

Process Simulation Software: User Interface

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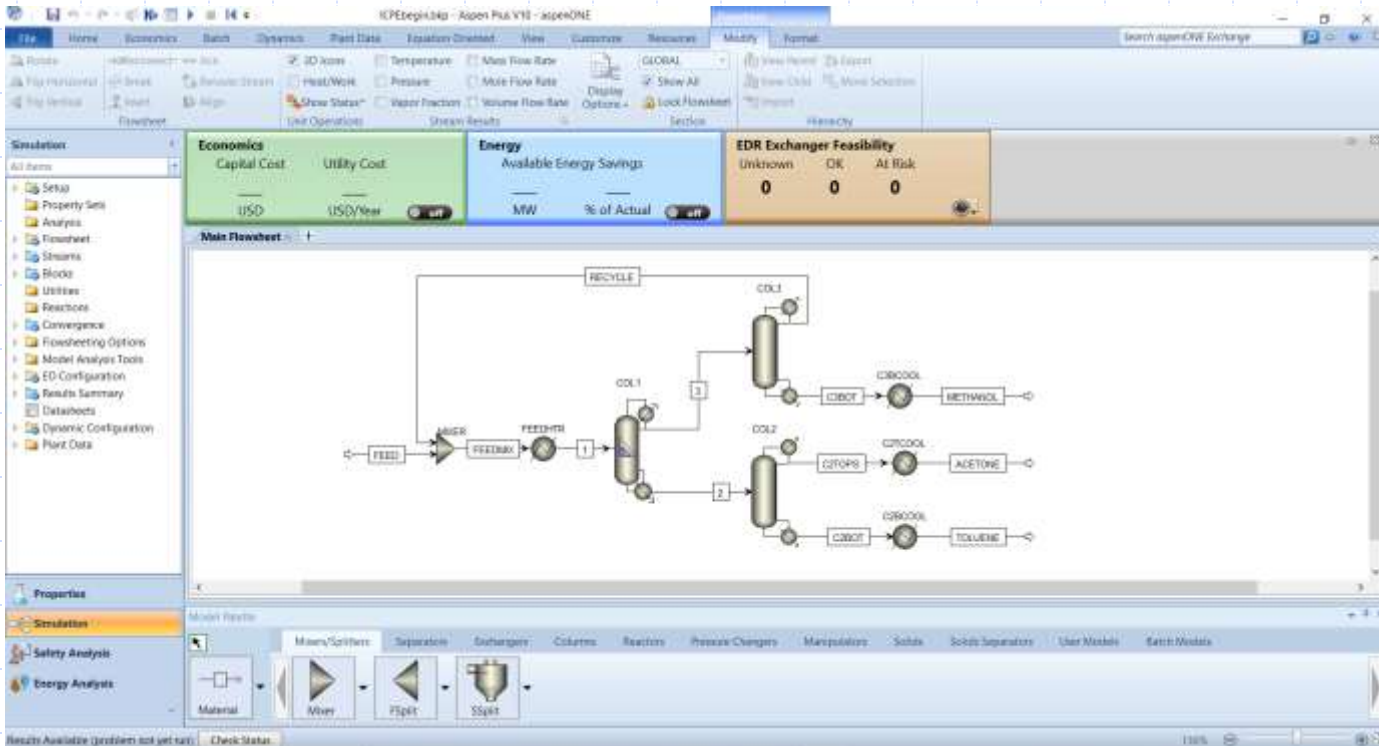
University of Trieste



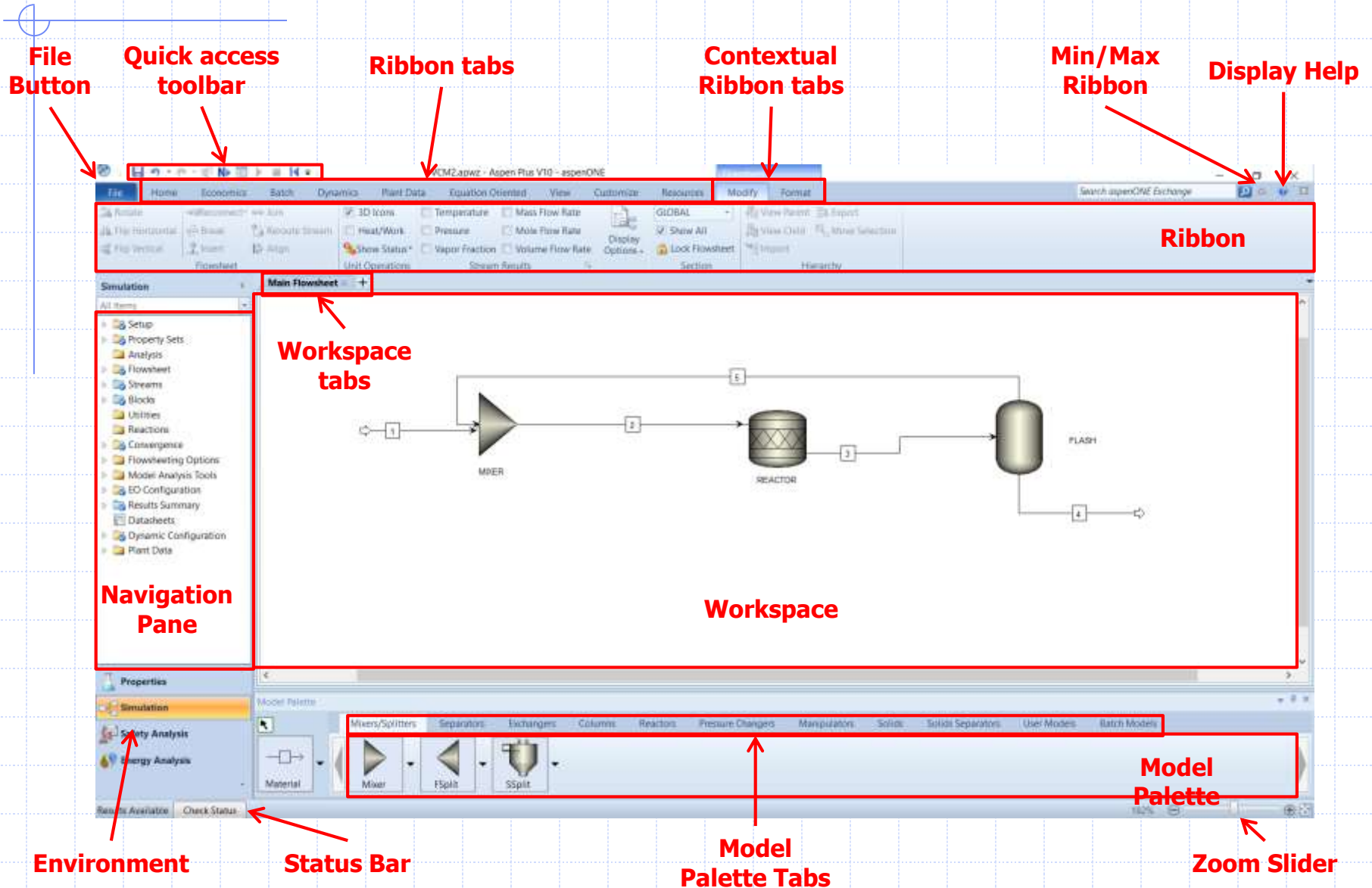
Agenda

- ◆ Aspentech SW: Aspen plus and Aspen properties
- ◆ COCO steady state simulation environment
- ◆ Super pro designer
- ◆ A survey of process simulation software

Aspen Plus



User interface



Aspen Plus Start Page

Simulation Examples

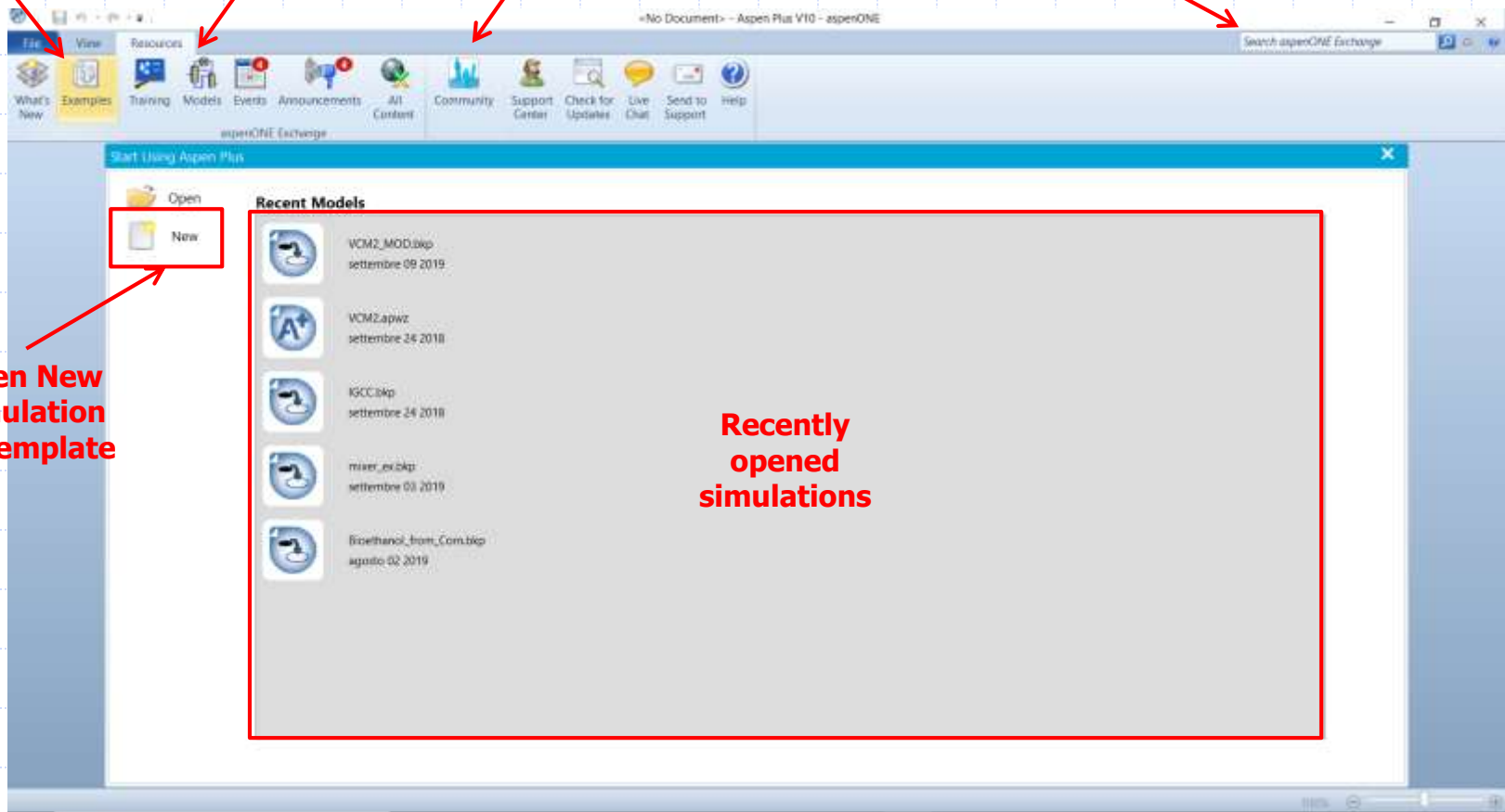
AspenONE Exchange

Community

Search in AspenONE Exchange

Open New Simulation or Template

Recently opened simulations



aspenONE Exchange

Search Filters

Search Categories

Preview items before download

Search in AspenONE Exchange

The screenshot shows the AspenONE Exchange web application interface. The browser address bar displays "Search: aspenONE Exchange". The application header includes a navigation menu with categories: Training, Documentation, Models, Literature, Tools, Events, Announcements, Blogs & Discussions, Learn About, and Related Features. The main content area is titled "Exchange" and features a search bar, a "Sort By" dropdown set to "Relevance", and a "Request new content" link. On the left, a "Filters" sidebar is expanded, showing sections for "Primary Product" (listing Aspen Plus, Aspen Shell & Tube Exch..., aspenONE Install, AES Install, Aspen Air Cooled Exchan..., Aspen HYSYS, Aspen Plus Dynamics, Aspen Shell and Tube Ex...), "Training Type" (listing Video Tutorials, Webinars, CBT, Best Practices, Instructor-Led, Documentation), and "Organization" (AspenTech). The "Search Results" section displays a list of items, each with a thumbnail and a title: "Distillation Improvement", "Getting Started with Aspen Simulation Workbook in Aspen Plus V8", "Welcome to the Training Center", "Getting Started with Aspen Dynamics V8", and "Getting Started with Activated Energy Analysis in Aspen Plus". The right sidebar contains "Learn About" (Batch Distillation Modeling, Entropy and Second Law of Thermodynamics, Granulation and Agglomeration, Advanced Solids Modeling, Modeling Physical Properties) and "Related Features" (Batch Process Development, Custom Modeling, Economic Evaluation, Solids Modeling, Exchanger Design And Rating). Red arrows point from the text labels to the corresponding UI elements: "Search Filters" points to the sidebar, "Search Categories" points to the top navigation menu, "Preview items before download" points to the search results list, and "Search in AspenONE Exchange" points to the browser address bar.

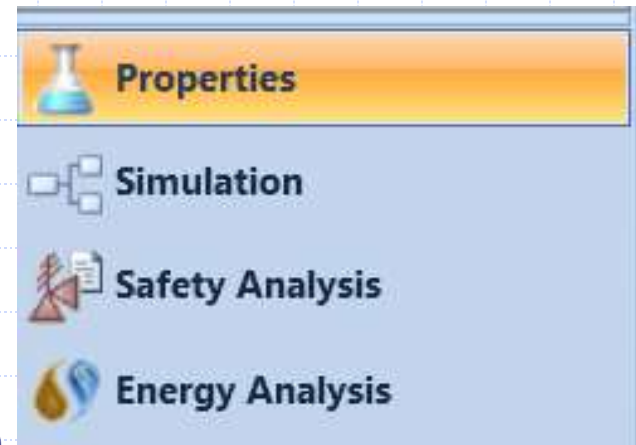
Aspen Plus Environments

◆ Properties Environment

- Define the physical properties
 - ◆ Component selection, generation and characterization
 - ◆ Thermodynamic methods and database
 - ◆ Collect experimental data
 - ◆ Property estimation
 - ◆ Property analysis
 - ◆ Data regression

◆ Simulation Environment

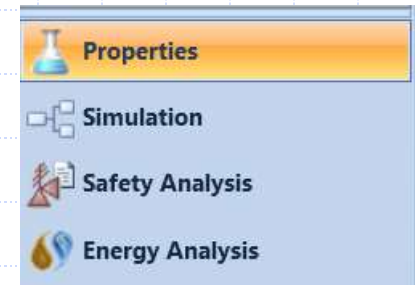
- Used to build and run the process model
 - ◆ Design and create process flowsheet
 - ◆ Perform interactive analysis (sensitivity, design spec.)
 - ◆ Fit models to process or experimental data
 - ◆ Preliminary equipment design, sizing and rating
 - ◆ Economic evaluation of the process design



Aspen Plus Procedure

◆ Properties Environment

- Select the components involved in the chemical process from databanks or generate the components using the specific interface
- Specify the thermodynamic methods suitable for the simulated system
- Collect experimental data
- Property estimation
- Property analysis
- Data regression



◆ Simulation Environment

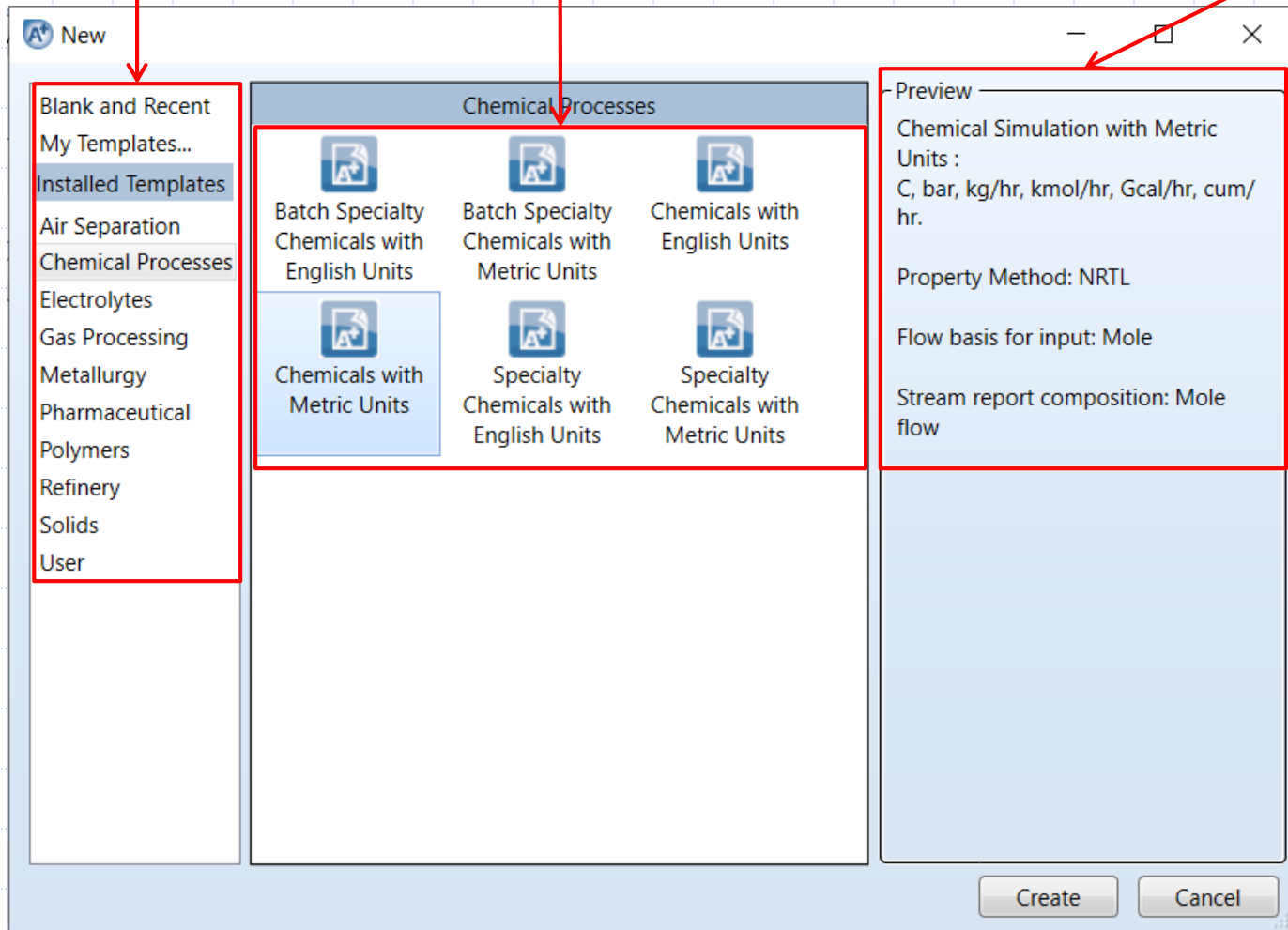
- Select the appropriate blocks to represent the process design
- Create the unit operations connected with streams
- Specify the streams condition, composition and flowrate
- Set the operative conditions of unit operation models
- Define the utilities and cost factor to perform energy and cost analysis

New Simulation

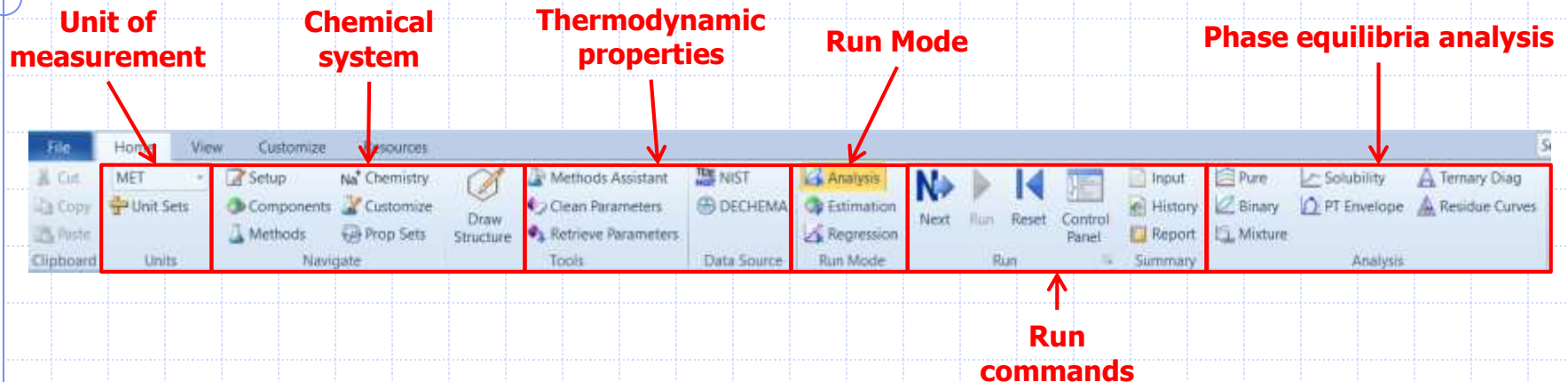
Process types

Templates available for category

Template characteristics

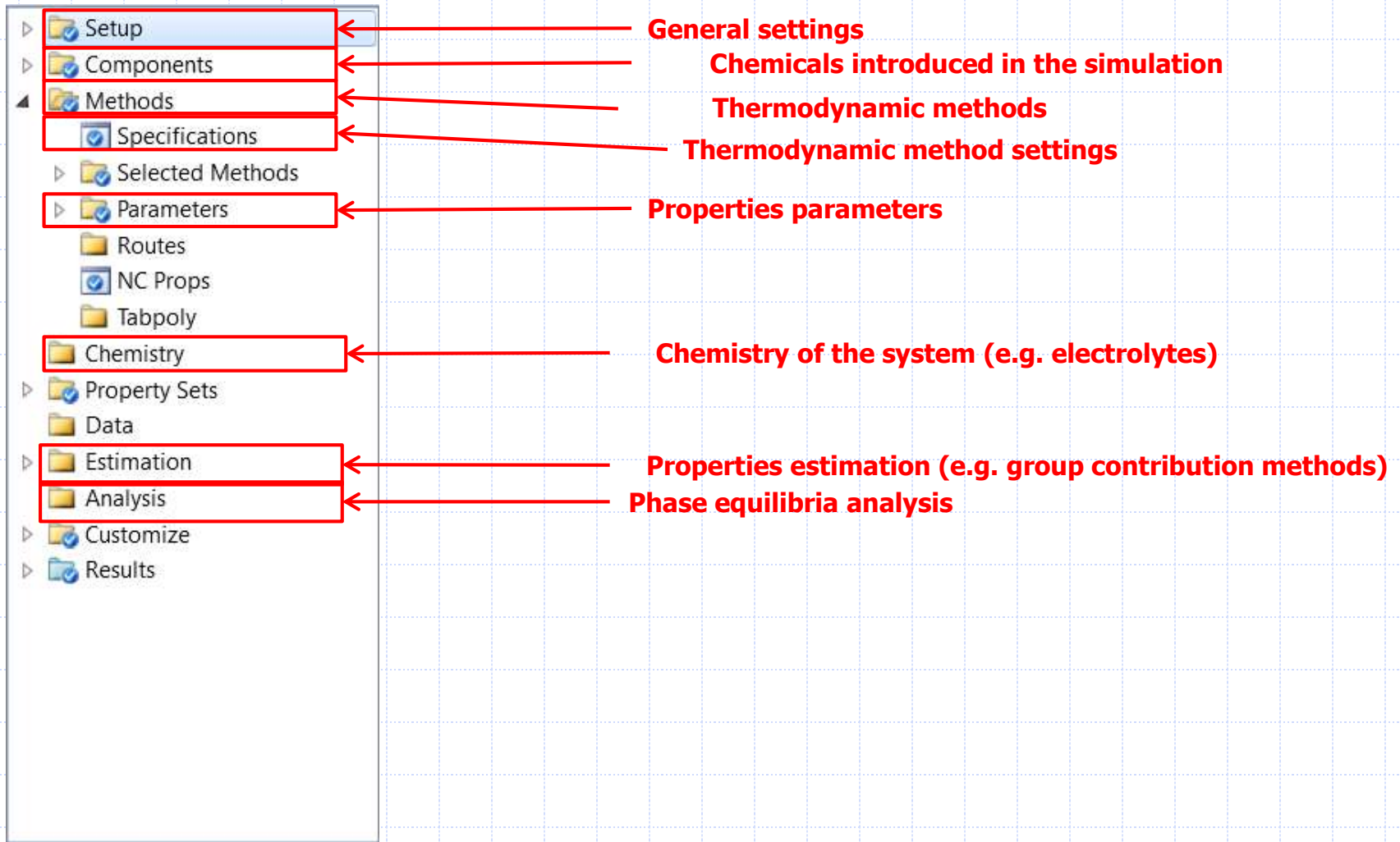


Properties Home Ribbon

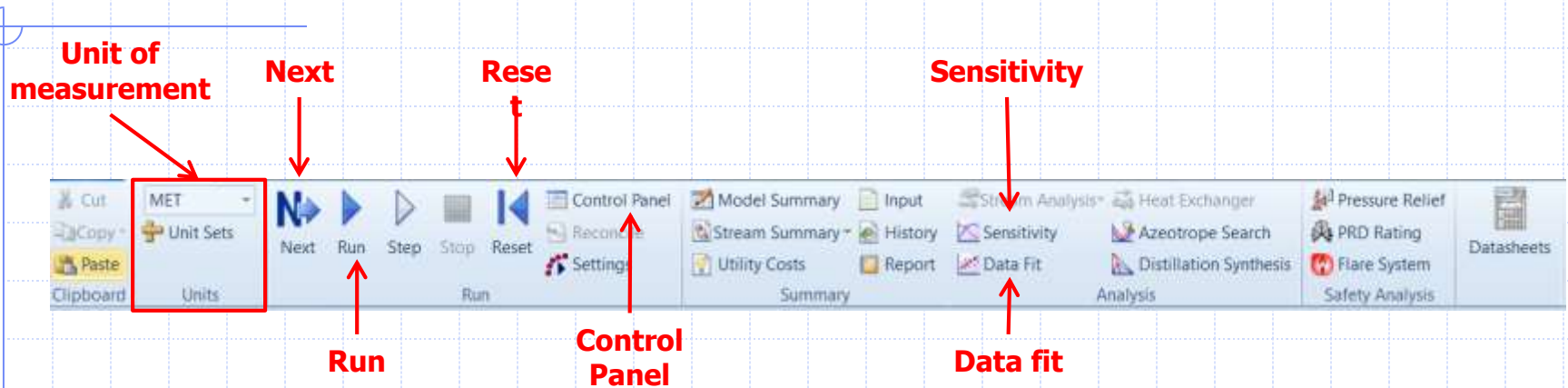


- ◆ **Unit of measurement:** select the appropriate set of UoM among the available ones or create your own
- ◆ **Chemical system:** define components involved
- ◆ **Thermodynamic prop:** set the thermodynamic method and parameters
- ◆ **Run mode:** specify the target of the simulation
- ◆ **Run commands:** perform calculations
- ◆ **Phase equilibria analysis:** perform analysis on thermophysical properties

Properties Navigation Pane

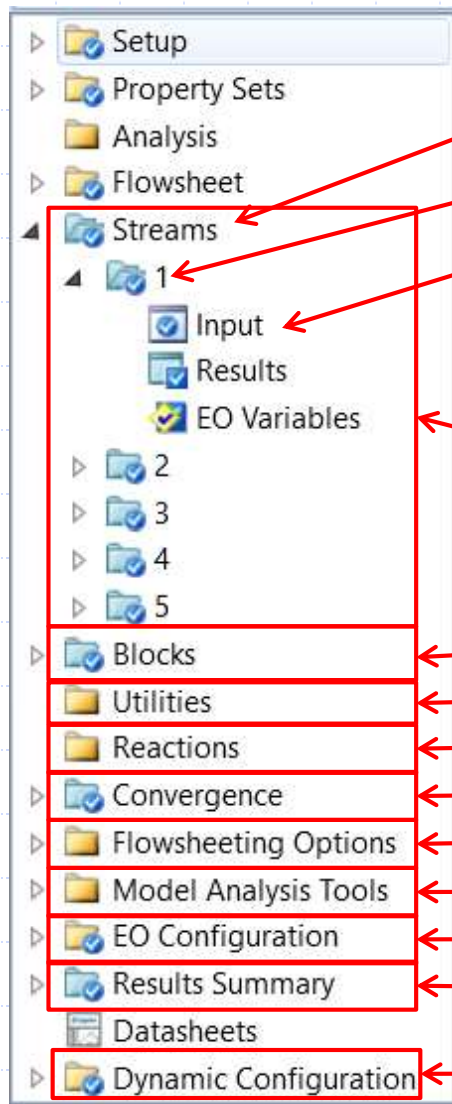


Simulation Home Ribbon



- ◆ **Unit of measurement:** select the appropriate set of UoM among the available ones or create your own
- ◆ **Next:** move to the next unspecified parameter
- ◆ **Run:** run the simulation
- ◆ **Reset:** purge simulation results. Very important when parameters have been modified between different runs
- ◆ **Control Panel:** shows convergence, warnings, errors and procedures during a run
- ◆ **Sensitivity:** perform sensitivity analysis
- ◆ **Data fit:** enable to fit real data to simulation results

Simulation Navigation Pane



Folders: refers to the root items in Nav Pane

Forms: used to enter data and view results

Sheets: can be selected using tabs

Streams list

Unit operations list

Utilities adopted

Reaction introduced

Convergence report & issues

Design Specification & Calculation

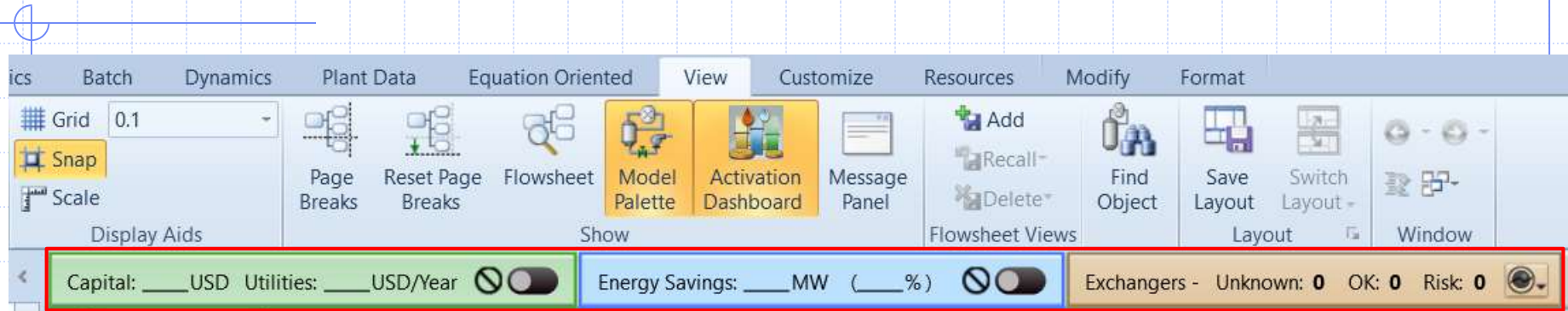
Sensitivity & Optimization

Equation Oriented approach

Results obtained

Dynamic parameters

Activated Analysis

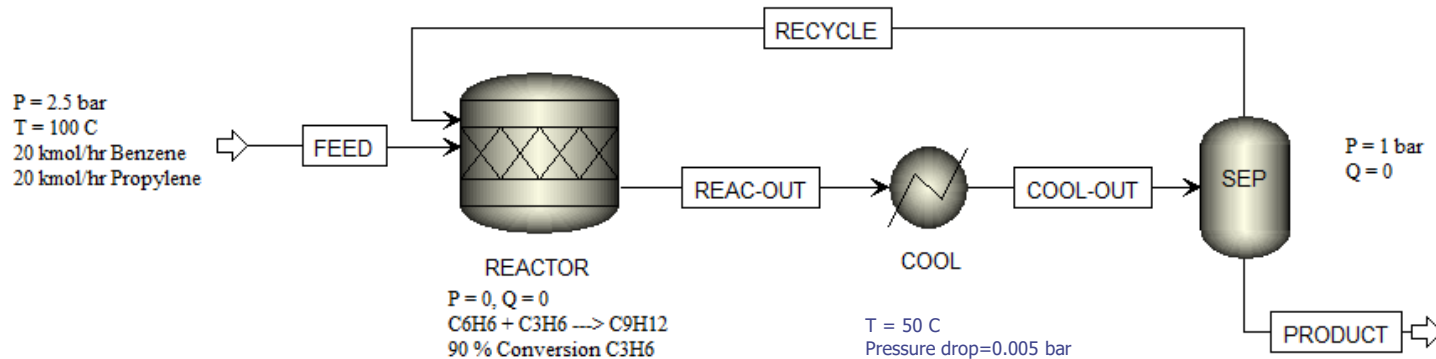


◆ Tools built-in to Aspen Plus to aid in process analysis and optimization

- **Activated Economic Analysis:** provides high level cost estimates useful for comparing process alternatives
- **Activated Energy Analysis:** looks for opportunities to reduce energy consumption using pinch technology
- **Activated Exchanger Analysis:** allows quick access to rigorous heat exchanger design and rating programs from Aspen Plus

Demo

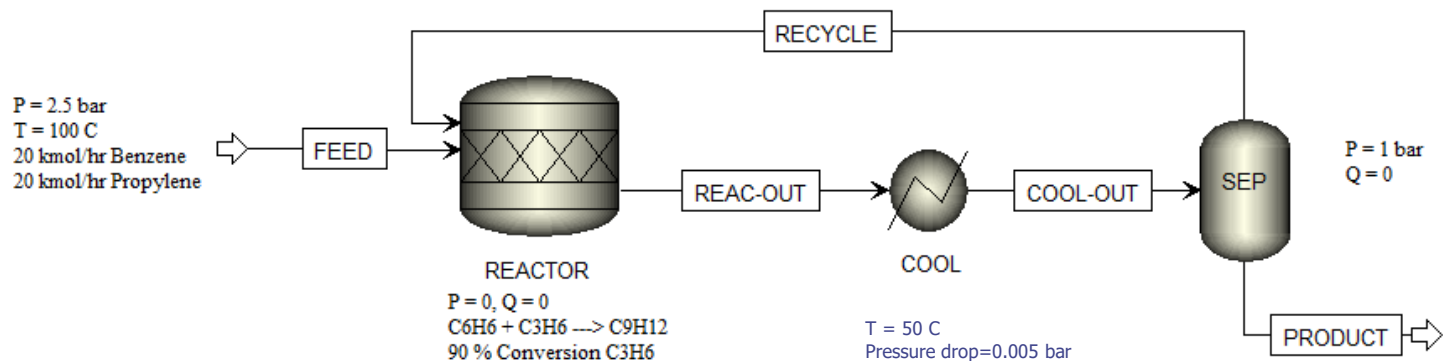
- ◆ Cumene production from propylene and benzene in a conversion reactor



Use the SRK property method.

Demo

◆ Cumene production from propylene and benzene in a conversion reactor



Design-Spec DS-1
Vary the Temperature of Block COOL such that the mole fraction of Cumene in stream PRODUCT = 0.98

Sensitivity S-1
Vary the Temperature of Block COOL from 30 to 130 C.
Tabulate the mole fraction of Cumene in PRODUCT.

Use the SRK property method.

Activate one or the other!

COCO-COFE a cape Open process simulator



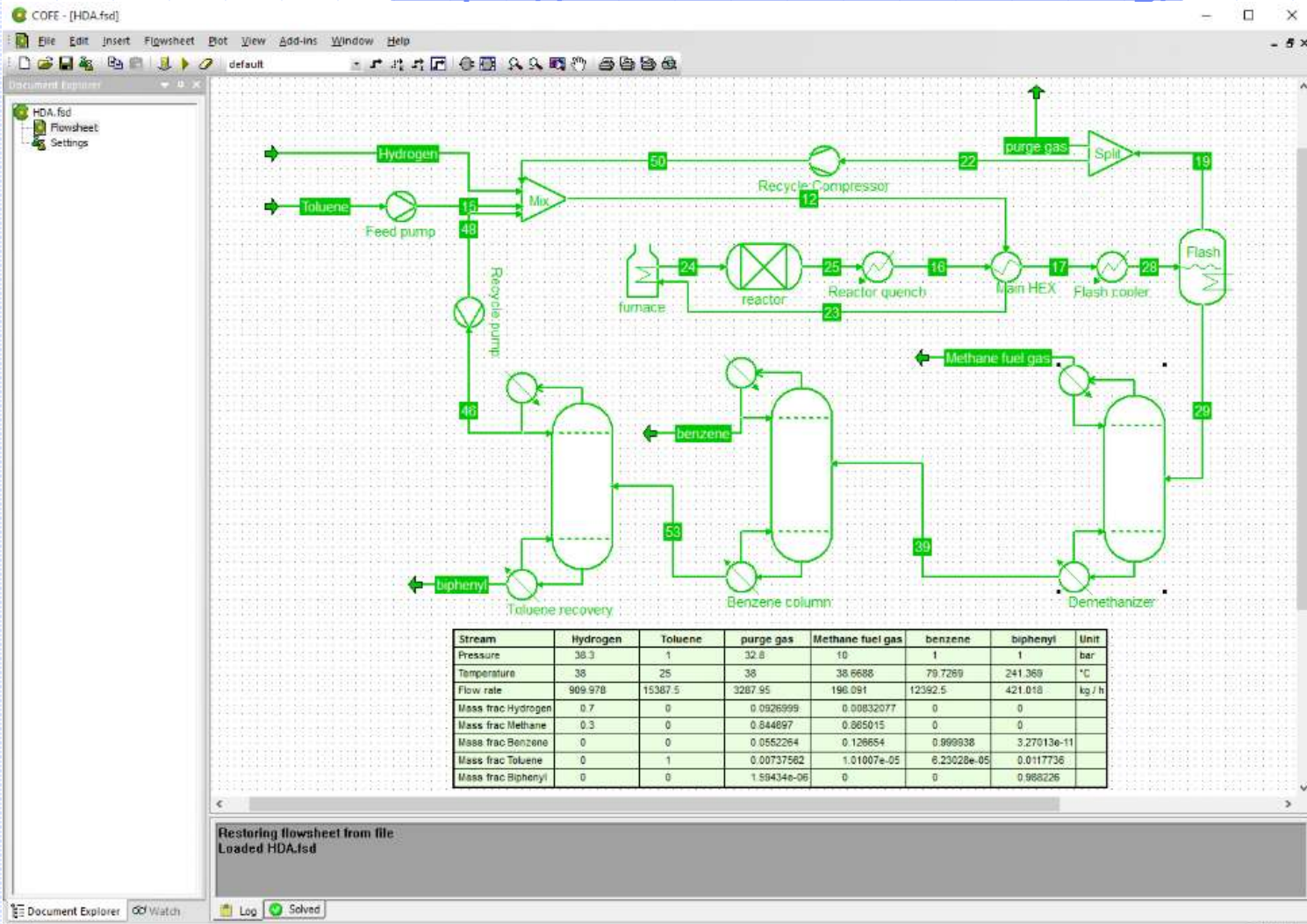
What is COCO?

↖ **CAPE-OPEN to CAPE-OPEN is a free-of-charge CAPE-OPEN compliant steady-state simulation environment**

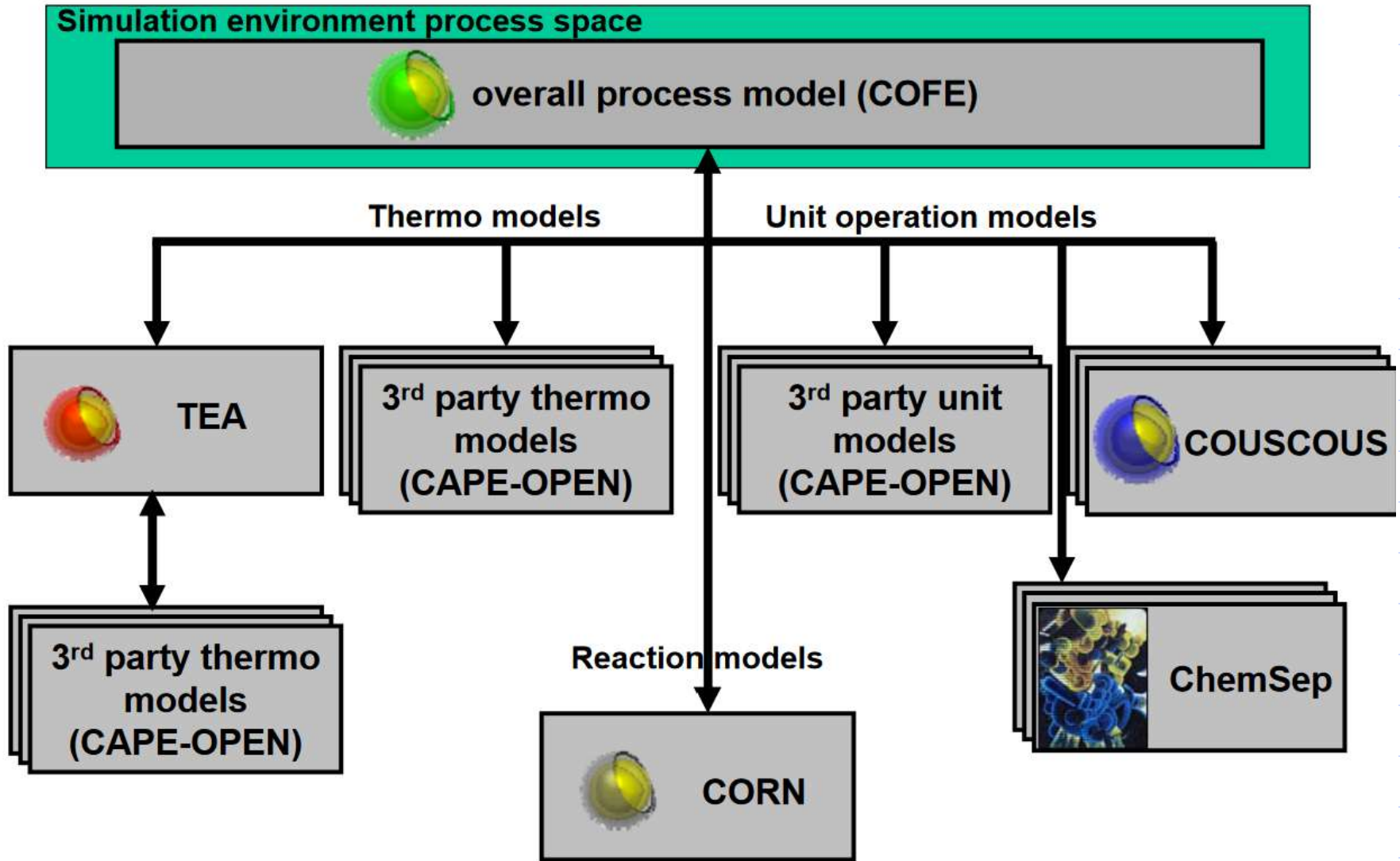
- COFE: CAPE-OPEN Flow-sheeting Environment
- TEA: ThermoDynamics for Engineering Applications
- COUSCOUS: CAPE-OPEN Unit-operations (Simple)
- CORN: CAPE-OPEN Reaction Numerics

COCO: a free-of-charge CAPE-OPEN compliant steady-state simulation environment

Available here: <https://www.cocosimulator.org/>

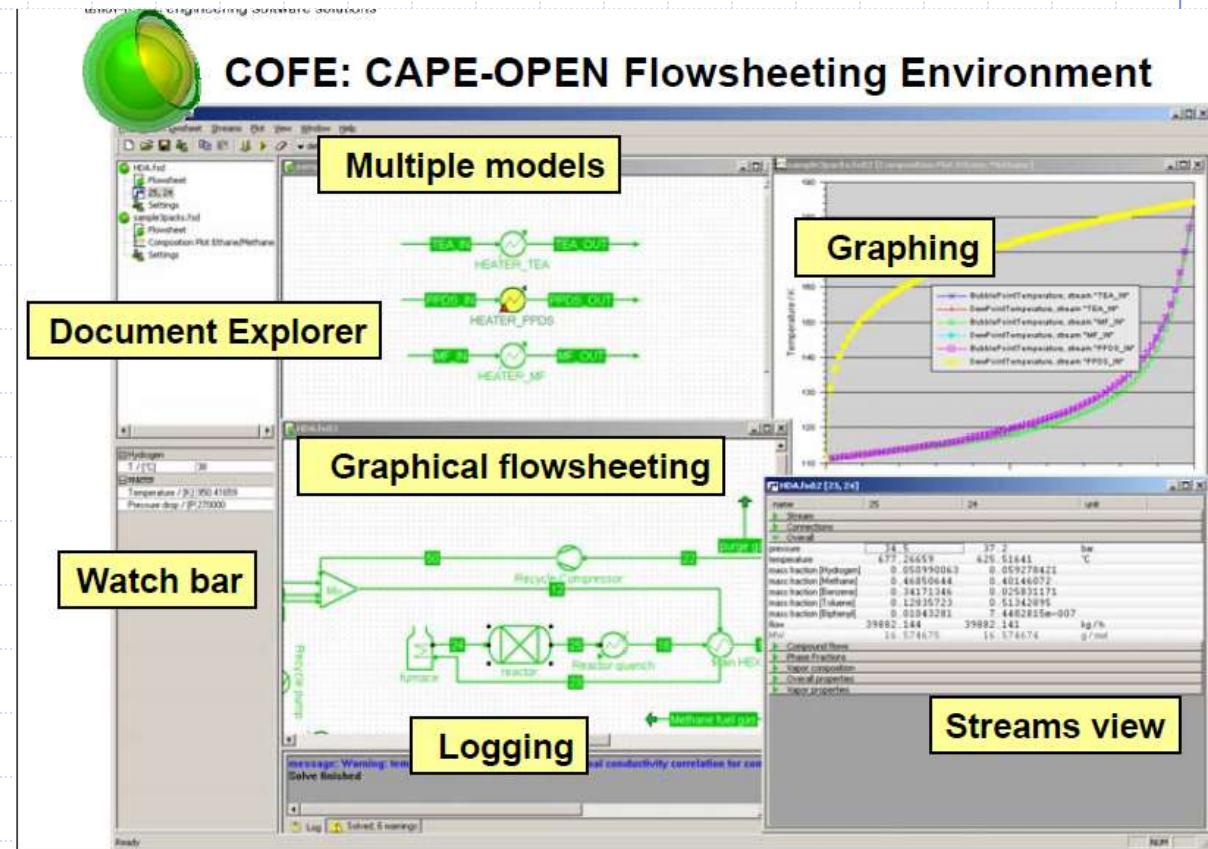


COCO-COFE a cape Open process simulator



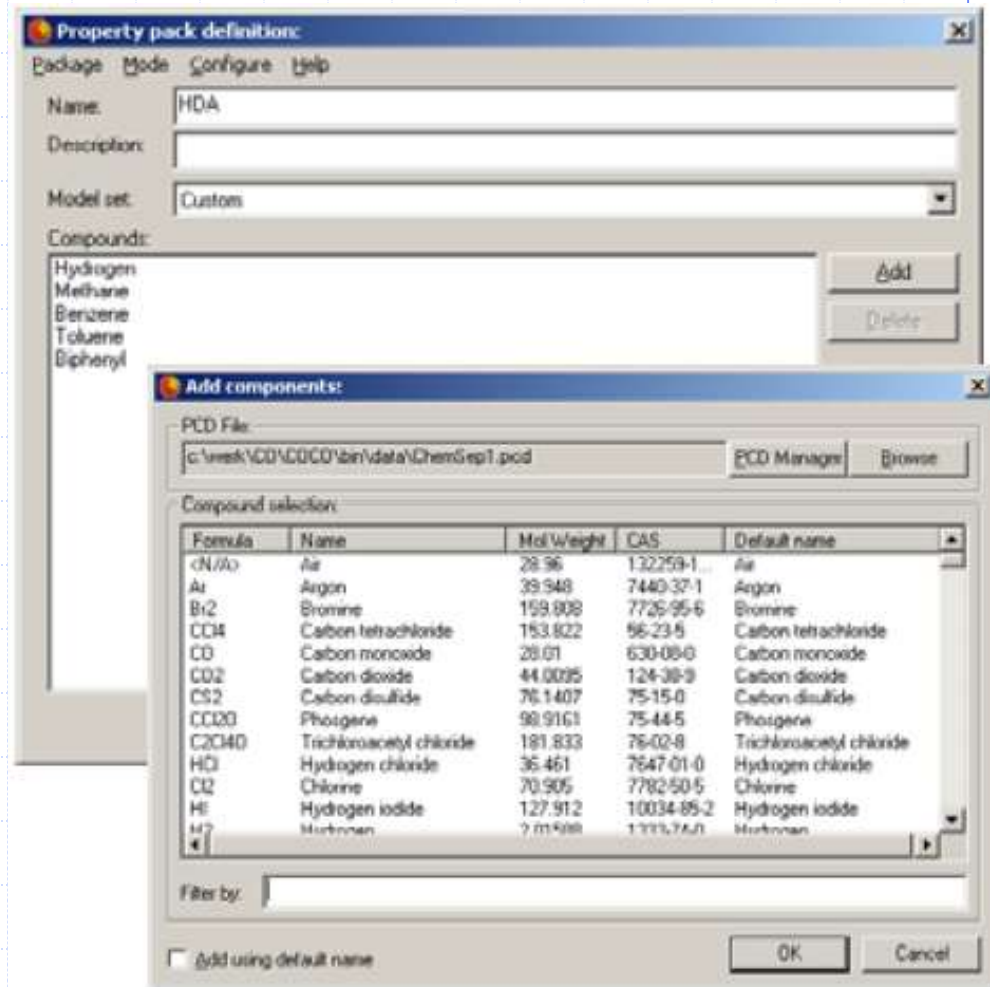
COFE: CAPE-OPEN Flowsheeting Environment

- ◆ Breaking recycles by **automatic tearing**
- ◆ **Solving recycles** by hybrid Newton / Wegstein
- ◆ **approach**, using reparameterization
- ◆ Support for **multiple material types**, with selection for thermo and sub-set of compounds
- ◆ Material, energy and information **streams**



TEA Thermodynamics for engineering calculations

- ◆ Pure compound data library
 - (extendible, or use DIPPR)
- ◆ 100+ Property calculation methods
 - (25+ different properties)
- ◆ Property derivatives
- ◆ Support of external property calculation routines and external equilibrium servers
- ◆ VLE equilibrium calculation
 - Large diversity of supported flash specifications
 - Inside-out approach
 - Post-checking of solution
 - Back-up full Newton approach

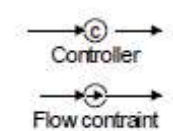
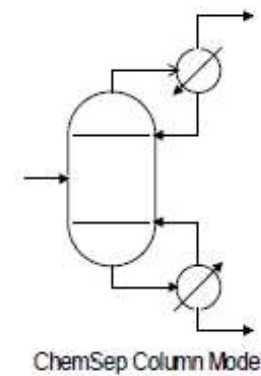
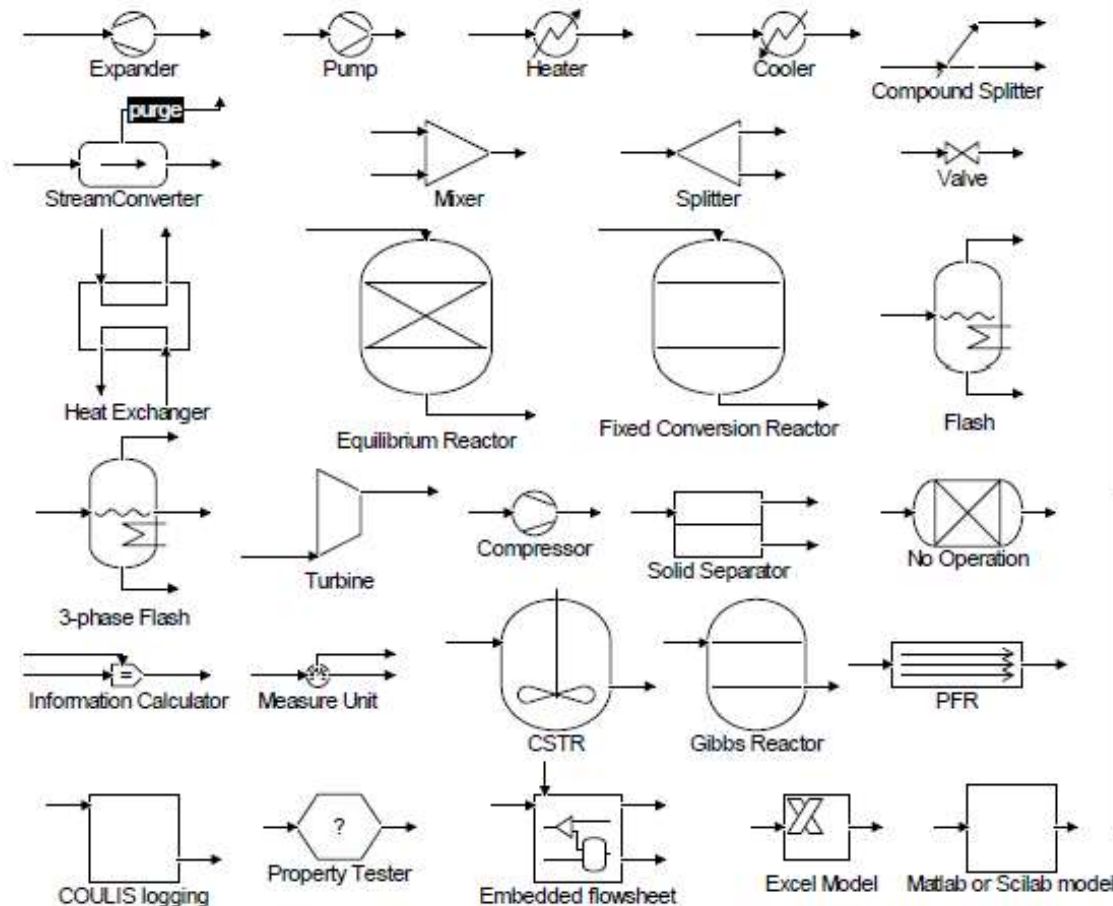


Thermodynamic models and compounds from ChemSep

COUSCOUS: simple unit operations



COUSCOUS: Simple unit operations



TEA: reasons to use it and not to use it

◆ Reasons to use it

- **Availability:** TEA comes free-of-charge with COCO
- TEA Thermo is **based on ChemSep** thermo
- ChemSep thermo, and therefore TEA thermo, has a history of **more than 10 years of validation**
- TEA is **actively being developed** by motivated people
- TEA is **highly configurable:** compound definitions, property calculations, plugging in external

◆ Reasons NOT to use it

- TEA's equilibrium routines **restricted to V-L** systems
- **All CAPE-OPEN thermo** is supported under COFE
- **Validate** your results
- **Availability**

Some other options



AspenProperties



Infochem
Multiflash



Simulis
Thermodynamics



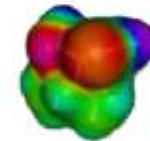
TUV/NEL
PPDS

ProSim



VMGThermo

Virtual Materials
Group



CosmoTherm



NIST REFPROP



AixCAPE

AixCAPE

Configuring TEA property packages

The image shows a Windows Start menu with the 'Programs' folder expanded to 'COCO', where 'ConfigureTEA' is highlighted. A red arrow points from the text 'ConfigureTEA' to this menu item. Below, the 'ConfigureTEA' dialog box is open, showing tabs for 'Flowsheet Options', 'Stream order', and 'Unit Operation order'. A red arrow points from the text 'ConfigureTEA' to the 'ConfigureTEA' dialog. In the foreground, the 'Property pack from TEA Property Pack Mana...' dialog is open, displaying a list of property packages. Red arrows point from the text 'New package' to the 'New' button and from 'Packages' to the 'Packages' button in this dialog. The list of packages includes: Alkanes, C1/C2 Amagat, C1/C2 PB, C1/C2 SRK, C1_C2, C1_C2 (EOS), HDA, n-deopropanizer, water ethanol test, and Water-nButanoHUNIQUAC.

ConfigureTEA

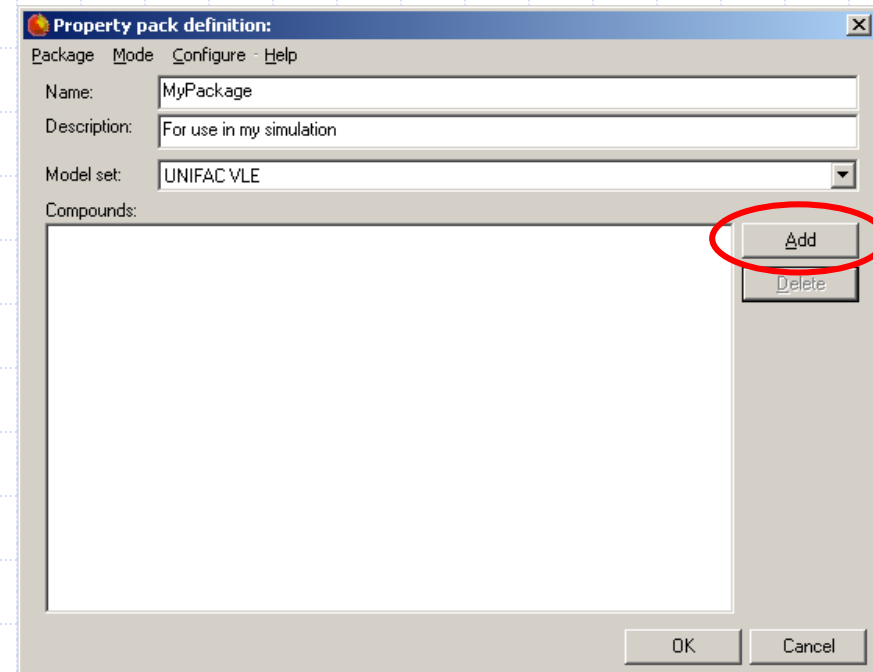
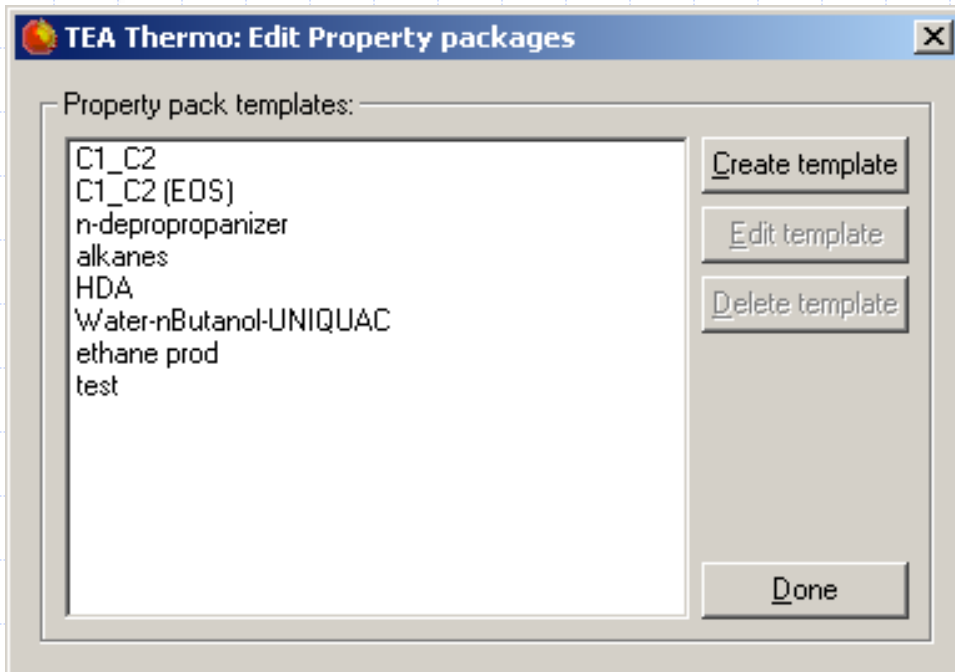
New package

Packages

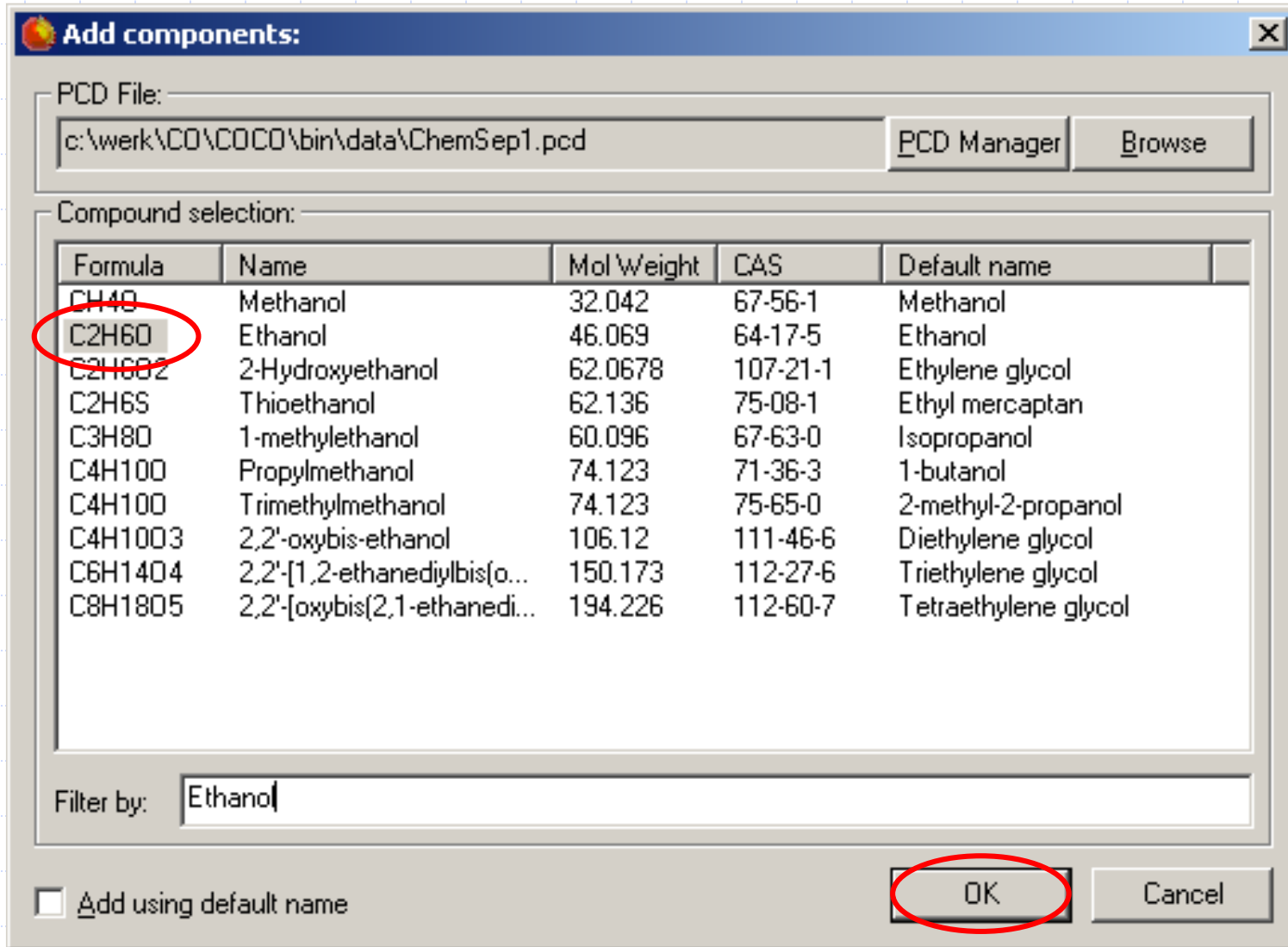
Configuring TEA property packages

◆ TEA packages configuration window

- Shows packages that already exist
- TEA property package instances are stored within a COFE document
- Inside the document you can change the compounds or property calculations of the TEA package used.
- The pre-configured property package templates are therefore called templates.



Configuring TEA property packages



Managing Pure Component Data (PCD) files

- ◆ PCD files are Pure Component Data files.
 - formula, name, critical pressure, coefficients to correlations for property calculations.
 - ChemSep (LITE) comes with a package to edit PCD files; **PCD manager**.
 - Load the PCD file at: C:\Program Files\ChemSepL8v23\pcd

The screenshot displays the ChemSep PCDmanager interface for editing the Benzene component. The window title is "ChemSep PCDmanager - chemsep1.pcd". The main area is divided into several sections:

- Information:** ChemSep v6 pure component data - adapted from Properties of Gases and Liquids 5th Ed.
- Components (194):** A list of components with "Benzene" selected. Other visible components include Isopentene, N-pentene, Neopentene, 1,2,4-trichlorobenzene, M-dichlorobenzene, O-dichlorobenzene, P-dichlorobenzene, Bromobenzene, Monochlorobenzene, Iodobenzene, Nitrobenzene, and Phenol.
- Benzene Component Data:** A table showing the ideal gas heat capacity correlation coefficients. The table has two columns: "Key" and "Value".

Key	Value
Eq.No.	16
T min (K)	200.0
T max (K)	1500
A	35345
B	-605.22
C	12.847
D	-0.00021029
E	0.0000000488

- Plot:** A graph titled "Ideal gas heat capacity (J/kmolK)" showing the heat capacity as a function of temperature (T in K). The x-axis ranges from 200 to 1400 K, and the y-axis ranges from 0.5 to 2.5 (1/ES). The curve shows a smooth, increasing trend.
- Buttons:** "Copy Data", "Copy Plot", "Mass densities", and "Ln" are visible.
- Search:** A search box with "not matched" and "Find Next" buttons.
- Footer:** "C:\ChemSep\pcd\chemsep1.pcd"

PCD manager contains:

◆ Basic info for components

- name, index number (index number of DIPPR), CAS number, SMILES string, structural formula, molecular weight, family (from the DIPPR list) and formula

◆ Critical properties

- Critical constants, normal boiling point, melting point, the triple point T and P.
- The critical constants are needed in any application of an equation of state to estimate thermodynamic properties.

◆ Estimation of missing properties

- missing value for heat of vaporization of benzene, and we can select several estimation methods from the drop down list

Benzen

Component | Critical | Molecular | T Correlations | Group Data | EOS | Miscellaneous | Log | Units | Paths

Key	Value
Name	Benzen
Index	501
CAS number	71-43-2
SMILES	c1ccccc1
Structure	-CHCHCHCHCHCH-
Molecular weight (kg/kmol)	78.11
Family	Inorganic bases
Formula	C6H6

synonyms:
benzol benzolene bicarburet of hydrogen carbon oil coal naphtha cyclohexatriene mineral naphtha motor benzol phenylhydride pyrobenzol

Benzen

Component | Critical | Molecular | T Correlations | Group Data | EOS | Miscellaneous | Log | Units | Paths

Key	Value
Critical temperature (K)	562.0
Critical pressure (Pa)	4.895E+06
Critical volume (m ³ /kmol)	0.2560
Critical compressibility factor (-)	0.2680
Normal boiling point (K)	353.2
Melting point (K)	278.7
Triple point temperature (K)	278.7
Triple point pressure (Pa)	4764

Click here to estimate properties

Order by property Order by method

Apply

Benzen

Component | Critical | Molecular | T Correlations | Group Data | EOS | Miscellaneous | Log | Units | Paths

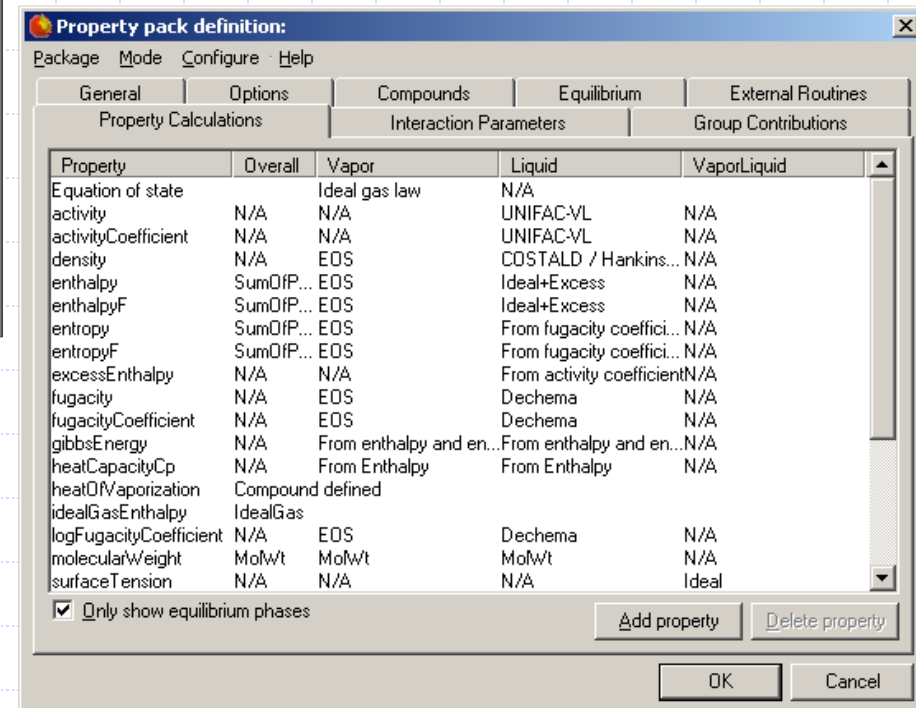
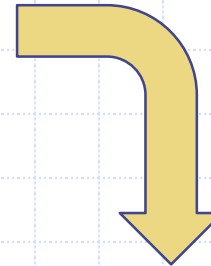
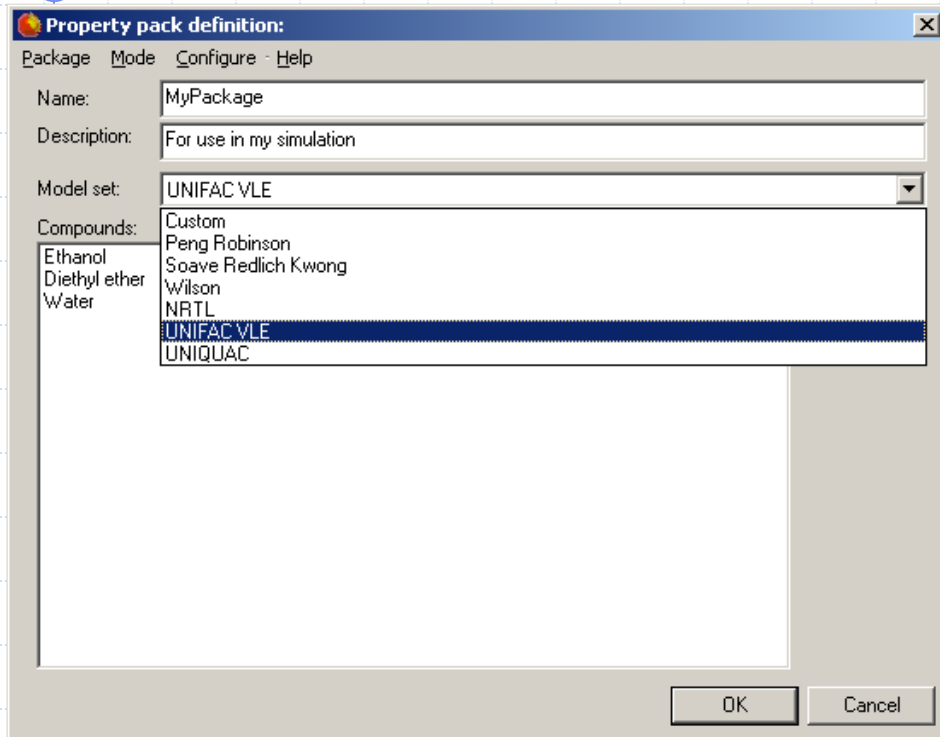
Key	Value
Liquid molar volume at normal boiling point (m ³ /kmol)	0.08341
Acentric factor (-)	0.2090
Radius of gyration (m)	3.004E-10
Solubility parameter (sqrt(J/m ³))	1.870E+04
Dipole moment (Coulomb.m)	0.0000
Van der Waals volume (m ³ /kmol)	0.04840
Van der Waals area (m ² /kmol)	6.000E+08
H _f heat of formation (J/kmol)	8.288E+07
H _f Gibbs energy of formation (J/kmol)	1.296E+08
H _f absolute entropy (J/kmol.K)	2.693E+05
Heat of fusion at melting point (J/kmol)	9.866E+06
Heat of vaporization at normal boiling point (J/kmol)	*
Standard net heat of combustion (J/kmol)	-3.138E+09

Click here to estimate properties

Order by property Order by method

Apply

Configuring TEA property packages

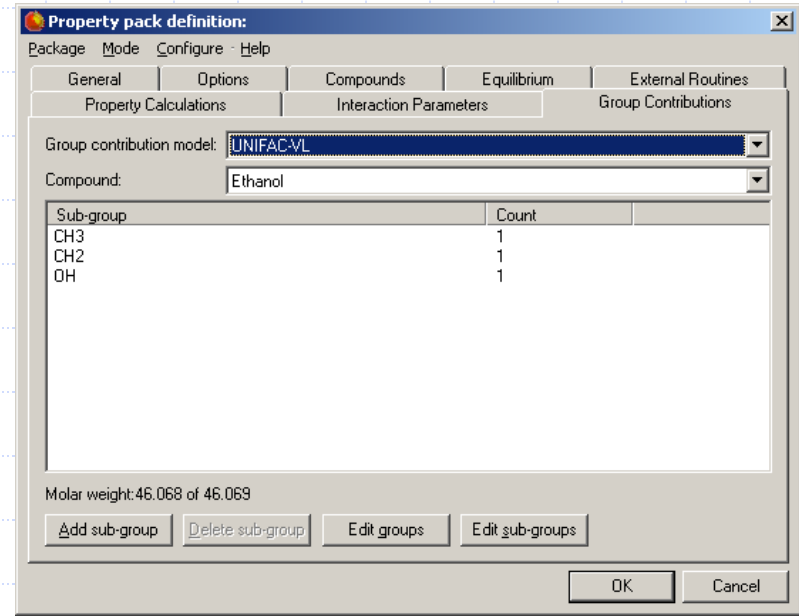
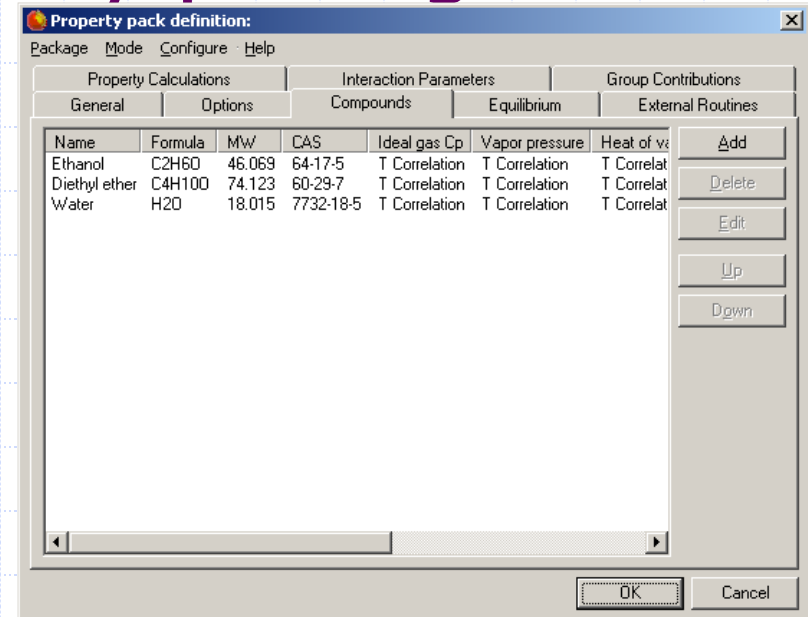


- ◆ Choosing Property Calculations from the Configure menu allows us to see which models are actually used for each property.
- ◆ We can add properties, remove properties, or change calculation methods.

Configuring TEA property packages

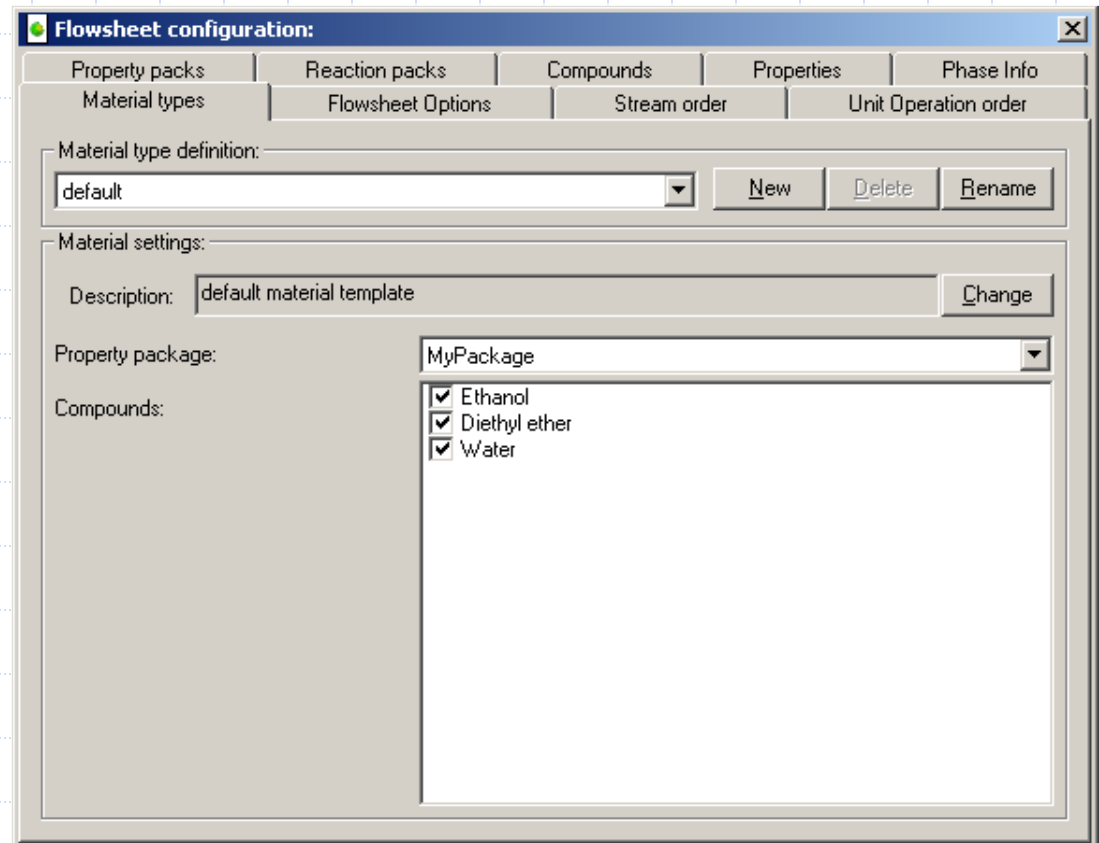
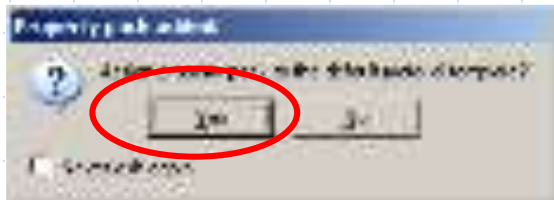
- ◆ some property calculations are defined per compound.
 - An example in the current package is vapor pressure.
 - Per-compound calculation details can be found on the Compounds tab.
 - For all compounds, vapor pressure is by default calculated from a temperature correlation.

- ◆ Parameters of models can also be inspected.
 - Here, we see the UNIFAC groups that define ethanol.
 - Group and sub-group parameters are available via the buttons.



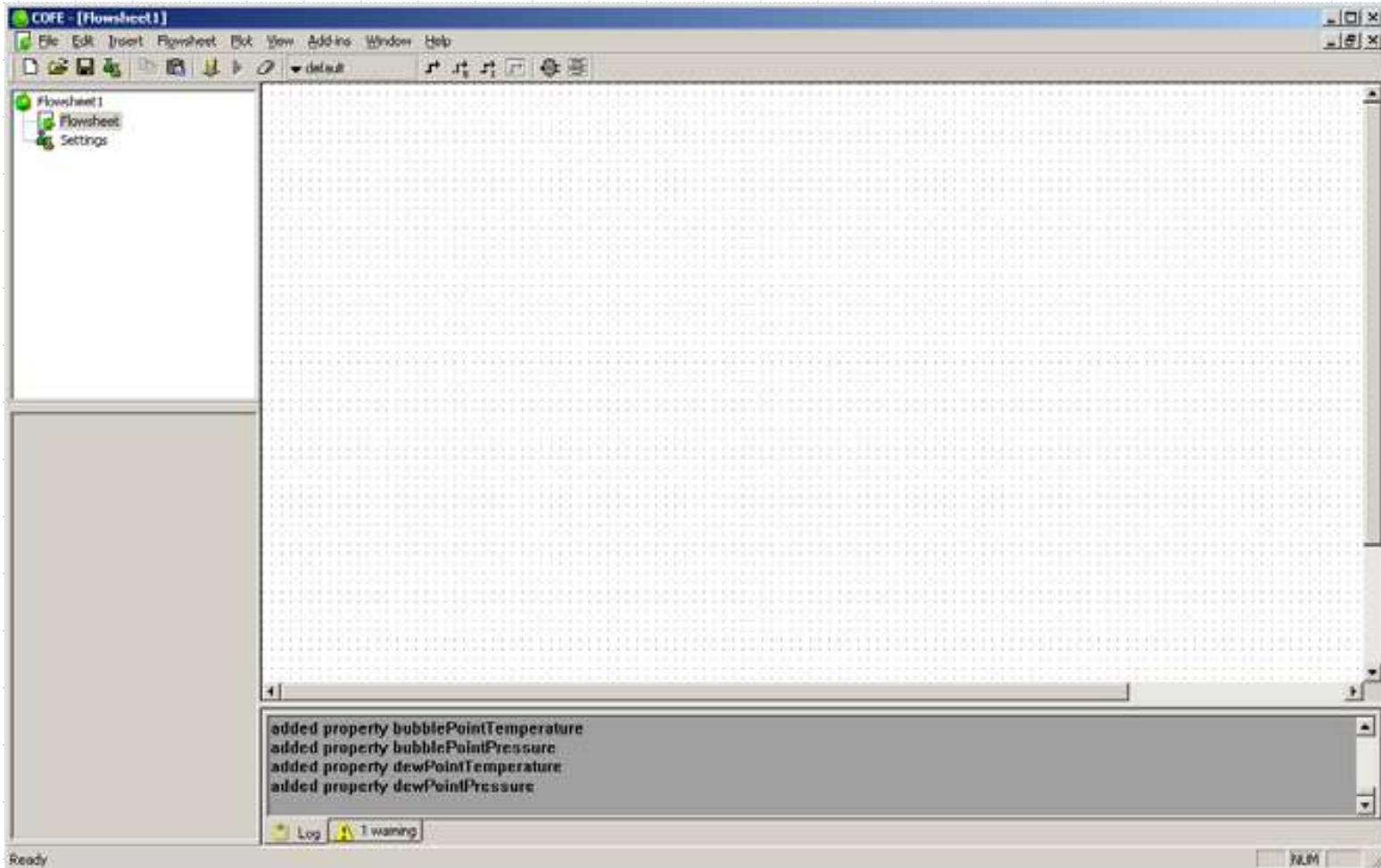
Configuring TEA property packages

- ◆ Finally we click OK to accept the Property Package configuration.
 - After it is inserted into COFE, we are asked whether we want to couple this to the default material template. We do.

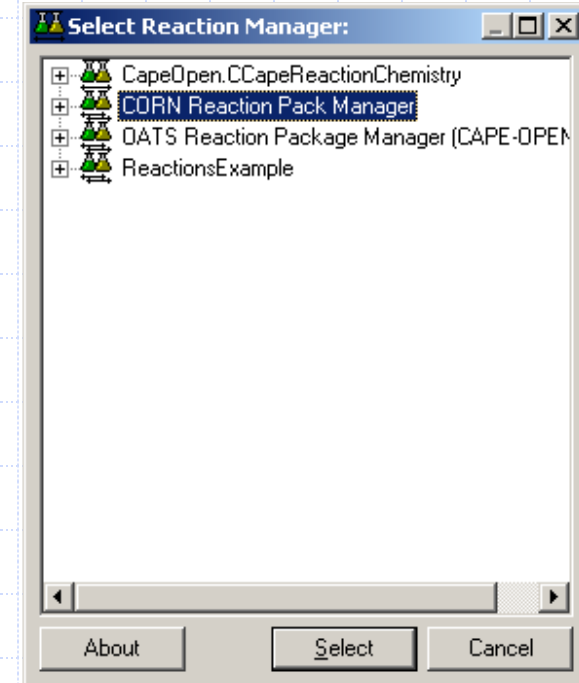
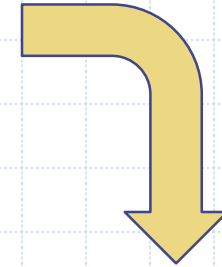
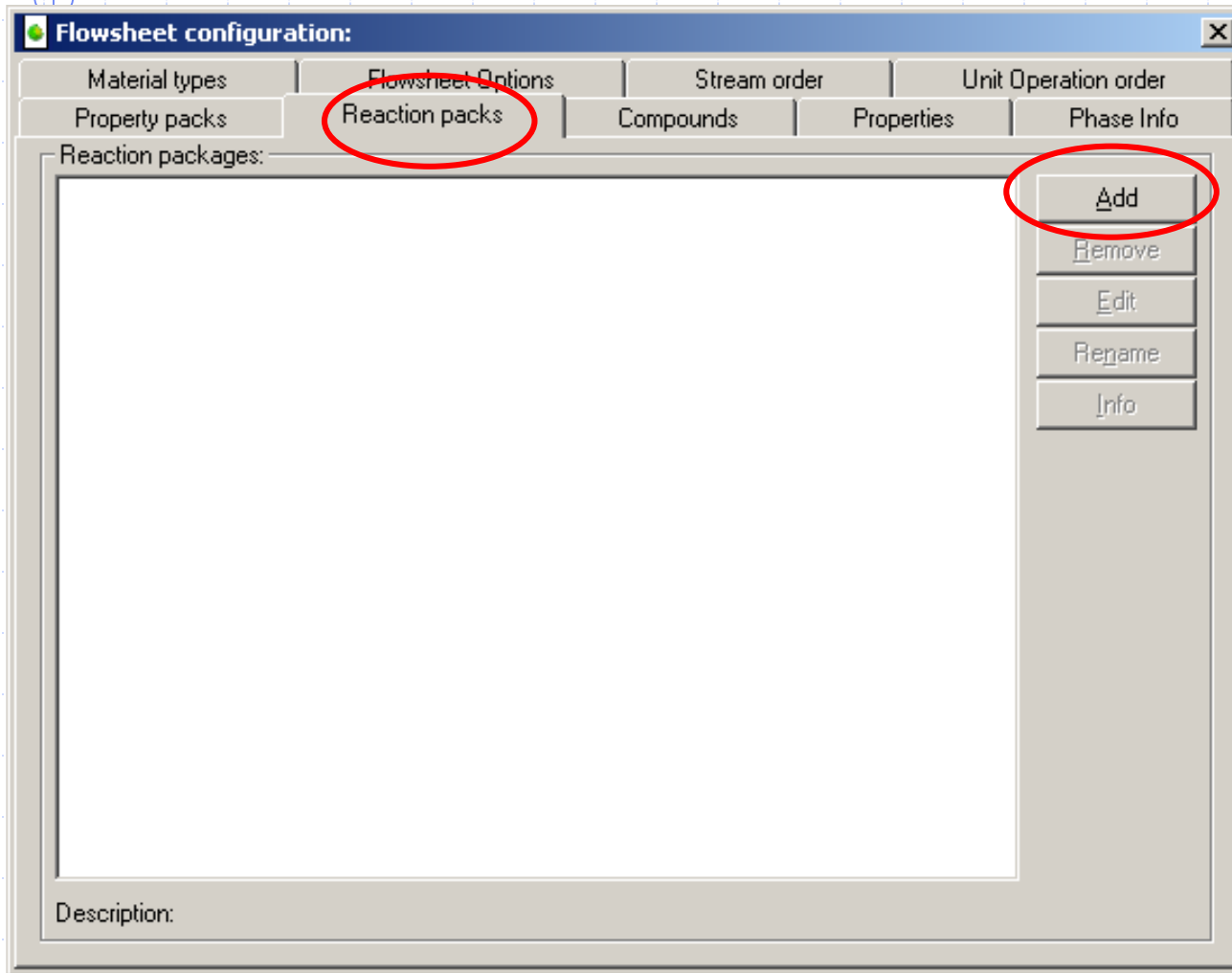


Setting up flowsheet with COFE

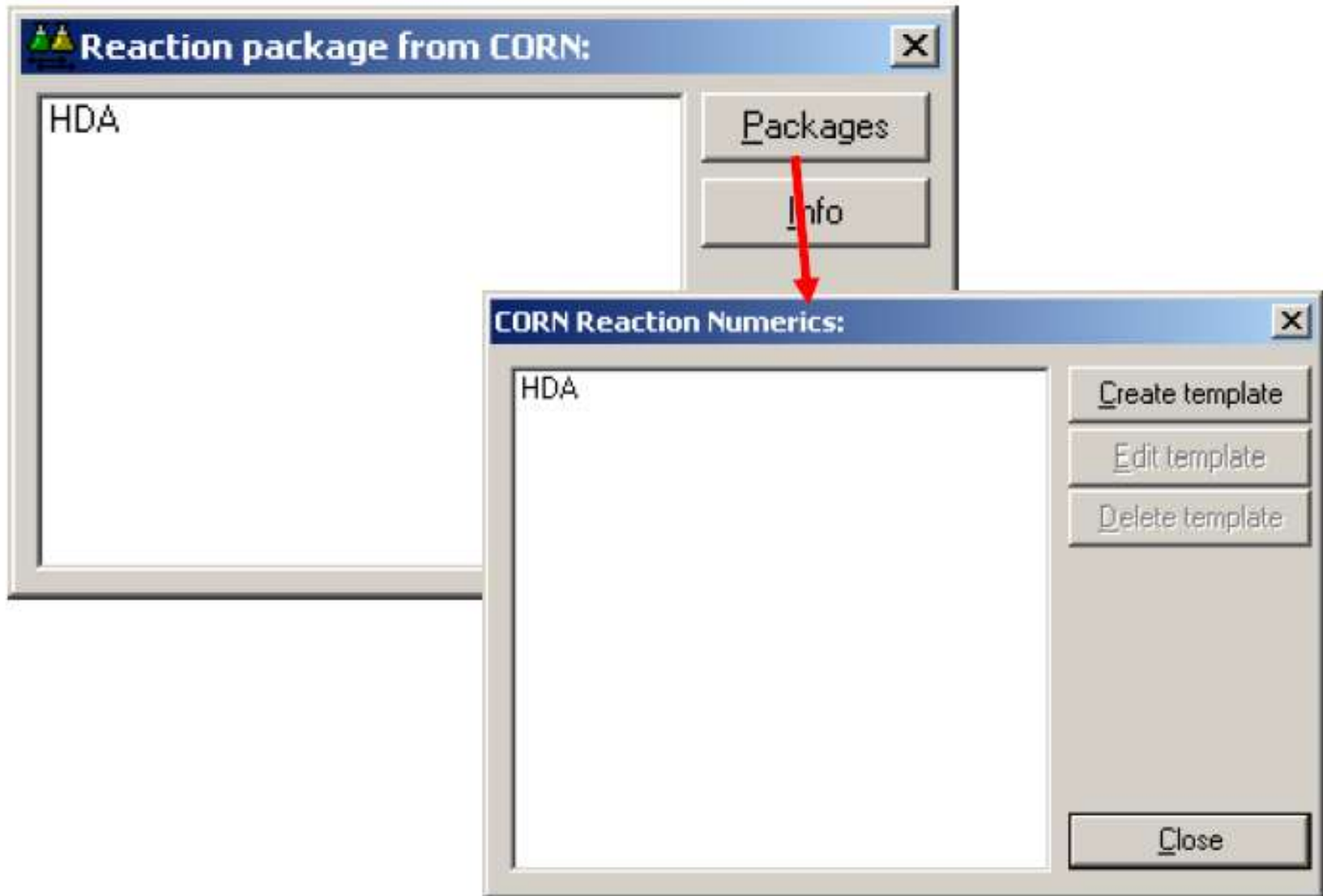
◆ Empty COFE document



Setting up reactions

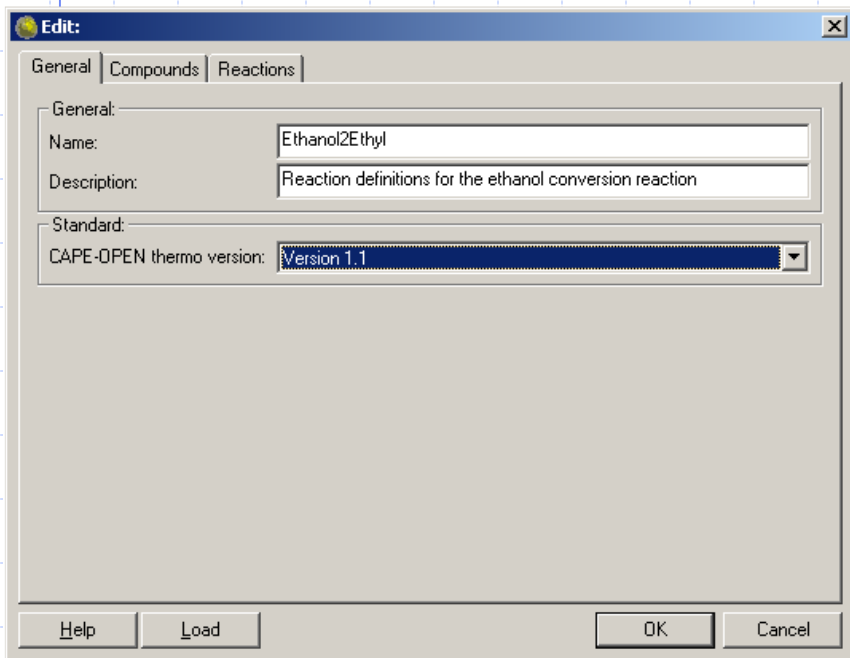


Setting up CORN



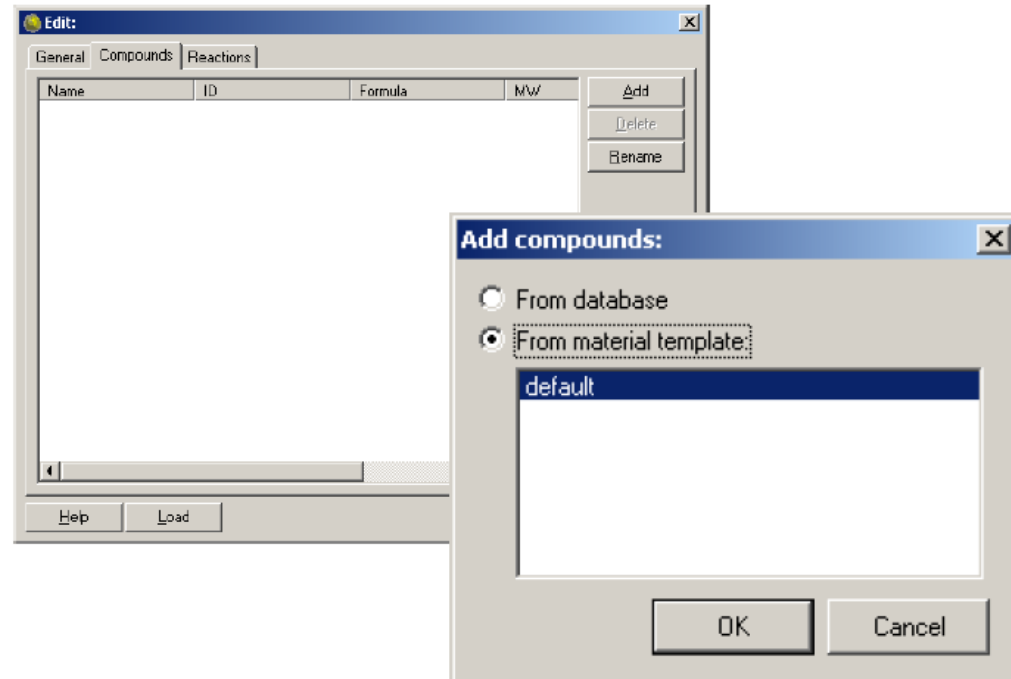
Editing a reaction package

- ◆ Create a name and description for the reaction package template



- ◆ add the compounds.

- Hit Add on the Compounds page.
- To use compounds defined in the simulation, choose a material template as the source for compounds and hit OK

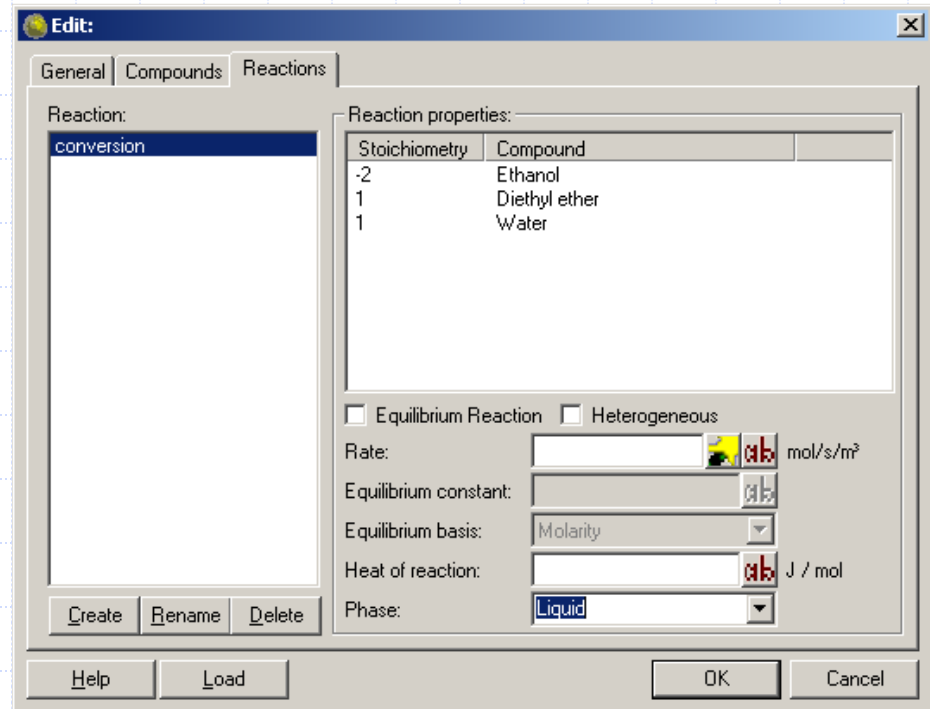
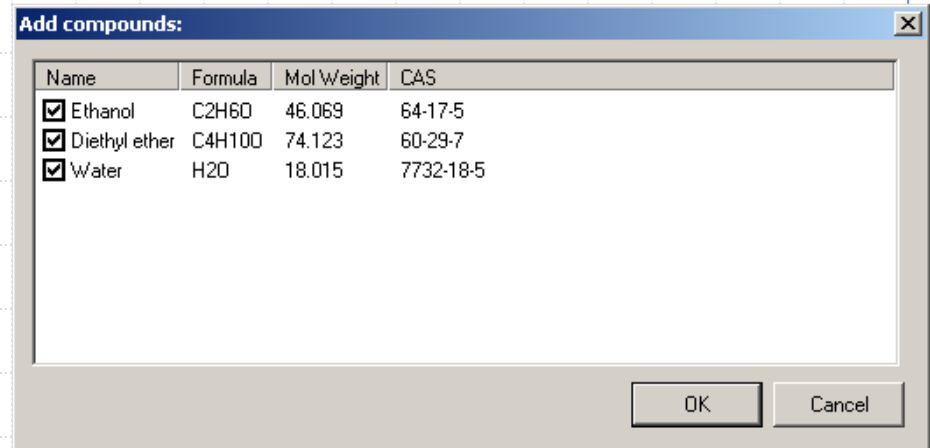


Editing a reaction package

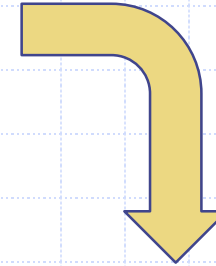
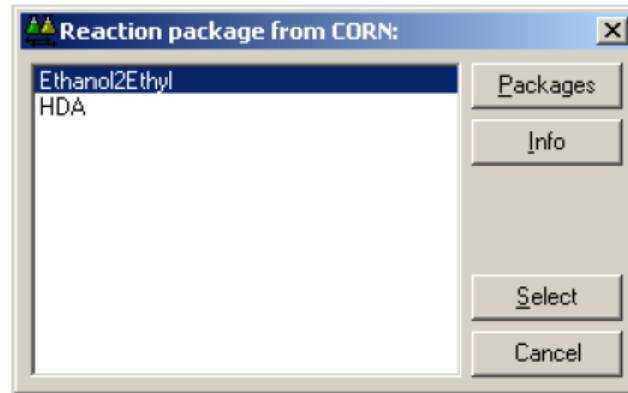
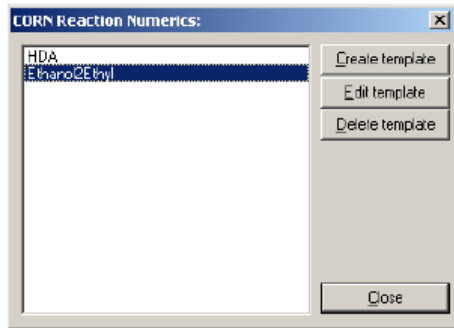
◆ Add all the components needed

◆ Define the reaction.

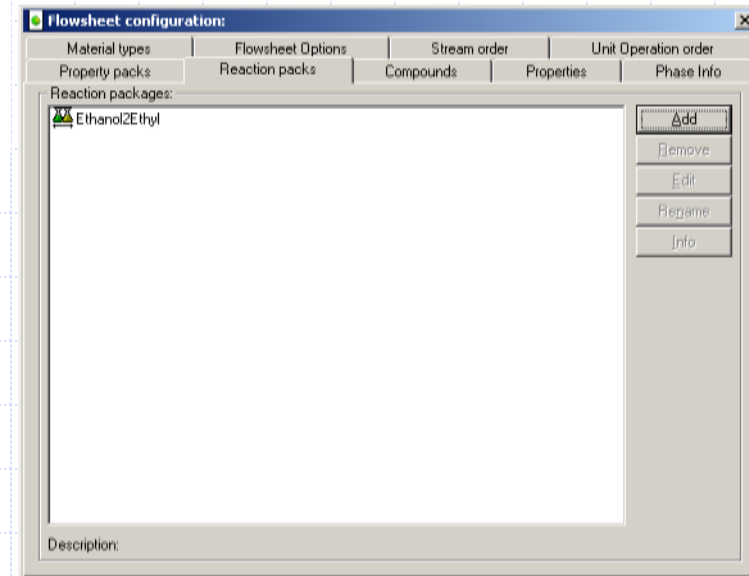
- On the reaction page, click Create and give a name.
- Define stoichiometry
- Select the reaction phase
- Define a reaction rate, equilibrium constant or heat of reaction.
- For conversion reactions no specification are needed



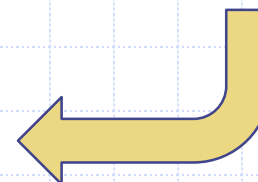
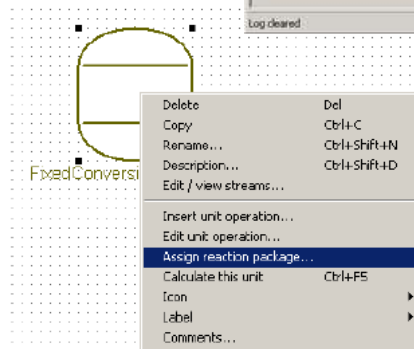
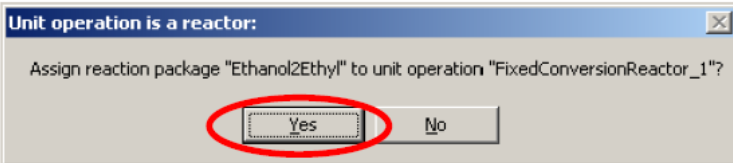
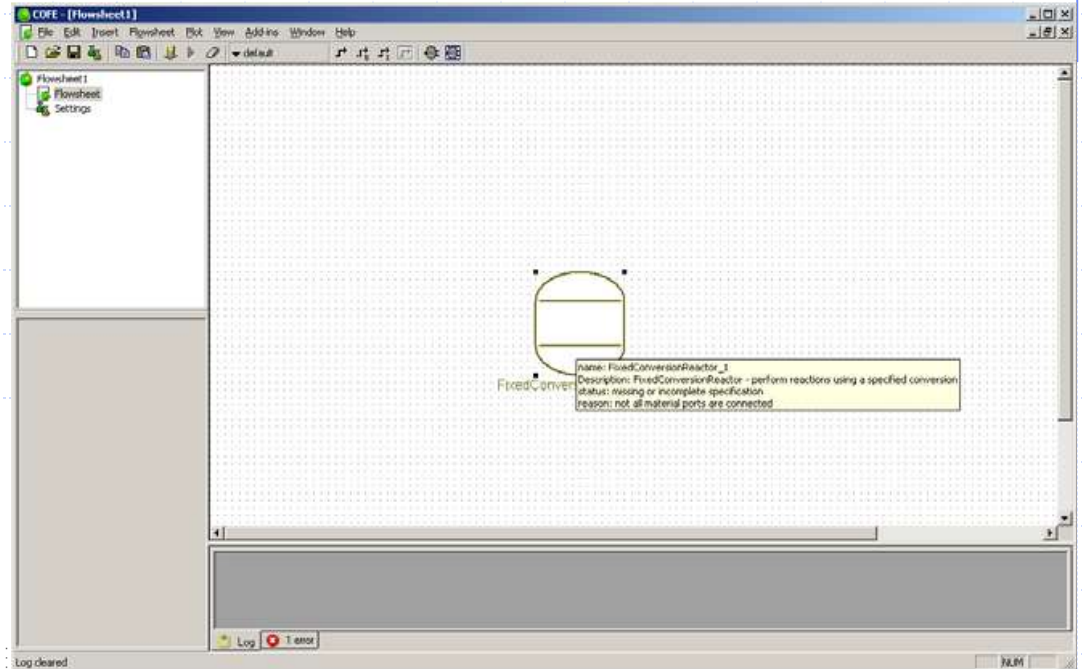
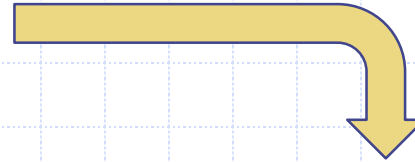
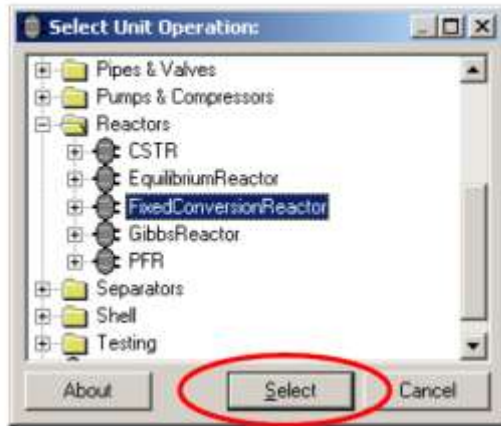
Add the reaction package to the simulation



Back to COFE

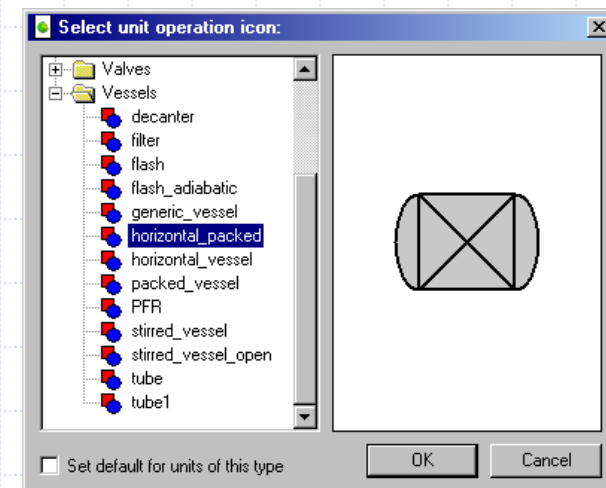
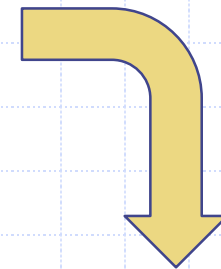
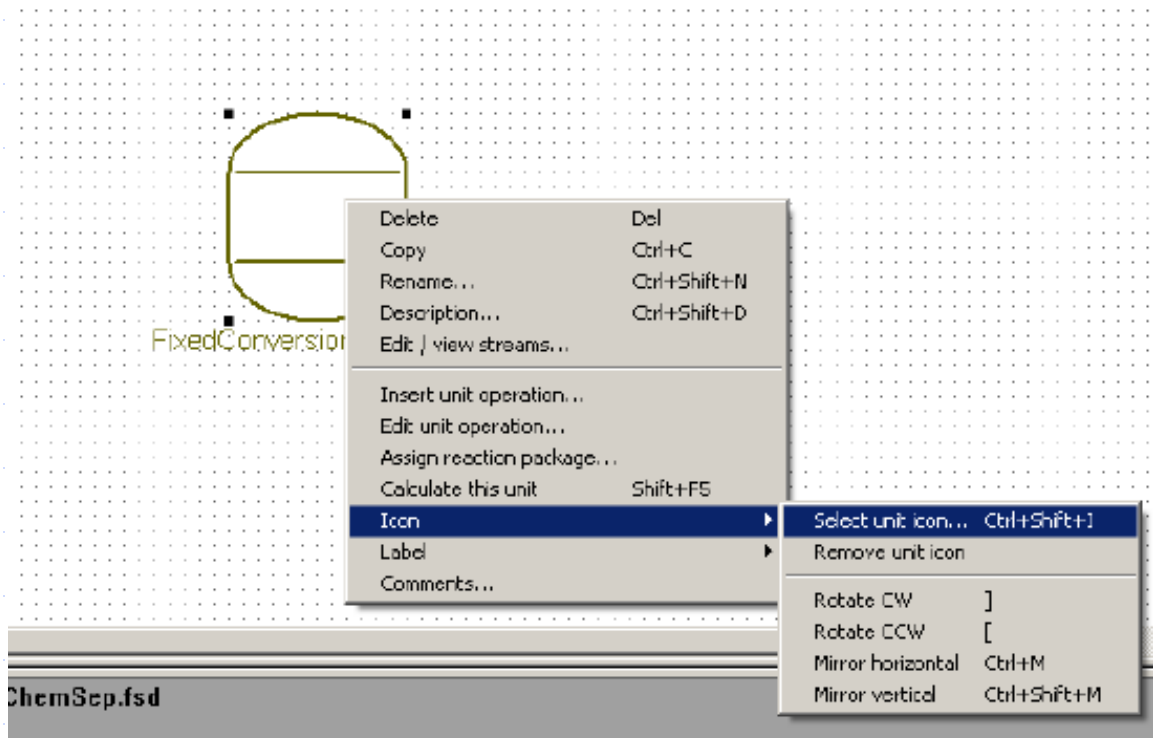


Inserting the reactor into COFE

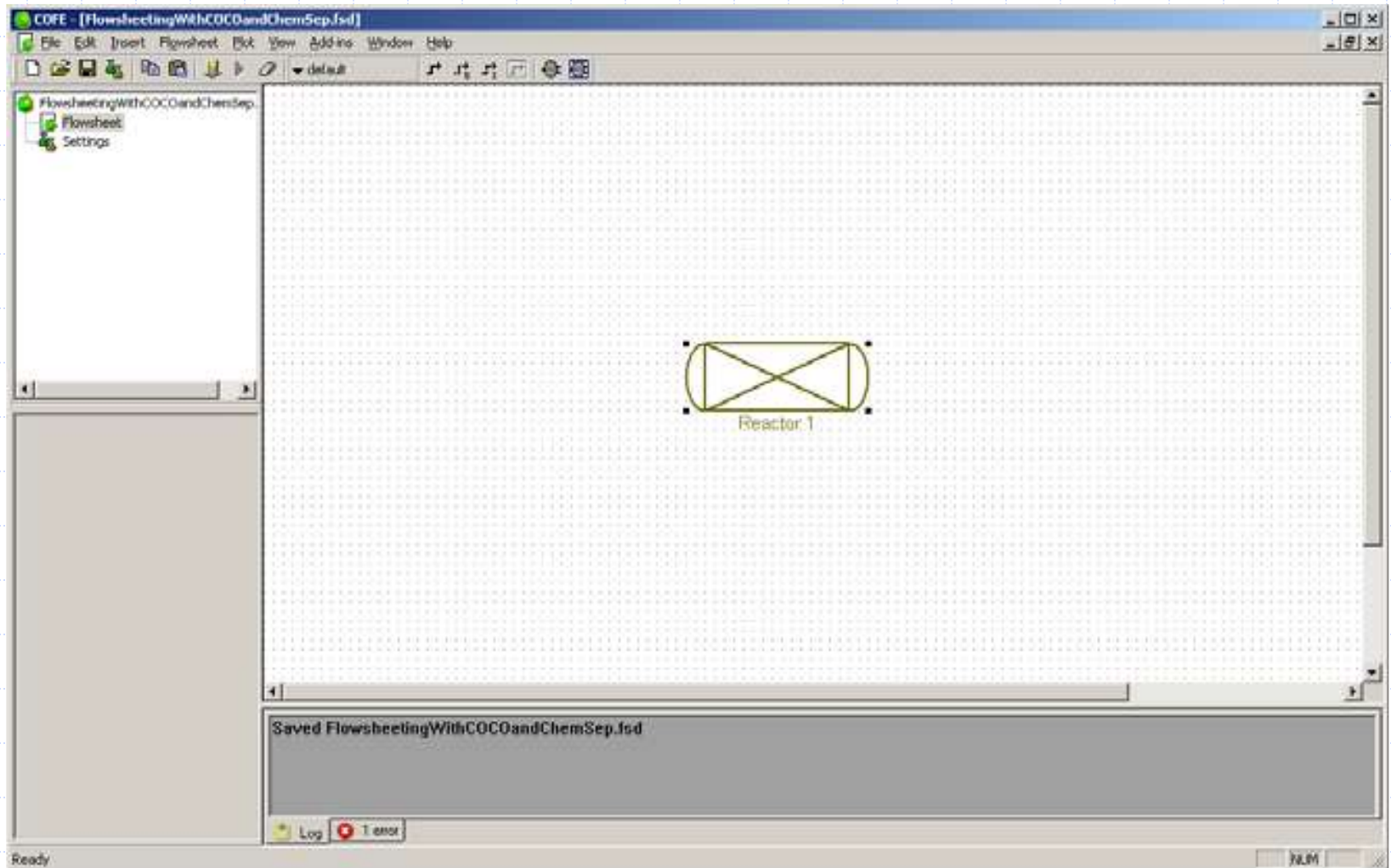


Changing the appearance of the reactor

- ◆ Right click on the reactor to pop up unit operation menu.
 - From the Icon sub menu, pick Select Unit Icon.

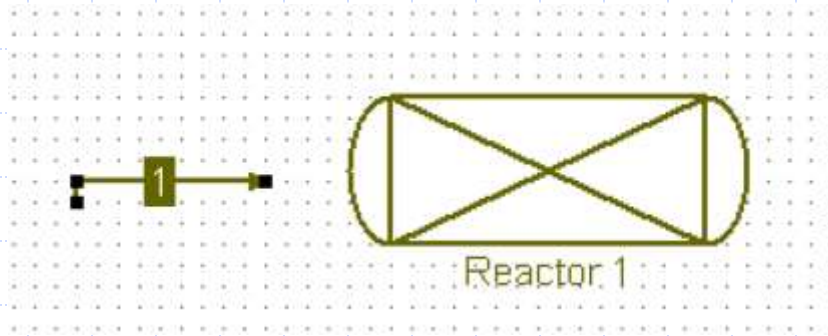


Inserting the reactor

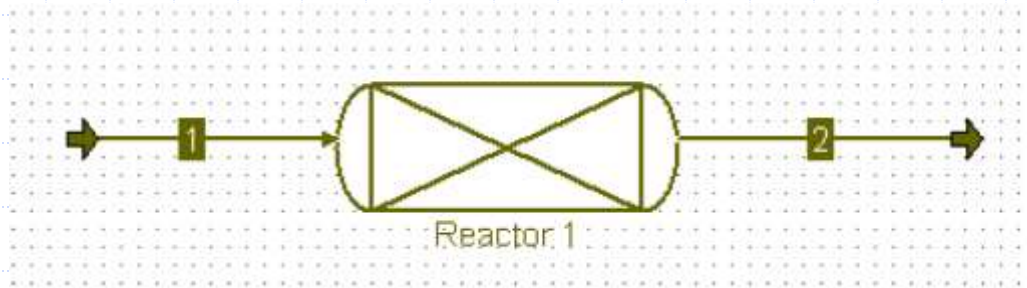


Inserting reactor feed and product stream

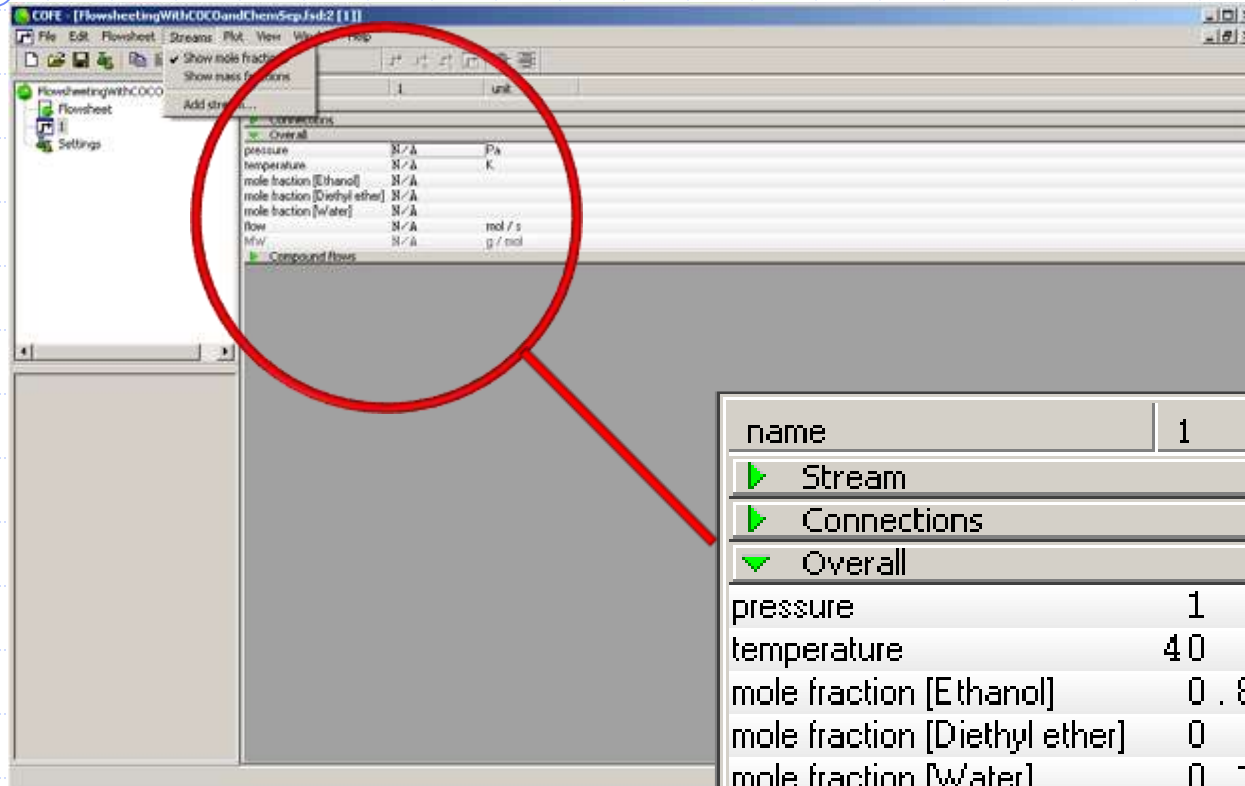
◆ Reactor feed stream



◆ Product stream



Specify the feed stream



name	1	unit
▶ Stream		
▶ Connections		
▼ Overall		
pressure	1	atm
temperature	40	°C
mole fraction [Ethanol]	0.85	
mole fraction [Diethyl ether]	0	
mole fraction [Water]	0.15	
flow	20	mol / s
M/w	41.8609	g / mol
▶ Compound flows		
▼ Phase Fractions		
molar phaseFraction [Liquid]	1	
▶ Liquid composition		
▶ Overall properties		
▶ Liquid properties		

Reactor's specification

Unit operation Reactor 1:

Parameter	Value	Unit
Pressure drop	0	Pa
Heat duty type	Isothermal	
Temperature	300	K
Heat duty	0	W
Enthalpy Type	Use EnthalpyF	
Thermo Version	1.1	

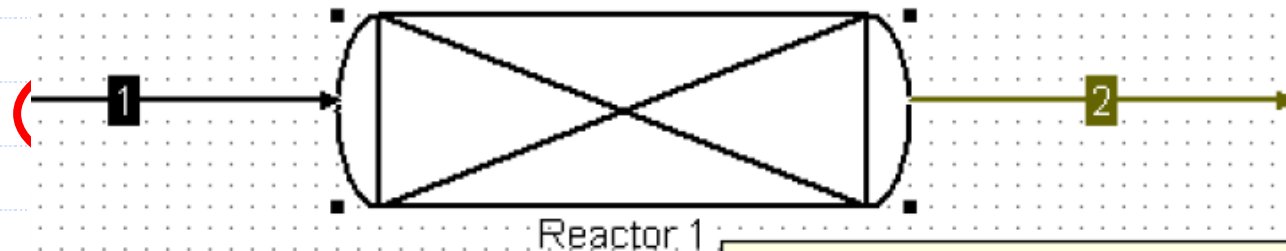
Unit Reactor 1:

General | Report | Operation | Reactions | About | Ports

Pressure drop: 0 Pa

Isothermal: 313.15 K

Heat duty: 0 J/s



Reactor 1

name: Reactor 1
Description: FixedConversionReactor - perform reactions using a specified conversion
status: specification complete

Specify reaction:

Reaction ID: conversion

Conversion: 0.5

Of compound: Ethanol

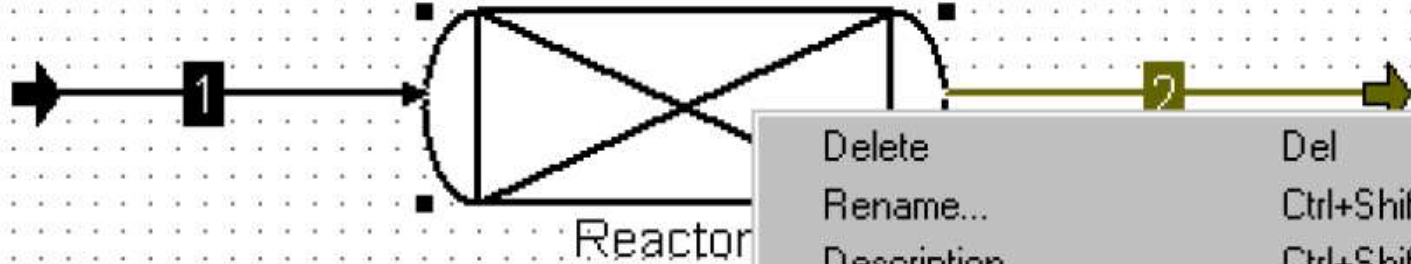
Serial reactions

Add Edit Delete Up Down

OK Cancel

Help

Calculate the reactor



- Delete Del
- Rename... Ctrl+Shift+N
- Description... Ctrl+Shift+D
- Edit / view streams...
- Insert unit operation...
- Edit unit operation...
- Assign reaction package...
- Calculate this unit Ctrl+F5**
- Icon ▶
- Label ▶
- Comments...

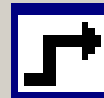
Calculate unit:

 Finished calculating unit Reactor 1

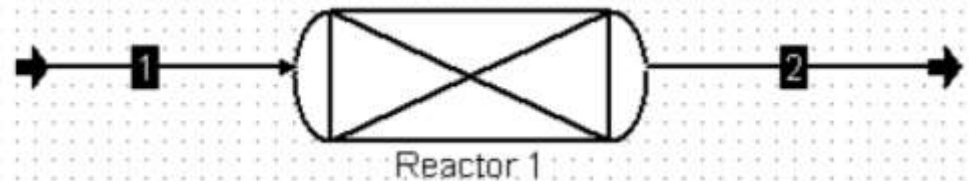
Ok

Never show this message again

Reactor's results



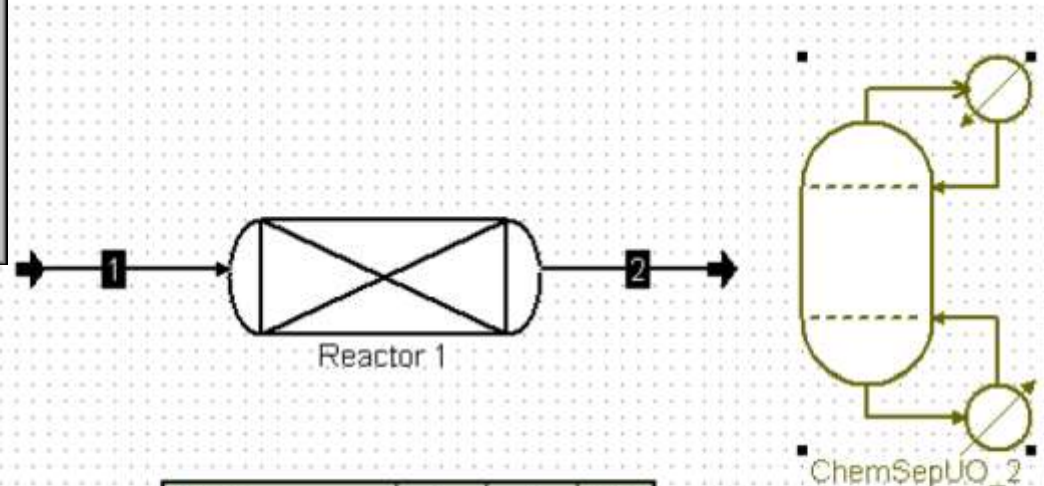
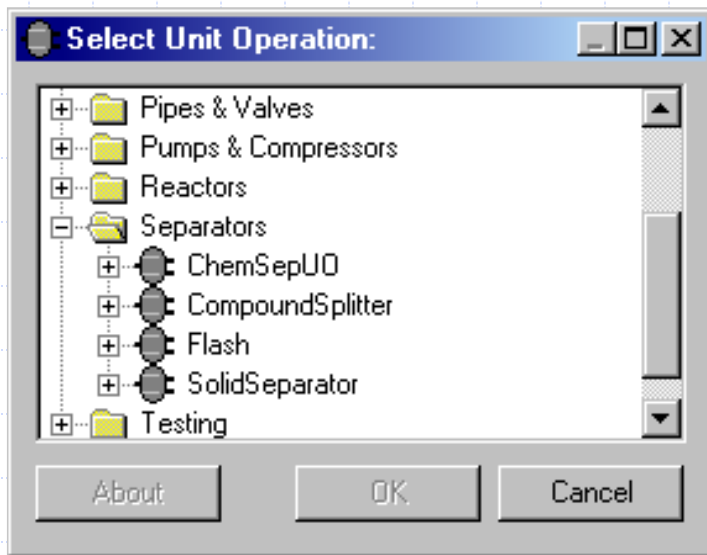
name	1	2	unit
▶ Stream			
▶ Connections			
▼ Overall			
pressure	1	1	atm
temperature	40	40	°C
mole fraction [Ethanol]	0.85	0.425	
mole fraction [Diethyl ether]	0	0.2125	
mole fraction [Water]	0.15	0.3625	
flow	20	20	mol / s
MW	41.8609	41.8609	g / mol
▶ Compound flows			
▼ Phase Fractions			
molar phaseFraction [Liquid]	1	1	
▶ Liquid composition			
▶ Overall properties			
▶ Liquid properties			



Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

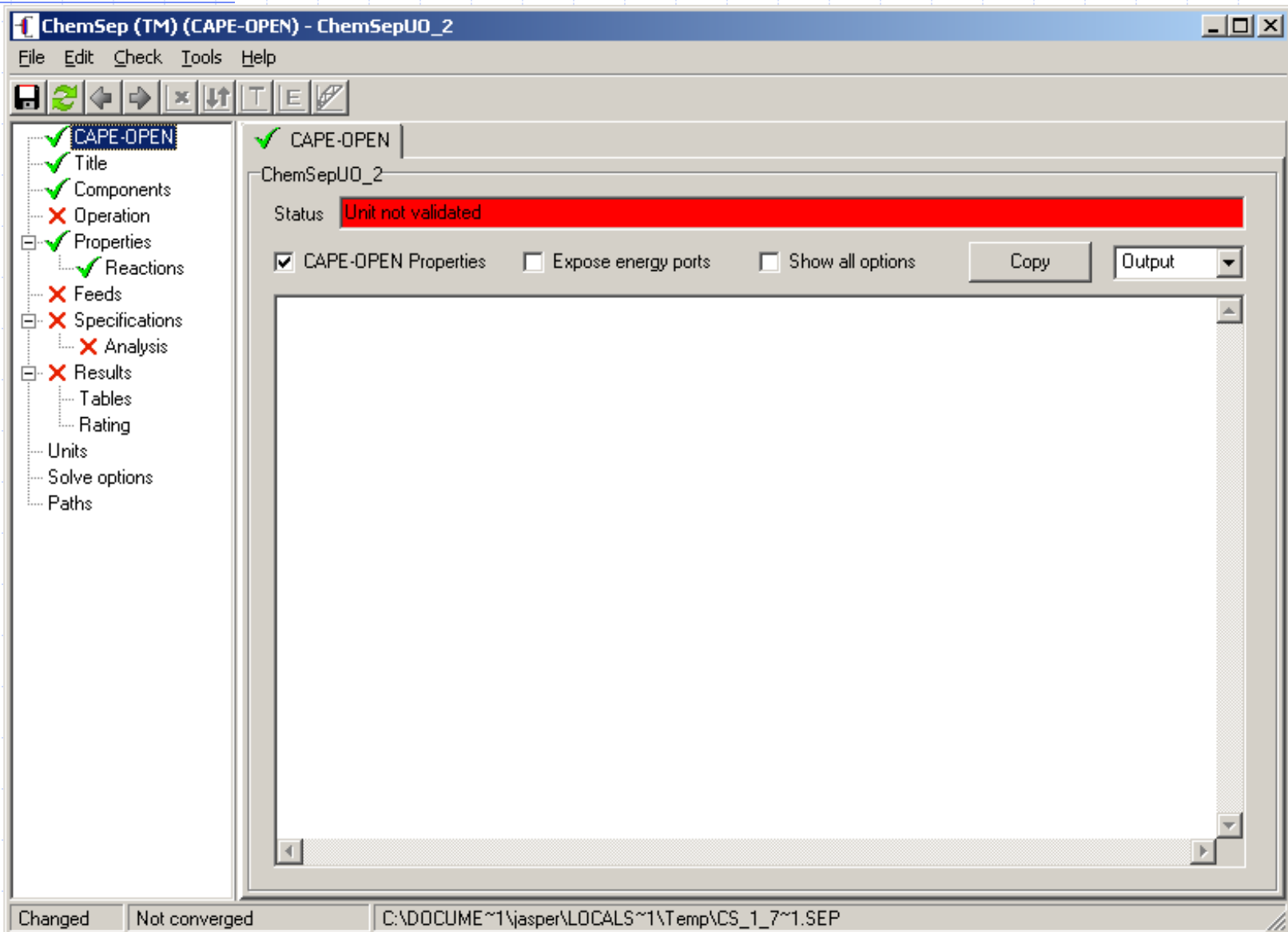
Using ChemSep in COFE

◆ Inserting ChemSep in COFE



Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

Inserting ChemSep column



Configuring ChemSep column

The screenshot displays the ChemSep (TM) (CAPE-OPEN) - ChemSepUO_2 software interface. The main window shows the configuration for a distillation column. The left sidebar contains a tree view with the following items:

- CAPE-OPEN
- Title
- Components
- Operation
- Properties
- Reactions
- Feeds
- Specifications
 - Analysis
 - Pressures
 - Heaters/Coolers
 - Efficiencies
 - Column specs
- Results
 - Tables
 - Graphs
 - McCabe-Thiele
 - Rating
- Units
- Solve options
- Paths

The main configuration area includes the following settings:

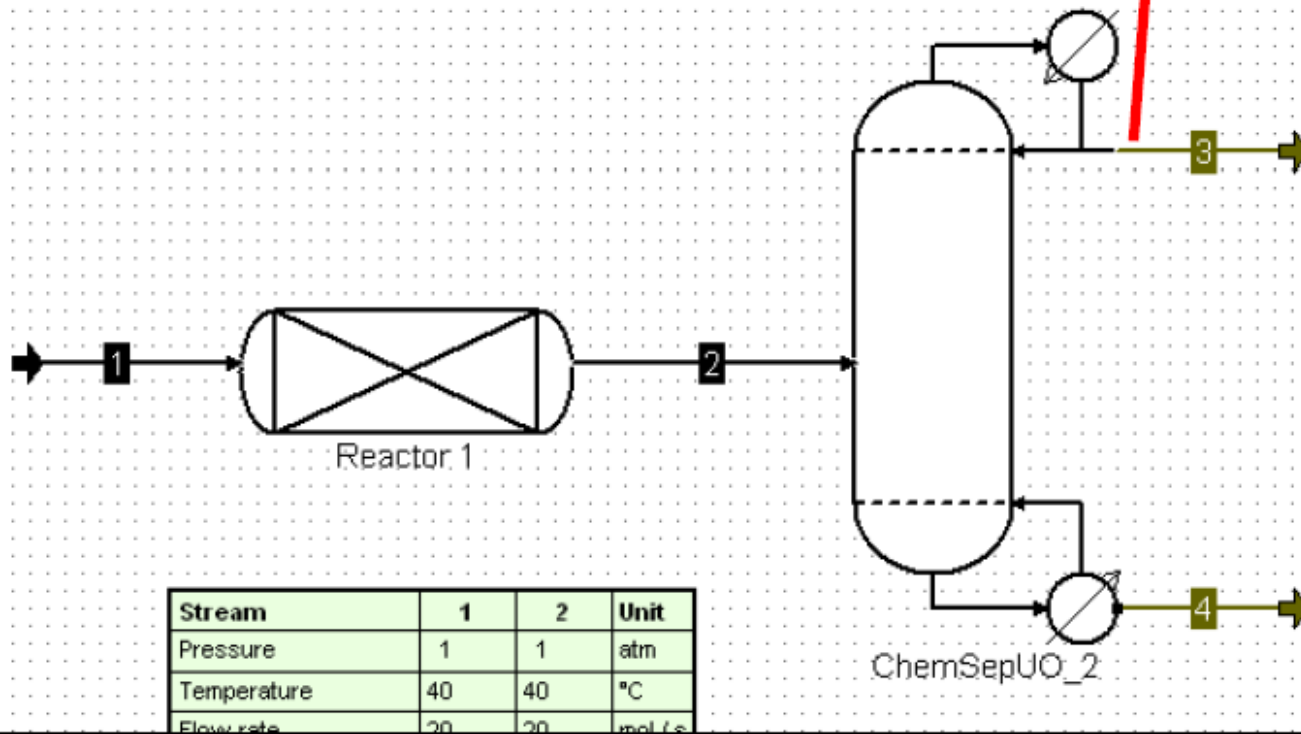
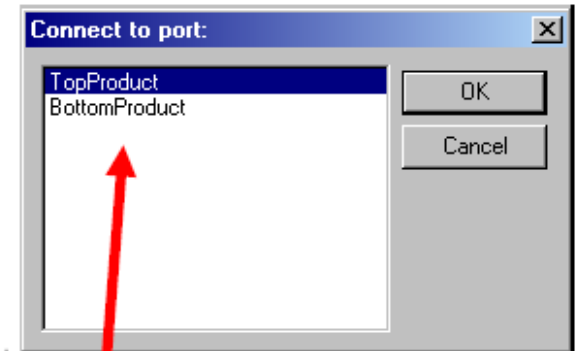
- Operation: Equilibrium column
- Configuration:
 - Operation: Simple Distillation
 - Condenser: Total (Liquid product)
 - Reboiler: Partial (Liquid product)
 - Number of stages (e.g. 10): 10
 - Feed stage(s) (e.g. 5,7): 7
 - Sidestream.stage(s) (e.g. 2,9):
 - Pumparound(s) (e.g. 6>8, 9>1):

Three confirmation dialog boxes are overlaid on the interface, each with the 'Yes' button circled in red:

- Confirm**: Problem specification is incomplete, are you sure you want to close this window. Buttons: Yes, No, Cancel.
- Confirm**: Do you want to save the current input in ChemSepUO_2. Buttons: Yes, No, Cancel.
- Update ChemSep icon:** The column configuration has changed. Update COFE icon? Buttons: Yes, No.

The status bar at the bottom shows 'Changed', 'Not converged', and the file path 'C:\DOCUME~1\jasper\LOCALS~1\Temp\CS_1_7~1.SEP'.

Connecting the ChemSep column



Configuring ChemSep column

✓ Pressures

Column Pressure Specifications

Condenser pressure (N/m²)

Column pressure

Top pressure (N/m²)

Pressure drop / stage (N/m²)

Bottom pressure (N/m²)

✓ Heaters/Coolers

Column and Stage Heat Duties

Column heat loss (J/s)

✓ Efficiencies

Specify Stage Efficiencies

Default stage efficiency (-)

- ✗ Results
- Tables
- Graphs
- McCabe-Thiele
- Rating
- Units

Configuring ChemSep column

✓ Column specs

Column Product Specifications

Top product name Condenser duty name

Top specification = (-)

Bottom product name Reboiler duty name

Bottom specification = (kmol/s)

Note: This bottom specification is just to get us started; later we will change it.

Run the column

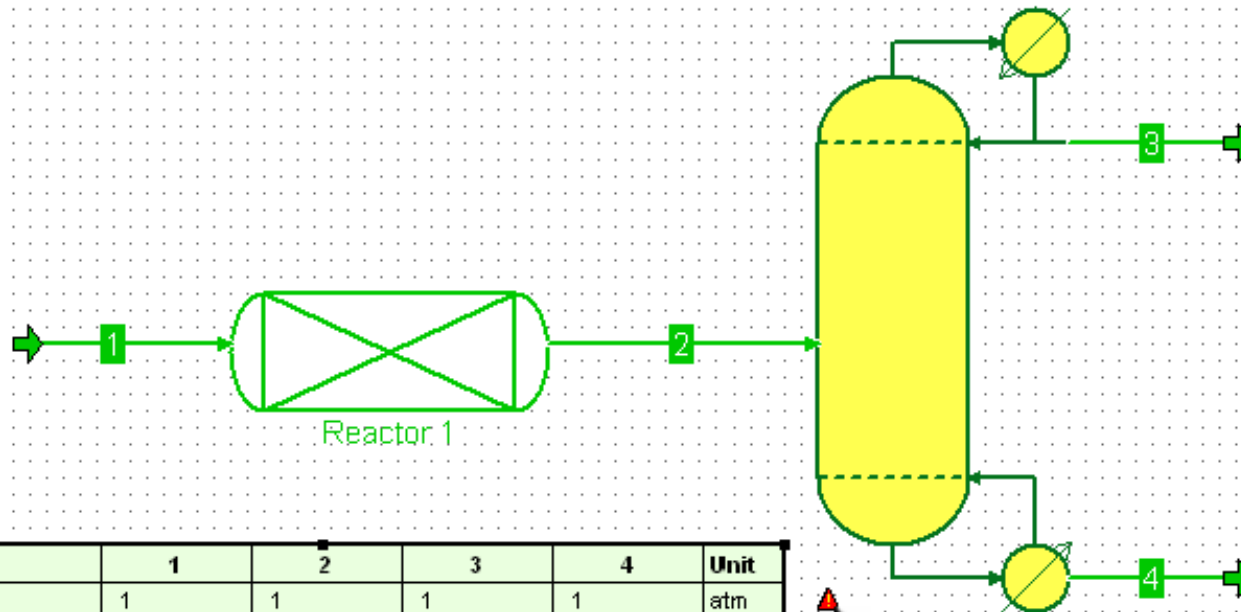
The screenshot shows a process simulation software window titled "CDPE - [FlowsheetingWithCOCCD...]. The toolbar contains a red circle around the "Run" button (a green play icon). The main workspace displays a process flow diagram with a reactor labeled "Reactor 1" and a distillation column labeled "ChemSepUQ_2".

Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.05	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

message: Warning: temperature out of range for liquid thermal conductivity correlation for compound Ethanol [T = 353.49 K, range = [159.05
message: Warning: temperature out of range for liquid thermal conductivity correlation for compound Ethanol [T = 353.30 K, range = [159.05
[last message repeated 1 time]
Solve finished in 2s, 125ms

Log Solved, 2 warnings

Checking column results

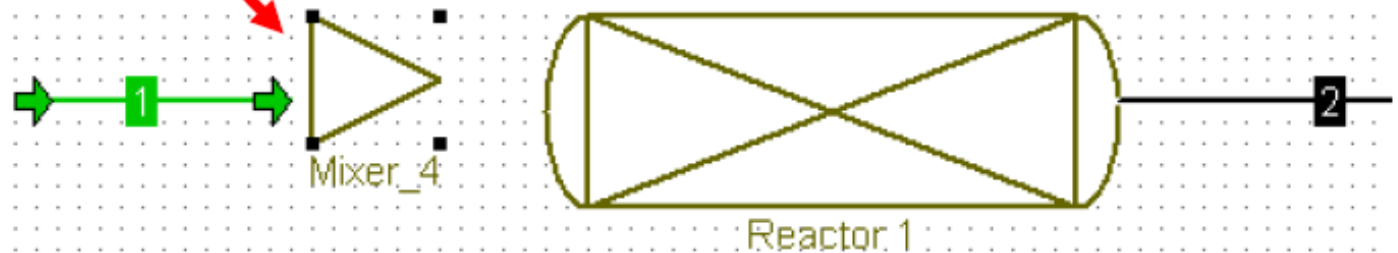
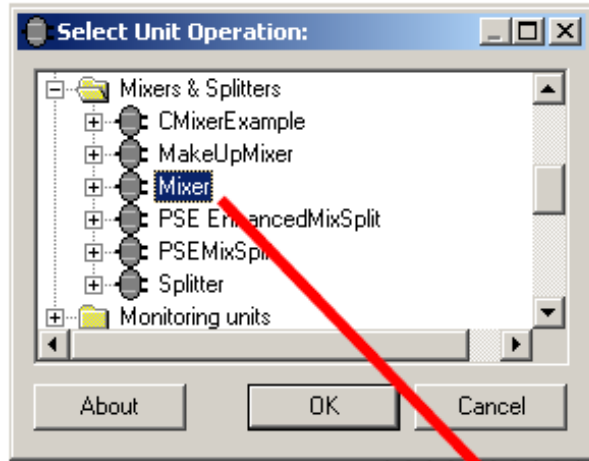


Stream	1	2	3	4	Unit
Pressure	1	1	1	1	atm
Temperature	40	40	36.3781	80.1532	°C
Flow rate	20	20	5	15	mol / s
Mole frac Ethanol	0.85	0.425	0.140139	0.519954	
Mole frac Diethyl ether	0	0.2125	0.849823	5.8839e-005	
Mole frac Water	0.15	0.3625	0.0100374	0.479988	

ChemSepUO_2

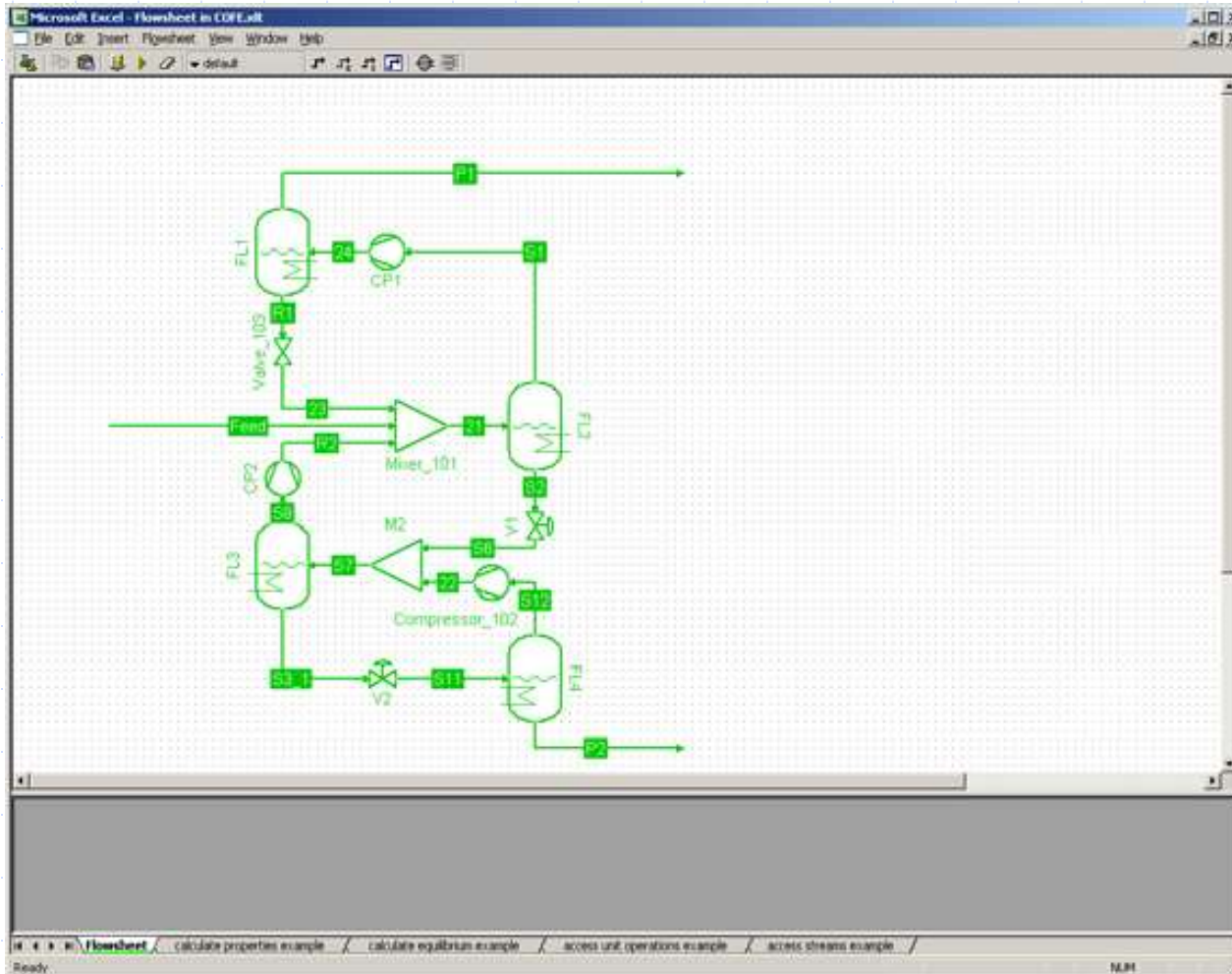
solve warnings:
 solving ChemSepUO_2
 message: Warning: temperature out of range for liquid thermal conductivity correlation for compound Ethanol (T = 353.49 K, range = [159.05 - 353.15] K)
 message: Warning: temperature out of range for liquid thermal conductivity correlation for compound Ethanol (T = 353.30 K, range = [159.05 - 353.15] K)
 (last message repeated 1 time)

Setting up the recycle



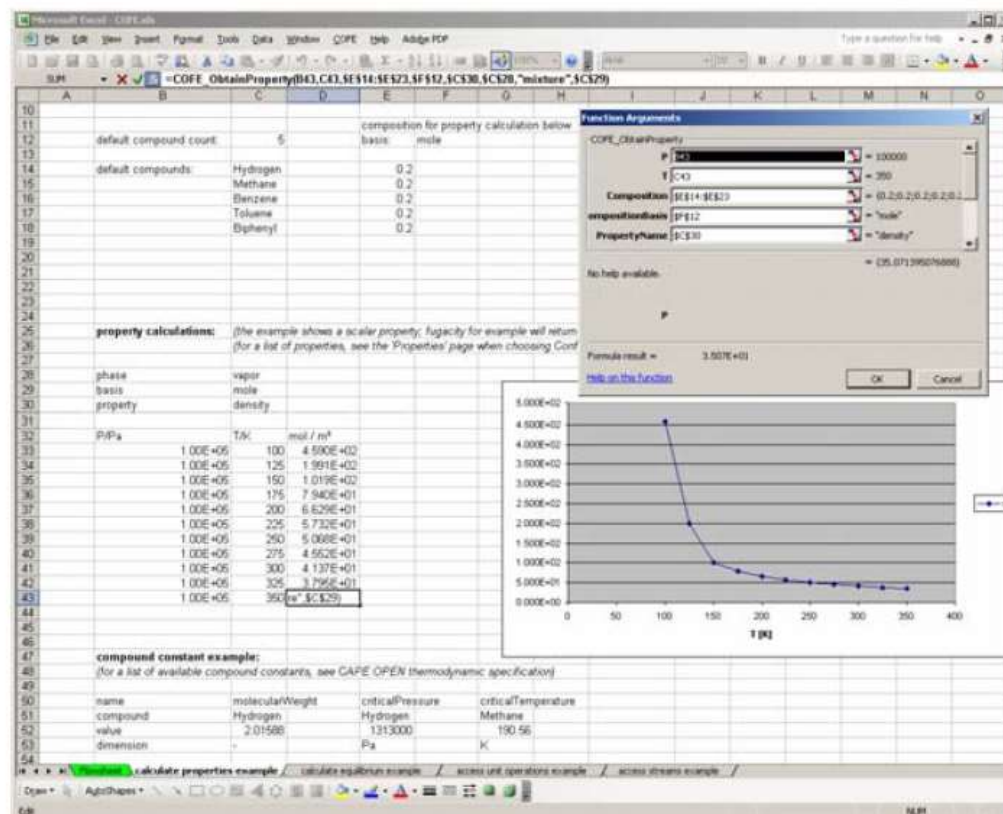
Embedding flowsheets in EXCEL

- ◆ COFE comes with an Excel template that you can use for creating a new flowsheet in Excel, or load an existing one.

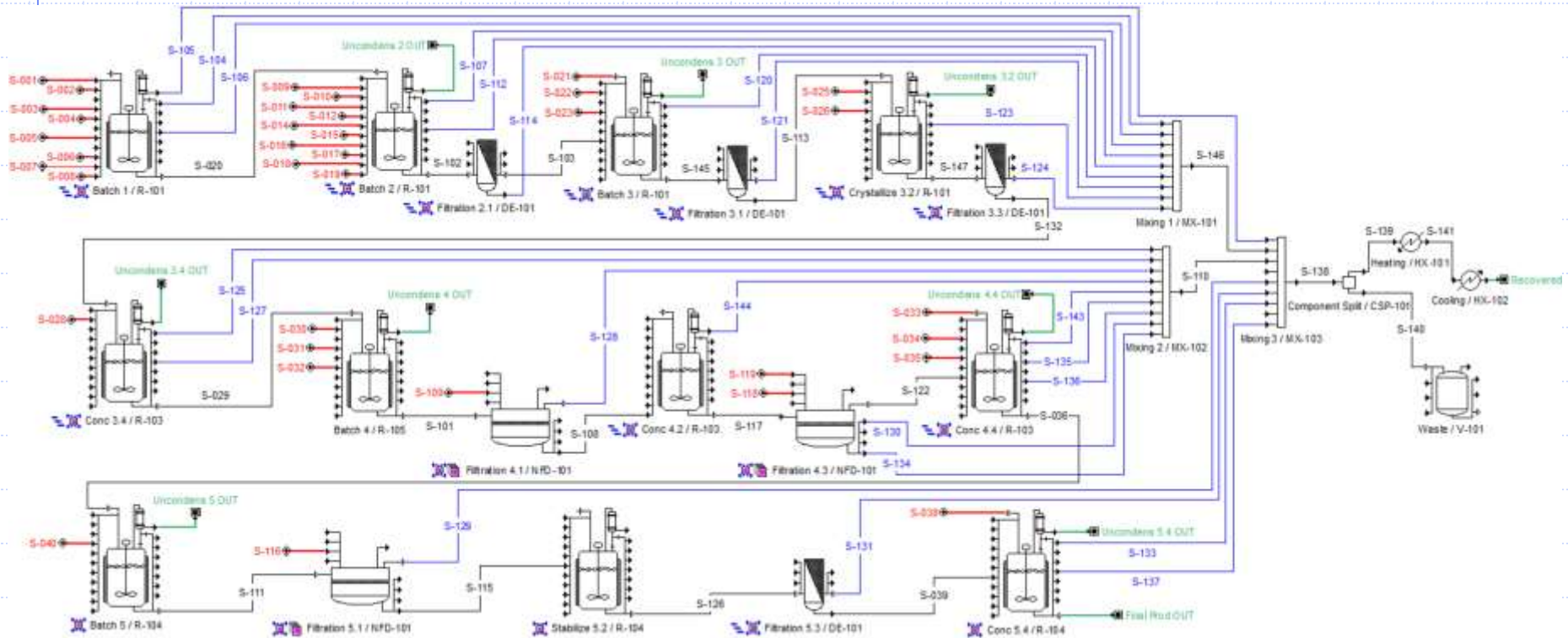


Embedding flowsheets in EXCEL

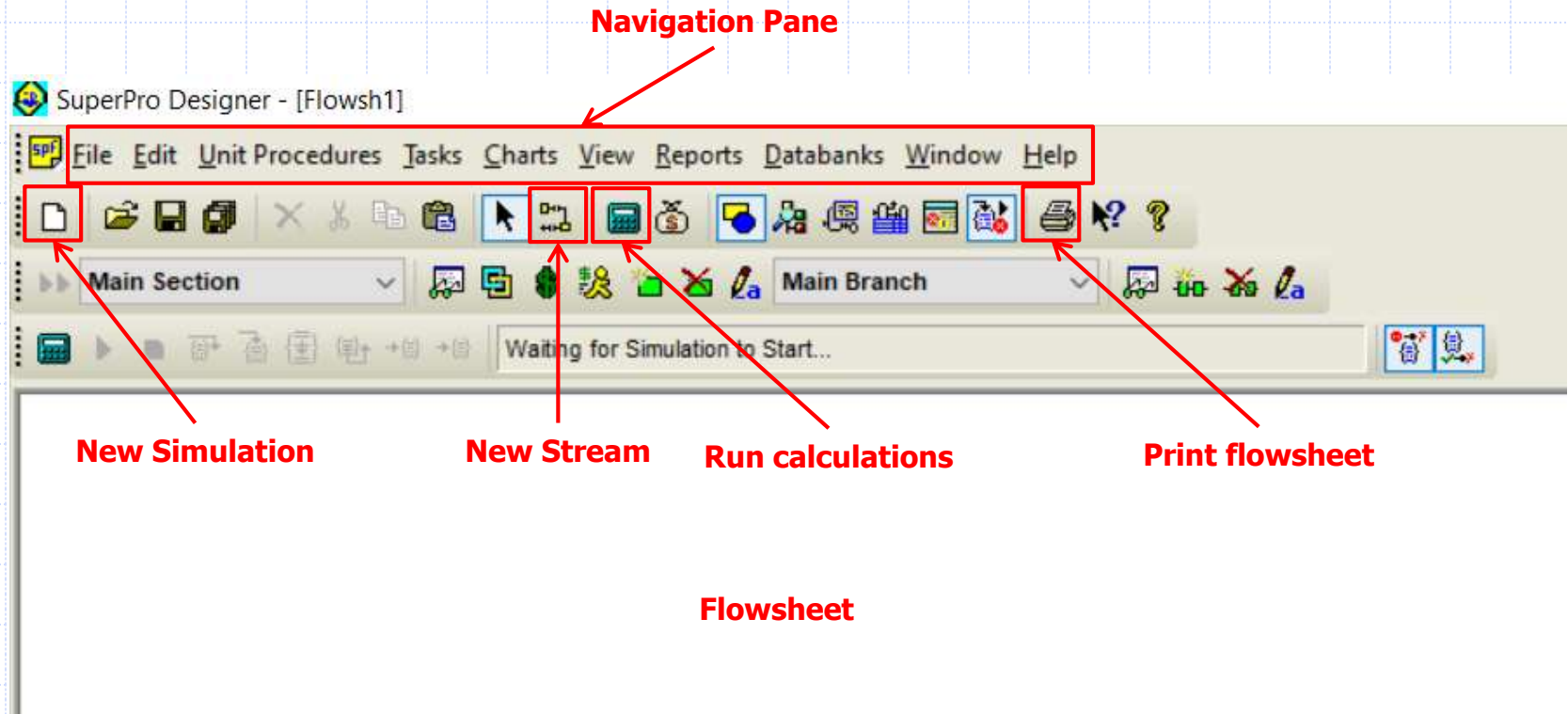
- ◆ Once the flowsheet is embedded in Excel, you can
 - **access all stream** and unit operation data.
 - perform thermodynamic **property calculations**, using whatever material types you have configured in the flowsheet.
- ◆ The Excel template comes with examples AND WIZARD



SuperPro Designer



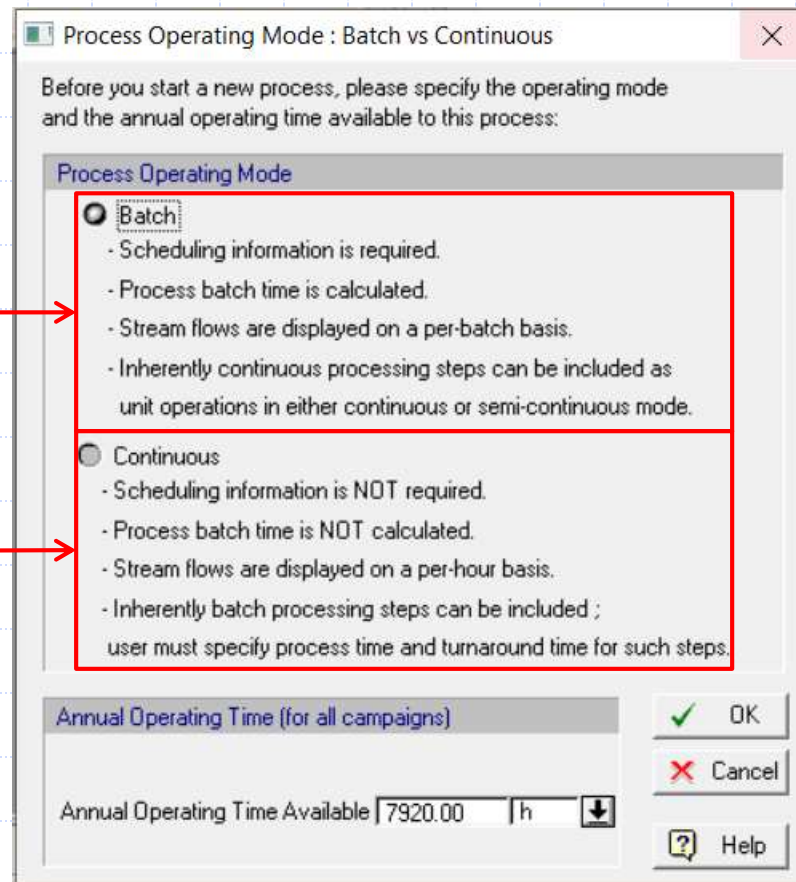
User interface



SuperPro Start Page

Batch Operating Mode

Continuous Operating Mode



SuperPro Procedure

- ◆ Start a new process file and the operation mode
- ◆ Define the default physical units
- ◆ Specify the components involved in the chemical plant
- ◆ Add any additional information regarding cost, physical property, existence of a mixture, etc...
- ◆ Insert the unit operations needed
- ◆ Connect the unit operations using streams
- ◆ Select the composition of charge streams at the battery limits
- ◆ Define the operation sequences within each unit operation
- ◆ Provide information about each operation sequence
- ◆ Check inconsistency and schedule
- ◆ Run simulation and review executive summary and Gantt
- ◆ Run economic evaluation
- ◆ Evaluate environmental impacts

SuperPro Unit Procedures

Unit Procedures	Tasks	Charts	View	...
Batch Vessel Procedure				
Continuous Reaction				
Inoculum Preparation				
Filtration				
Centrifugation				
Homogenization/Milling				
Chromatography/Adsorption				
Drying/Granulation				
Sedimentation				
Phase Change				
Distillation				
Extraction				
Absorption/Stripping				
Storage/Blending				
Heat Exchange				
Mixing				
Splitting				
Washing				
Size Reduction				
Formulation & Packaging				
Transport (near)				
Transport (far)				
Pressure Drop (Valves)				
Power Generation				
Generic Boxes				
Design Spec				

Reactors

**Solid-Liquid
separation**

Flash, Condenser, Evaporator

Liquid-Liquid separation

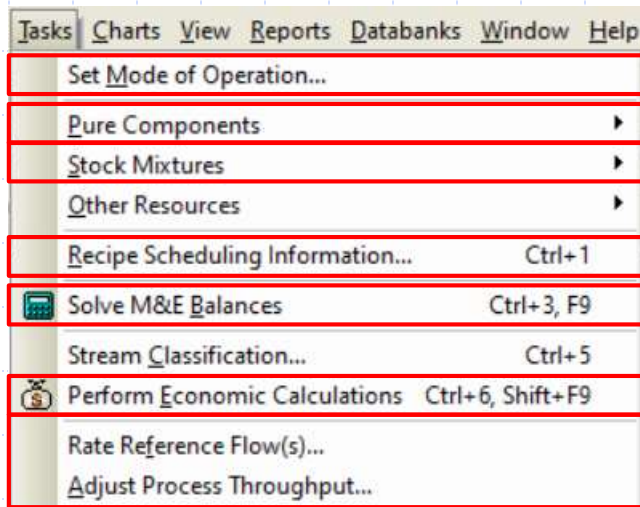
**Vapor-Liquid
separation**

Streams operations

Post-Production

Design Specification

SuperPro Tasks



Batch/Continuous mode

Add components to simulation

Add mixtures to simulation

Batches, Time, bottlenecks

Run command

Perform economic calculations

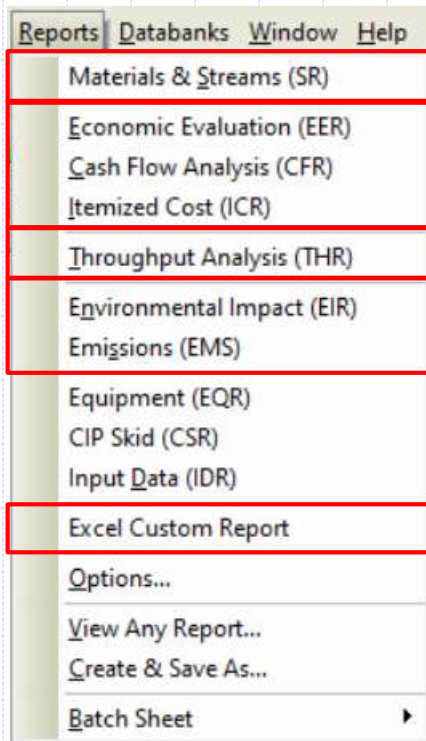
Production potentiality

SuperPro Charts

The image shows a screenshot of the 'Charts' menu in SuperPro. The menu items are: Equipment Occupancy, Gantt Charts, Materials, Labor, Heat Transfer Agents, Power, Storage Units, Aux Equipment Demand, and Throughput Analysis. Red arrows point from text labels to specific menu items: 'Time-depedent occupancy of equipment' points to 'Equipment Occupancy', 'Sequence of operations' points to 'Gantt Charts', 'Balances' points to 'Heat Transfer Agents', and 'Efficiency of equipment utilization' points to 'Throughput Analysis'. The menu items 'Materials', 'Labor', and 'Power' are grouped together and are not pointed to by any label.

Menu Item	Description
Equipment Occupancy	Time-depedent occupancy of equipment
Gantt Charts	Sequence of operations
Materials	
Labor	
Heat Transfer Agents	Balances
Power	
Storage Units	
Aux Equipment Demand	
Throughput Analysis	Efficiency of equipment utilization

SuperPro Reports



Mass Balance

**Economic
evaluation**

Mass Balance 2

Environmental evaluation

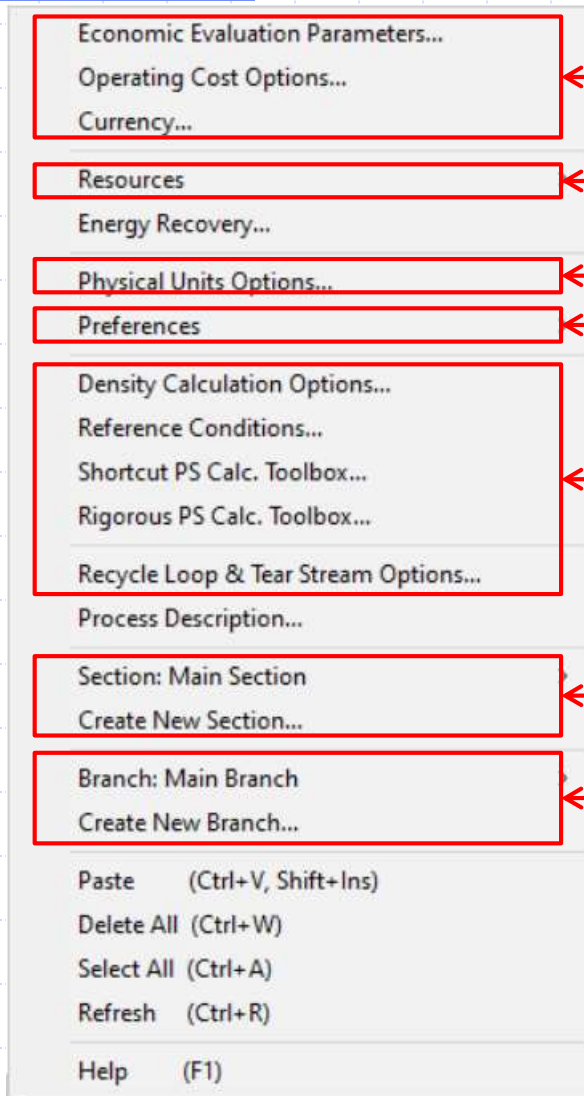
Excel export

SuperPro Databanks

The image shows a screenshot of the 'Databanks' menu in SuperPro. The menu items are listed on the left, and red arrows point from each item to a corresponding description on the right. The descriptions are in bold red text.

Menu Item	Shortcut	Description
Pure Components...	F2	Pure Components
Stock Mixtures...	Shift+F2	Predefined Mixtures
Binary Coefficients...	Shift+Ctrl+F2	Thermodynamic parameters
Heat Transfer Agents...	F3	Utilities
Labor Types...	Shift+F3	Employees
Power Types...	Shift+Ctrl+F3	Electricity
Sites and Resources...	F5	
Consumables...	Shift+F5	Equipment Consumables
Currencies...	Ctrl+F5	
Equipment		Equipment Databank
Processes		Processes Databank
Availability, Passwords & Locations...		
Import Data into the Active User DB...		
Upgrade a Past Version User DB File...		

SuperPro Flowsheet Right-Click



Financial aspects

Streams info

Definition of physical units

Report information

Calculation methods and parameters

Flowsheet sections

Plant Branches

DWSIM: Cape-Open compliant chemical process simulator

- ◆ How to get it:
<http://dwsim.inforside.com.br/wiki/index.php?title=DWSIM>

The screenshot displays the DWSIM software interface for a distillation column simulation. The main window shows a process flow diagram with two distillation columns, pumps, and various streams. The left panel contains configuration options for the 'Methanol Column (1 atm)'. The bottom panel shows a table of estimates for the distillation stages.

General Info

- Object: Methanol Column (1 atm)
- Status: Calculated (01/01/2001 00:00:00)

Column Specs

- General: Condenser, Reboiler
- Absorber Operating Mode: [Dropdown]
- Number of Stages: 40
- Solver: Wang-Henke (Bubble Point)
- Solving Scheme: Direct Rigorous
- Maximum Number of Iterations: 1000
- Convergence Tolerance: 0.002
- Maximum Temperature Change: 10.0 K
- Property Package: PP_1
- Rash Algorithm: Default

Column Configuration

- Connections: Stages, Initial Estimates, BP Solver

Estimates

Stage	Temperature (K)	Vapor Flow (mol/h)	Liquid Flow (mol/h)
0	327.84061	0.0005	83.69429
1	328.08249	84.15289	76.56626
2	328.55104	77.06486	68.17435
3	329.45256	68.67295	59.23208
4	331.00118	59.75068	51.49619
5	333.0238	51.99478	46.3247

Information

Date	Type	Message
12/06/2019 10:10:11	Tip	If some windows are missing, click on 'View' > 'Restore Layout'.
12/06/2019 10:10:11	Tip	To view detailed results of the calculations in real time, enable console redirection and select a debug mode. You must restart DWSIM for the changes to take effect.
12/06/2019 10:10:11	Tip	Use the quick connection tool on the toolbar to quickly connect objects by pressing the CTRL key and dragging the cursor from the first to the second object.
12/06/2019 10:10:11	Tip	Press F5 on any area inside the flowsheet to start a full calculation.
12/06/2019 10:10:11	Tip	Hold SHIFT during DWSIM initialization to reset the settings to their default values.
12/06/2019 10:10:10	Message	File C:\Program Files\DWSIM5\samples\Extractive Distillation.dwsim loaded successfully.

A survey of process simulation software

Steady state simulators and batch

- Aspen Plus (Aspentech)
- Hysys.Process (Aspentech)
- PRO II (Sim Sci)
- COCO (AmsterChem)
- DWSIM (open source)
- Chem CAD
- Process
- Prode simulator (Prode SW)
- ProSim
- Super Pro designer
-

Dynamic simulators

- Speedup→Aspen Dynamics (Aspentech)
- Batch model - DynSim (Sim Sci)
- Hysys.Plant (Aspentech)
- gPROMS (PSE)
- Batches
- ASSETT (Kongsberg digital)
- JADE (GSE systems)
-