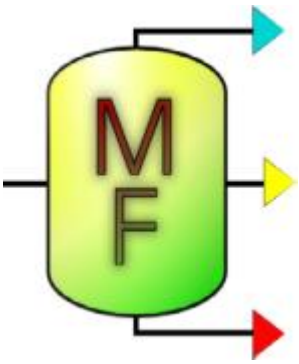
Multiflash 6.1 CAPE-OPEN Components

FOR MS WINDOWS OPERATING SYSTEMS

Infochem/KBC Advanced Technologies plc

Version 6.1

June 2016



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Introduction

The CAPE-OPEN (CO) project has established a set of open interface specifications for process modelling software components. The CAPE-OPEN Laboratories Network (CO-LaN) disseminates information and maintains and develops the interface standards. For further information and the latest versions of all CO documents see the website at www.colan.org .

The Multiflash CO components support versions 1.0 and 1.1 of the Thermodynamics and Physical Properties specification. They are implemented as Windows COM objects. The two versions provide similar basic capabilities for vapour and liquid phases but version 1.1 also supports a wider range of phases, properties and phase equilibrium calculations. The names and functionality of the software components are summarised in the following table.

Version 1.1	Version 1.0	purpose
Property Package Manager	Thermo System	provides a means of selecting a Multiflash CO Property Package
Property Package	Property Package	• describes a fixed set of chemical species and phases • calculates properties of pure species and mixtures in one or more phases. • performs phase equilibrium calculations

A Multiflash Property Package (PP) is configured using the Multiflash Windows GUI that provides an interactive environment for selecting the chemicals, models and phases in the PP. Once a PP has been configured it can be exported and will then be available through the Property Package Manager (PPM) or Thermo System (TS).

Changes

The Multiflash CO components were re-written for version 3.8. A full list of changes in Multiflash is given in Appendix A.

System requirements

- Operating System: Microsoft Windows (XP or more recent versions).
- The Multiflash Windows GUI and dll must be installed.
- The CO components must be licensed – they are an additional option for Multiflash.
- A port driver and license server are required to interact with the licensing system, if using USB Dongles.

Acknowledgements

We would like to express our thanks to the following organisations that have provided assistance and feedback on the contents of this document.

- AspenTech
- BP Exploration
- CAPE-OPEN Laboratories Network (CO-LaN)
- CoCo simulator
- SimSci-Esscor
- Process Systems Enterprise
- Prosim

Installation

The CAPE-OPEN interface is installed by default with Multiflash. The CapeOpen Components will be registered automatically.

Since Multiflash 4.4, a 64bit version of the CapeOpen DLL is also included.

Support Files

Support files for users of the CO components are installed with Multiflash in the standard installation directory.

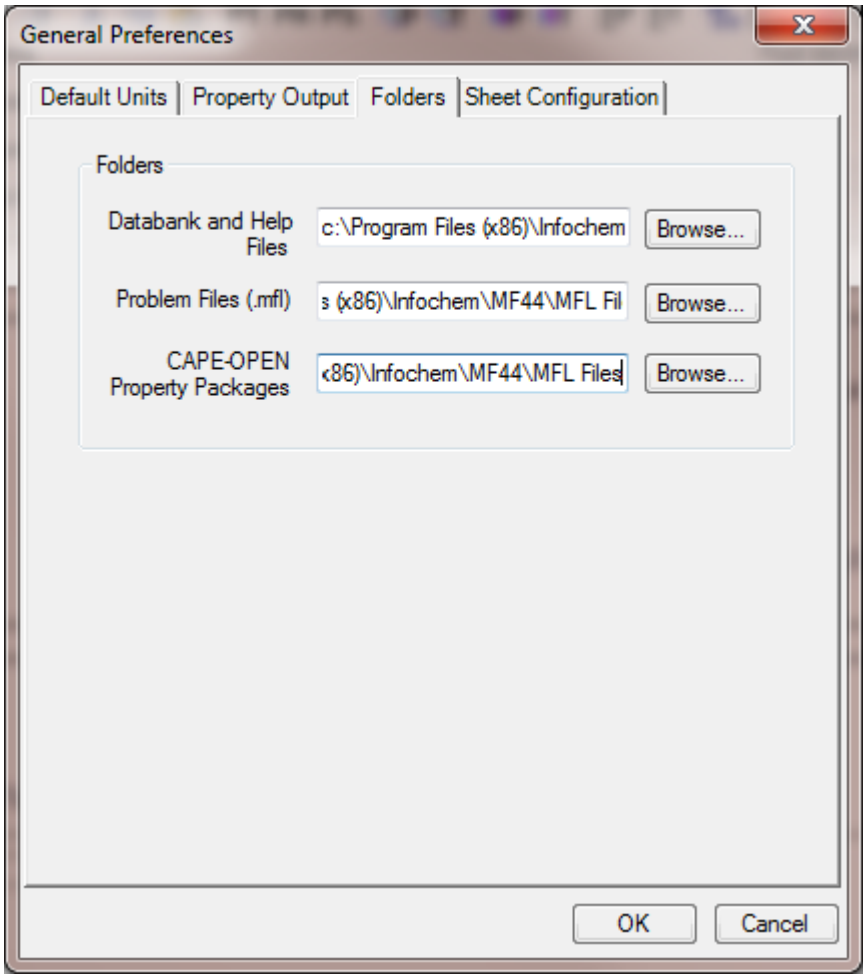
MF CO Manual.pdf	this document (Adobe Acrobat PDF format).
MF_CAPEOPEN.dll	Multiflash CAPE-OPEN components for versions 1.0 and 1.1Property Package component.
MF_CAPEOPEN64.dll	Multiflash CAPE-OPEN components for versions 1.0 and 1.1Property Package component (64bit).
c3c5.mfl	sample Property Package
HDA.mfl	sample Property Package

Configuration

Folder for Multiflash CO Property packages

The folder where Multiflash PPs are stored should be set using the Multiflash GUI. The Tools/Preferences/General menu item displays a tabbed dialog box (see below). Click on the Folders tab and enter a location for storing the CO PPs. The location is stored in the Windows Registry and is used by the PPM/TS when searching for PPs.

For Multiflash versions prior to 3.6 the CO PP location was set using an environment variable (MF_CODIR). If the Registry value is not set the environment variable will still be used if it is present.



Logging and diagnostics

Debug information may be logged to a file by setting an environment variable MF_CO_LOG. A value of FALSE means no logging and TRUE will turn on logging.

The log file name is <temp_dir>\Multiflash_Cape_open(<app_name>).log

<temp_dir> is the directory set by the TEMP environment variable.

<app_name> is the name of the application that is using the Multiflash CO components.

Diagnostics from Multiflash can be written using the methods of the ICapeDiagnostic interface (if implemented by the application) by setting an environment variable MF_CO_DIAGNOSTICS. A value of FALSE means no diagnostics TRUE will turn on diagnostics.

Neither logging nor diagnostics should be turned on for normal operation because they will significantly slow down the application.

Installing Multiflash CAPE-OPEN interface in Windows Vista and 7

Because of security implementations of Windows Vista and higher, COM objects that are registered for the current user cannot be detected by applications that run with elevated privileges. By default, the Infochem Multiflash CAPE-OPEN COM object

is registered only for the current user. If you need to access the Multiflash CAPE-OPEN functionality from elevated applications, you can use the RegMFCAPEOPEN.exe utility to register the Multiflash CAPE-OPEN for all users.

The RegMFCAPEOPEN.exe utility allows for registering and unregistering the Infochem Multiflash CAPE-OPEN interface COM object, for the current user or for all users. When run the user will be shown the following:



Current user registrations are seen before all-user registrations, so in case the all-user and current user registrations are both present, the CAPE-OPEN interface as registered by the current user will be used.

Technical support

If you need further assistance contact us at:

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Creating a Multiflash CO Property Package

A Multiflash CO PP is created using the Multiflash Windows GUI. You should be reasonably familiar with the Multiflash GUI before attempting to create a PP for use in another environment. Information on using the GUI is given in the *User Guide for Multiflash for Windows*.

A Multiflash PP can be created by launching the GUI directly in the usual way or the GUI can be launched from within a Process Modelling Environment (PME) using the Edit method of the ICapeUtilities interface which is provided by all Multiflash CO components. Not all PMEs support the use of Edit.

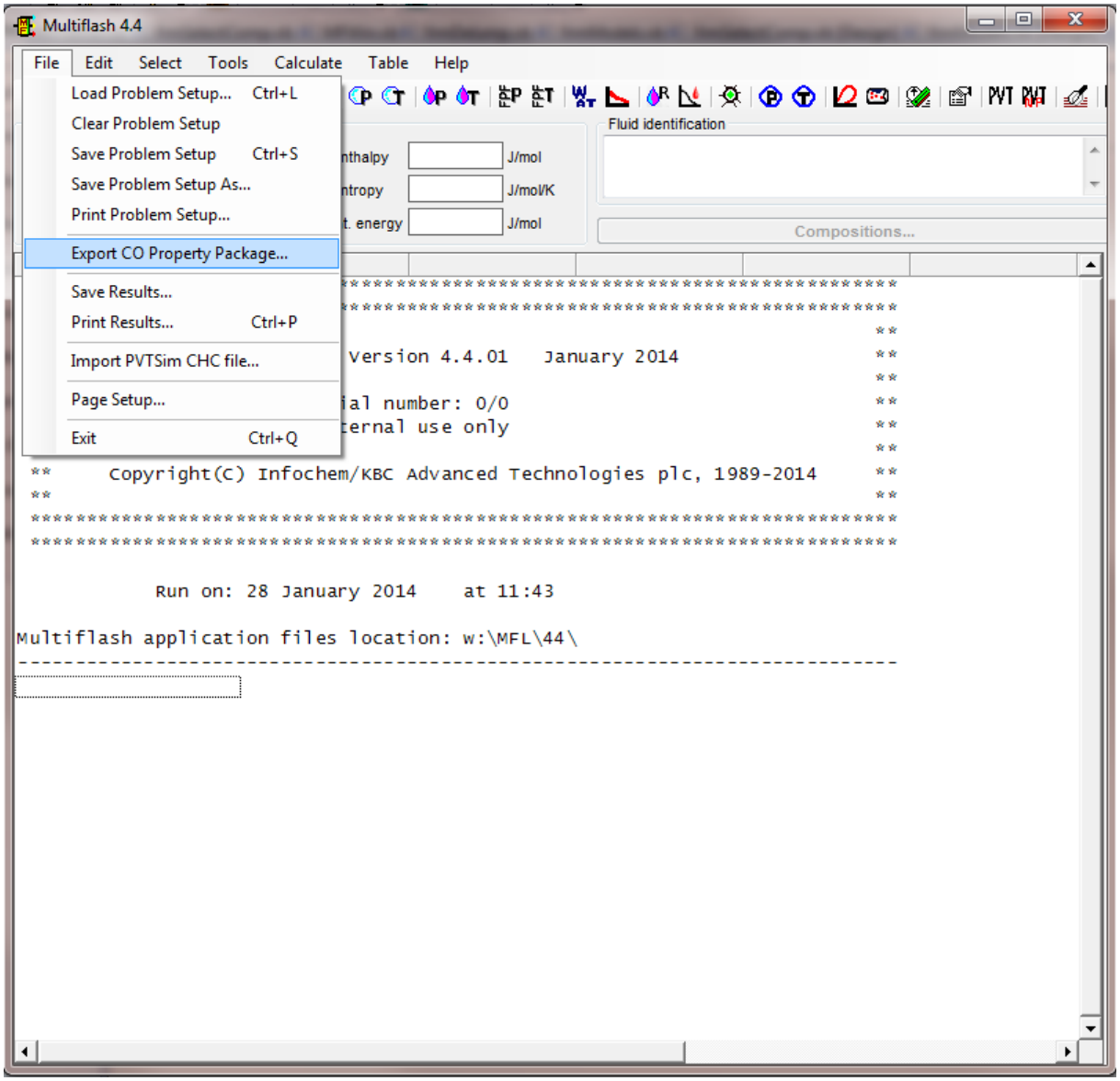
To set up a CO PP it is necessary to define the following:

- The **compounds** (substances) that are included. These may be any compounds from databanks supported by Multiflash or petroleum fraction pseudocomponents. Use the Select/Components menu item.
- The **thermodynamic/physical property models** that will be used to evaluate properties such as volume, enthalpy, fugacity coefficients, transport properties etc. Use the Select/Model Set menu item.
- The **binary interaction parameters** (BIPs) that will be used by the model(s). BIPs for Multiflash models can come from external BIP databanks, internal model-specific correlations or they can be entered directly using the Tools/BIPs menu option.
- The **phases** that may be included. The phases in Multiflash are selected in the same dialogue as the models. You should be aware that the CO 1.0 specification only allows for a vapour and one liquid phase. If you select more phases for Multiflash only the first liquid phase will be available in the CO PP.

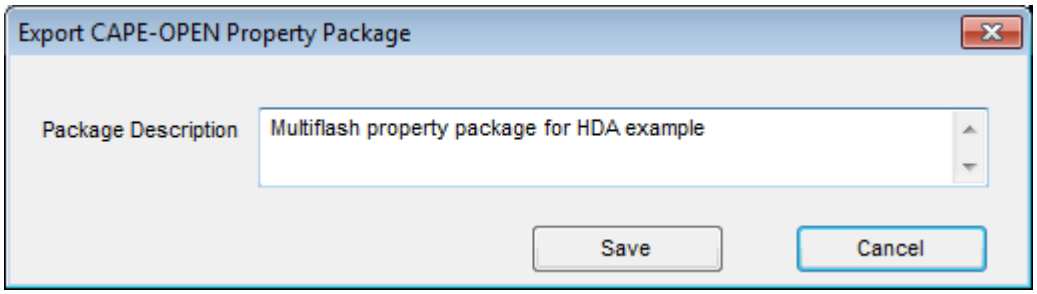
Once the CO PP information has been defined it is advisable to test the setup by carrying out some calculations. To do this you will also need to enter a composition and specify conditions such as temperature and pressure. Multiflash allows you to work in a wide range of units but the choice of units in the GUI does not affect how the PP behaves when used by another application.

A description for the PP can be entered in the 'Fluid identification' field on the GUI main window or when the PP is saved (see below). The description will be saved with the PP and may be displayed by an application that uses the PP.

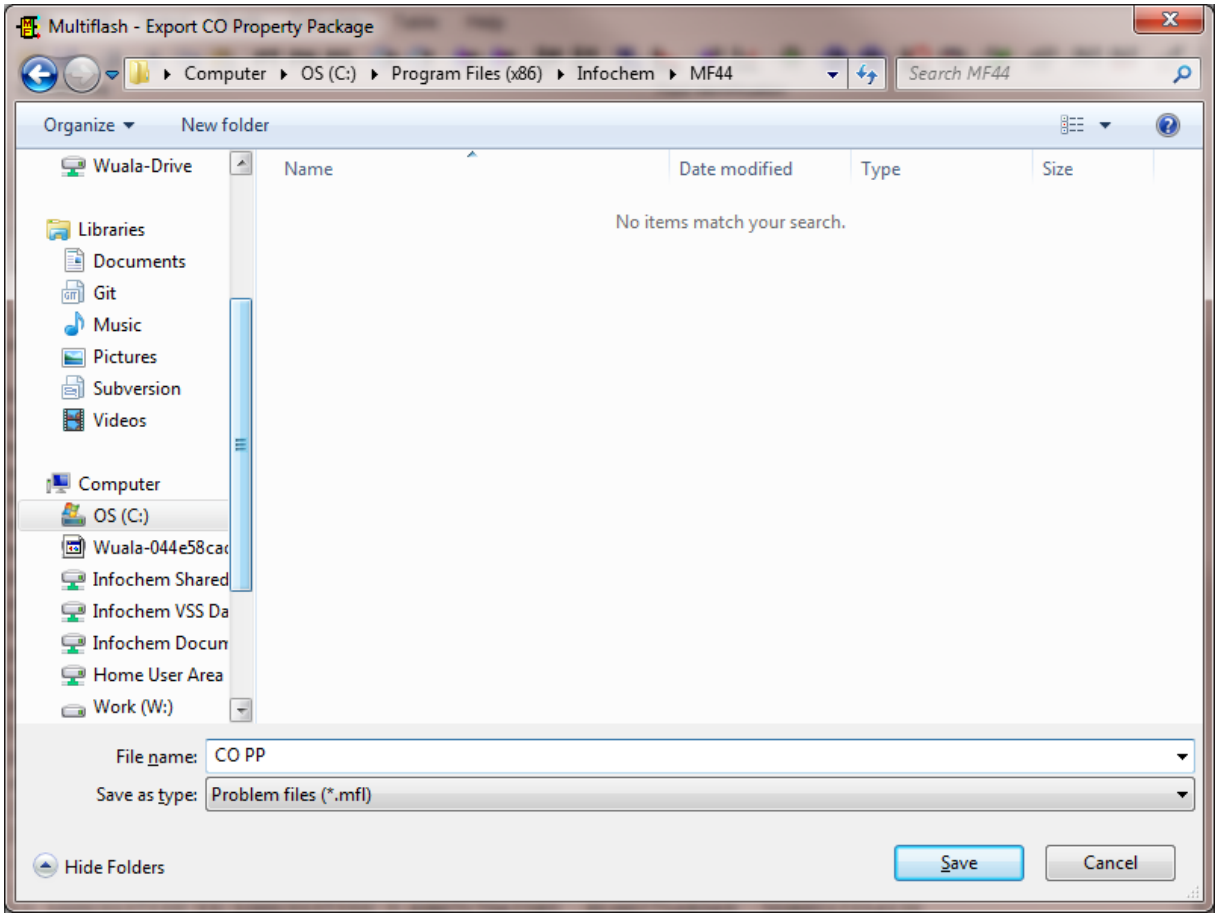
To save the CO PP use the ‘File/Export CO Property Package’ menu item



This displays the PP description which may be amended before saving the PP.

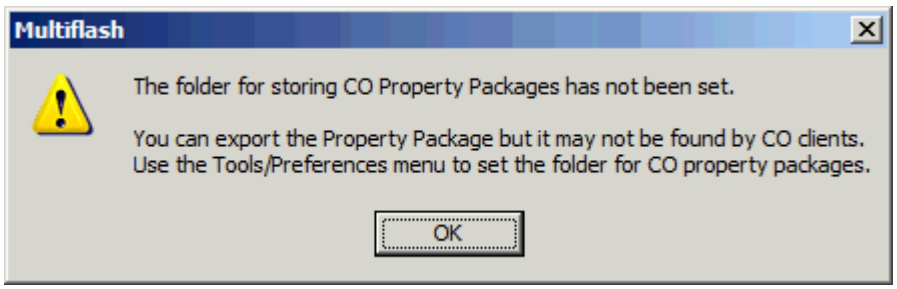


The File Save dialog allows the PP file to be given a name and saved:



A Multiflash CO PP is simply a text file that describes the compounds, models etc. using the Multiflash command language. This is the same format as is used to record the Multiflash problem setup when using the Multiflash GUI or Multiflash Excel interface. The files can therefore be loaded into the GUI (using the File/Load problem Setup menu item) and changed as necessary. Although users should not normally need to understand the Multiflash command language it is described in the *Multiflash Command Reference* manual.

If the folder for CO PPs is not set the Multiflash GUI will display a warning message:



As this message explains the PP may be saved but the PPM/TS may not be able to find it. It is strongly recommended that the folder is set (as described on p.5) so that the GUI and PPM can interact as intended.

Supported CAPE-OPEN Features

The calculations, properties and phases supported by a Multiflash Property Package depend on the configuration chosen and also on the information stored for compounds in the selected databanks. The following lists assume that a complete set of models has been selected and that there is no missing information for pure compounds. The identifiers listed below are defined in the CO specification documents.

Pure Compound Constant Properties: String-Valued

casRegistryNumber
iupacName
chemicalFormula

Pure Compound Constant Properties: Real-Valued

acentricFactor
associationParameter
charge
criticalCompressibilityFactor
criticalDensity
criticalPressure
criticalTemperature
criticalVolume
dipoleMoment
gyrationRadius
heatOfFusionAtNormalFreezingPoint
idealGasEnthalpyOfFormationAt25C
idealGasGibbsFreeEnergyOfFormationAt25C
liquidDensityAt25C
liquidVolumeAt25C
molecularWeight
normalBoilingPoint
normalFreezingPoint
parachor
refractiveIndex
solubilityParameter
specificGravity
standardEntropyGas
standardFormationEnthalpyGas
triplePointPressure
triplePointTemperature
vanderwaalsArea
vanderwaalsVolume

Pure Compound Temperature-Dependent properties

property id version 1.1	property id. version 1.0	derivatives
heatCapacityOfLiquid		
heatCapacityOfSolid		
heatOfVaporization	heatOfVaporization	dT
idealGasEnthalpy	idealGasEnthalpy	
IdealGasEntropy		
IdealGasHeatCapacity	IdealGasHeatCapacity	
surfaceTensionSatLiquid		
thermalConductivityOfLiquid		
thermalConductivityOfVapor		
vaporPressure	vaporPressure	dT
virialCoefficient	virialCoefficient	
viscosityOfLiquid		
viscosityOfVapor		
volumeOfLiquid		dT

Pure Compound Pressure-Dependent properties

None is supported.

Non-constant Single-phase Mixture properties

property id version 1.1	property id. version 1.0	derivatives
compressibilityFactor	compressibilityFactor	
density	density	
enthalpy	enthalpy	dT, dP, dn
enthalpyF	enthalpyF	dT, dP, dn
enthalpyNF	enthalpyNF	dT, dP, dn
entropy	entropy	dT, dP, dn
entropyF	entropyF	dT, dP, dn
entropyNF	entropyNF	dT, dP, dn
fugacityCoefficient	fugacityCoefficient	dT, dP, dn
gibbsEnergy	gibbsFreeEnergy	
heatCapacityCp	heatCapacity	
heatCapacityCv	heatCapacityCv	
InternalEnergy	energy	dT, dP, dn
logFugacityCoefficient	logFugacityCoefficient	dT, dP, dn
molecularWeight	molecularWeight	
speedOfSound	speedOfSound	
thermalConductivity	thermalConductivity	dT, dP, dn
viscosity	viscosity	dT, dP, dn
volume	volume	dT, dP, dn

Non-constant Two-phase Mixture properties

property id version 1.1	property id. version 1.0	derivatives
kvalue	kvalues	dT, dP, dn
logKvalue	logKvalues	dT, dP, dn
surfaceTension	surfaceTension	

Derivatives

In the above tables supported derivatives are denoted by the following codes.

code	CO derivative id
dT	.Dtemperature
dP	.Dpressure
dn	.Dmoles

The identifier for the derivative is made up of the property identifier and the derivative identifier. For example, the temperature derivative of the enthalpy is denoted by ‘enthalpy.Dtemperature’.

Phases

Multiflash can support any number and any types of phases. The phase labels for the 1.1 PP are defined by the Multiflash phase descriptor names.

The CO 1.0 specification allows a single vapour phase identifier (Vapor) and the special phase identifiers Overall and VaporLiquid. Multiple liquid and solid phase identifiers can be specified in the format LiquidX or SolidX where X can be any string. A typical set of phase identifiers would be:

Overall
Vapor
Liquid
Liquid2
Solid
VaporLiquid

Flash Types

Version 1.1 PP

The following pairs of property identifiers are supported to specify a phase equilibrium calculation in CalcEquilibrium method. The order in which the properties are specified is not significant.

property 1	property 2
pressure	temperature
pressure	enthalpy
pressure	enthalpyF
pressure	enthalpyNF
pressure	entropy
pressure	entropyF
pressure	entropyNF
pressure	volume
pressure	internalEnergy
pressure	phaseFraction
temperature	enthalpy
temperature	enthalpyF
temperature	enthalpyNF
temperature	entropy
temperature	entropyF
temperature	entropyNF
temperature	volume
temperature	internalEnergy
temperature	phaseFraction
internal energy	volume
entropy	volume
entropyF	volume
entropyNF	volume
enthalpy	entropy
enthalpyF	entropyF
enthalpyNF	entropyNF

Version 1.0 PP

The supported CO 1.0 flash types are:

flash type identifier	fixed quantities
TP	temperature and pressure
PH	pressure and enthalpy
TH	temperature and enthalpy
TVF	temperature and vapour fraction
PVF	pressure and vapour fraction
PT	temperature and pressure (synonym for TP)
PS	pressure and entropy
TS	temperature and entropy
HS	enthalpy and entropy
UV	internal energy and volume
SV	entropy and volume
PV	pressure and volume
TV	temperature and volume
PSF	pressure and entropyF
PSNF	pressure and entropyNF
PHF	pressure and enthalpyF
PHNF	pressure and enthalpyNF
THF	temperature and enthalpyF
THNF	temperature and enthalpyNF
TSF	temperature and entropyF
TSNF	temperature and entropyNF
HFSF	enthalpyF and entropyF
HNFSNF	enthalpyNF and entropyNF
SFV	entropyF and volume
SNFV	entropyNF and volume

Limitations

There is a practical limit on the number of Multiflash PPs that can be created by a single application as components, phases and model storage are limited. Each new property package will add those items to the Multiflash DLL global storage.

Using a Multiflash CO Property Package

A Multiflash Property Package should be useable in any application that implements the CO Version 1.1 Property Package Manager and Property Package sockets or the CO Version 1.0 Thermo System and Property Package sockets. Each application will typically have its own way of handling the selection of CO Property packages. Below we describe how to use a CO Property Package in KBC's PetroSIM5, Aspen Hysys, Aspen Plus, COFE, gPROMS, PRO/II and Simulis Thermodynamics.

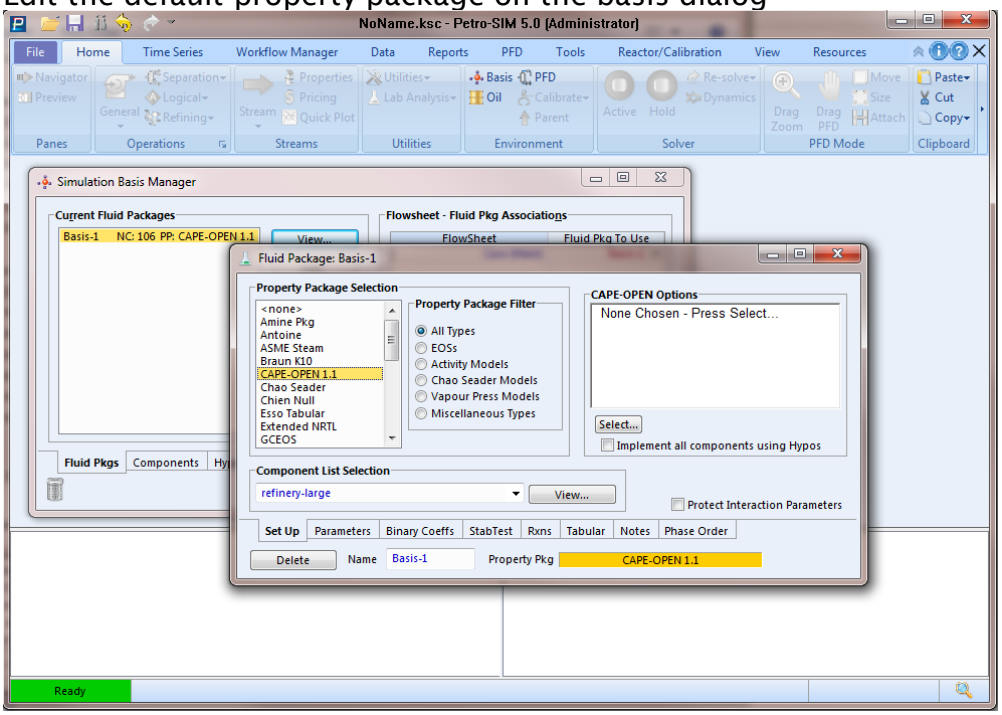
The Multiflash CO components have also been used with Predici (www.cit-wulkow.de), COMSOL (www.comsol.com) and DWSIM http://dwsim.inforside.com.br). Other applications should have equivalent facilities. The application supplier should provide full information on how to use a CO Property Package.

PetroSIM 5

The following procedure applies to PetroSIM 5 (http://www.kbcat.com/technology/process-simulation-software), KBC's process simulator. Only Sockets for version 1.1 are supported.

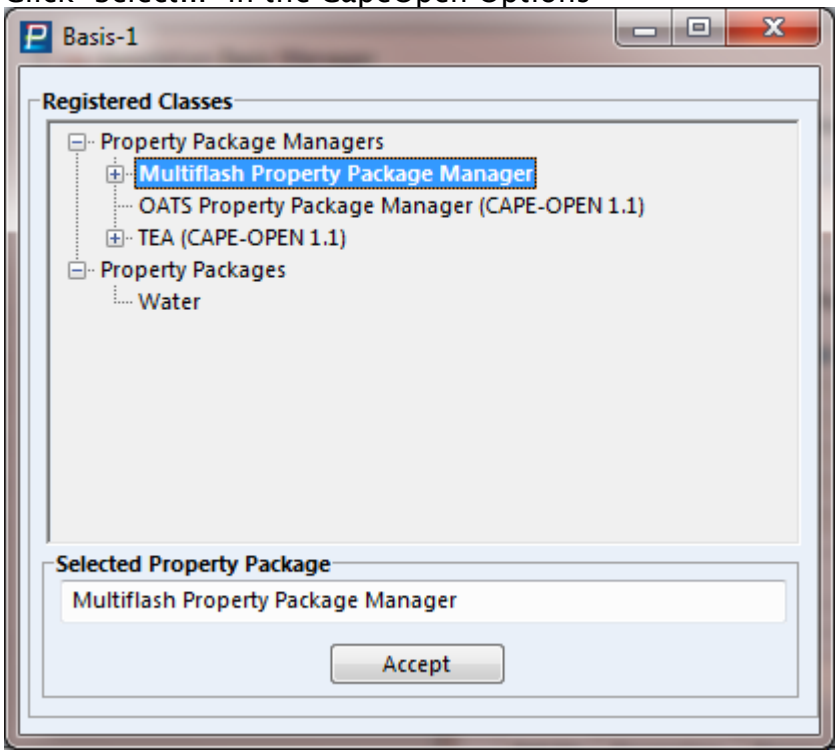
Using Multiflash on a new case

1. Create a new case
   It is not important if it is a refinery case or a production case.
2. Edit the default property package on the basis dialog



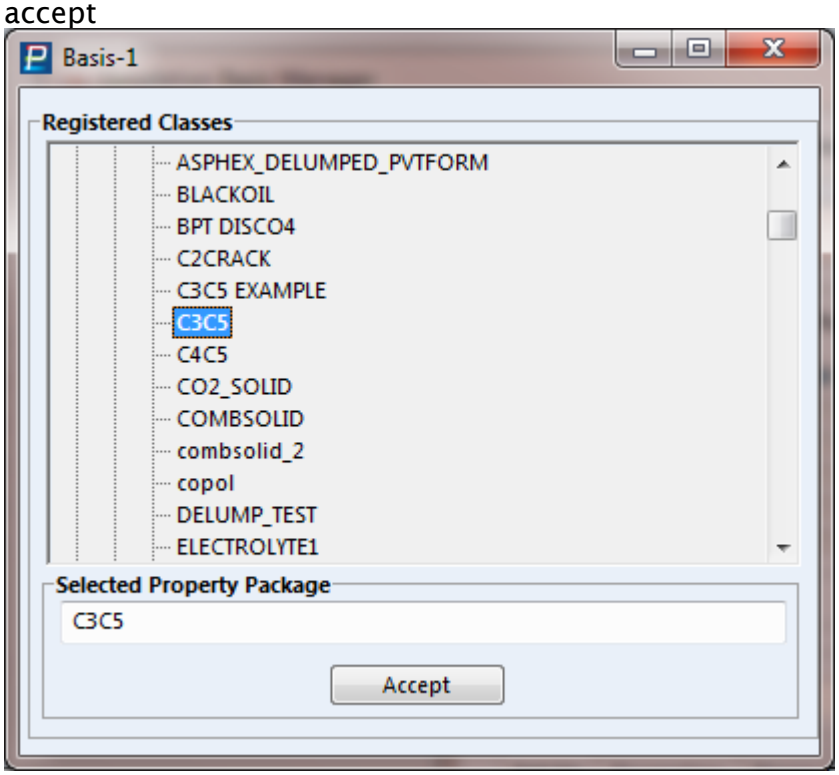
and select Cape-OPEN 1.1.

3. Click "Select..." in the CapeOpen Options



Multiflash should appear in the list of registered classes of property package providers.

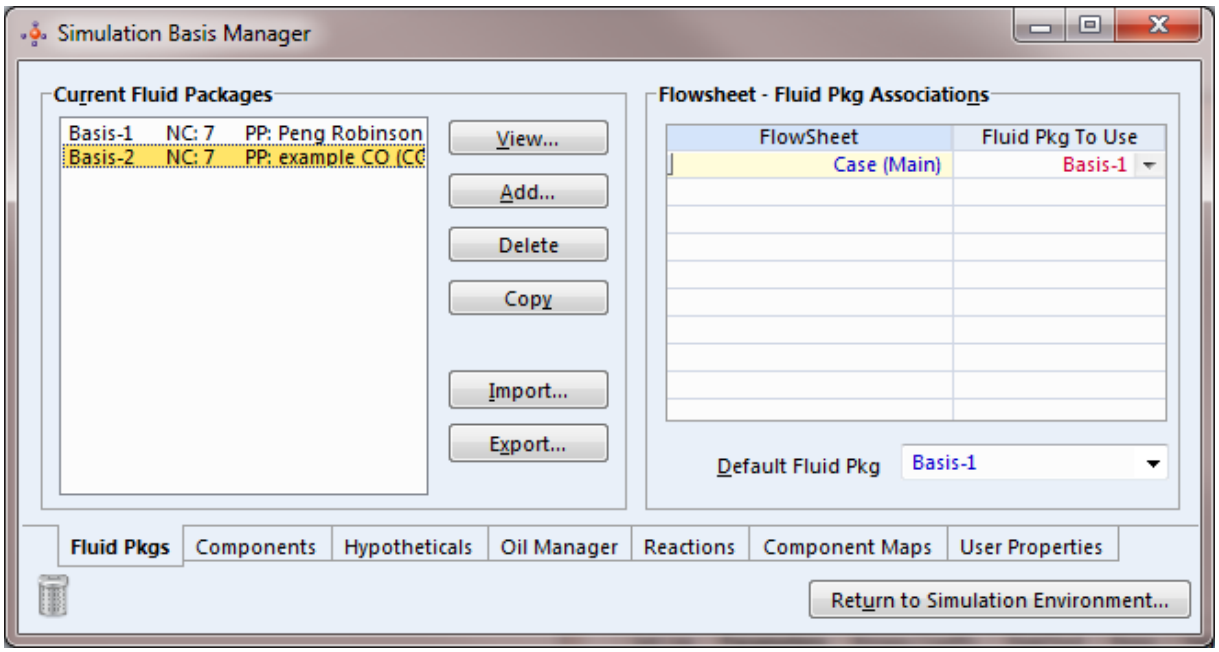
4. Select the desired Multiflash property package created previoulsy and click accept



5. The property package is ready to use

Change an existing property package into a CapeOpen one

1. Create an MFL file with the same component order of the current PP.
2. Add a new fluid package in the basis where the CO PP will be setup.

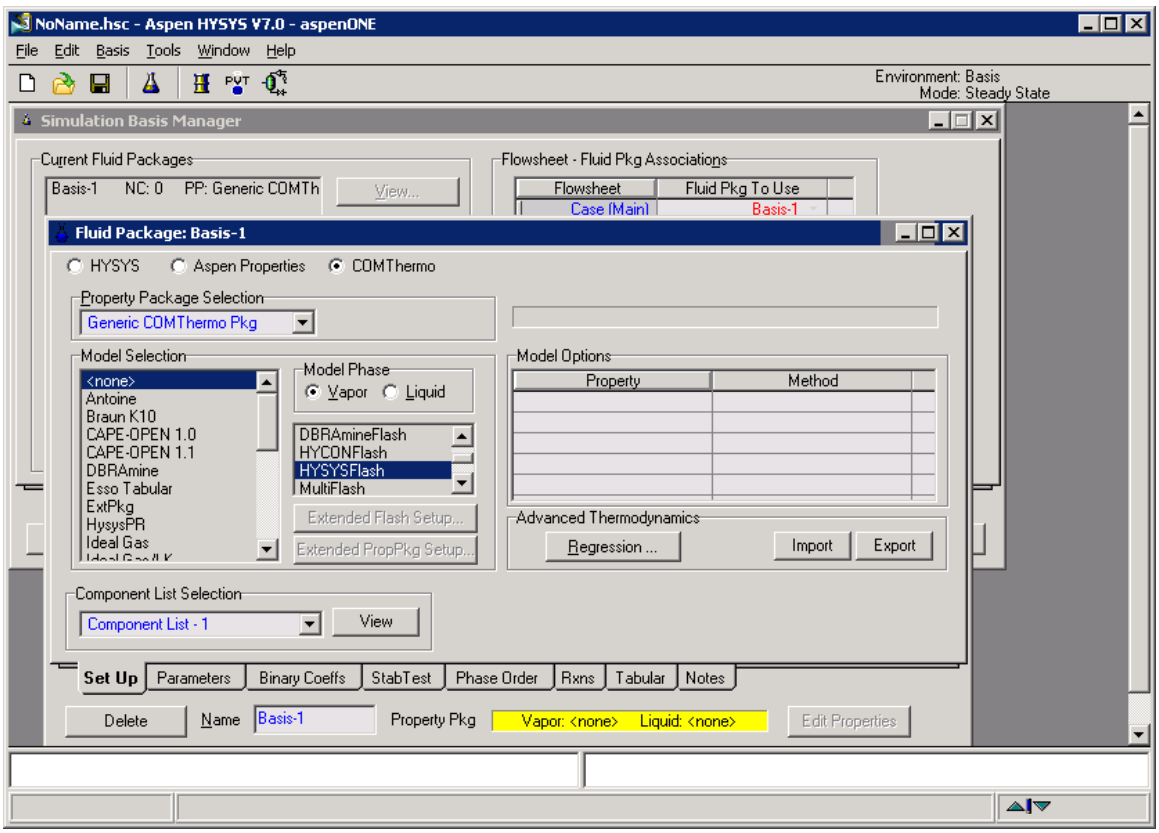


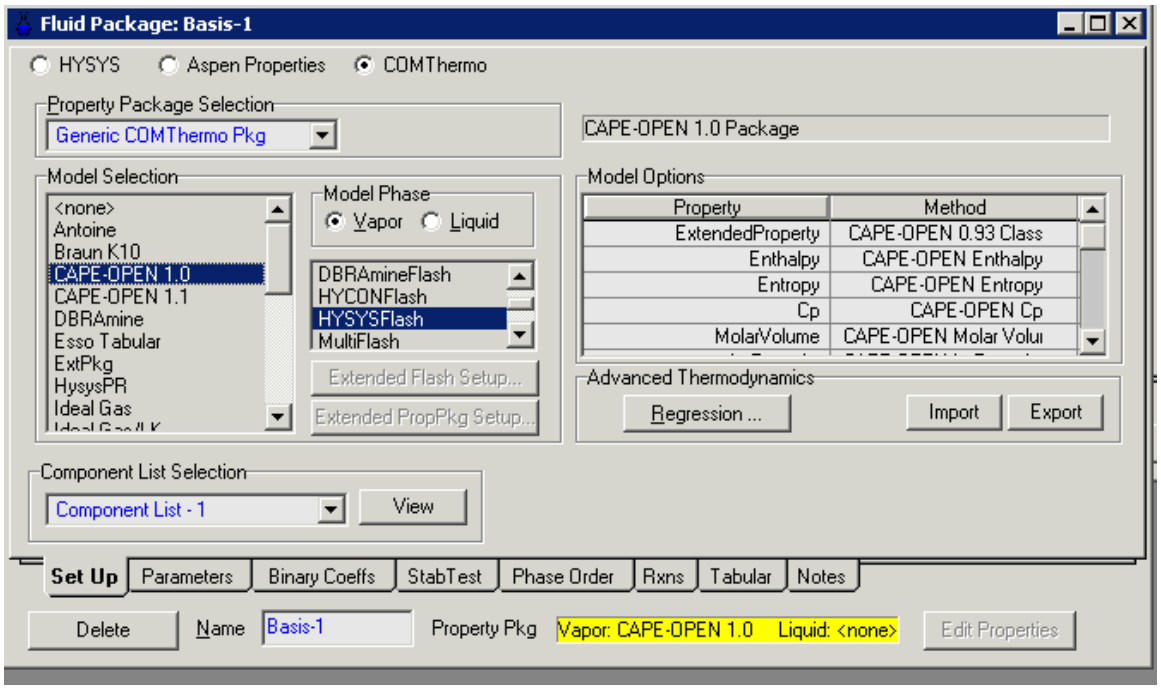
6.
7. delete the old property package
   Accept the warning that exiting unit operations will be using the new fluid package.
3. Return to the simulation environment. If the solver is active, the case should converge.

Aspen Hysys

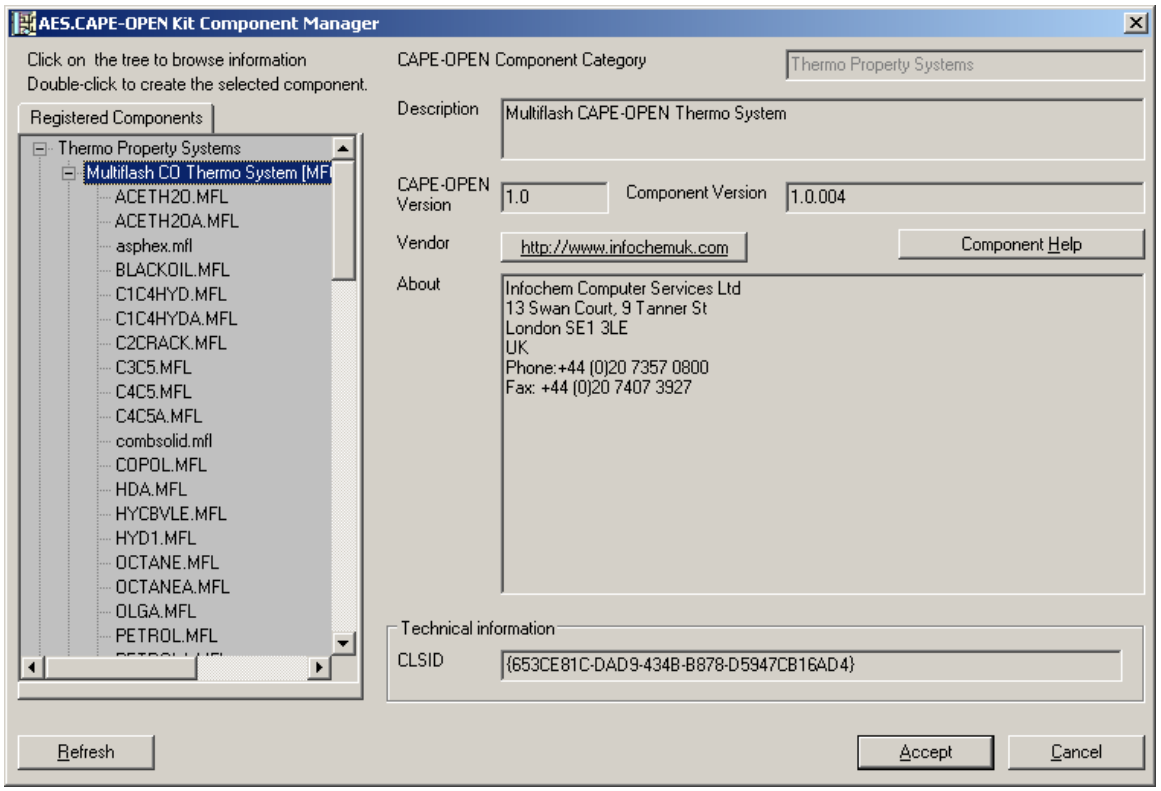
The following description applies to the AspenTech (www.aspentech.com) Aspen Hysys V.7.1 process simulator. The CO 1.0 and 1.1 sockets are supported.

Creating a new simulation case in Hysys will display the Basis Environment that allows either a standard Hysys package or a CO Property package to be selected. Select the 'Fluid Pkgs' tab and click on 'Add'. Select COMThermo Pkg from the Property Package Selection list and click on COMThermo Setup in the Advanced Thermodynamics frame





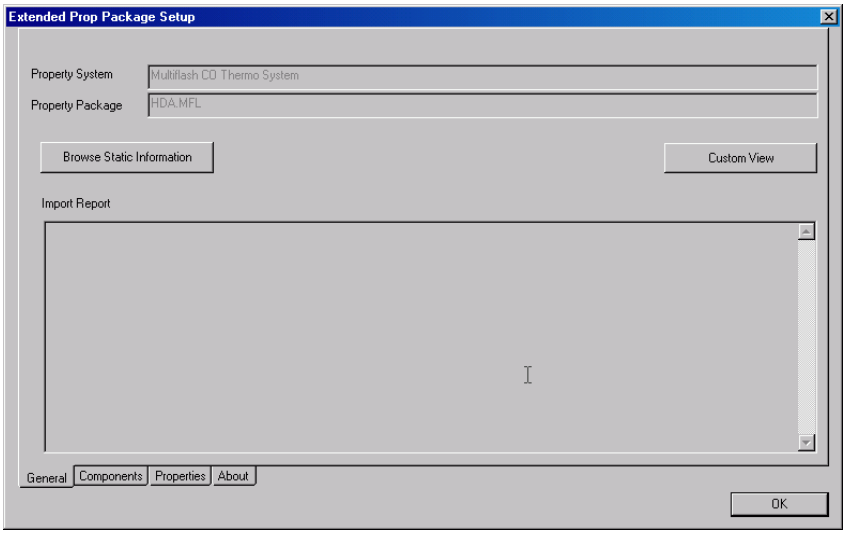
Select CAPE-OPEN 1.0 in the Model Selection list and then in the Model Phase frame click the Liquid button and again select CAPE-OPEN 1.0. A list of CO Thermo Systems and stand-alone Property Packages is now displayed.



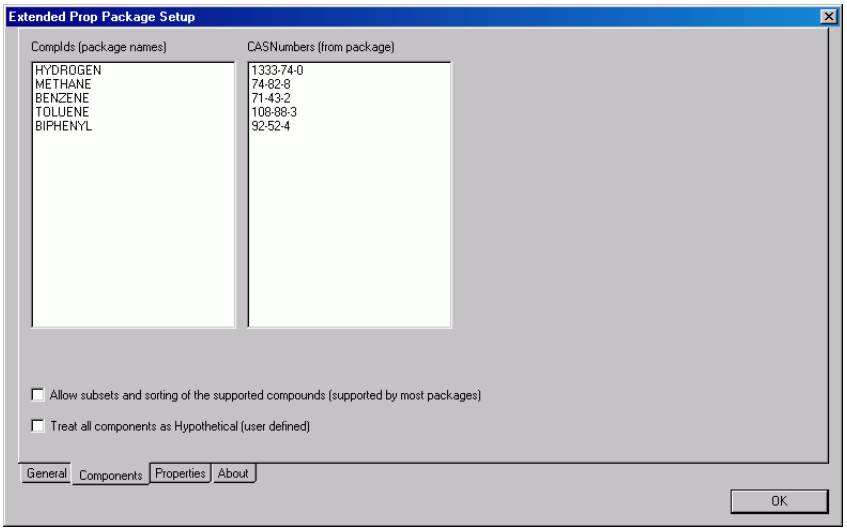
The Multiflash Thermo System provides a list of available Property Packages. To select a package such as HDA highlight the name and click Accept.

It is necessary to click the Extended PropPkg Setup button and then Finish Setup which shows some information about the package.

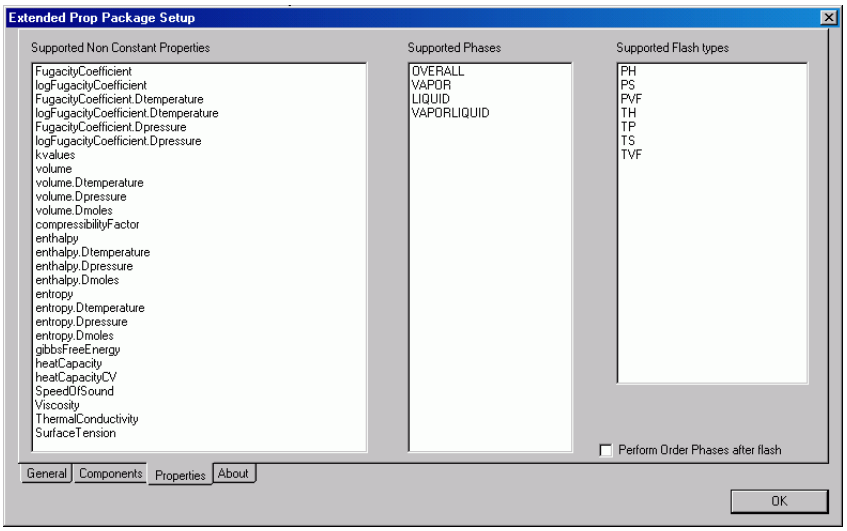
The General tab just shows the package name



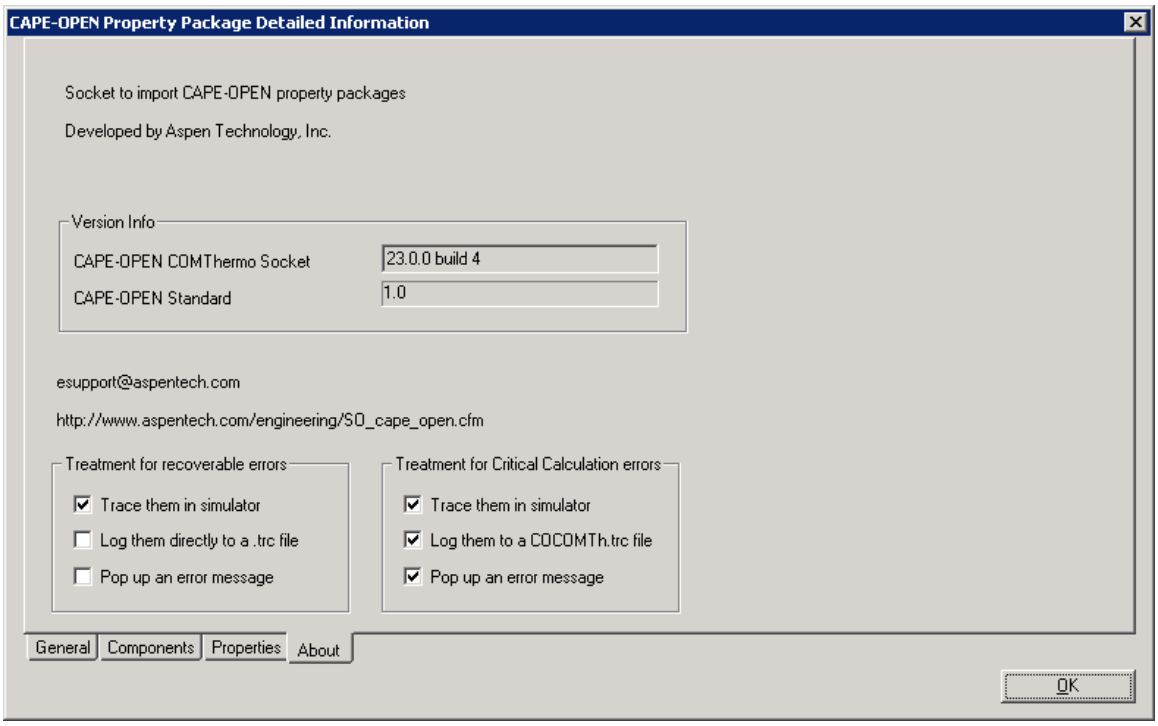
The Components tab shows the compounds in the package:



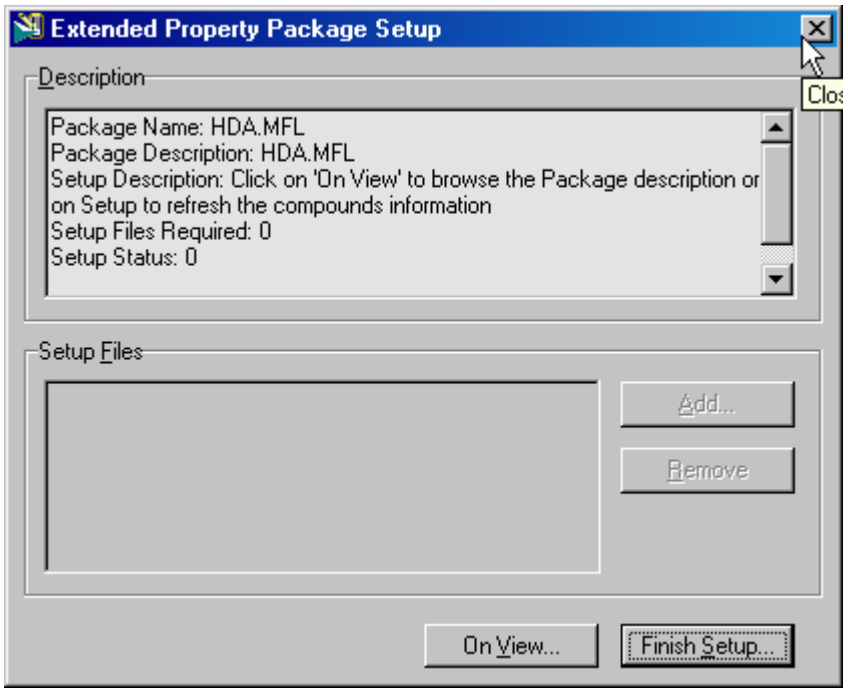
The Properties tab lists the properties that the package can calculate, the phases supported and the flash types available



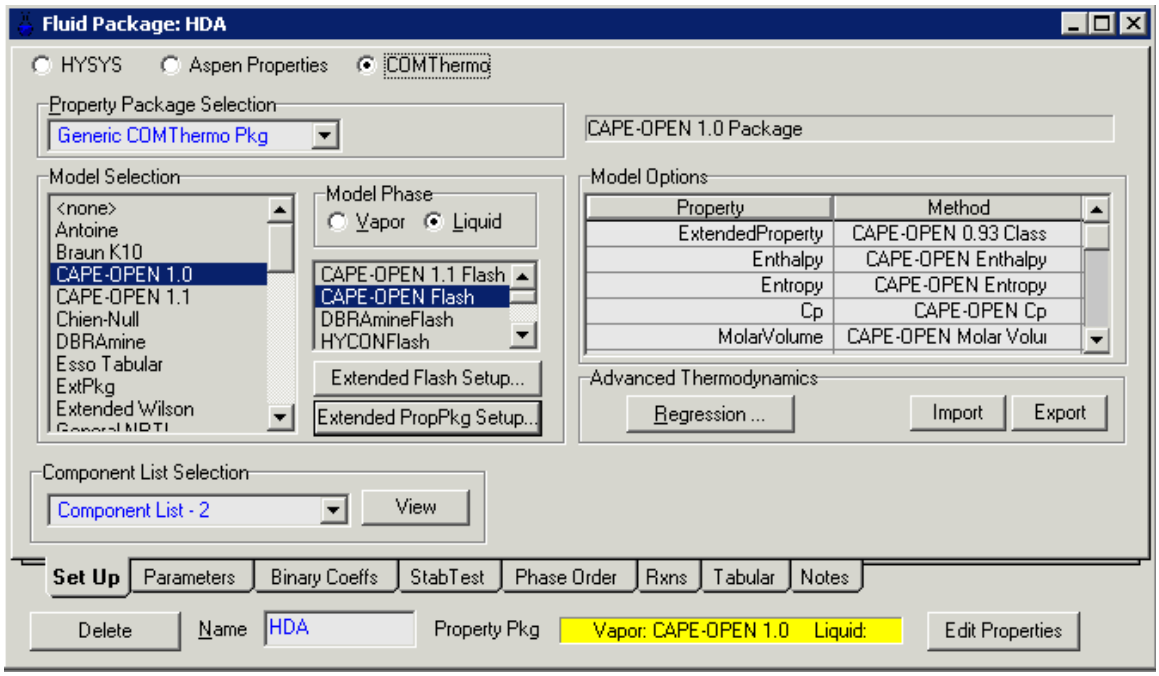
The About tab gives information about the CO socket and allows the user to choose how errors are handled.



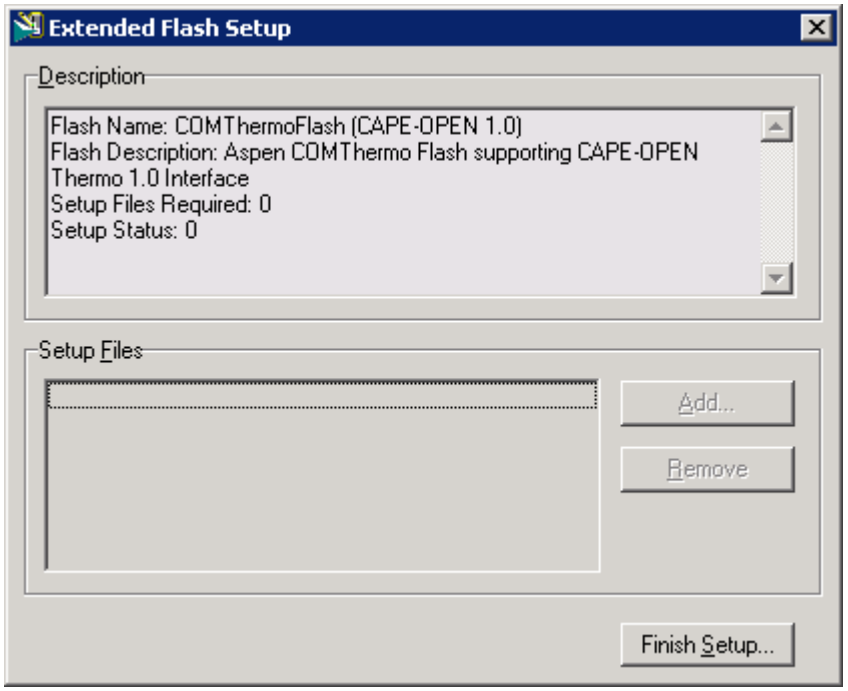
Finally, clicking OK and then the Close button (top RH corner) will return to the Simulation Basis Manager.



A Multiflash CO Property Package can be used with the Hysys flash or with the Multiflash phase equilibrium routines via the Cape-Open interface. The Multiflash flash works more efficiently with the Multiflash property package but you should note that it may return more phases (or types of phases) than Hysys or other simulators can deal with. To use the Multiflash flash select the CAPE-OPEN Flash from the dialog



and click on the Extended Flash Setup button and then on Finish Setup

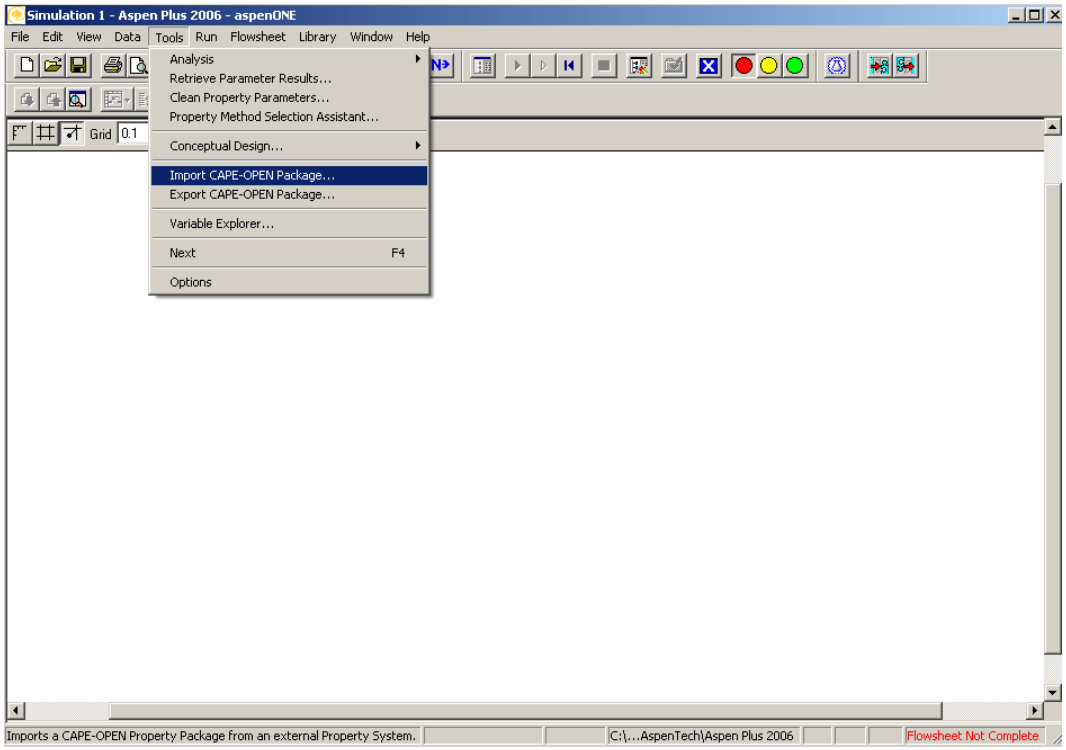


The Basis that contains the CO Property Package can then be associated with the whole flowsheet or a sub-flowsheet in the Hysys simulation.

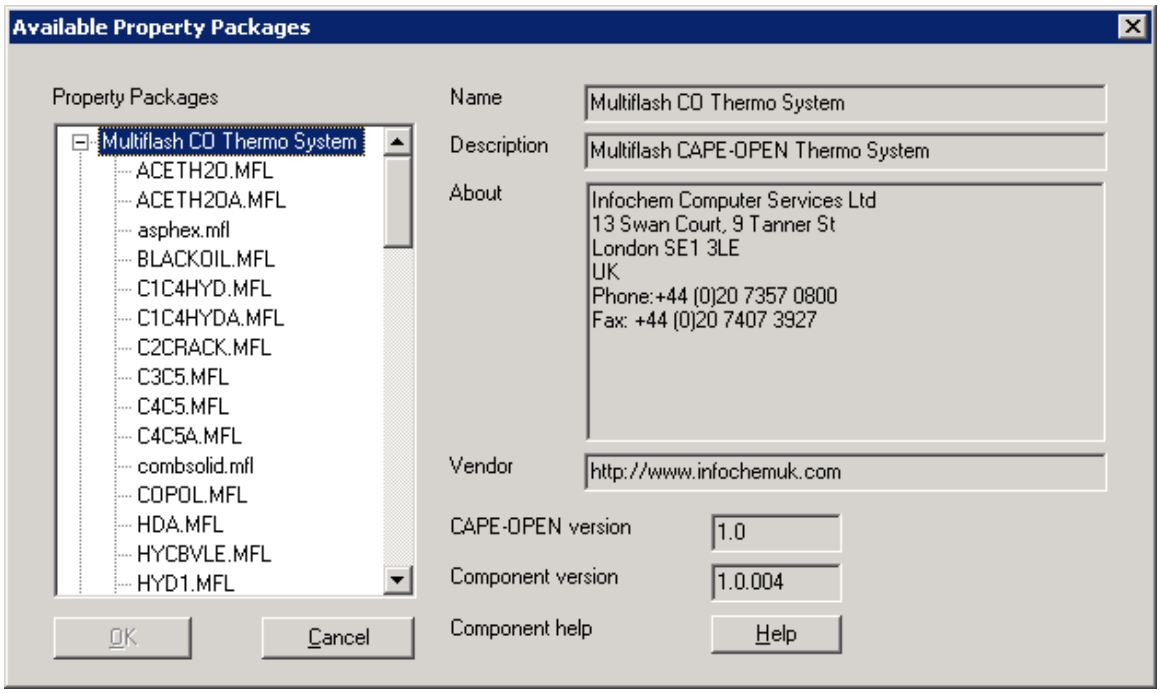
Aspen Plus

The following section shows how a Multiflash Property Package is selected in the AspenTech (www.aspentech.com) Aspen Plus V.7.1 process simulator. The proc. The CO 1.0 sockets are supported.

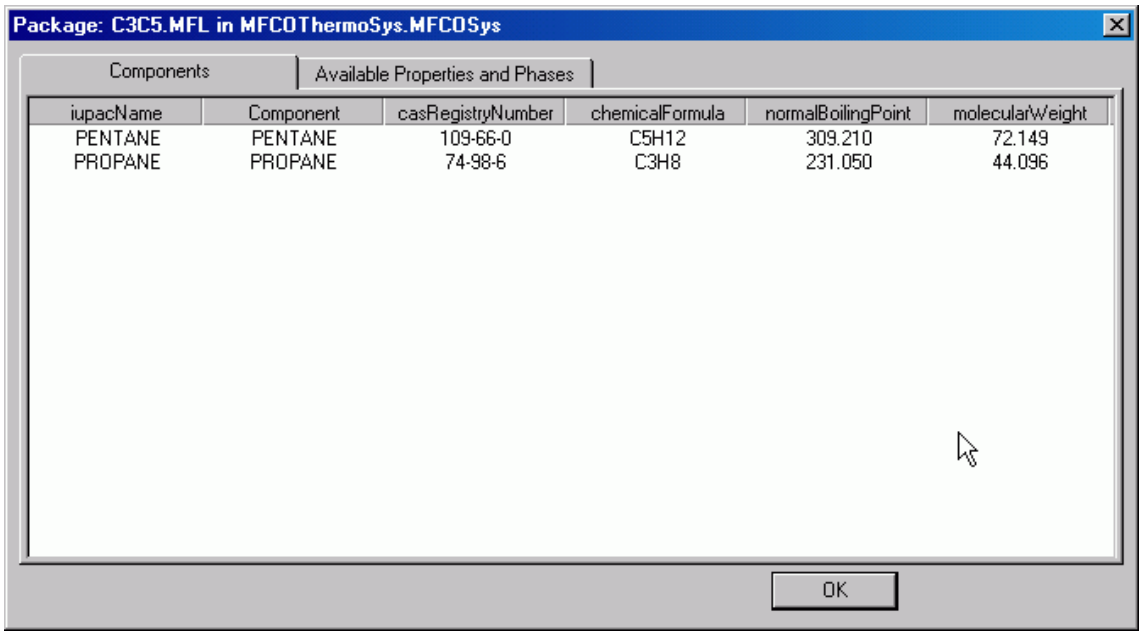
Create a new flowsheet or open an existing simulation. The Tools menu allows you to import a CO Property Package



Click on the [+] symbol by the Multiflash CO Themo System to display the list of available property packages. The package names correspond to the Multiflash .mfl configuration files saved by the Multiflash GUI.

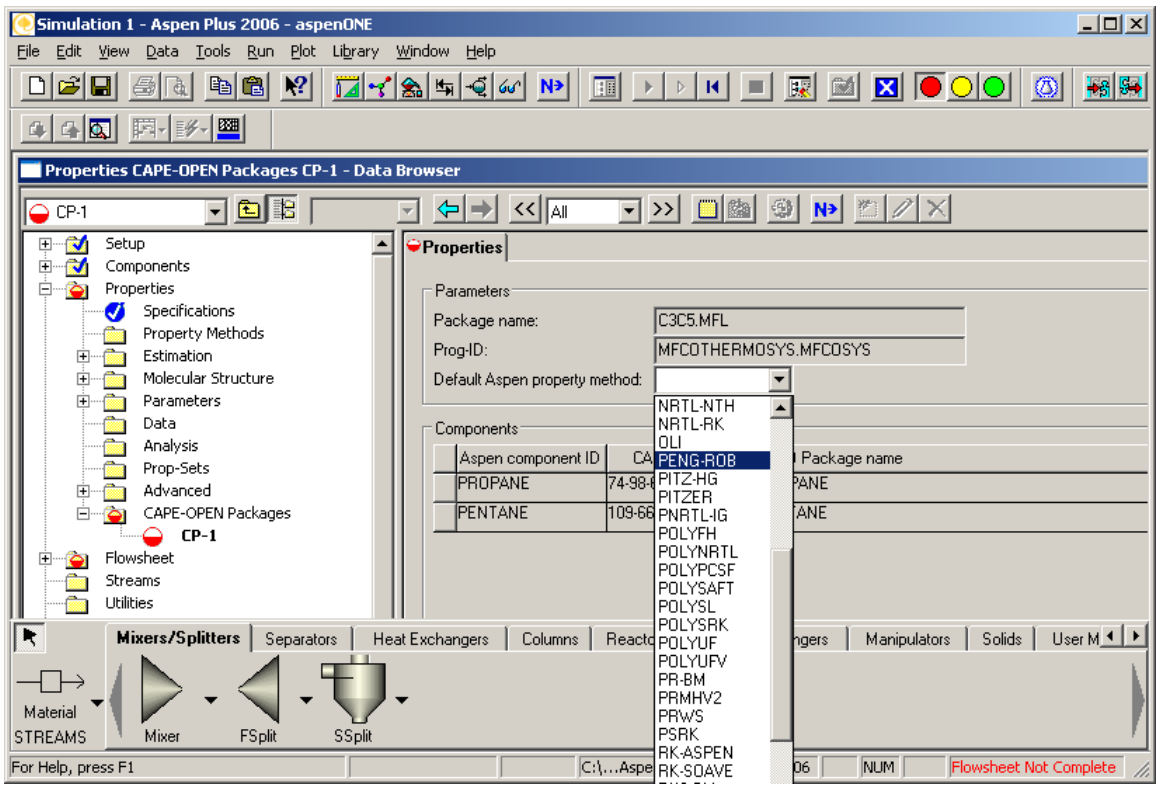


To view the compounds and properties supported by a package click on the name and then on the Package Details button.



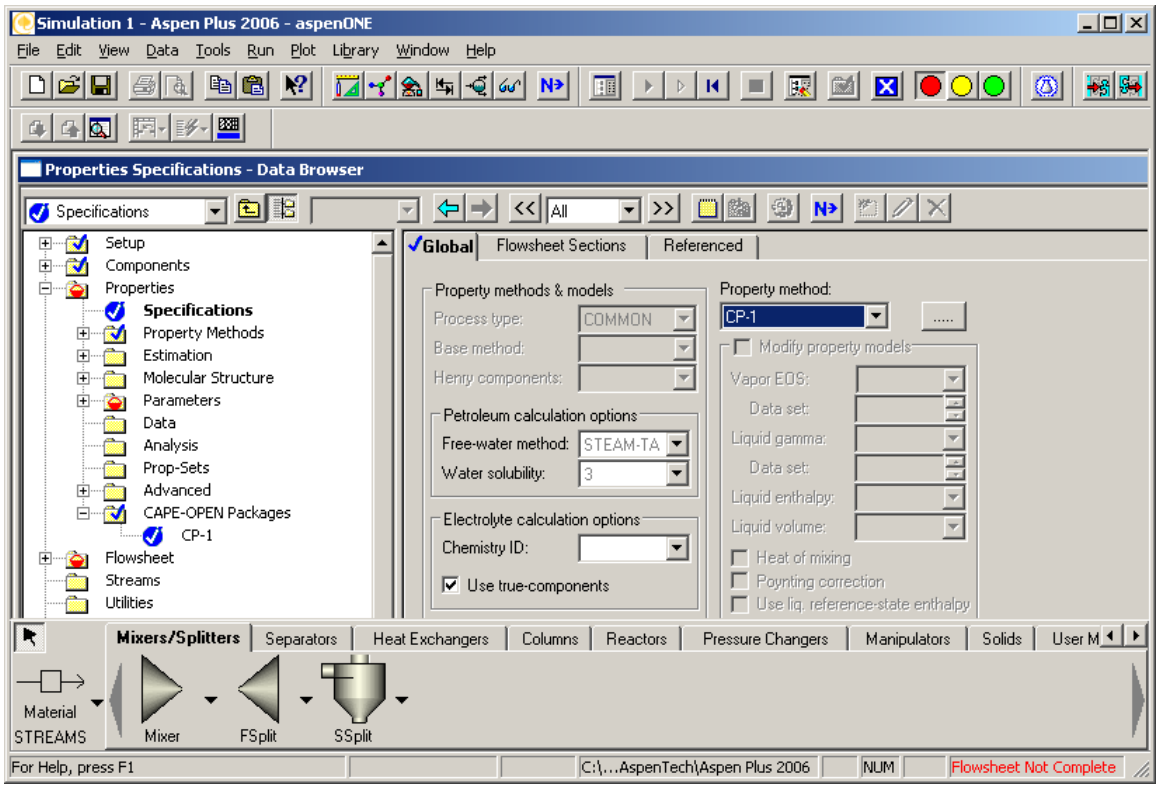
To select a package click on the name and then OK in the Available Property Packages window.

To complete the package setup you must define a default Aspen property method that will be used to calculate any properties not supported by the CO package. This is done using the Data menu and selecting Properties and then the CO package (CP-1 in the next screenshot)



The drop-down list can be used to choose the default package. Depending on your choice you may need to set up additional information such as interaction parameters for the default package.

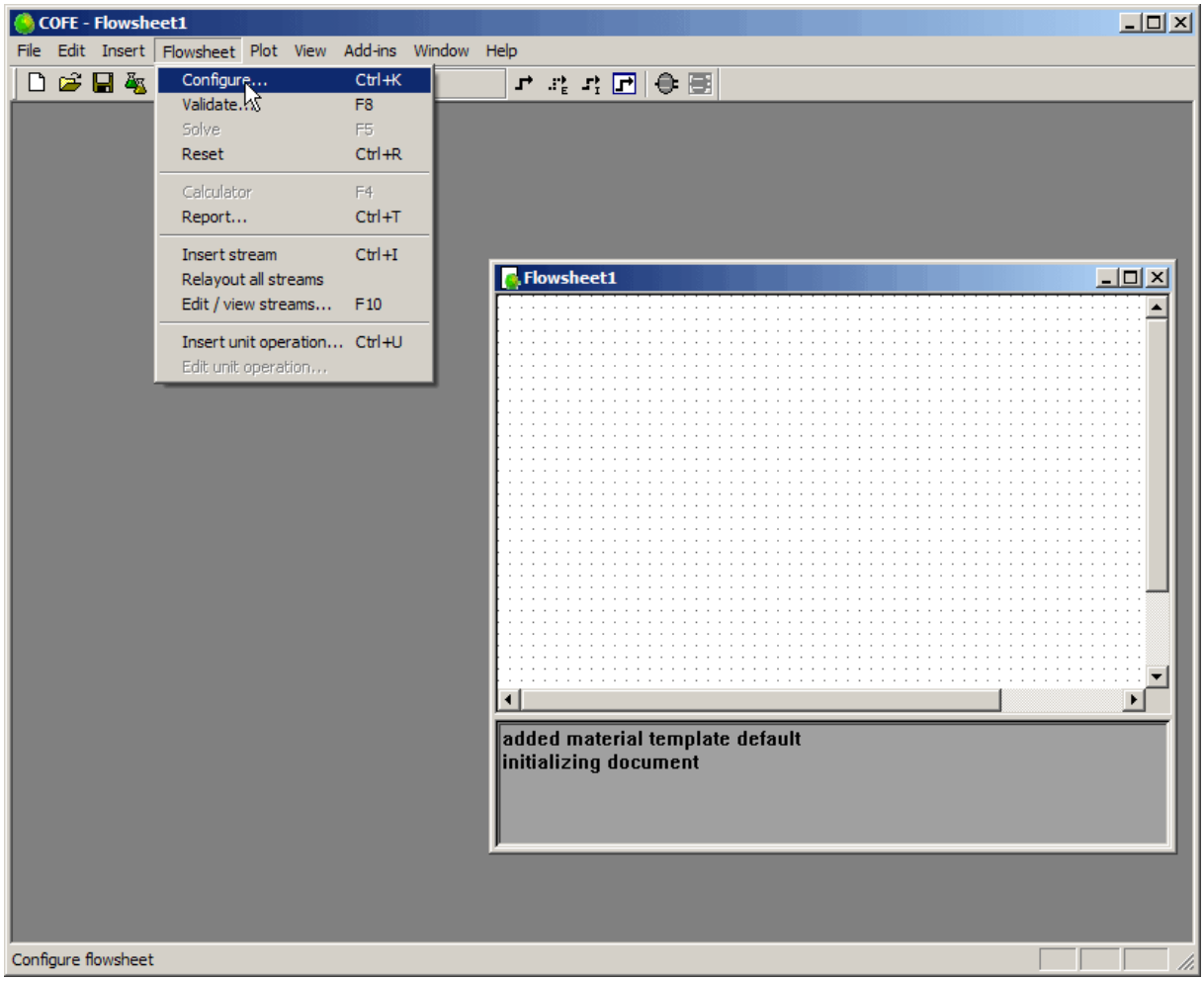
The Specifications item under Properties can then be used to make the CO Property Package the Global property method for the simulation.



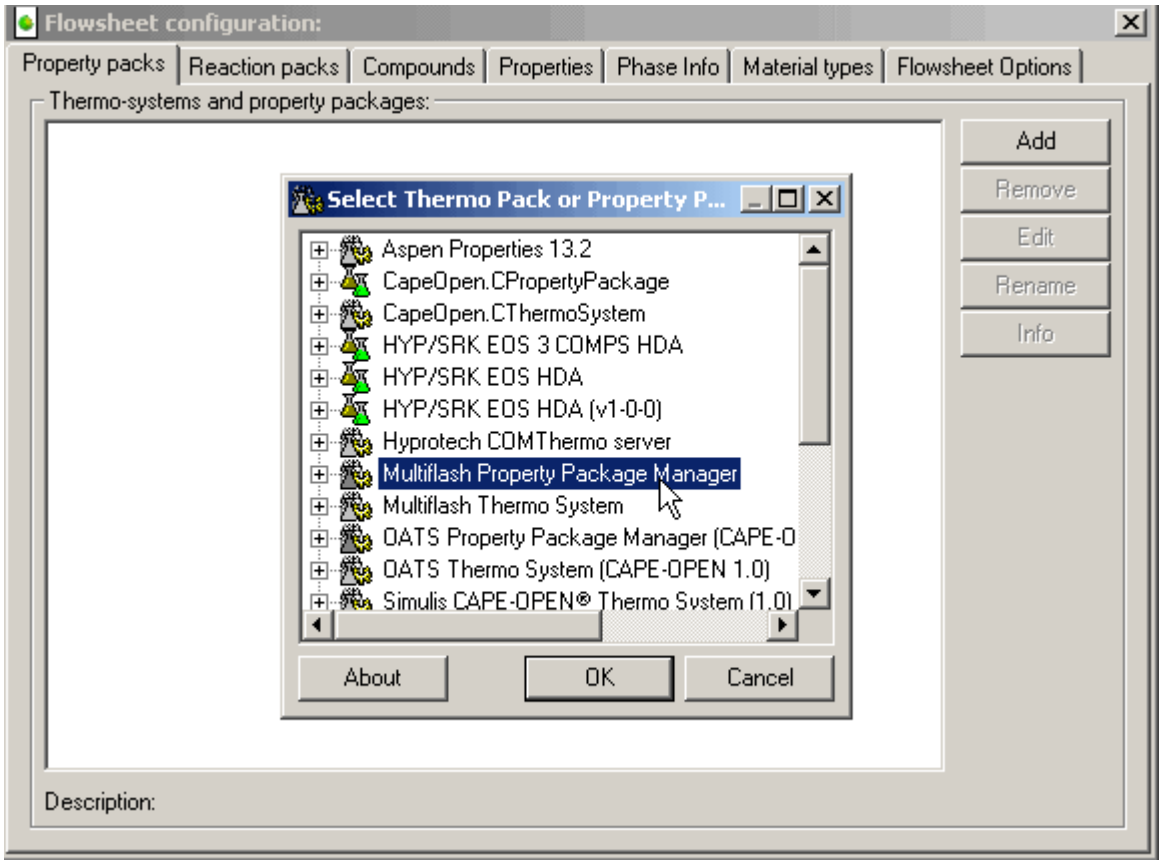
COFE

COFE is the Cape-Open Flowsheeting Environment which is part of the COCO (CAPE-OPEN to CAPE-OPEN) steady-state simulation environment (www.cocosimulator.org). The following screenshots are taken from COFE 1.16 which supports sockets for version 1.1 and 1.0 of the CO components.

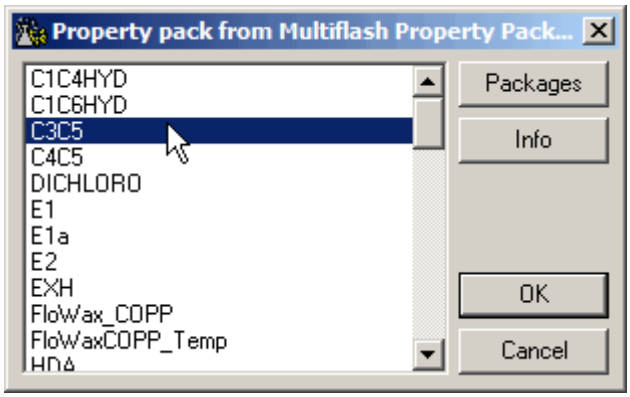
To set up a CO PP click on Configure on the Flowsheet menu



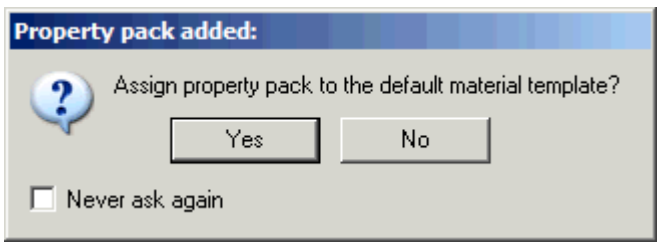
On the Property Packs tab click Add and choose the Multiflash Property Package Manager from the list shown and click OK



A list of available PPs is shown



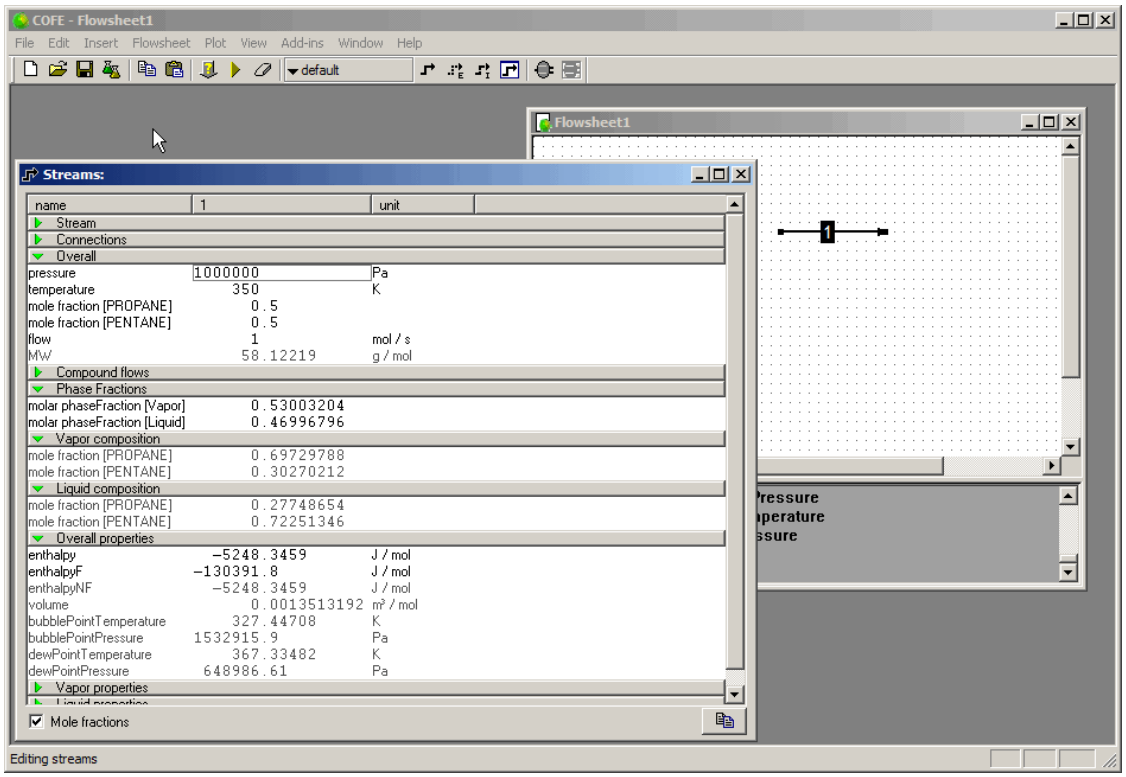
Select the required package and click OK. Click Yes in the following dialog box



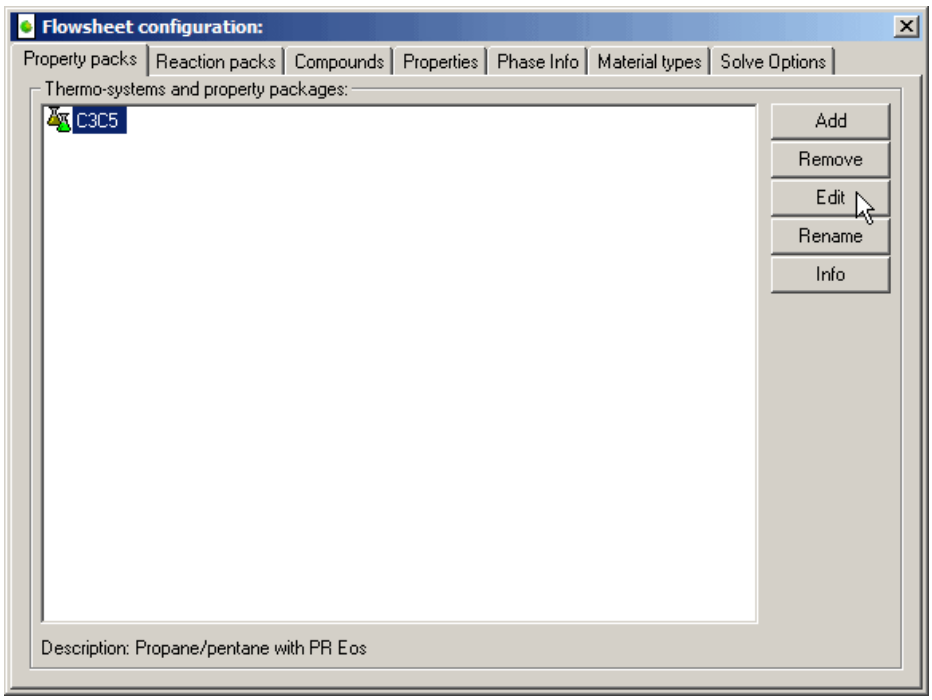
You may then add other PPs, configure other options or exit from the configuration dialog.

The following example uses the C3C5.mfl PP which contains propane and pentane with gas and liquid phases. Enter a stream in the flowsheet and set the

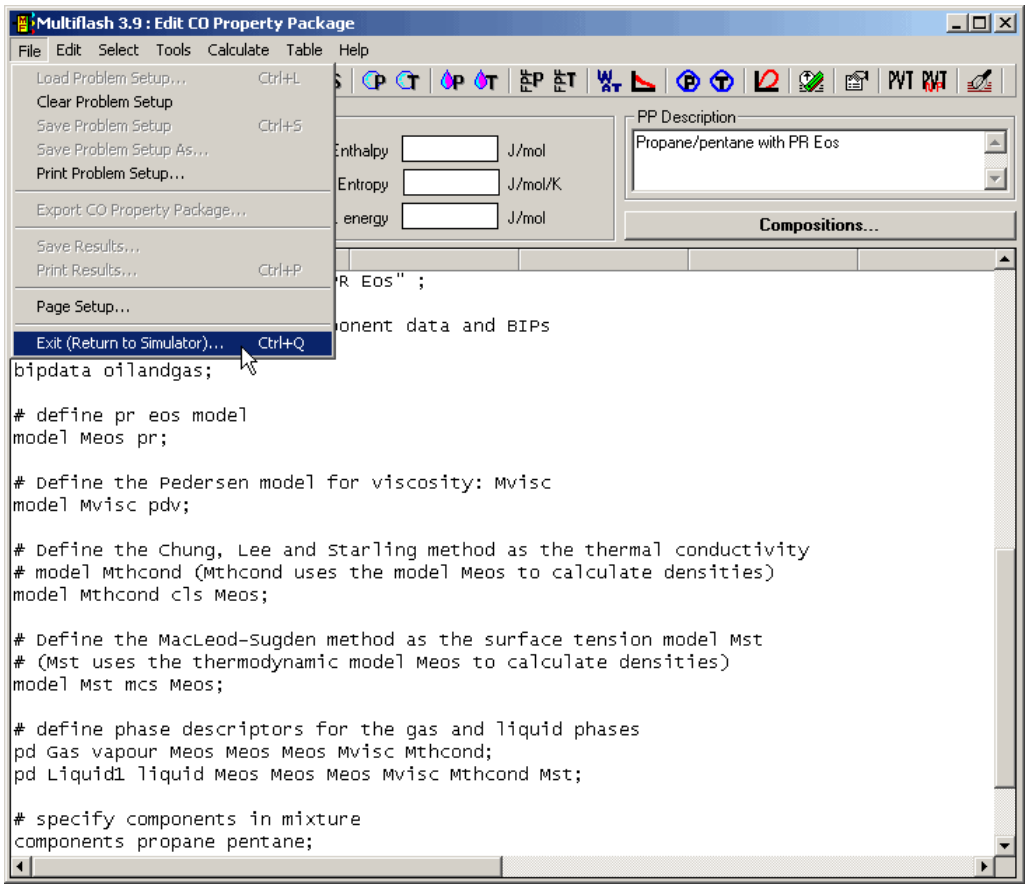
composition, flowrate, temperature and pressure. The calculated properties are displayed.



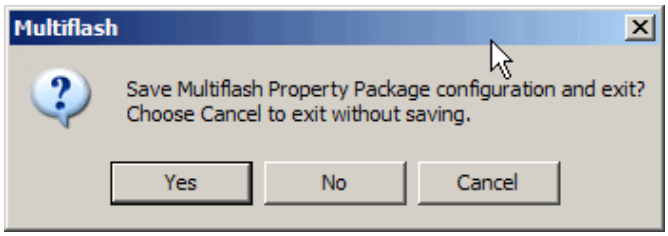
CoCo allows for editing of Property Packages. To edit a Multiflash PP open the Flowsheet Configuration window, select the PP and click Edit.



This will launch the Multiflash GUI. The PP configuration may edited and the updated PP is returned to the using the File/Exit menu option

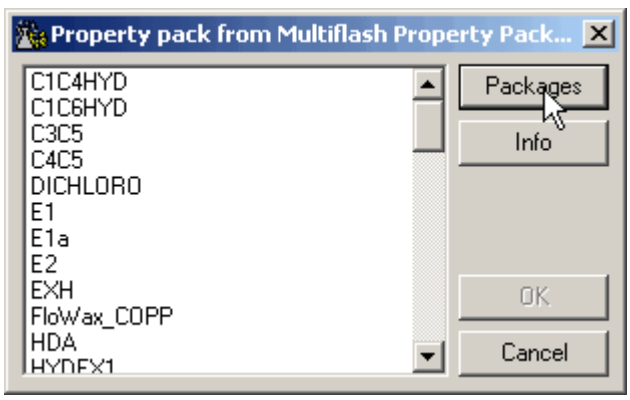


You then have the choice of saving the PP or returning to the PME without saving any changes

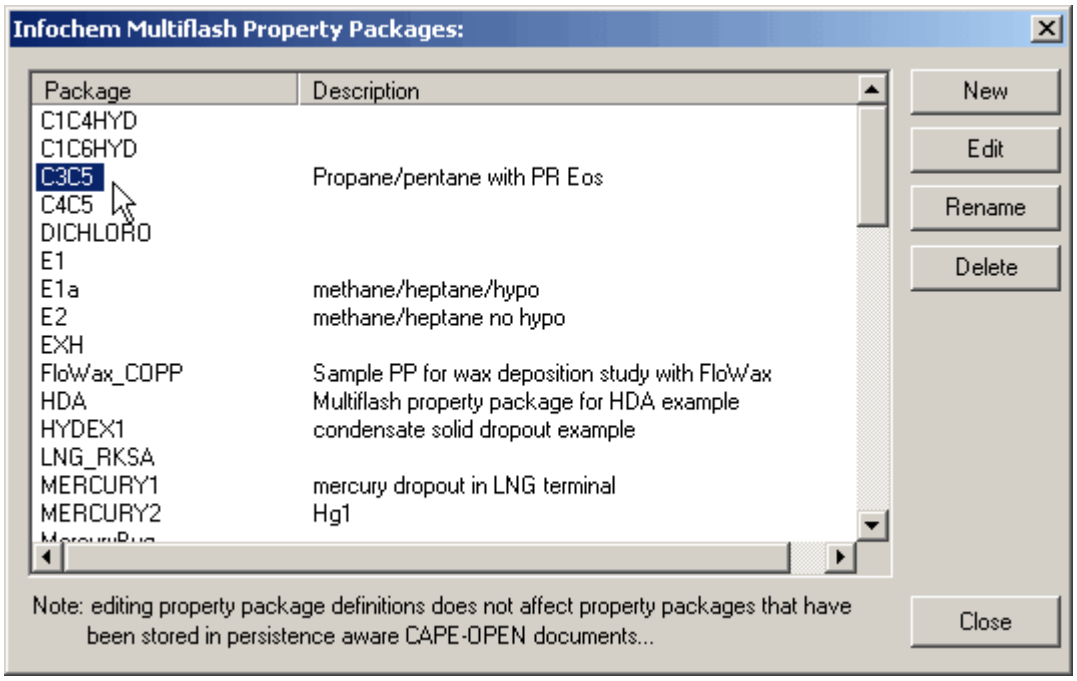


The edit operation only affects the copy of the Multiflash PP saved with the COFE simulation not the file on which it is based.

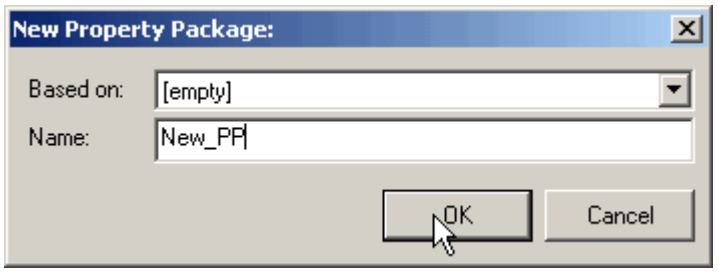
It is also possible to set up a new Multiflash PP from COFE.



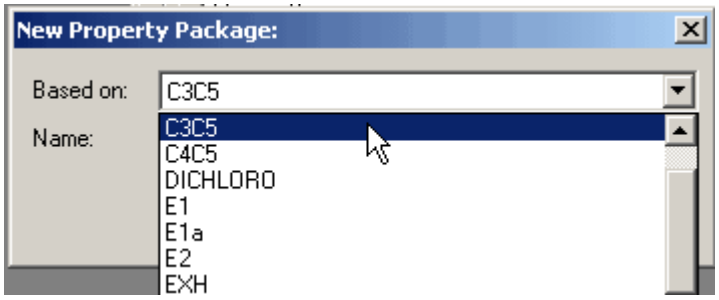
Clicking the ‘Packages’ button in the Property Package Manager window displays a list of existing PPs



Clicking ‘Edit’ will edit the selected PP as above but the edit operation will affect the saved PP. ’New’ will create a new a new PP. Enter a name and click OK to create a new PP from scratch



or select an existing PP on which to base the new one, enter a name and click OK.



gPROMS

gPROMS® is an advanced process modelling environment from Process Systems Enterprise Ltd. (www.psenterprise.com). The following description applies to gPROMS 3.1 which supports the CO 1.0 socket.

When using a flowsheet built from the gPROMS PML (Process Model Library) you setup a CO PP by double-clicking on a "Source" unit and specifying that it should use "COThermoFO" physical properties.

The format of this specification is one of:

COThermoFO::*ThermoSystemProgID*<*PackageName*>

To use a named package from a thermo system with properties and calculations on a molar basis

COThermoFO::*ThermoPackageProgID*

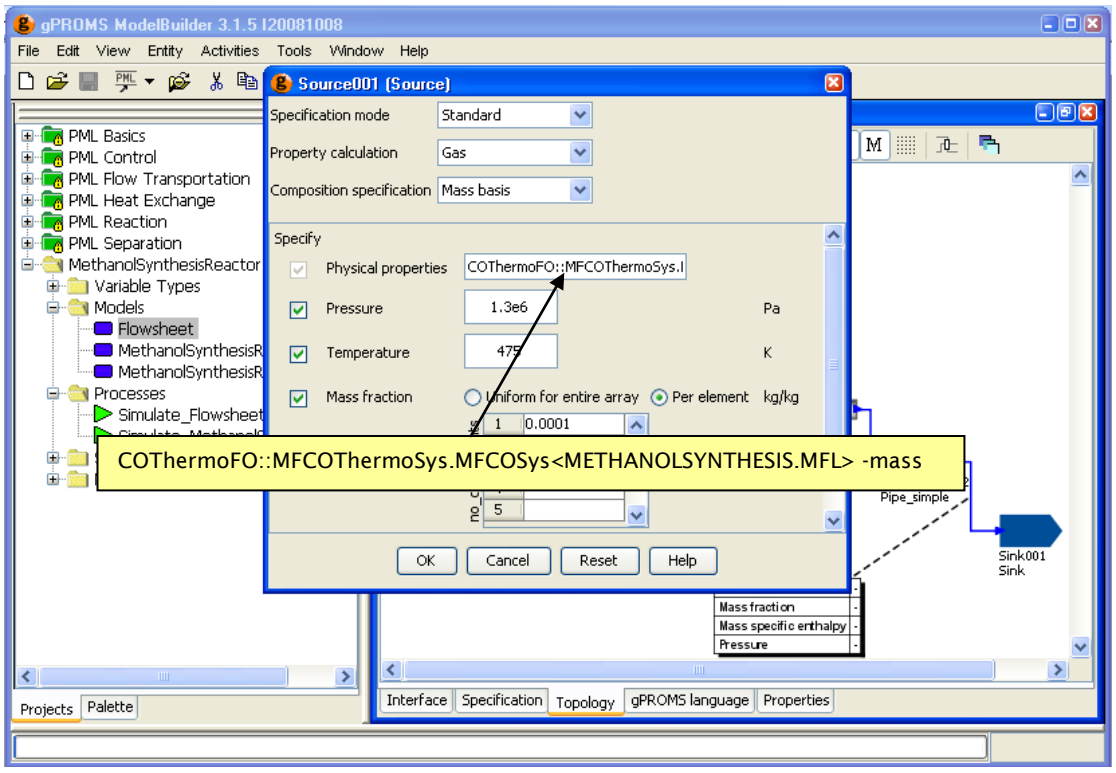
To use a thermo package with properties and calculations on a molar basis

COThermoFO::*ThermoSystemProgID*<*PackageName*> -mass

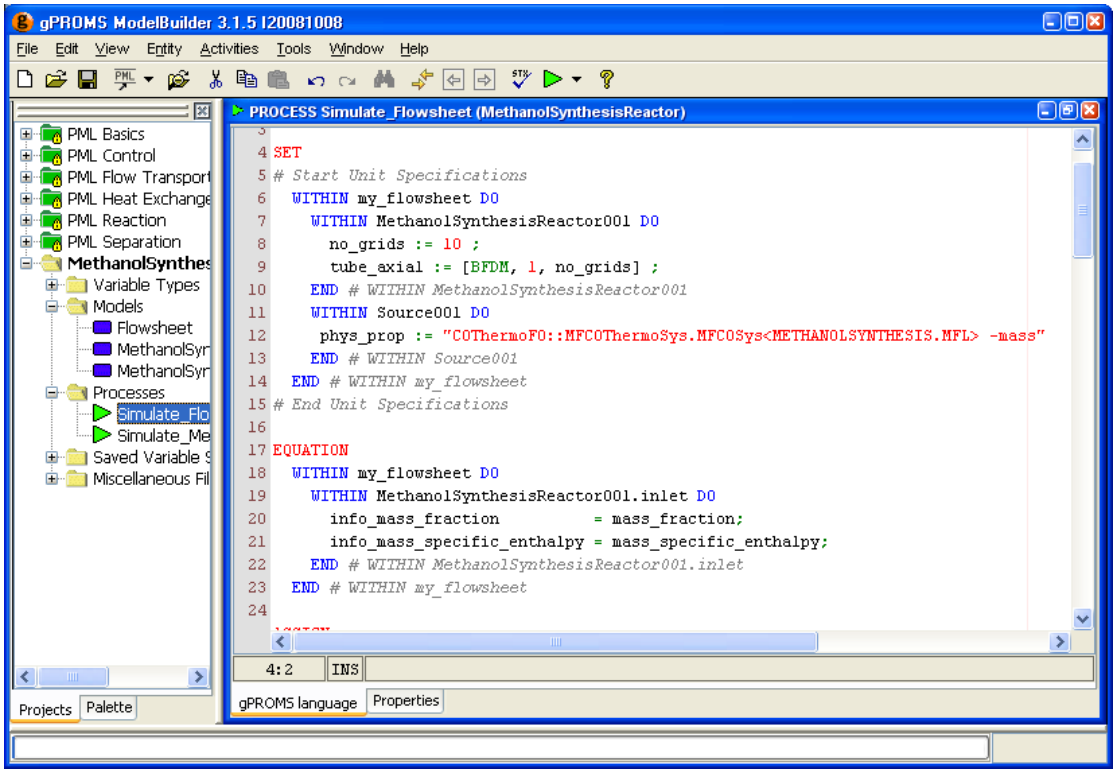
To use a named package from a thermo system with properties and calculations on a mass basis

COThermoFO::*ThermoPackageProgID* -mass

To use a thermo package with properties and calculations on a mass basis



A CO PP can also be specified explicitly directly in the gPROMS modelling language:

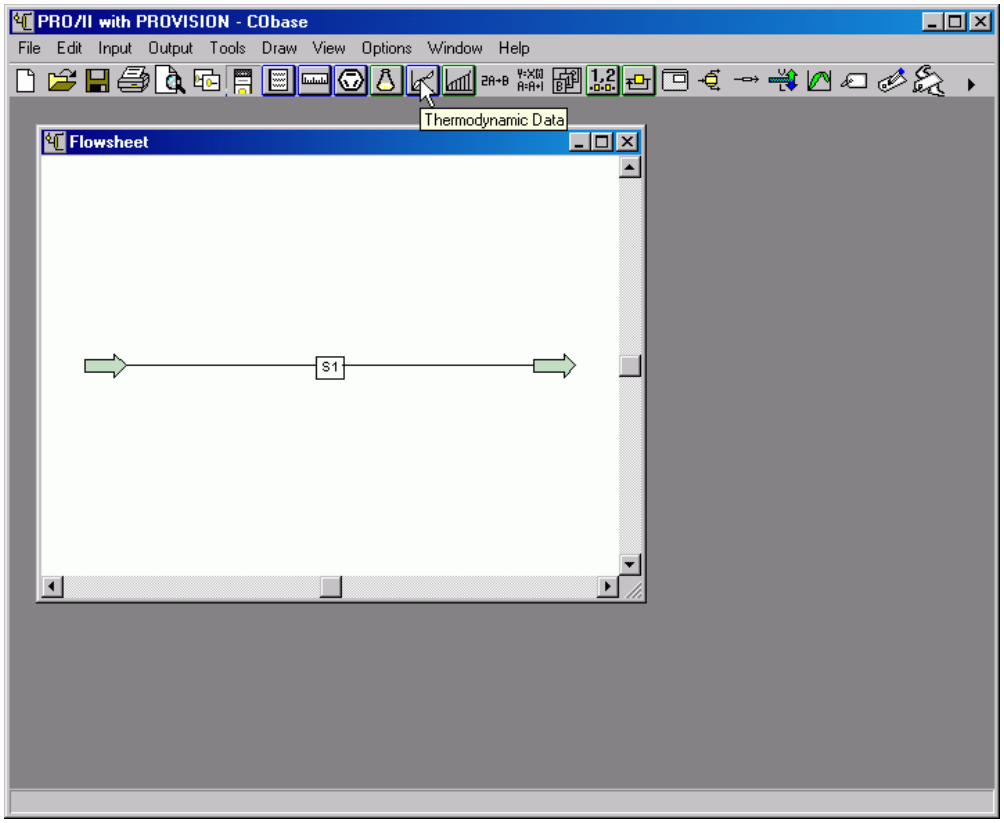


Note that the '-mass' flag is only one of several options controlling the behaviour of the COThermoFO; see the file README_CAPEOPEN.txt in your gPROMS installation for the complete list of options.

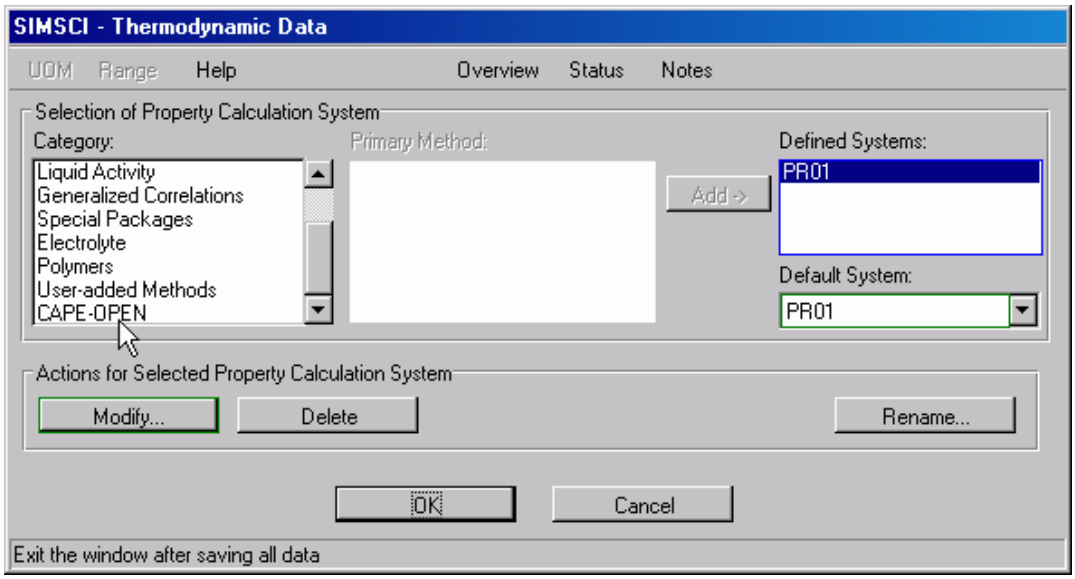
PRO/II

The following example shows how a Multiflash Property Package is selected in the PRO/II version 8.2 process simulator from SimSci-Esscor (www.simsci-esscor.com). The CO 1.0 sockets are supported.

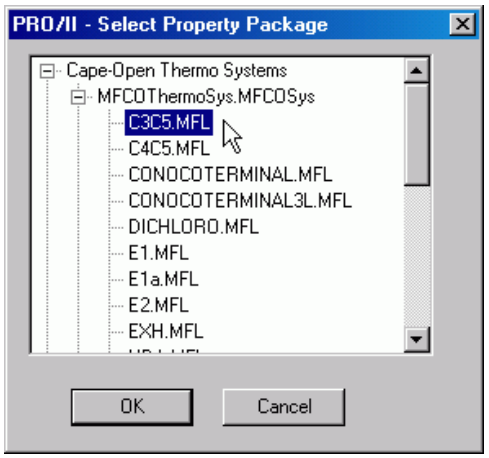
Open an existing simulation or create a flowsheet. Click on the Thermodynamic Data toolbar button



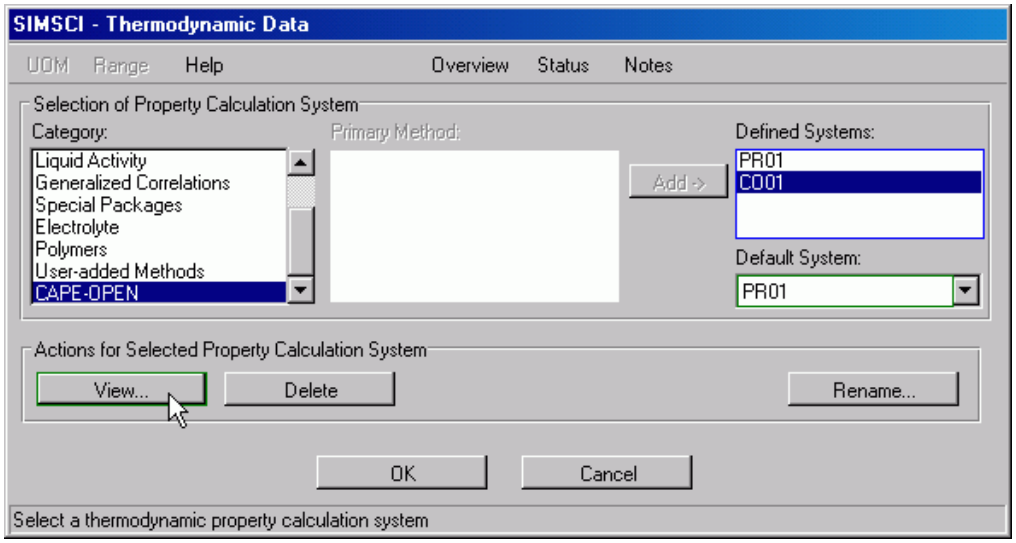
The Thermodynamic Data window is displayed. Scroll down the Category list and click on CAPE-OPEN.



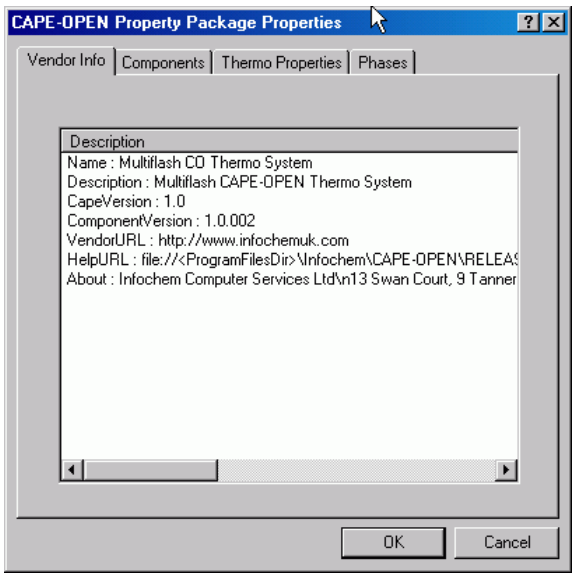
The Select Property Package window is displayed and clicking on the [+] symbols will show the list of available Thermo Systems and Property packages. Select the required package and click OK.

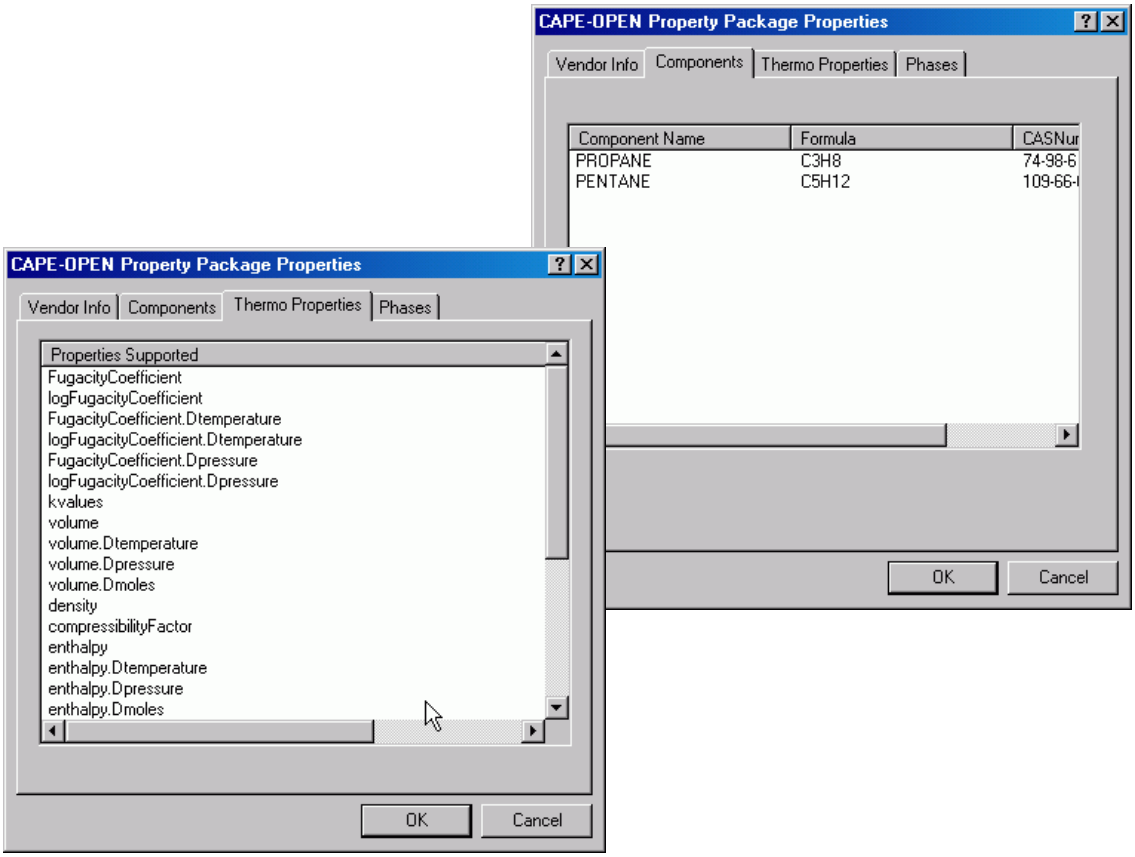


A CO package will be added to the list of defined systems

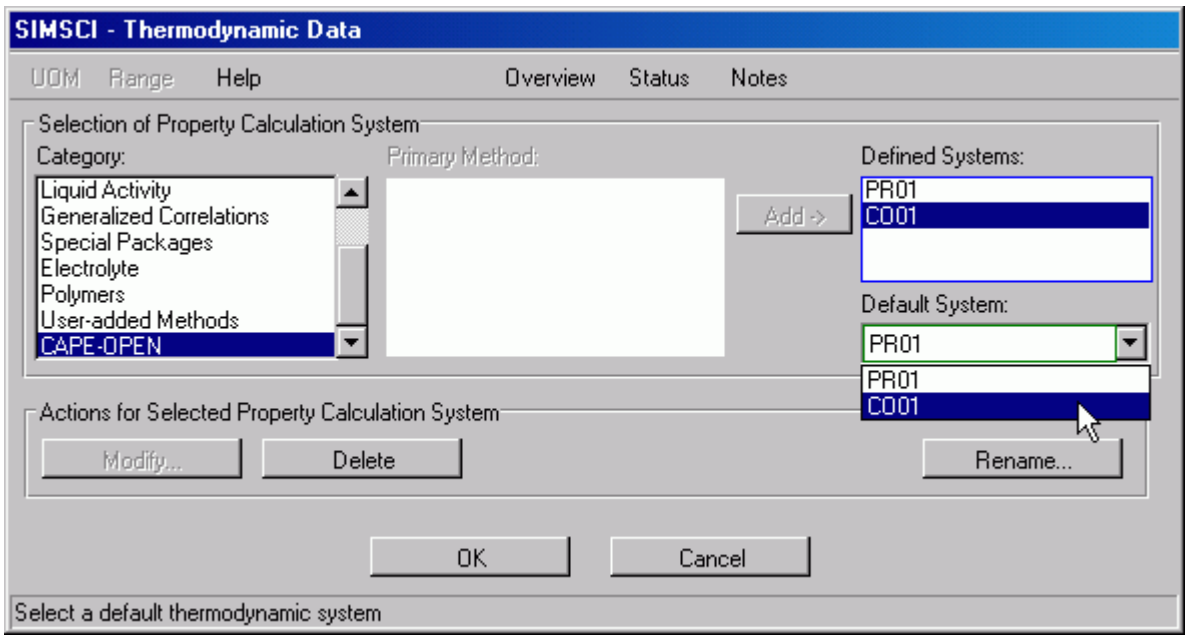


Clicking on the View button displays information about the package





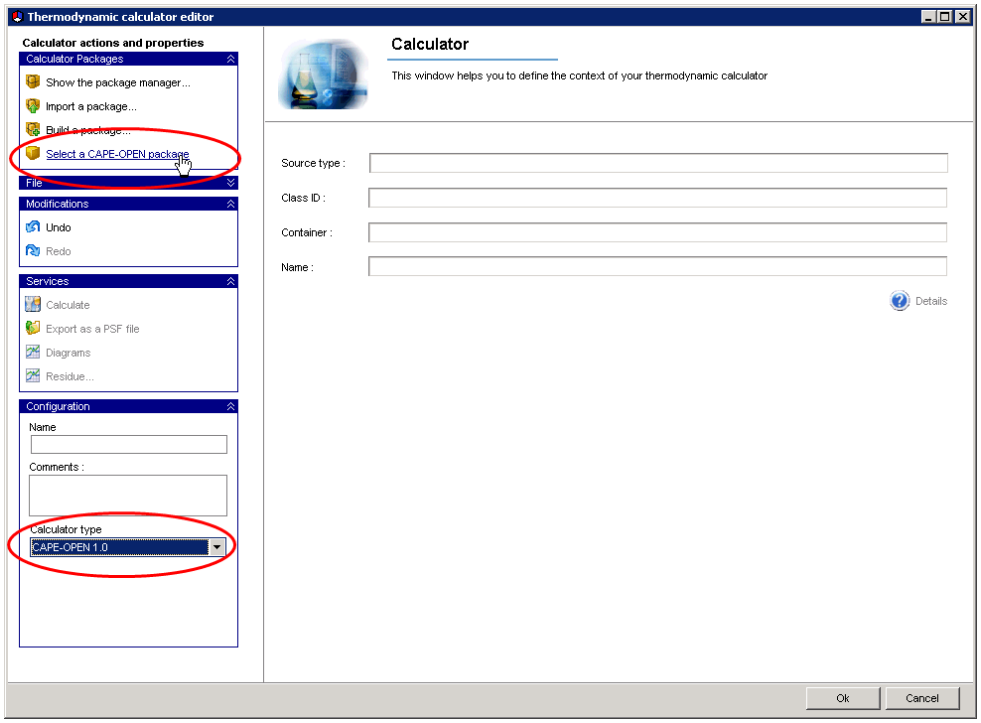
You can make the CAPE-OPEN package the default system for the simulation or, alternatively, it can be selected for parts of the flowsheet.



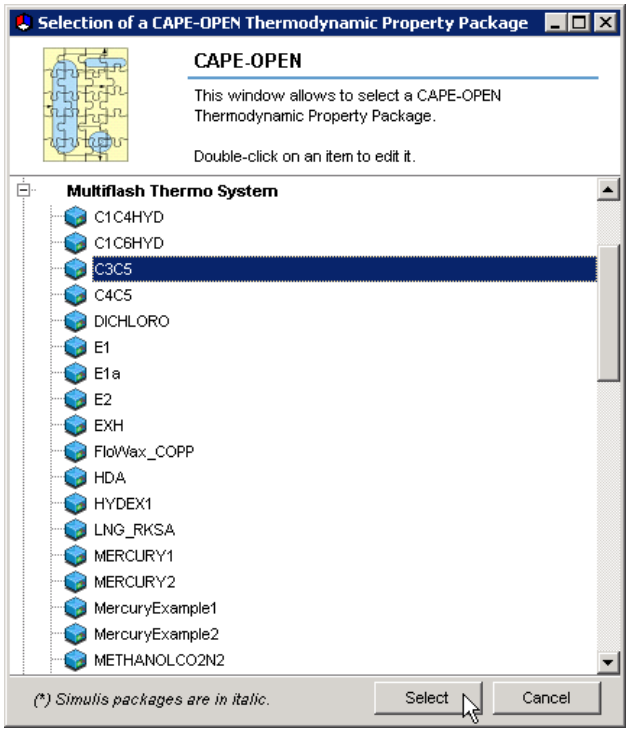
SIMULIS Thermodynamics

Simulis® Thermodynamics is a product of ProSim SA (www.prosim.net). Simulis 1.3 supports both the CO 1.0 and 1.1 sockets.

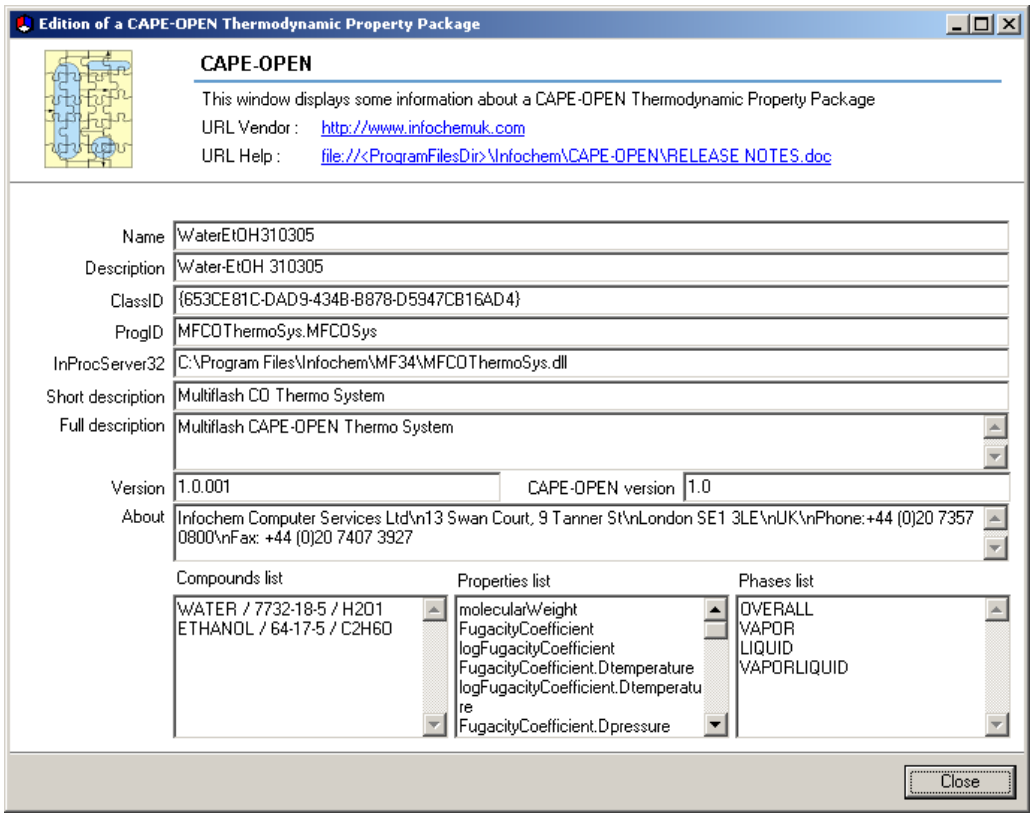
A CAPE-OPEN Property Package is selected using the Thermodynamic Calculator Editor. Select the Calculator type as CAPE-OPEN 1.0 or 1.1 and then click on 'Select a CAPE-OPEN package'.



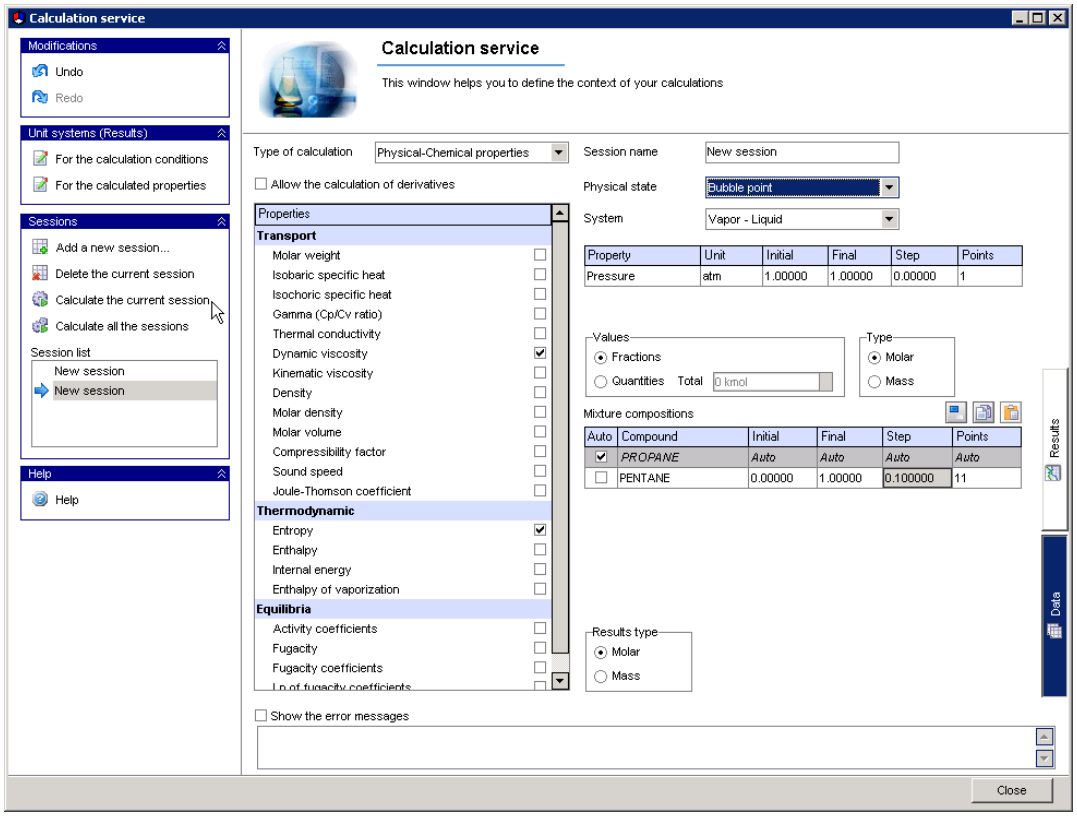
The Property packages available via various CAPE-OPEN Thermo Systems will be displayed. Select the required packaged from the list.

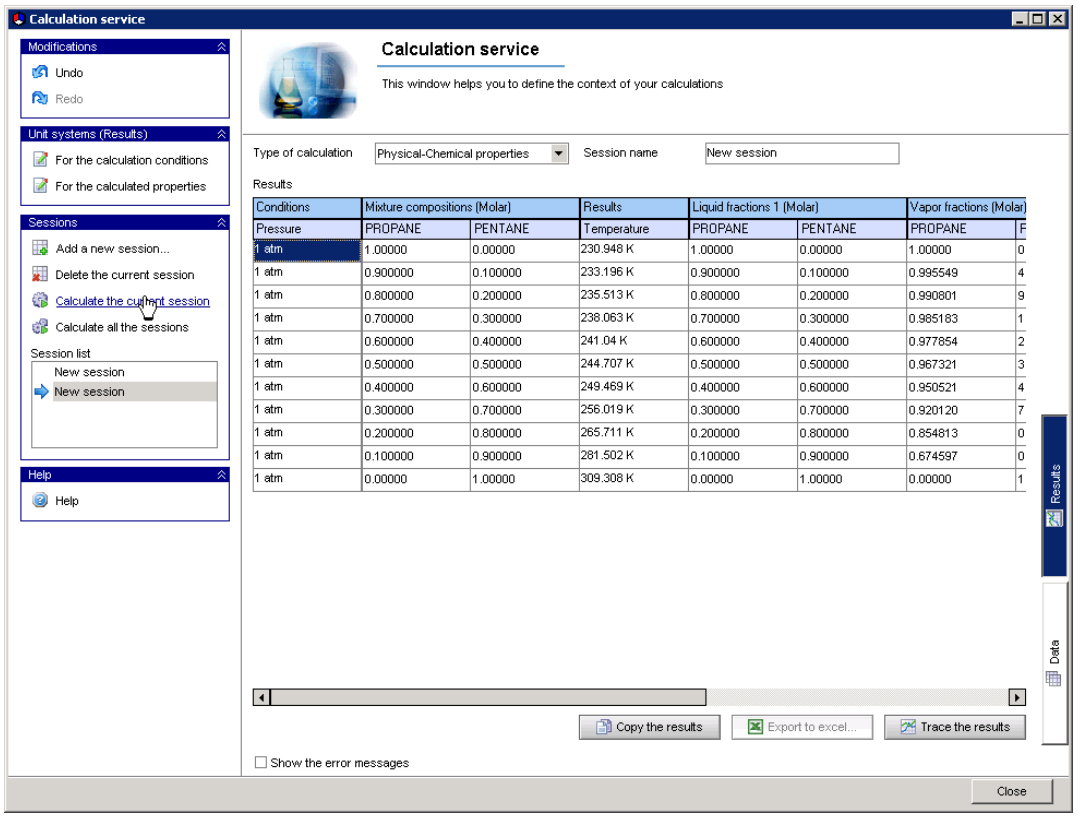


Information on the selected package is displayed and more details can be displayed by clicking on the 'Details' button as shown below

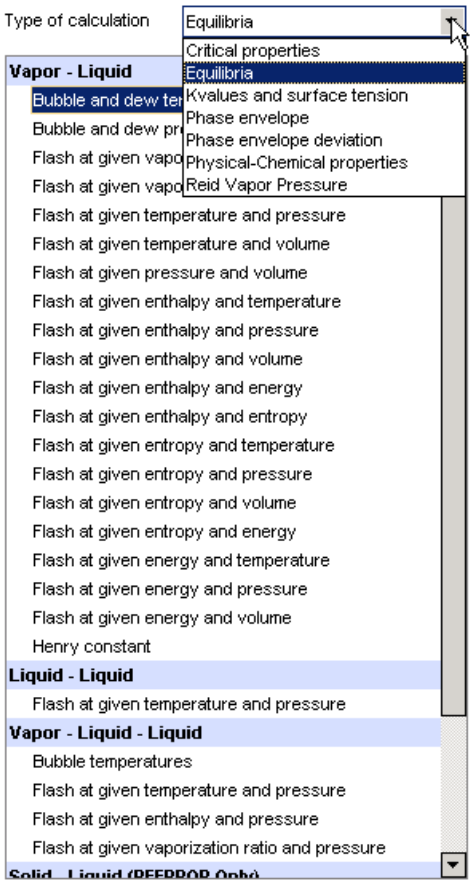


Properties and flashes are carried out using the Calculate facility.





A range of flash types and other calculations is available



Appendix A: Changes since previous version

Version 6.1

No changes were made to the Multiflash CAPE-OPEN in 6.1

Version 6.0

No changes were made to the Multiflash CAPE-OPEN in 6.0

Version 4.4

The 64bit version of the CapeOpen interface is distributed as well.

Version 4.3

No changes were made to the Multiflash CAPE-OPEN interface in 4.3.

Version 4.2

No changes were made to the Multiflash CAPE-OPEN interface in 4.2.

Version 4.1

No changes were made to the Multiflash CAPE-OPEN interface in 4.1.

Version 4.0

No changes were made to the Multiflash CAPE-OPEN interface in 4.0.

Version 3.9

Maximum number of models is increased from 40 to 100

Added support for two-phase surface tension models in Multiflash.

Version 3.8

The Multiflash CO components have been re-written for version 3.8. The principal functional changes are as follows.

1. Improved performance in the CO interface which is now implemented in C++ instead of VB6.
2. All software components for versions 1.0 and 1.1 of the CO Thermo interfaces are contained in a single dll for improved ease of installation and maintenance.

3. Support of Edit method of ICapeUtilities in PP, TS and PPM allows existing PPs to be edited or created from within a PME.
4. Support for persistence of PPs saved by a PME.
5. Improved ease of debugging through a new logging facility. See the section *Logging and diagnostics* on p. 6.
6. Diagnostic messages from Multiflash may be written to the ICapeDiagnostic interface of the PME (if supported). See the section *Logging and diagnostics* on p. 6.
7. Hierarchical configuration options using the Windows Registry and/or environment variables. See *Appendix B: Configuration details* on p.41.
8. The following new properties have been added:
   enthalpyF, enthalpyNF, entropyF, entropyNF and, kvalue. Dtemperature, Dpressure and Dmoles derivatives of these properties are also provided.

   Dtemperature, Dpressure and Dmoles derivatives of fugacityCoefficient, thermalConductivity, viscosity, kvalue.

   Dtemperature derivatives of heatOfVaporization and vaporPressure for 1.0 PPs.

   charge compound constant property.
9. The following new flash calculations have been added:
   pressure plus enthalpyF, enthalpyNF, entropyF, or entropyNF
   temperature plus enthalpyF, enthalpyNF, entropyF, or entropyNF
   volume plus entropyF, or entropyNF
   enthalpyF plus entropyF

Appendix B: Configuration details

A summary of configuration options is given in the section *Configuration* on p. 5. This appendix gives details of all the alternative configuration options that might be used.

Multiflash dll

The location of the Multiflash dll (full pathname) that will be used by the CO components may be specified as follows (in order of precedence):

1. Registry key HKCU\Software\Infochem\Multiflash\CAPE-OPEN\DLL

where HKCU means HKEY_CURRENT_USER

2. Registry key HKLM\Software\Infochem\Multiflash\CAPE-OPEN\DLL

where HKLM means HKEY_LOCAL_MACHINE

3. Environment variable MF_CO_DLL

The Multiflash installation package uses method 2.

Property Packages

The TS/PPM will look for PP configuration files (.mfl) in a location that may be specified as follows (in order of precedence):

1 HKCU\Software\Infochem\Multiflash\CAPE-OPEN\PPpath

2. HKCU\Software\Infochem\Multiflash\version x.y\GUI\Paths\CapeOpen

(with x and y determined from the Multiflash dll version)

3. HKLM\Software\Infochem\Multiflash\CAPE-OPEN\PPpath

4. HKLM\Software\Infochem\Multiflash\version x.y\GUI\Paths\CapeOpen

5. Environment variable MF_CODIR

6. HKCU\Software\Infochem\Multiflash\version x.y\GUI\Paths\CaseFiles

7. HKLM\Software\Infochem\Multiflash\version x.y\GUI\Paths\CaseFiles

The Multiflash installation package uses method 4.

Multiflash Databanks

The location of the Multiflash databank files is specified as follows (data bank path is considered valid if "infodata.bin" is present). In order of precedence:

1. HKCU\Software\Infochem\Multiflash\CAPE-OPEN\DBPath

2. HKCU\Software\Infochem\Multiflash\Version x.y\GUI\Paths\InstallLoc

3. HKLM\Software\Infochem\Multiflash\CAPE-OPEN\DBPath

4. HKLM\Software\Infochem\Multiflash\Version x.y\GUI\Paths\InstallLoc

5. Environment variable MFxyAPP

The Multiflash installation package uses method 4.

Multiflash GUI

In MF 3.9 and higher it is possible to edit a PP provided that this operation is supported by the PME. To allow editing the CO dll needs to locate the Multiflash GUI. The GUI is searched for in the following locations (in order of precedence):

1. HKCU\Software\Infochem\Multiflash\Version x.y\GUI\Paths\InstallLoc
2. HKLM\Software\Infochem\Multiflash\Version x.y\GUI\Paths\InstallLoc
3. Environment variable MFxyAPP

The Multiflash installation package uses method 1.

Logging

Debug information may be logged to a file by setting one of the following:

1. Registry key HKCU\Software\Infochem\Multiflash\CAPE-OPEN\log
2. Environment variable MF_CO_LOG

(value "0" or "FALSE" means *off*, other values mean *on*)

The log file name is <temp dir>\Multiflash_CapeOpen(<appname>).log

<temp_dir> is the directory set by the TEMP environment variable.

<app_name> is the name of the application that is using the Multiflash CO components.

CO Diasgnostics

Diagnostic messages from Multiflash can be written to ICapeDiagnostic (if implemented by the PME) by setting one of the following:

1. Registry key HKCU\Software\Infochem\Multiflash\CAPE-OPEN\diagnostics
2. Environment variable MF_CO_DIAGNOSTICS

(value "0" or "FALSE" means *off*, other values mean *on*).

Appendix C: Converting a Hysys model to use a Multiflash PP

The following notes have been contributed by Malcolm Woodman, BP Exploration. They describe a procedure for converting an existing HYSYS v2006.5 model to use a Multiflash Property Package via CAPE-OPEN Thermo 1.0 For all or part of the flowsheet.

1. Pre-requisites: Multiflash, the license control software and the CAPE-OPEN components must be installed and working.
2. Create a Multiflash CAPE-OPEN Property Package as described in the section on page 8. The PP should contain all the compounds in the flowsheet. The pseudocomponent names need not be the same as in the base model, but the pseudo definition must be equivalent.
3. Open a new case in HYSYS 2006.5 CP3.
4. In Simulation Basis Manager, Add a new Fluid Package.
5. Choose “COMThermo Pkg”
    a. Select CAPE-OPEN 1.0 for Vapour phase
    b. Select CAPE-OPEN 1.0 for Liquid phase
    c. In the pop-up window, select the CO Property Package exported in step 2 above, click on Accept
    d. Click on “Extended PropPkg Setup…”
    e. Click on “Finish Setup…”
    f. Click on OK
    g. Select “CAPE-OPEN Flash” in the small scrollable window
    h. Click on “Extended Flash Setup…”
    i. Click on “Finish Setup…”
    j. Close “COMThermo Setup” window
    k. Close Fluid Package window
    l. Add the base fluid package from the existing HYSYS model, including any user over-rides, e.g. binary coefficients
    m. Set base model to original fluid package, including for Case (Main)
    n. “Enter Simulation Environment…”
    o. Put model on hold
    p. Save the new model
6. Open the existing HYSYS model.
    a. Select the entire flowsheet
    b. “Copy selected objects” (right click, choose “Cut/Paste Objects…”)
    c. Paste into new model created in step 7
    d. Open Simulation Basis Manager, delete newly created Fluid Package (Basis-2), click on OK on the pop-up warning
    e. Delete newly created component list (Component List – 1)
    f. Return to Simulation Environment, save model
7. Copy the composition of all feed streams containing pseudocomponents from the existing model to the new model.
    a. Required because, even if the Multiflash pseudos have the same name, they are treated as different compounds in HYSYS. Therefore, the cut-and-paste of the flowsheet objects will not copy these compositions.

b. In existing model, open the worksheet for the feed stream, switch to composition view. Highlight all compositions (not just the pseudos), copy with ctrl-c
c. In new model, open the worksheet for the same feed stream, switch to composition view and edit. Highlight all the compositions, use ctrl-v to paste.
d. Also need to update the split factors for pseudos in any splitter block in the flowsheet
e. Release solver
f. Save

8. The new model is now complete, with the original base model being used for all objects. Now switch relevant objects to use Multiflash, but note that great care should be taken with the transfer basis (right click on sub-flowsheet, "View Properties", "Transfer Basis" tab).
    a. Default transfer basis is P-H flash. This is unlikely to be correct, because the two different fluid packages (Multiflash and built-in HYSYS) will probably use different reference states for the enthalpy. This should be changed to T-P flash for any streams which cross the boundary where the fluid package changes
    b. Note: a -PVF flash may be the best option for some streams, e.g. where the degree of saturation is critical.
9. To move objects into a sub-flowsheet in HYSYS and change the property method:
    a. Put model on hold
    b. Select objects to be moved, point at one of them, right click. Select "Cut/Paste Objects ➔ Combine into sub-flowsheet".
    c. In Basis Manager, change the fluid package
    d. In the Sub-flowsheet Environment, select all objects, point at one of them and right click. Select "Change Fluid Package…" and change to the required package.
    e. Release solver