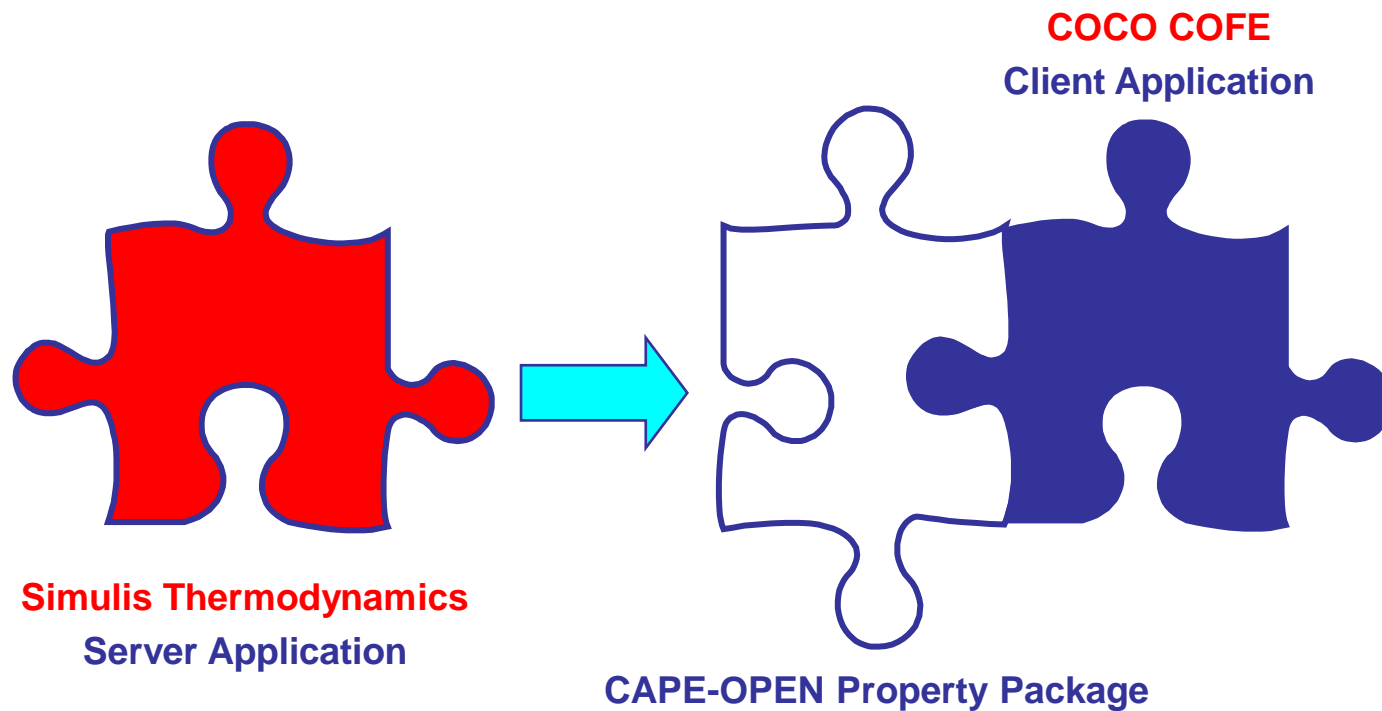


Calculation with TEA P.P. using Simulis Thermodynamics features within Microsoft Excel

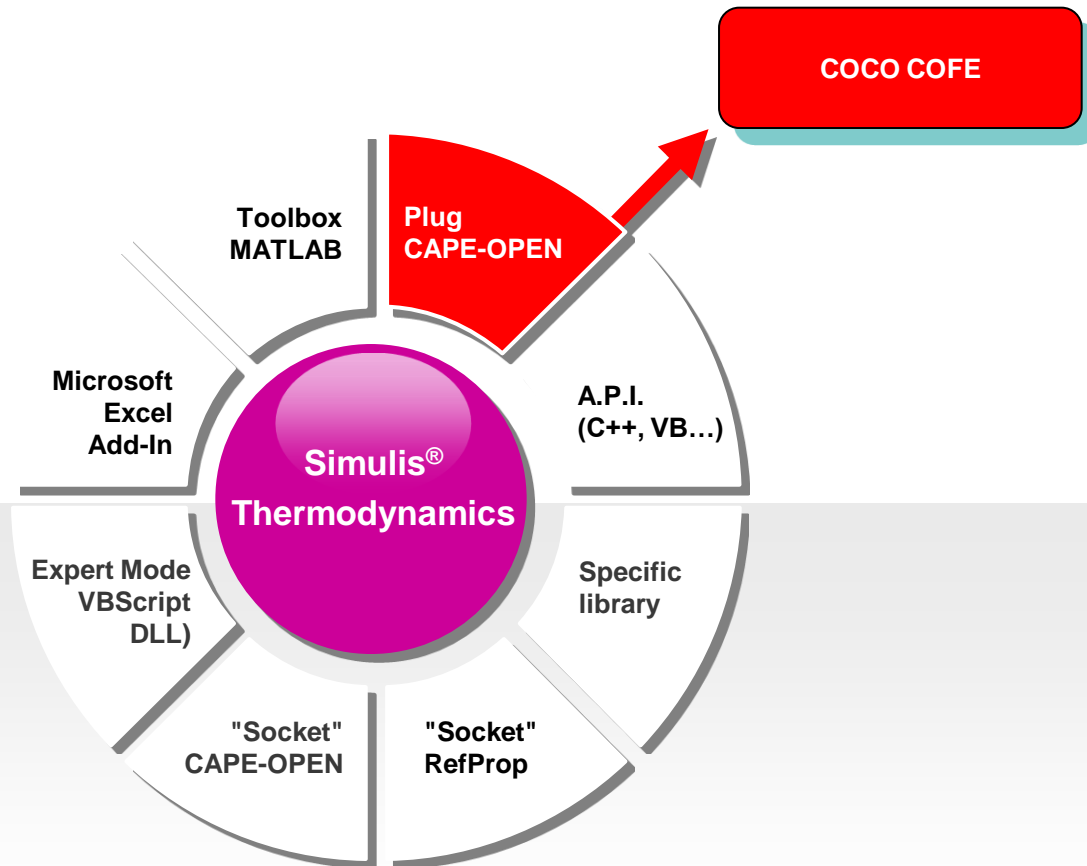


« Thermodynamic plug »

Demos



Demonstration 1



Creation of a Simulis Thermodynamics P.P. (compliant 1.1 and 1.0) based on native models

The screenshot displays the ProSim software interface. On the left, a sidebar contains menu items: 'Import', 'Build a package...', 'Select a CAPE-OPEN package', 'File', 'Modifications', 'Services', 'Calculate', 'Export as a PSF file', 'Diagrams', 'Residue...', 'Export as a PVT file', and 'Stream...'. Below this is the 'Configuration' section with a 'Name' field, a 'Comments' field, a 'Calculator type' dropdown menu set to 'Native' (circled in red), and a 'Show the expert mode' checkbox. The main window shows 'Compounds actions' (Import, Edit, Add, Delete, Clone, Remove, Create pseudo-compounds, Temperature dependent properties, Editor array, Compare with the original, Compare the compounds), 'File' (Open, Save as, Publish), 'Order', and 'Compounds Packages' tabs. A table lists compounds:

#	IUPAC Name	Registry Cas Number
1	WATER	7732-18-5
2	ETHANOL	64-17-5

The 'Creation of a Simulis Package' dialog box is open, showing 'Package properties'. It includes a brief instruction: 'Use this window to set the properties of your package. Some fields are mandatory (in bold), the others can be used freely.' The fields are: 'File' (C:\Users\alain.vacher.PROSIM2003\Desktop\PackageDemo1.dll), 'Name' (Demo 1 (Water-Ethanol NRTL)), 'Description', 'Vendor URL', 'Help URL', and 'About'. 'Create' and 'Cancel' buttons are at the bottom.



The image shows a screenshot of the COFE software interface. The main window is titled "COFE - [Flowsheet1]" and contains a menu bar (File, Edit, Insert, Flowsheet, Plot, View, Add-ins, Window, Help) and a toolbar. A "Document Explorer" pane on the left shows a tree view with "Flowsheet1", "Flowsheet", and "Settings". A "Flowsheet configuration:" dialog box is open, displaying tabs for "Material types", "Flowsheet Options", "Stream order", "Unit Operation order", "Property packs", "Reaction packs", "Compounds", "Properties", and "Phase Info". Under "Thermo-systems and property packages:", "StarDust® Thermodynamic Calculator" is listed. A "Select Thermo Pack or Prop..." dialog box is also open, showing a list of thermo packs. The "Show:" dropdown is set to "CAPE-OPEN 1.1". The list includes "Demo 1 (Water-Ethanol NRTL) (CO Thermo v1.1)", "Demo CAPE-OPEN 2011 (CO Thermo v1.1)", "Package Bender Kiwi (Simulis) (CO Thermo v1.1)", "Simulis CAPE-OPEN® Thermo System (1.0) / P.P.M. (", "TEA (CAPE-OPEN 1.1)", "Water", "Water-Ethanol (REFPROP) (CO Thermo v1.1)", and "Water-Ethanol NRTL (Simulis) (CO Thermo v1.1)". The "Demo 1" option is selected. Buttons for "About", "Select", and "Cancel" are visible at the bottom of the dialog.

**Selection of this Simulis Thermodynamics P.P.
within COCO COFE**



COFE - Flowsheet1

File Edit Flowsheet Streams Plot View Window Help

Document Explorer

- Flowsheet1
 - Flowsheet
 - 1
 - Settings

Use of this Simulis Thermodynamics P.P. for calculating properties of a stream within COCO COFE

1

Flowsheet1:2 [1]

name	1	unit
▶ Stream		
▶ Connections		
▼ Overall		
pressure	101325	Pa
temperature	355	K
mole fraction [WATER]	0.5	
mole fraction [ETHANOL]	0.5	
flow	10	mol / s
MW	0.03204185	kg / mol
▶ Compound flows		
▼ Phase Fractions		
molar phaseFraction [Vapor]	0.77396047	
molar phaseFraction [Liquid]	0.22603953	
▶ Vapor composition		
▼ Liquid composition		
mole fraction [WATER]	0.74665381	
mole fraction [ETHANOL]	0.25334619	
▶ Overall properties		
▼ Vapor properties		
viscosity	1.1273015e-005	Pa s
thermalConductivity	0.021668042	W / m K
internalEnergy	137.94975	J / mol
enthalpy	3089.5777	J / mol
entropy	15.147145	J / mol K

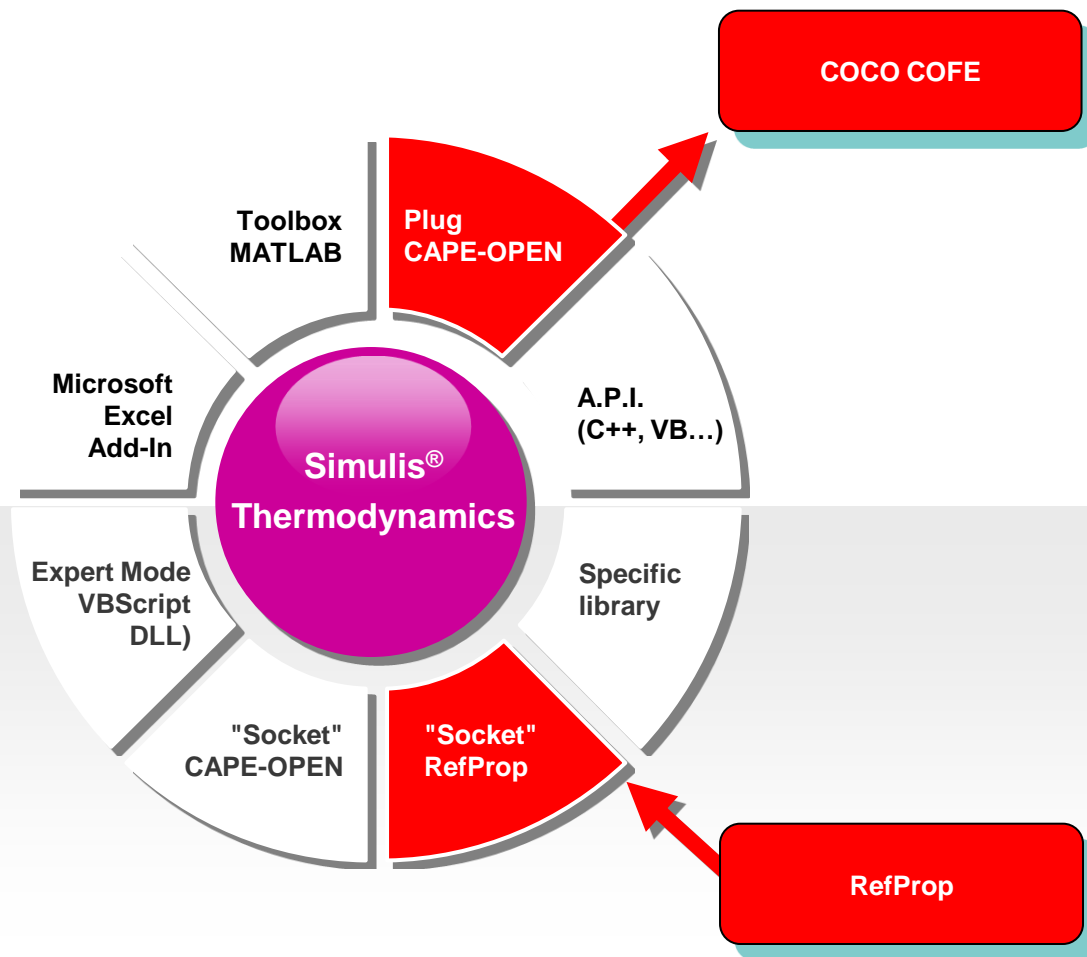
Document Explorer Watch

Ready

CAP NUM SCRL



Demonstration 2



Creation of a Simulis Thermodynamics P.P. (complaint 1.1 and 1.0) based on REFPROP models

Warning: RefProp does not support simultaneous calculations on different calculators.

Parameters and mixture file: HMX.BNC

Fluids	x0
WATER.FLD	0
ETHANOL.FLD	0

Fluids available in the mixture file

- 1BUTENE.FLD
- ACETONE.FLD
- AIR.PPF
- AMMONIA.FLD
- ARGON.FLD

Creation of a Simulis Package

Package properties

Use this window to set the properties of your package. Some fields are mandatory (in bold), the others can be used freely.

File: C:\Users\valain.vacher.PROSIM2003\Desktop\PackageDemo2.dll

Name: Demo2 (Water-Ethanol REFPROP)

Description:

Vendor URL: Help URL:

About:

Create Cancel

Reference state

Enthalpy and entropy

- Use the default reference state
- Enthalpy, entropy= 0 for the saturation state
- Enthalpy, entropy= 0 for the saturation state at 200 K
- Enthalpy= 200 kJ/kg, entropy= 1 kJ/kg.K
- Specify the reference state value

Calculator type: RefProp

COFE - [Flowsheet1]

File Edit Insert Flowsheet Plot View Add-ins Window Help

Document Explorer

- Flowsheet1
 - Flowsheet
 - Settings

Selection of this Simulis Thermodynamics P.P. within COCO COFE

Flowsheet configuration:

Material types | Flowsheet Options | Stream order | Unit Operation order

Property packs | Reaction packs | Compounds | Properties | Phase Info

Thermo-systems and property packages:

- StarDust® Thermodynamic Calculator

Add

Select Thermo Pack or Prop...

Show: CAPE-OPEN 1.1

- Demo 1 (Water-Ethanol NRTL) (CO Thermo v1.1)
- Demo CAPE-OPEN 2011 (CO Thermo v1.1)
- Demo2 (Water-Ethanol REFPROP) (CO Thermo v1.1)**
- Package Bender Kiwi (Simulis) (CO Thermo v1.1)
- Simulis CAPE-OPEN® Thermo System (1.0) / P.P.M. (
- TEA (CAPE-OPEN 1.1)
- Water
- Water-Ethanol (REFPROP) (CO Thermo v1.1)
- Water-Ethanol NRTL (Simulis) (CO Thermo v1.1)

About Select Cancel

SCRL

Description:

Document Explorer

Ready



COFE - Flowsheet1

File Edit Flowsheet Streams Plot View Window Help

Document Explorer

Flowsheet1
Flowsheet
1
Settings

Use of this Simulis Thermodynamics P.P. for calculating properties of a stream within COCO COFE

Flowsheet1:2 [1]

name	1	unit
▶ Stream		
▶ Connections		
▼ Overall		
pressure	101325	Pa
temperature	355	K
mole fraction [water !full name]	0.5	
mole fraction [ethyl alcohol !full name]	0.5	
flow	10	mol / s
MW	0.032041854	kg / mol
▶ Compound flows		
▼ Phase Fractions		
molar phaseFraction [Vapor]	0.76592833	
molar phaseFraction [Liquid]	0.23407167	
▼ Vapor composition		
mole fraction [water !full name]	0.43189324	
mole fraction [ethyl alcohol !full name]	0.56810676	
▼ Liquid composition		
mole fraction [water !full name]	0.72285131	
mole fraction [ethyl alcohol !full name]	0.27714869	
▶ Overall properties		
▶ Vapor properties		
▶ Liquid properties		

Document Explorer Watch

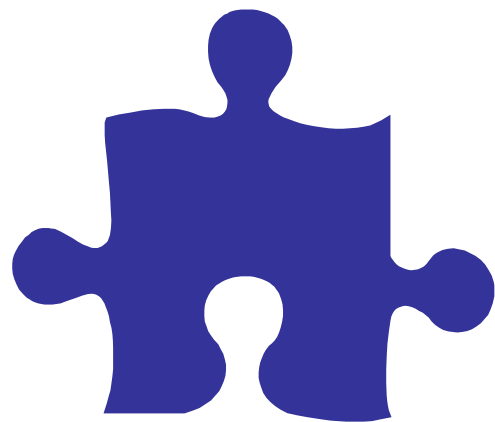
Ready

CAP NUM SCRL

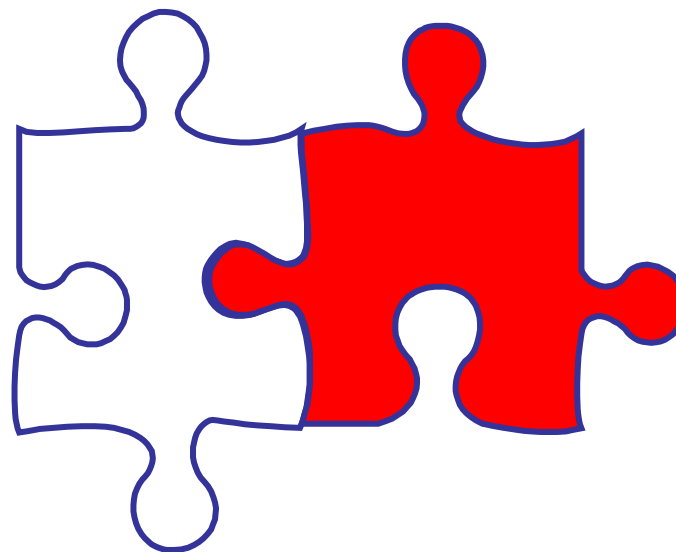
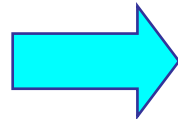


« Unit socket »

Demo



COCO COUSCOUS
Server Application



ProSimPlus
Client Application

CAPE-OPEN Unit Operation



ProSimPlus Standard - Unnamed.pmp3

File Edit Configuration Flowsheet Tools Simulation Windows Help

Name of the item:

Selection of a CAPE-OPEN Component

CAPE-OPEN

This window allows to select a CAPE-OPEN component.

Right click on an item to obtain some details.

Selection of a CAPE-OPEN flash belonging to the COUSCOUS library within ProSimPlus

Library Tree view

- Absorbers
- Feed / Product stream
- Controls
- 2-phase distillation
- 3-phase distillation
- Heat exchangers
- Liquid-liquid extraction
- Flashes and decanters
- Compressor/Expander/Pump
- Mixers / Splitters / Separators
- User defined unit operations
 - Windows Script
 - CAPE-OPEN unit operation**
 - User defined unit operation UTI
- Reactors
- Liquid-solid separation
- Strippers
- Utilities
- Subflowsheet

Main

FixedConversionReactor

Flash

GibbsReactor

HeatExchanger

HeatOfCombustionUnit

HeaterCooler

InformationCalculator

MakeUpMixer

Material eater

MeasureUnit

...

URL Vendor: <http://www.cocosimulator.org/>

URL Help: [<none>](#)

Name	Flash
Description	Flash - separate input stream into vapor and remaining phases
ClassID	{BD25A684-3814-4212-84CD-76D752E106EE}
ProgID	COCO_COUS.Flash.1
InProcServer32	C:\Program Files\COCO\COCOCOUS.dll
Short description	Flash
Full description	Split inlet stream into vapor and liquid outlet stream
Version	2.4.0.0
CAPE-OPEN version	1.0
About	CAPE-OPEN 1.0 unit operation - Copyright 2011 www.cocosimulator.org

Close

Full page




ProSimPlus Standard - V:\Archives\Présentations IEP\COUSCOUS vers ProSimPlus\COUSCOUS toPSP.pmp3 Modified

File Edit Configuration Flowsheet Tools Simulation Windows Help

Name of the item: _____

Library Tree view

- ▼ Absorbers
- ▼ Feed / Product stream
- ▼ Controls
- ▼ 2-phase distillation
- ▼ 3-phase distillation
- ▼ Heat exchangers
- ▼ Liquid-liquid extraction
- ▼ Flashes and decanters
- ▼ Compressor/Expander/Pump
- ▼ Mixers / Splitters / Separators
- ▲ User defined unit operations
 - WS Windows Script
 -  CAPE-OPEN unit operation
 - U User defined unit operation UTI
- ▼ Reactors
- ▼ Liquid-solid separation
- ▼ Strippers
- ▼ Utilities
- ▼ Subflowsheet

Main

Use of this CAPE-OPEN flash within ProSimPlus

77.14 %

Streams		1	2	3
From		Alimentation...	Flash	Flash
Partial flows		kg/h	kg/h	kg/h
ETHANOL		230.34	203.96	26.381
WATER		90.077	59.672	30.405
Partial flows		kmol/h	kmol/h	kmol/h
ETHANOL		5	4.4273	0.57266
WATER		5	3.3123	1.6877
Total flow	kg/h	320.42	263.63	56.786
Total flow	kmol/h	10	7.7396	2.2604
Temperature	°C	355	355	355
Vapor molar fraction		0.77396	1	0



Thank you...



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ProSim