Process Simulation Software: User Interface

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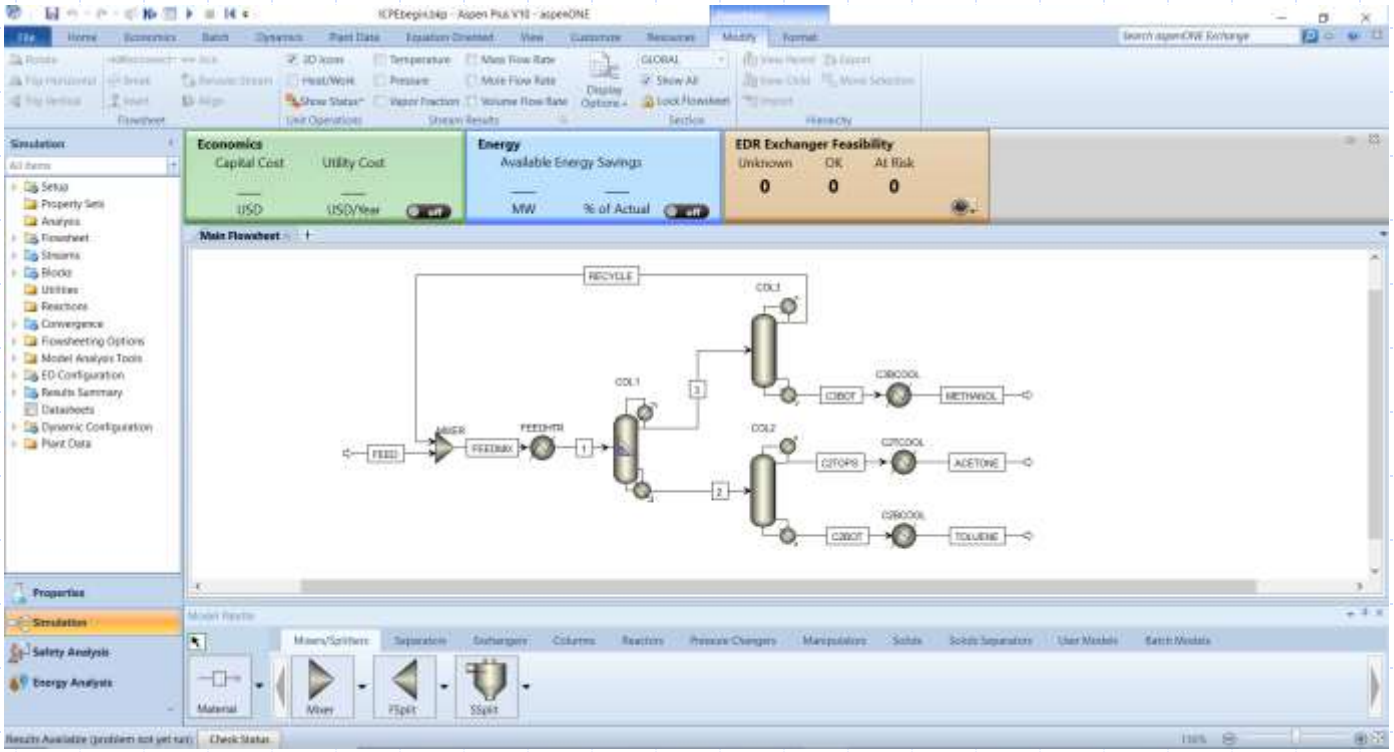
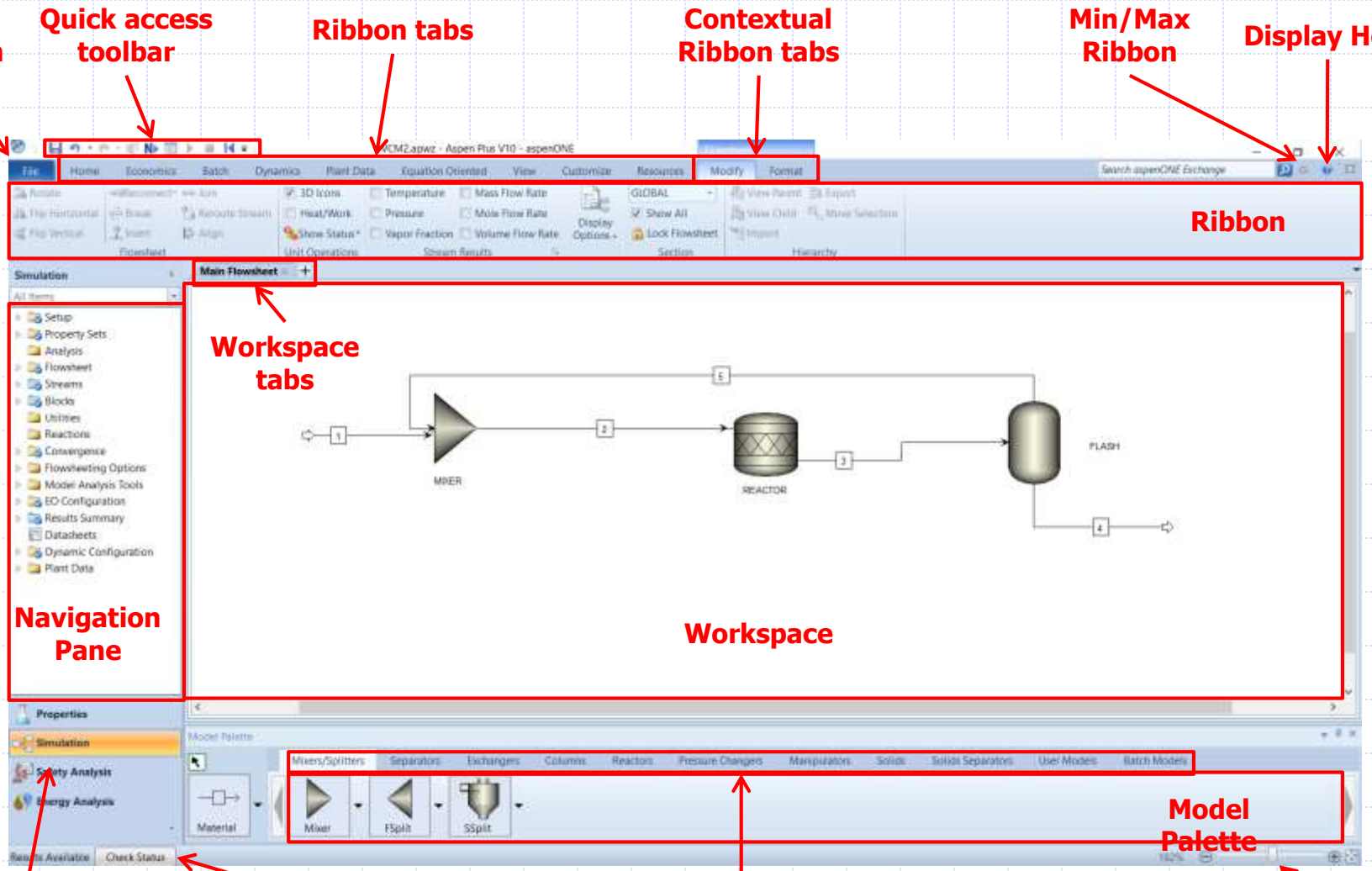
Agenda

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

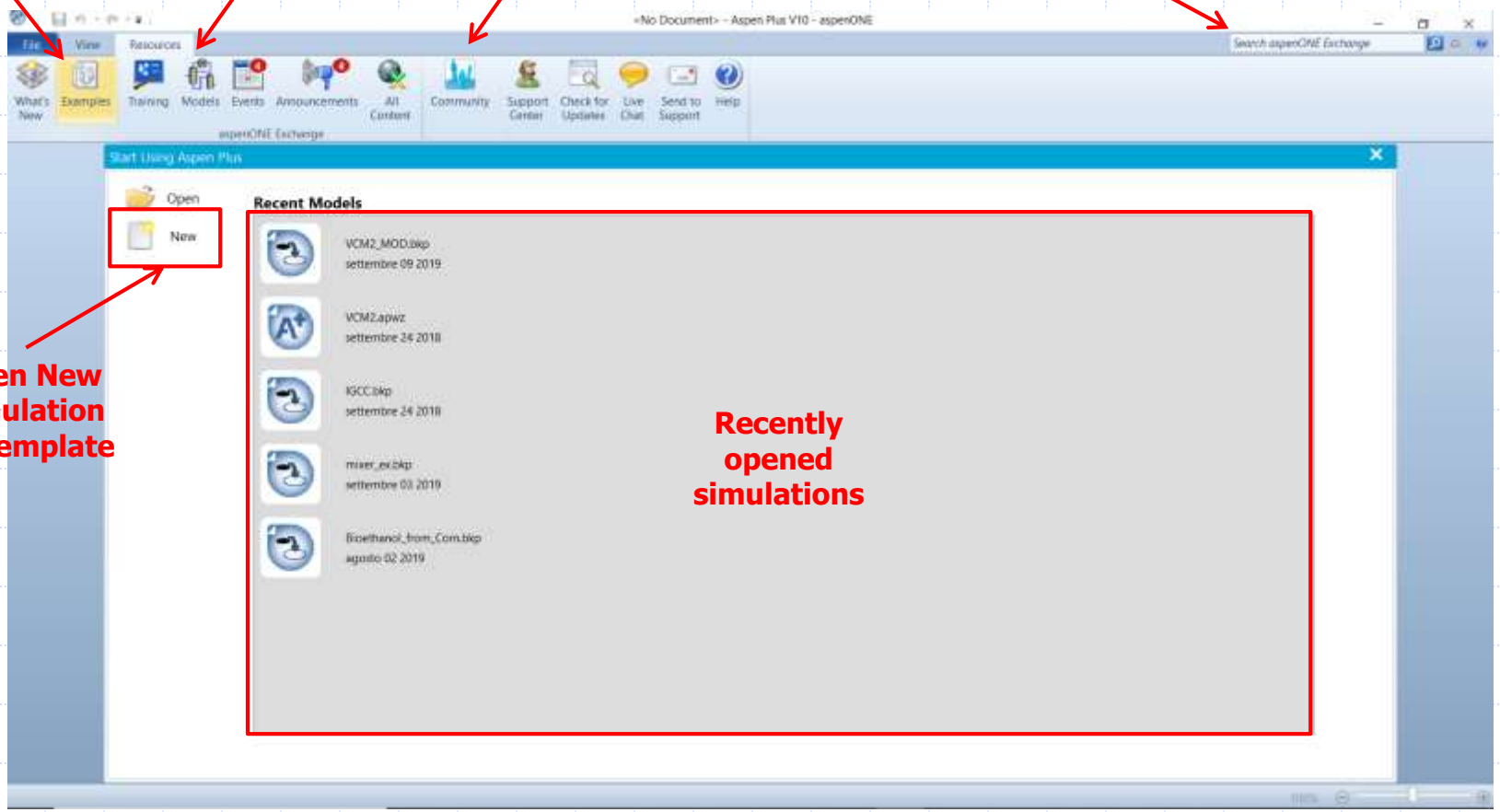
Aspen Plus


Economics
Capital Cost
Utility Cost
USD
USD/Year
Energy
Available Energy Savings
MW
% of Actual
EDR Exchanger Feasibility
Unknown
OK
At Risk
0
0
0
Main Flowsheet
RECYCLE
COL1
COL2
C3BOT
METHANOL
C2TOPS
ACETONE
TOLUENE
FEED
Properties
Simulation
Safety Analysis
Energy Analysis
Material
Mixer
FSplit
SSplit

User interface



Aspen Plus Start Page



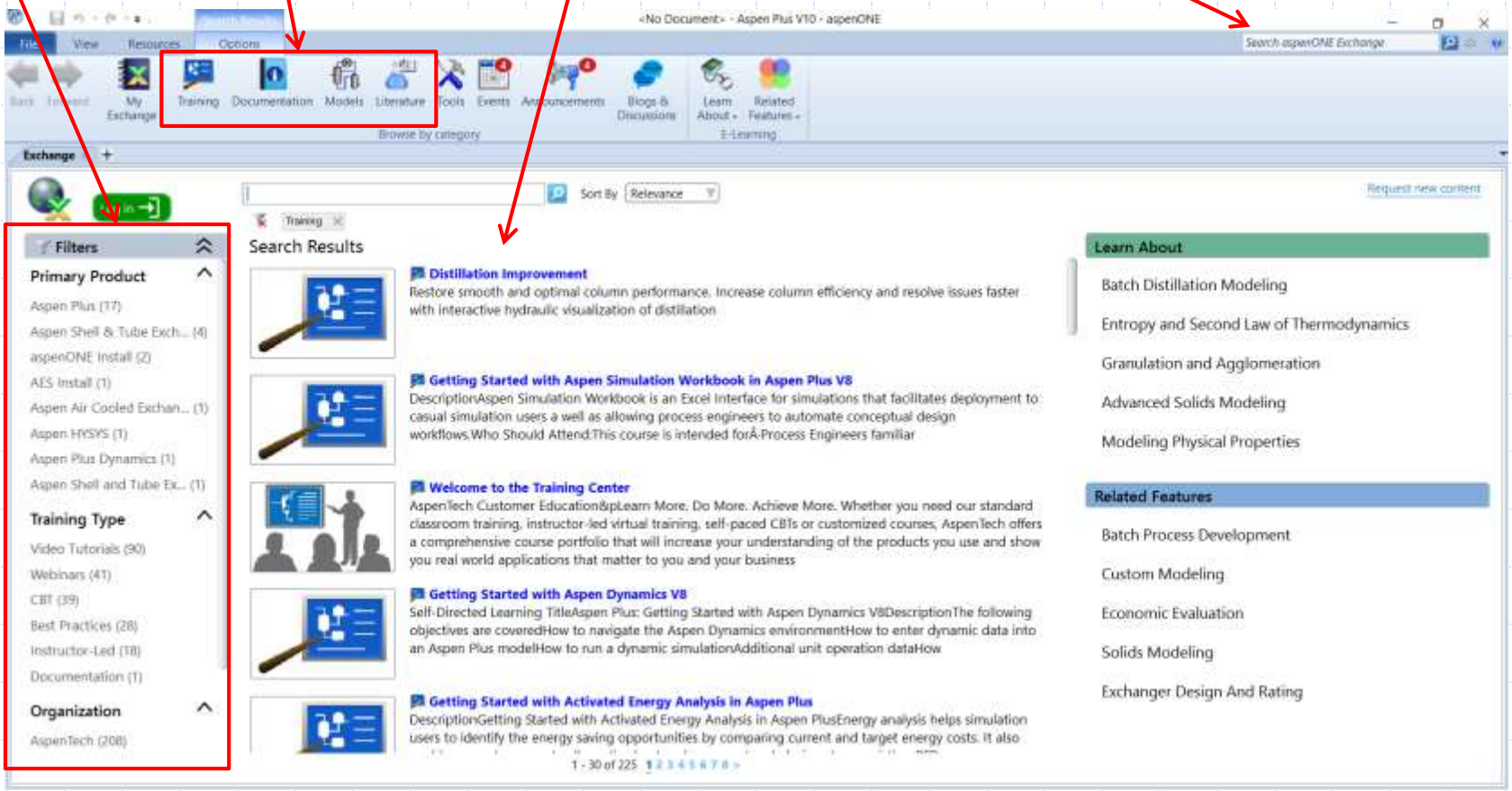
aspenONE Exchange

Search Filters

Search Categories

Preview items before download

Search in AspenONE Exchange



Aspen Plus Environments

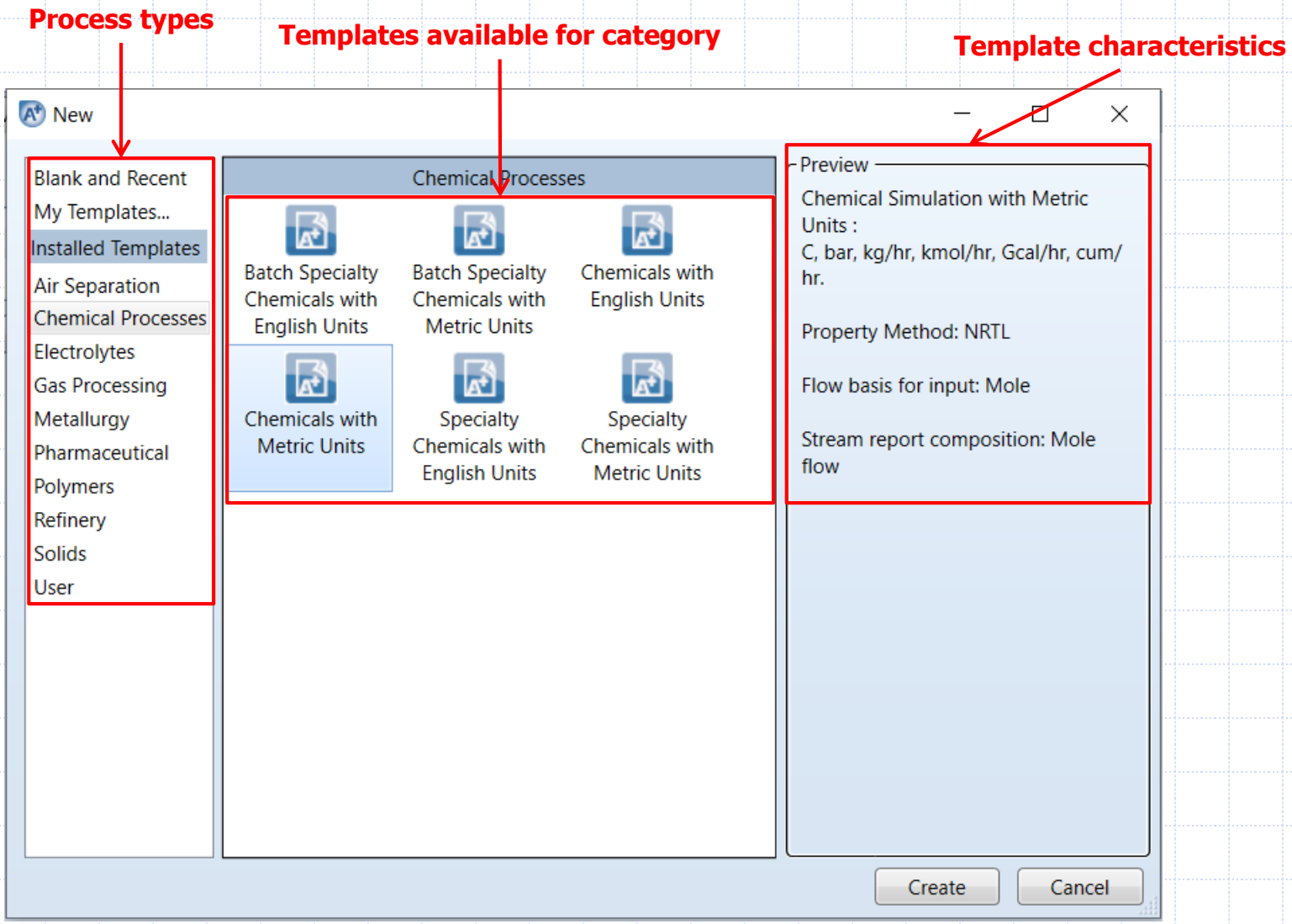
- Properties Environment
  - Define the physical properties
    - Component selection, generation and characterization
    - Thermodynamic methods and database
    - Collect experimental data
    - Property estimation
    - Property analysis
    - Data regression
- Simulation Environment
  - Used to 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

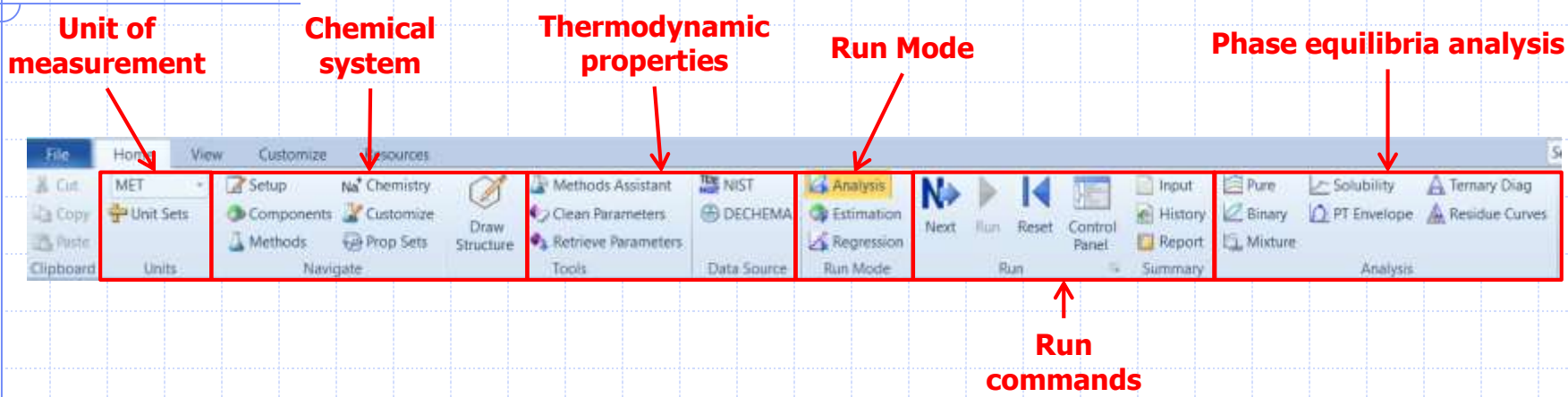
- Properties Environment
  - Select the components involved in the chemical process from databanks or generate the components using the specific interface
  - Specify the thermodynamic methods suitable for the simulated system
  - Collect experimental data
  - Property estimation
  - Property analysis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

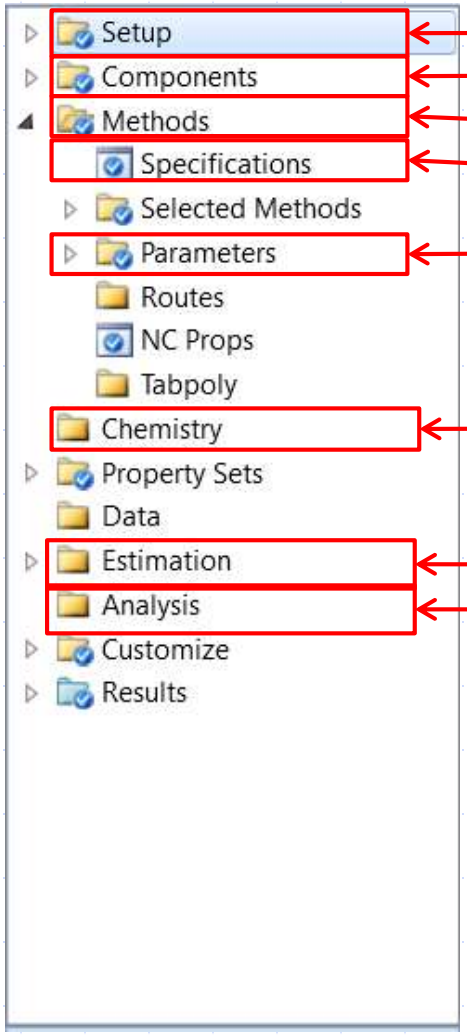


Properties Home Ribbon



- **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



General settings

Chemicals introduced in the simulation

Thermodynamic methods

Thermodynamic method settings

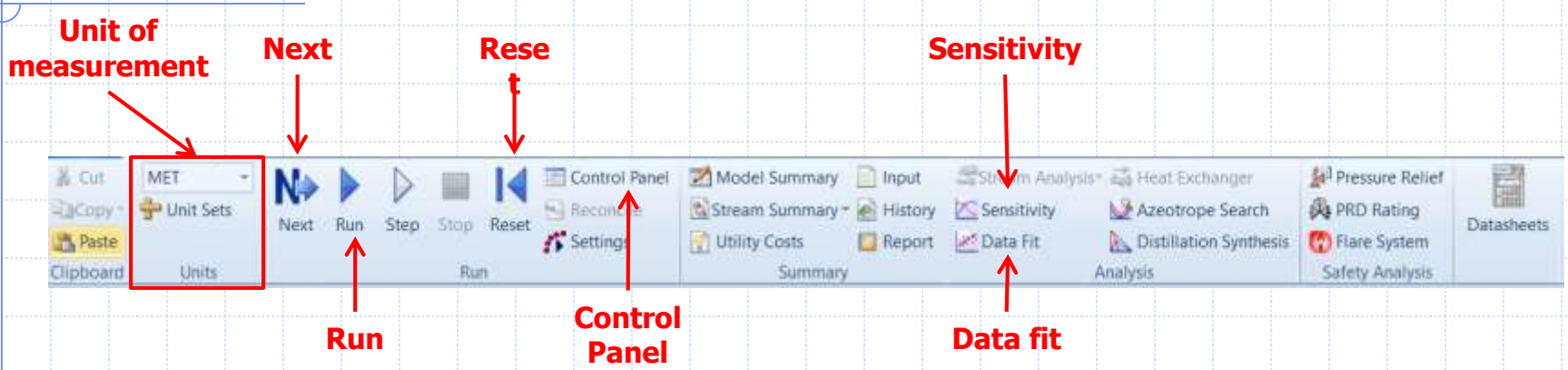
Properties parameters

Chemistry of the system (e.g. electrolytes)

Properties estimation (e.g. group contribution methods)

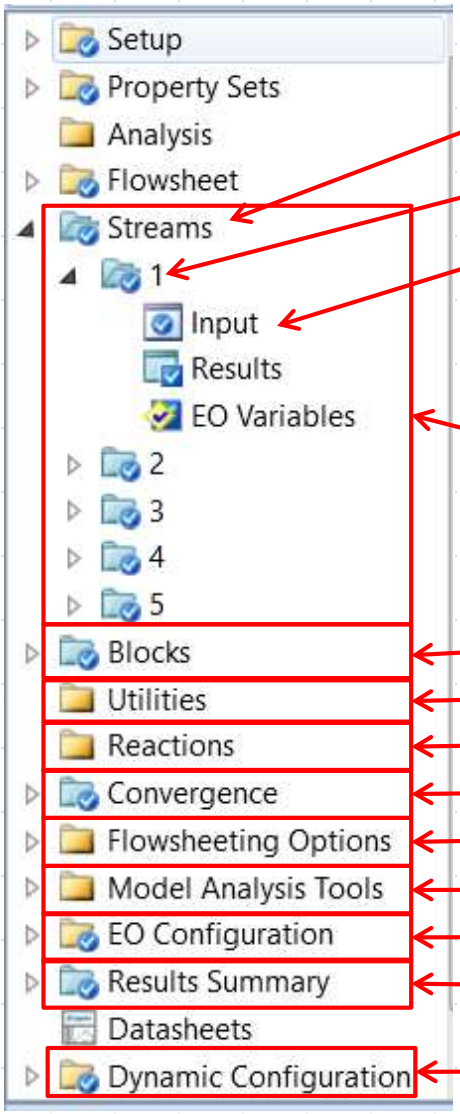
Phase equilibria analysis

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

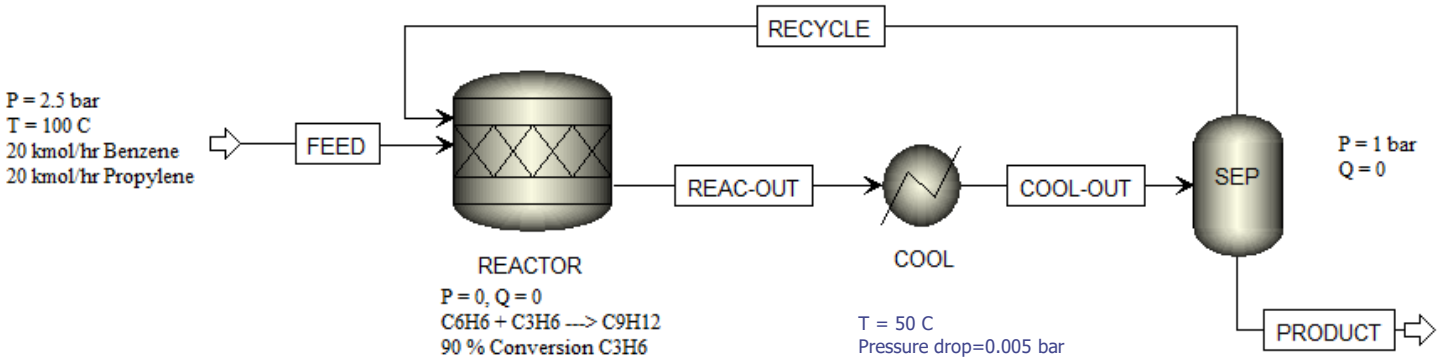
Dynamic parameters

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

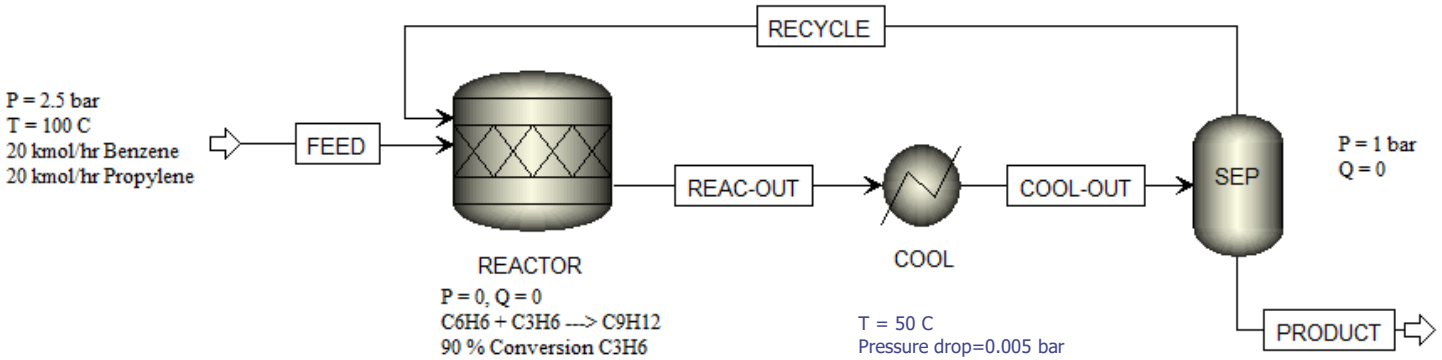
- Cumene production from propylene and benzene in a conversion reactor



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

Activate one or the other!

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.

COCO-COFE a cape Open process simulator

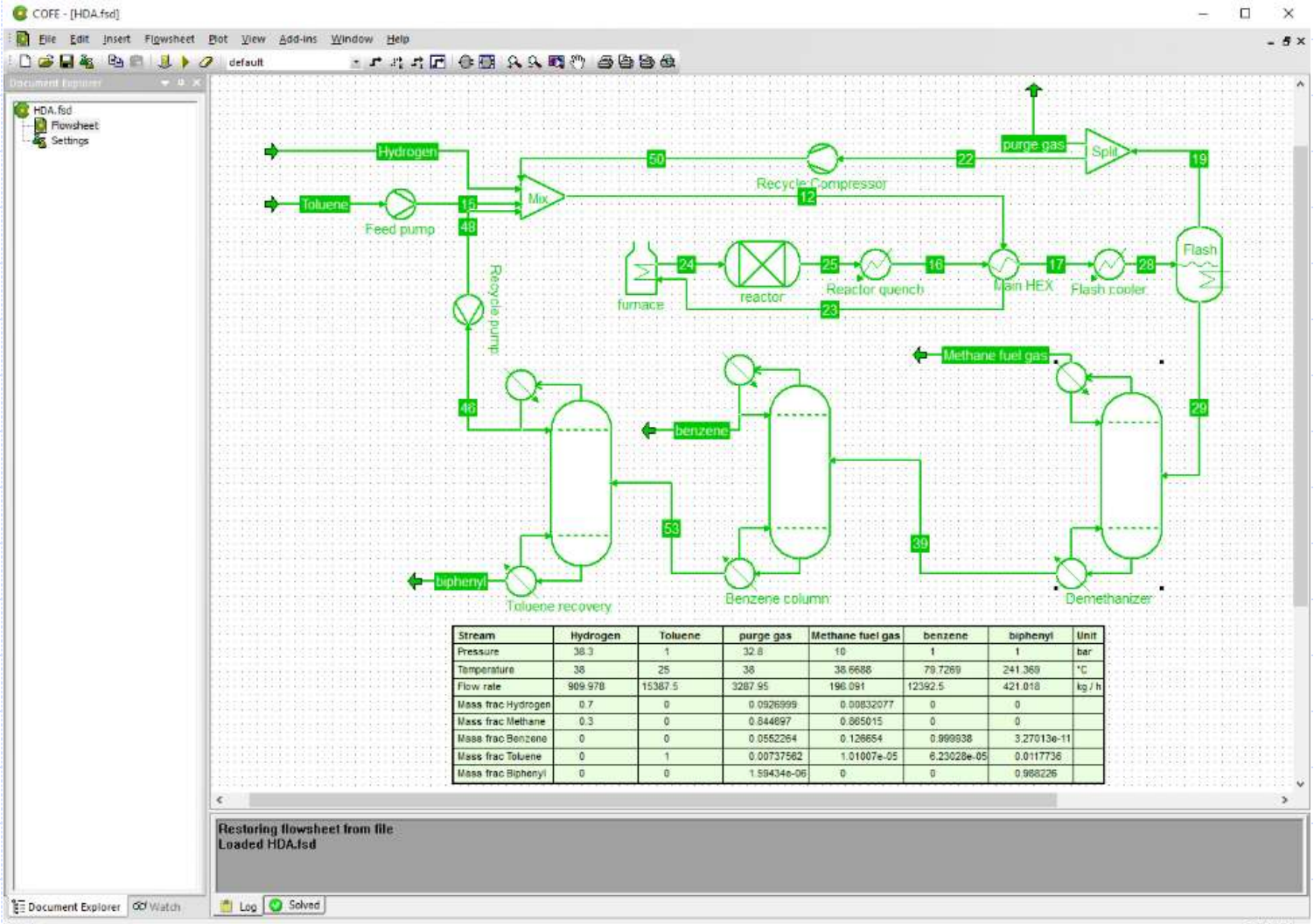
What is COCO?

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 Engeering Applications
- COUSCOUS: CAPE-OPEN Unit-operations (Simple)
- CORN: CAPE-OPEN Reaction Numerics

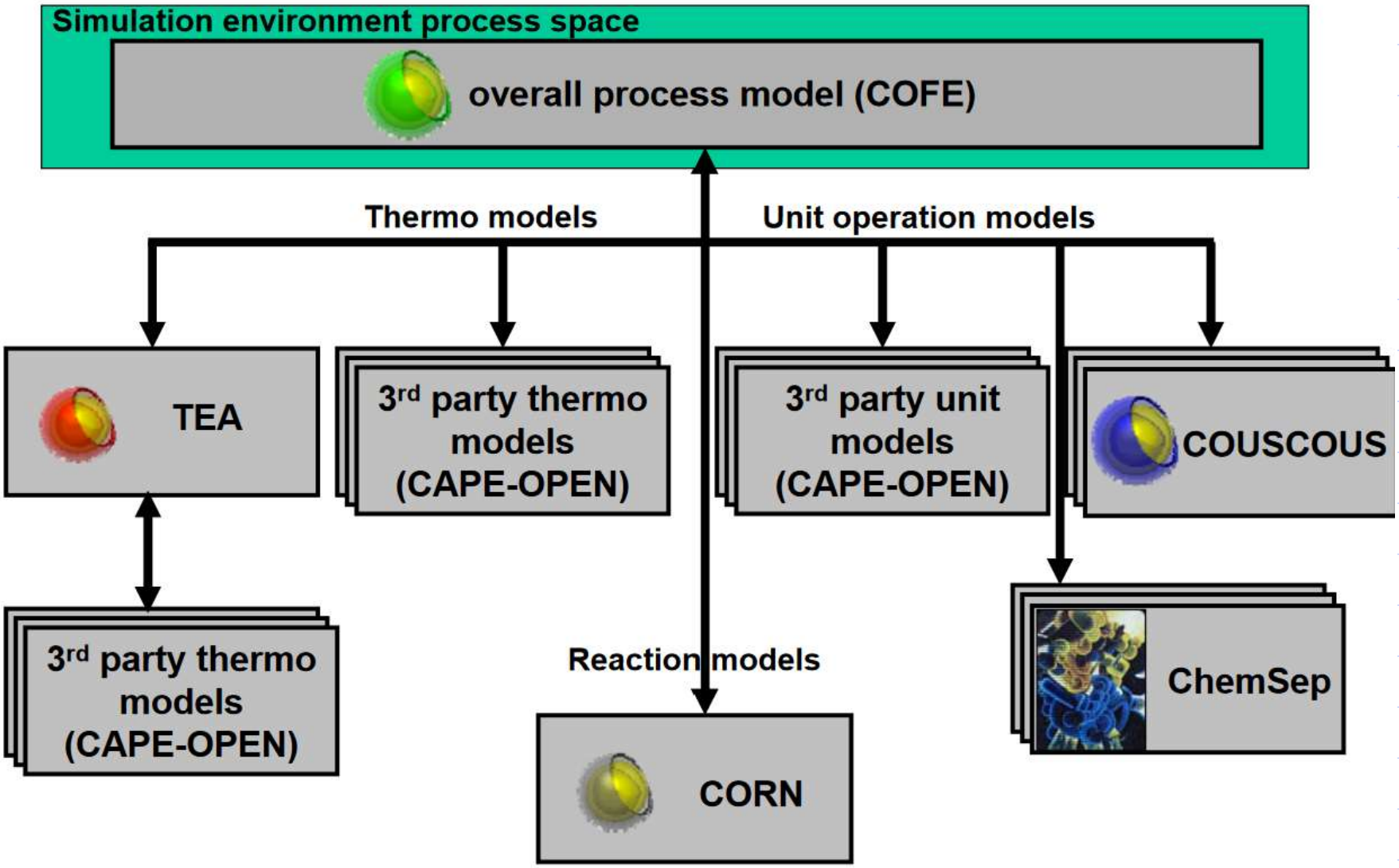
COCO: a free-of-charge CAPE-OPEN compliant steady-state simulation environment

- Available here: https://www.cocosimulator.org/



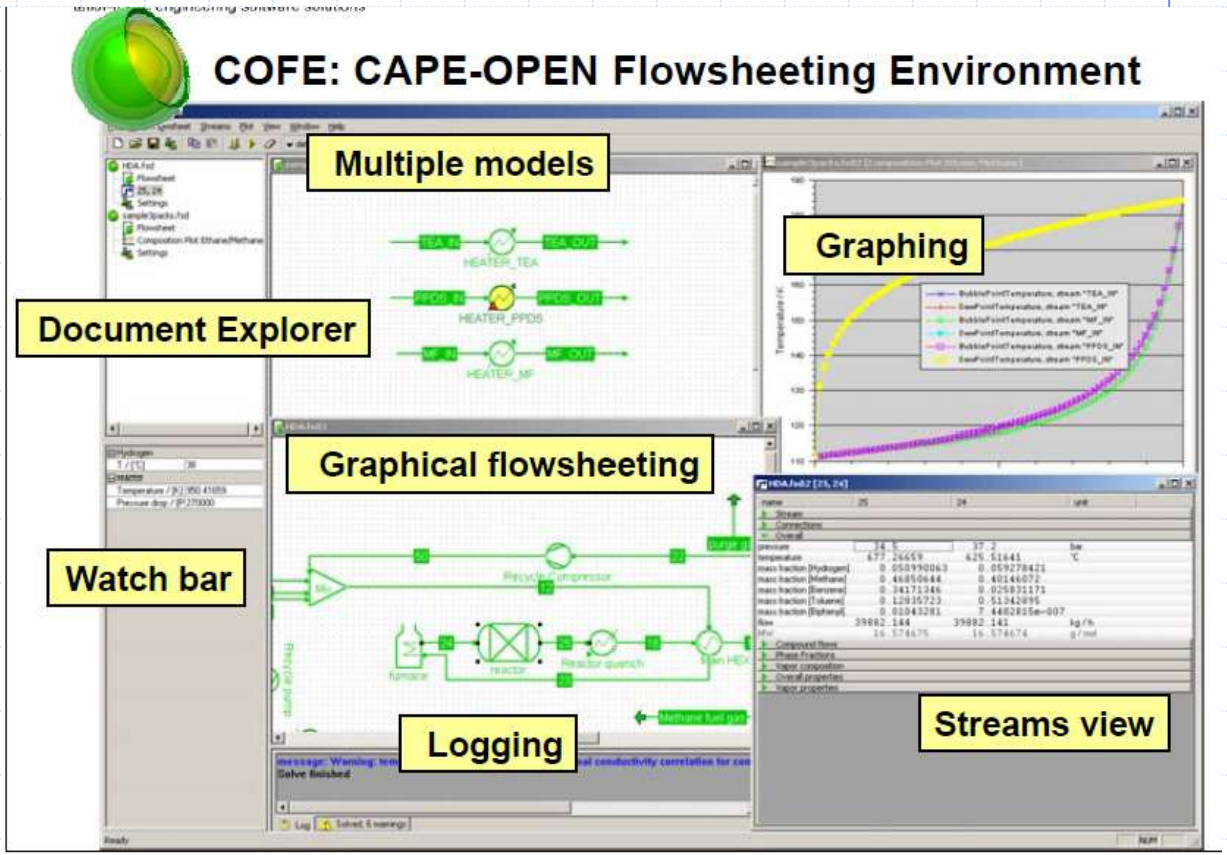
Stream	Hydrogen	Toluene	purge gas	Methane fuel gas	benzene	biphenyl	Unit
Pressure	38.3	1	32.8	10	1	1	bar
Temperature	38	25	38	38.6688	79.7269	241.369	°C
Flow rate	909.978	15387.5	3287.95	196.091	12392.5	421.018	kg / h
Mass frac Hydrogen	0.7	0	0.0926999	0.00832077	0	0	
Mass frac Methane	0.3	0	0.844697	0.865015	0	0	
Mass frac Benzene	0	0	0.0552264	0.126654	0.999938	3.27013e-11	
Mass frac Toluene	0	1	0.00737562	1.01007e-05	6.23028e-05	0.0117736	
Mass frac Biphenyl	0	0	1.59434e-06	0	0	0.988226	

COCO-COFE a cape Open process simulator



COFE: CAPE-OPEN Flowsheeting Environment

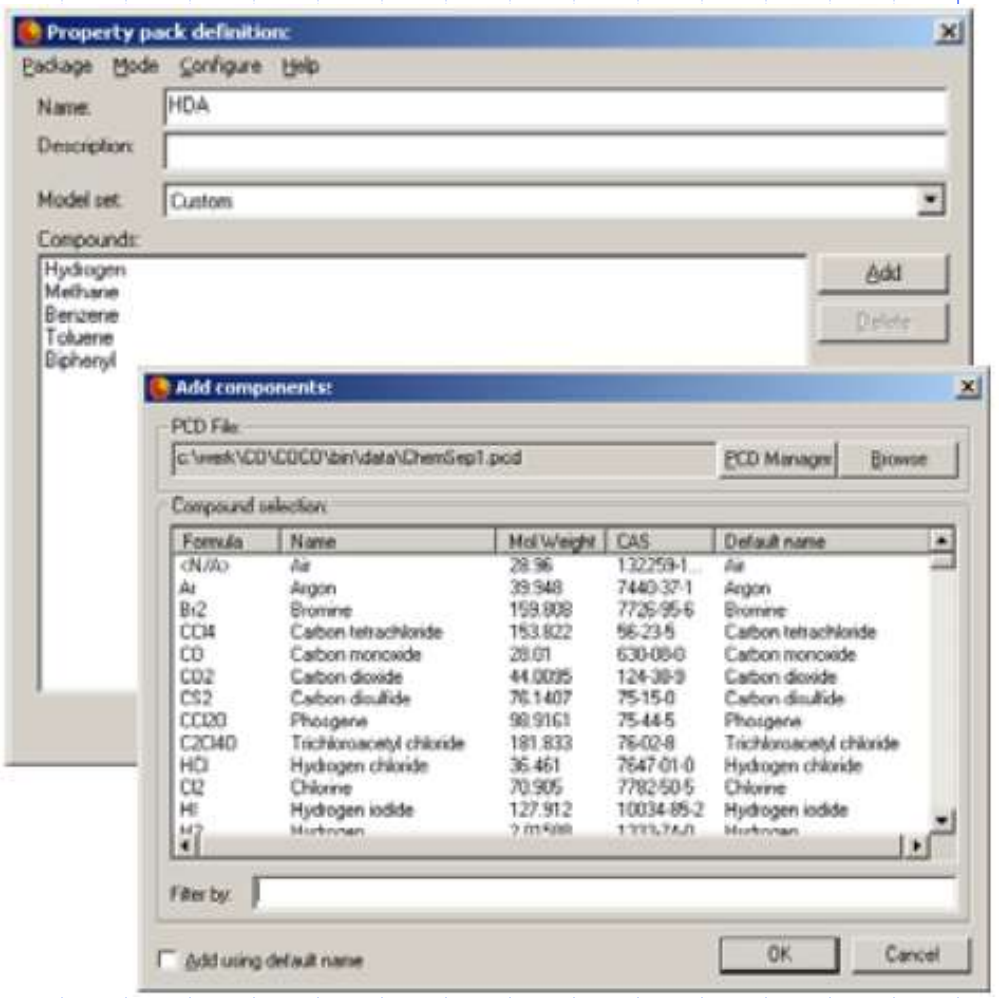
- Breaking recycles by **automatic tearing**
- **Solving recycles** by hybrid Newton / Wegstein
- **approach**, using re parameterization
- Support for **multiple material types**, with selection for thermo and sub-set of compounds
- Material, energy and information **streams**



TEA Thermodynamics for engineering calculations

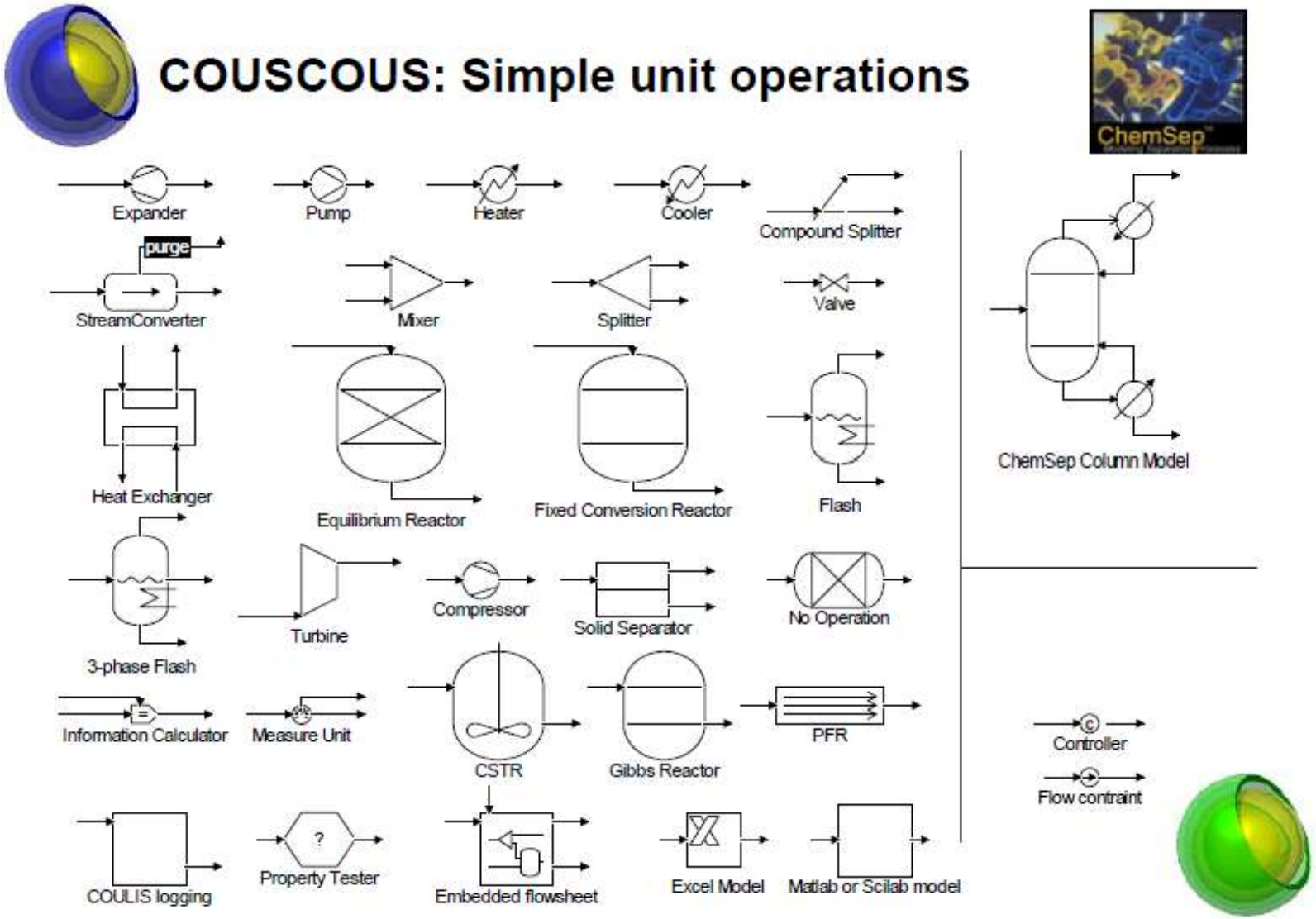
- Pure compound data library
  - (extendible, or use DIPPR)
- 100+ Property calculation methods
  - (25+ different properties)
- Property derivatives
- Support of external property calculation routines and external equilibrium servers

- 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

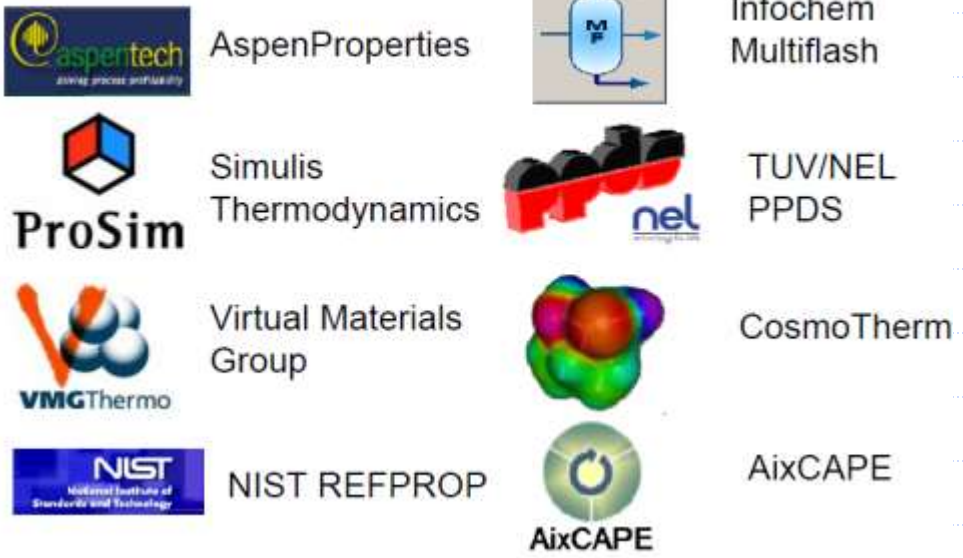
COUSCOUS: simple unit operations



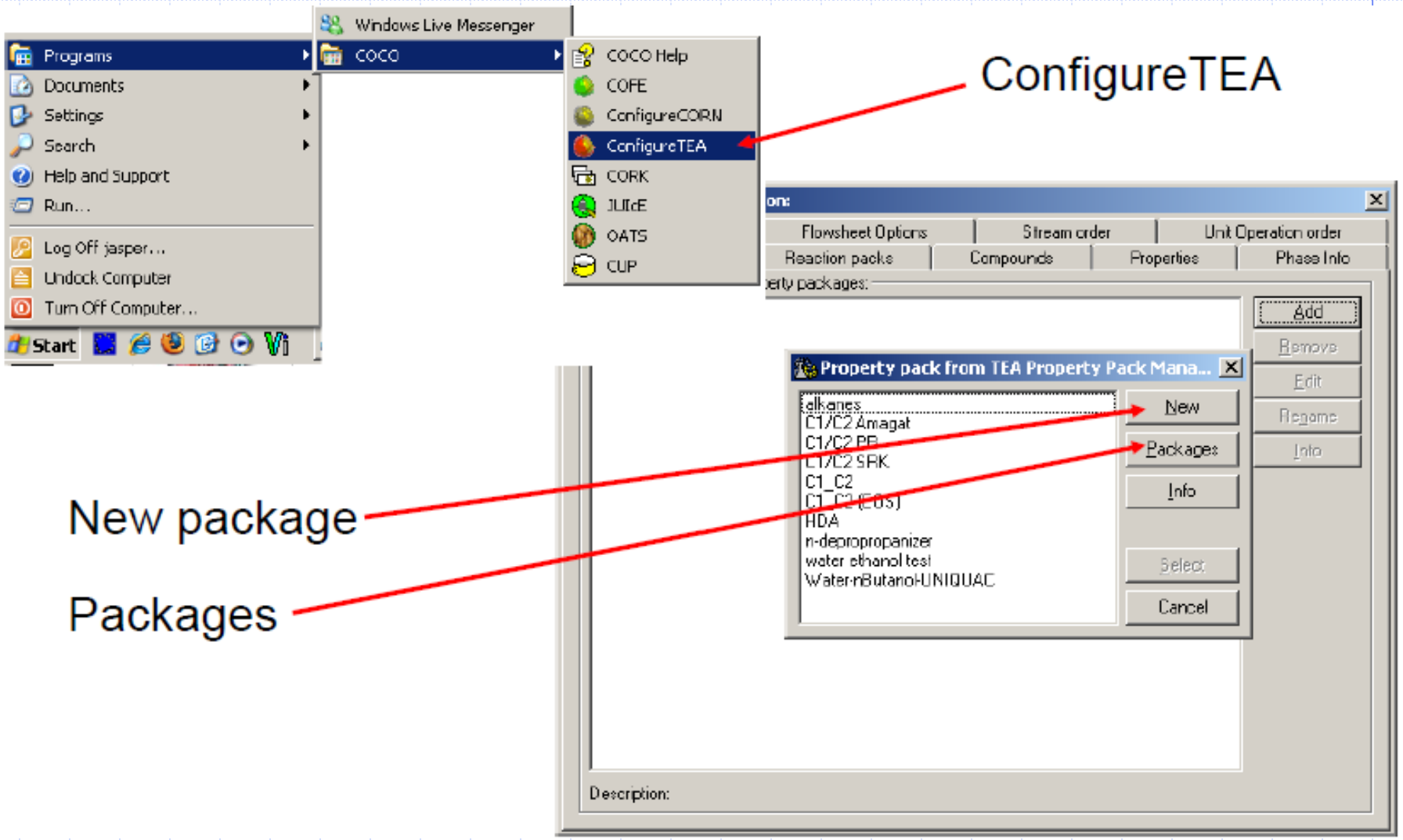
TEA: reasons to use it and not to use it

- 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 externa
- 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

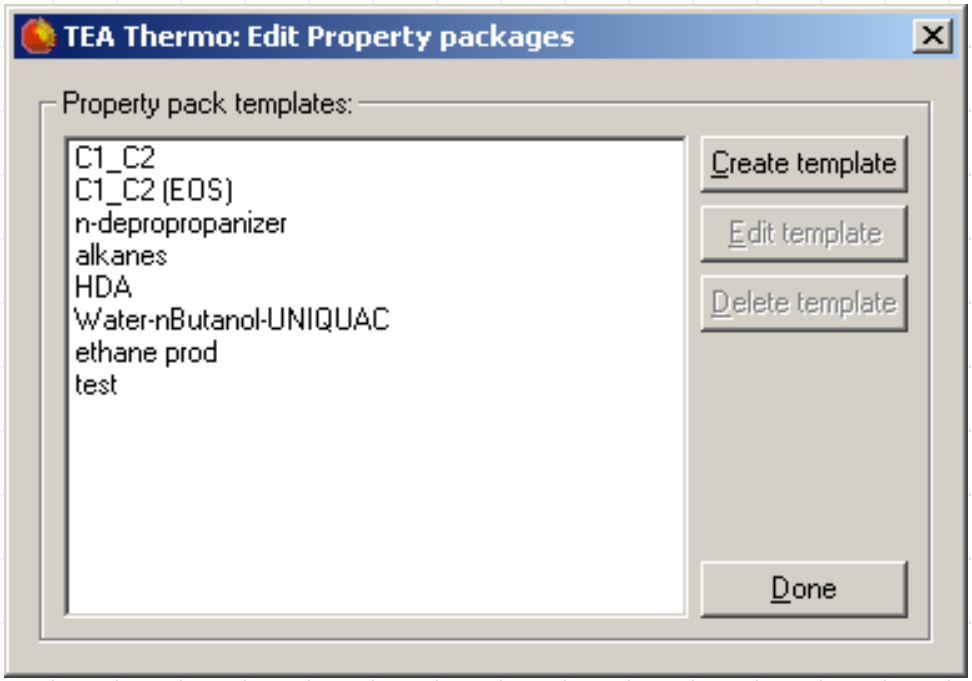


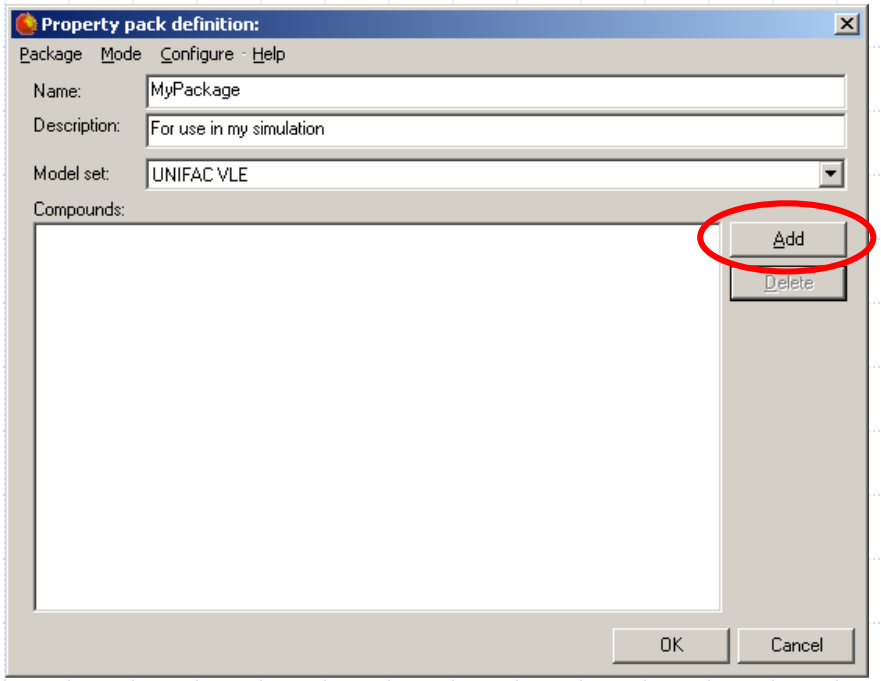
Configuring TEA property packages



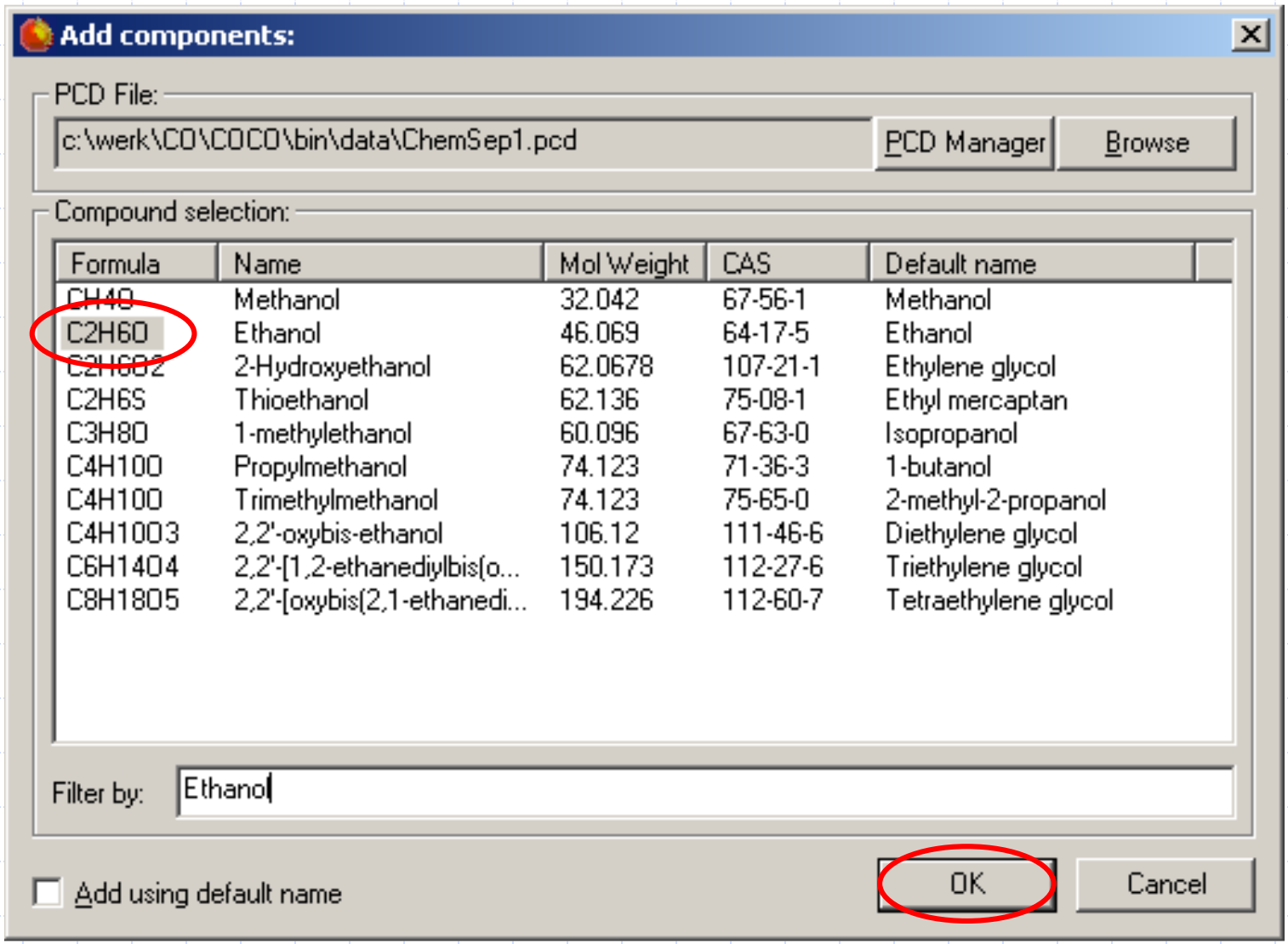
Configuring TEA property packages

- 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.



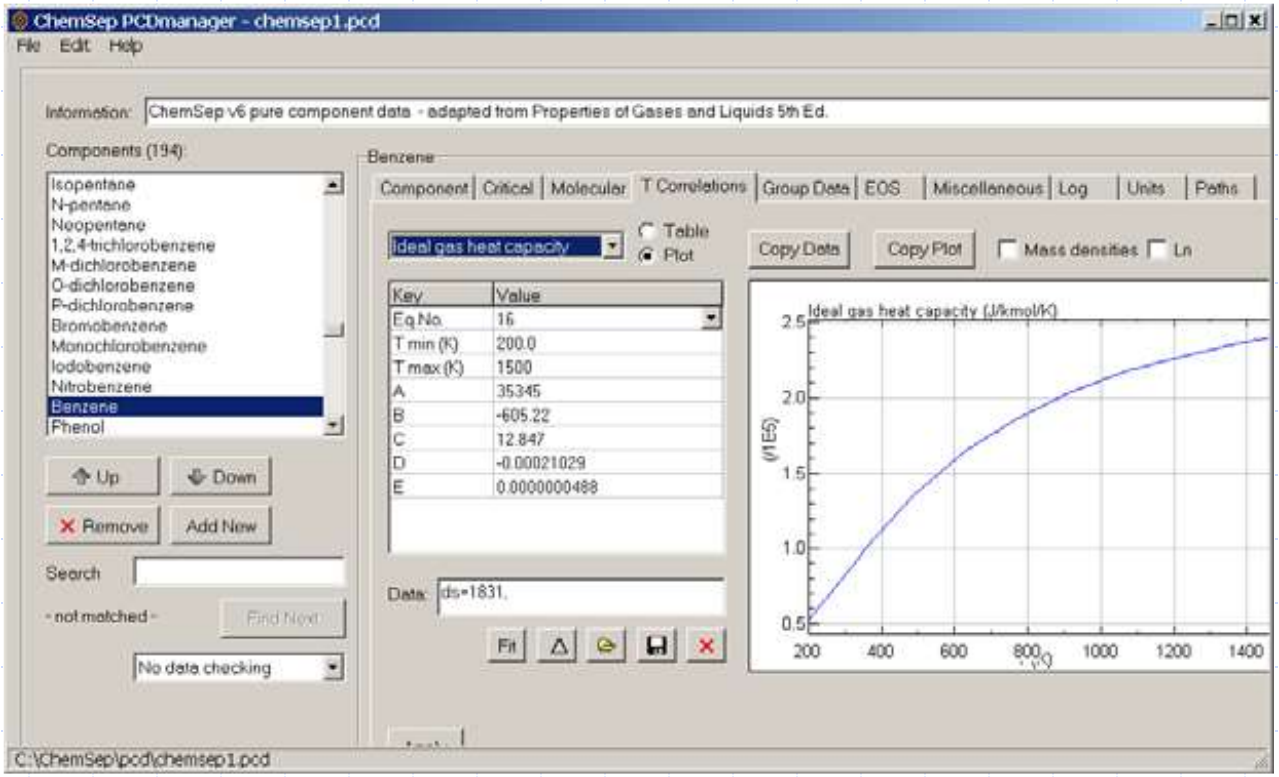


Configuring TEA property packages



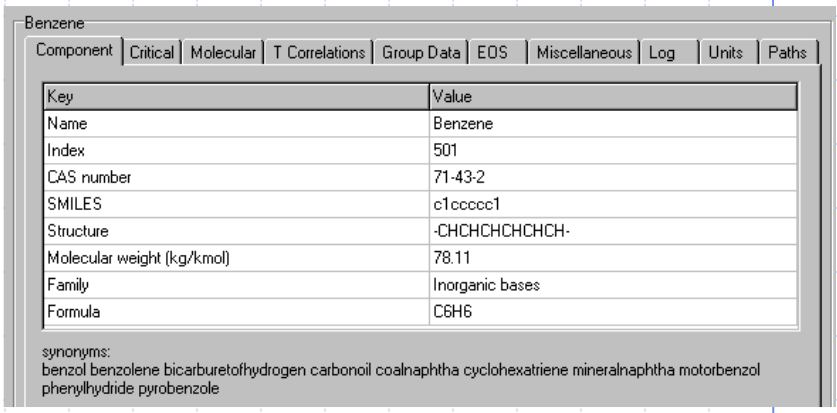
Managing Pure Component Data (PCD) files

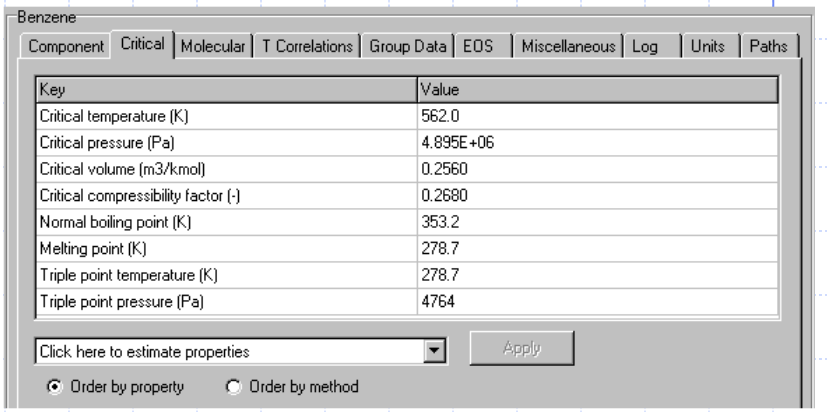
- PCD files are Pure Component Data files.
  - formula, name, critical pressure, coefficients to correlations for property calculations.
  - ChemSep (LITE) comes with a package to edit PCD files; **PCD manager.**
  - Load the PCD file at: C:\Program Files\ChemSepL8v23\pcd

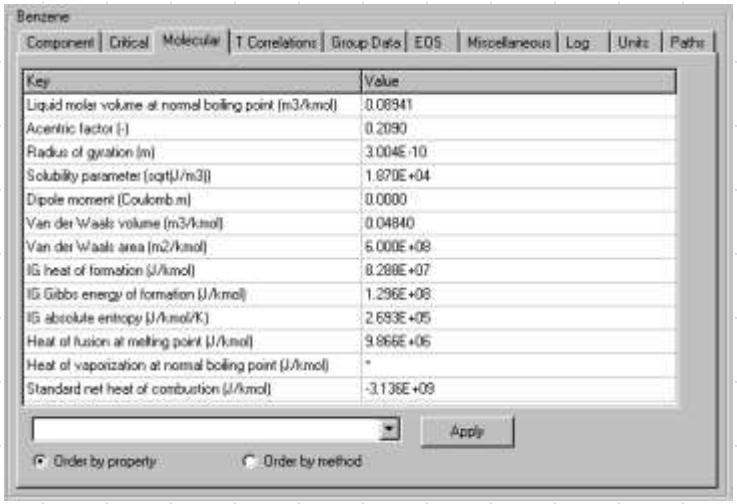


PCD manager contains:

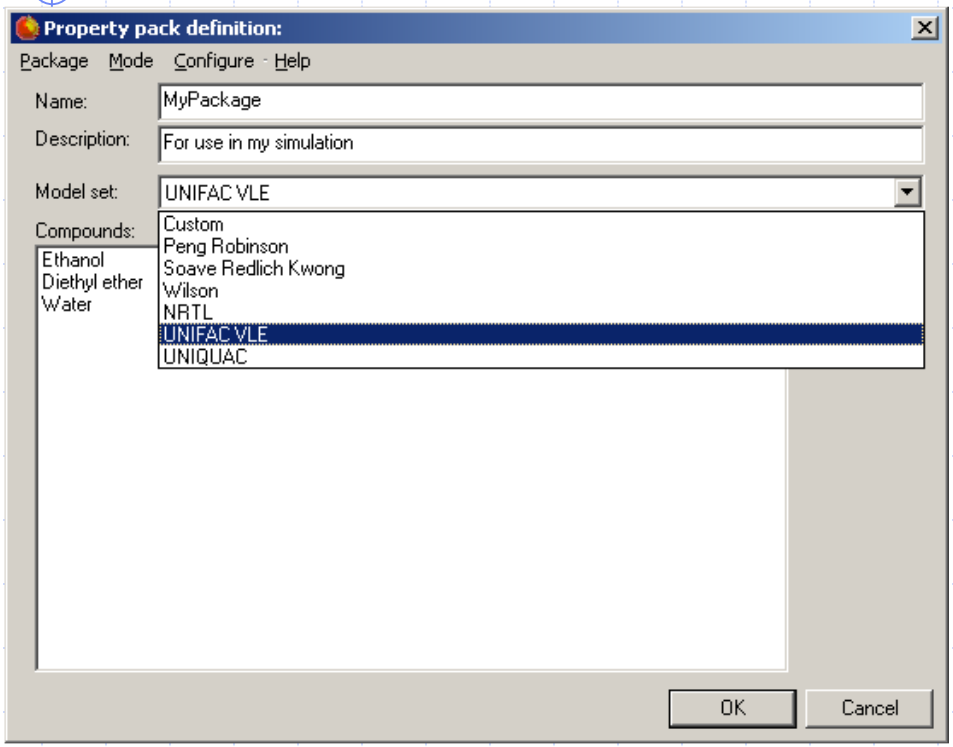
- Basic info for components
  - name, index number (index number of DIPPR), CAS number, SMILES string, structural formula, molecular weight, family (from the DIPPR list) and formula
- Critical properties
  - Critical constants, normal boiling point, melting point, the triple point T and P.
  - The critical 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

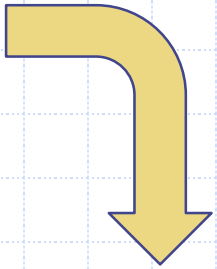


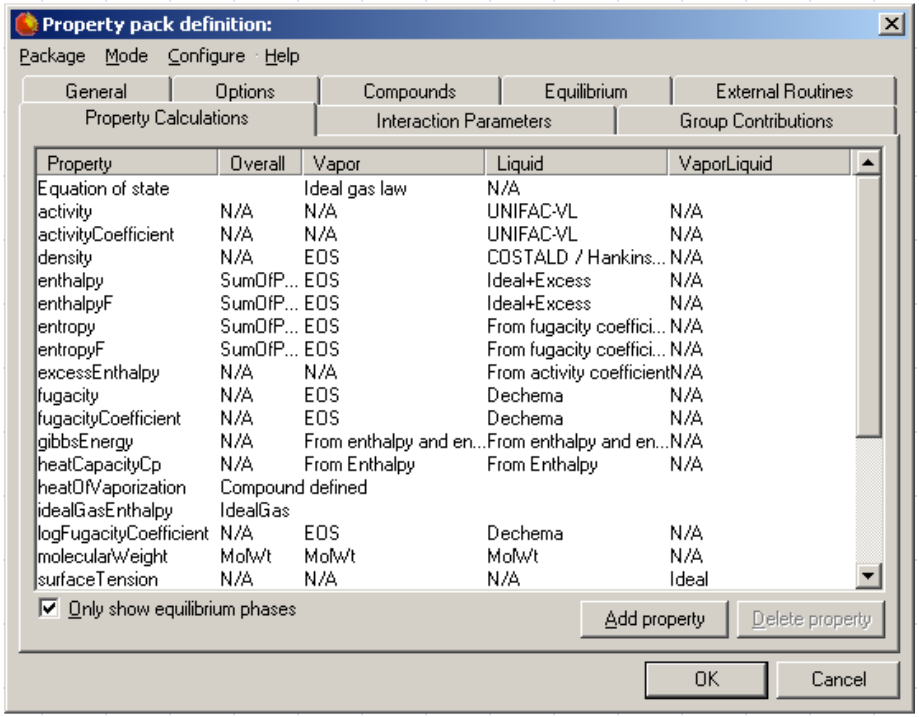




Configuring TEA property packages



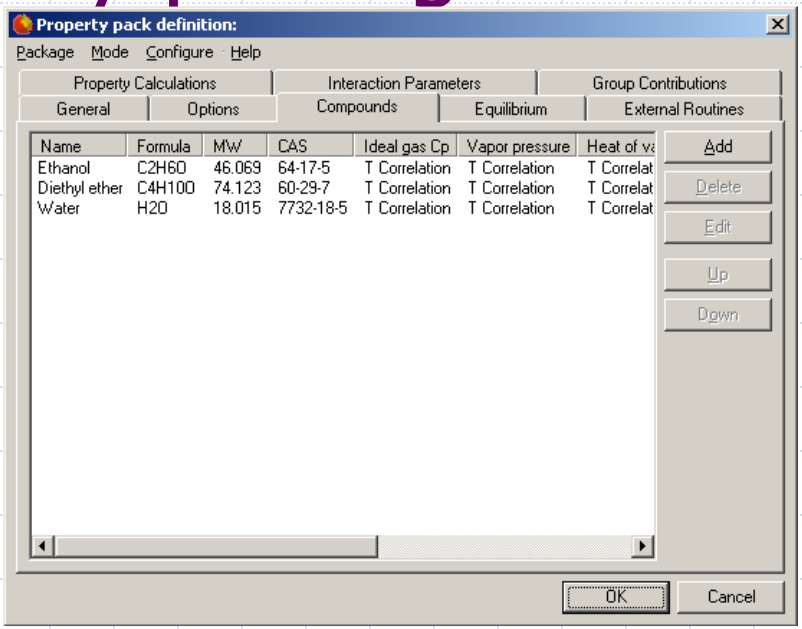




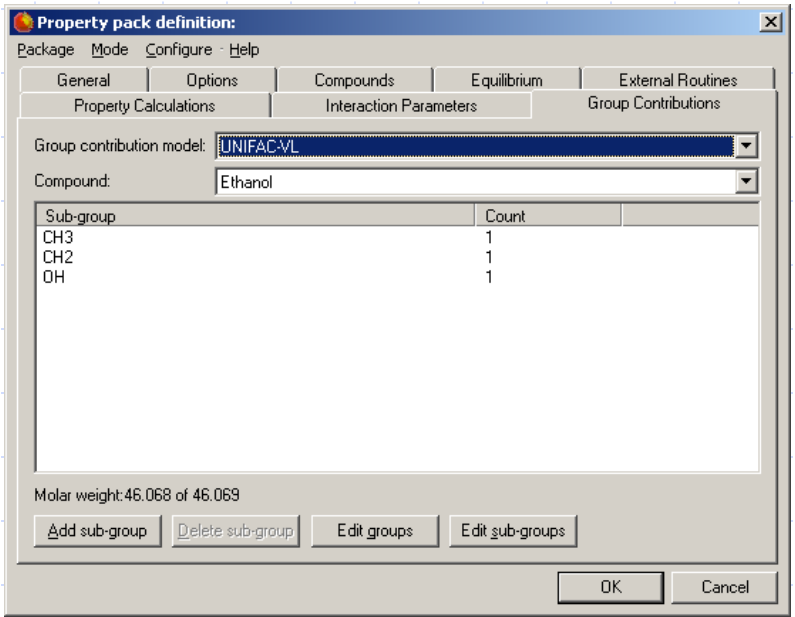
- Choosing Property Calculations from the Configure menu allows us to see which models are actually used for each property.
- We can add properties, remove properties, or change calculation methods.

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.

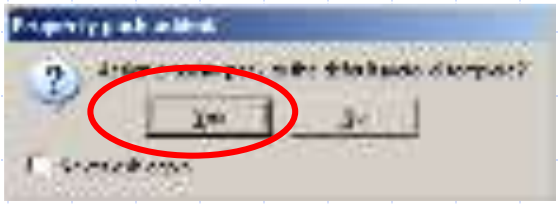


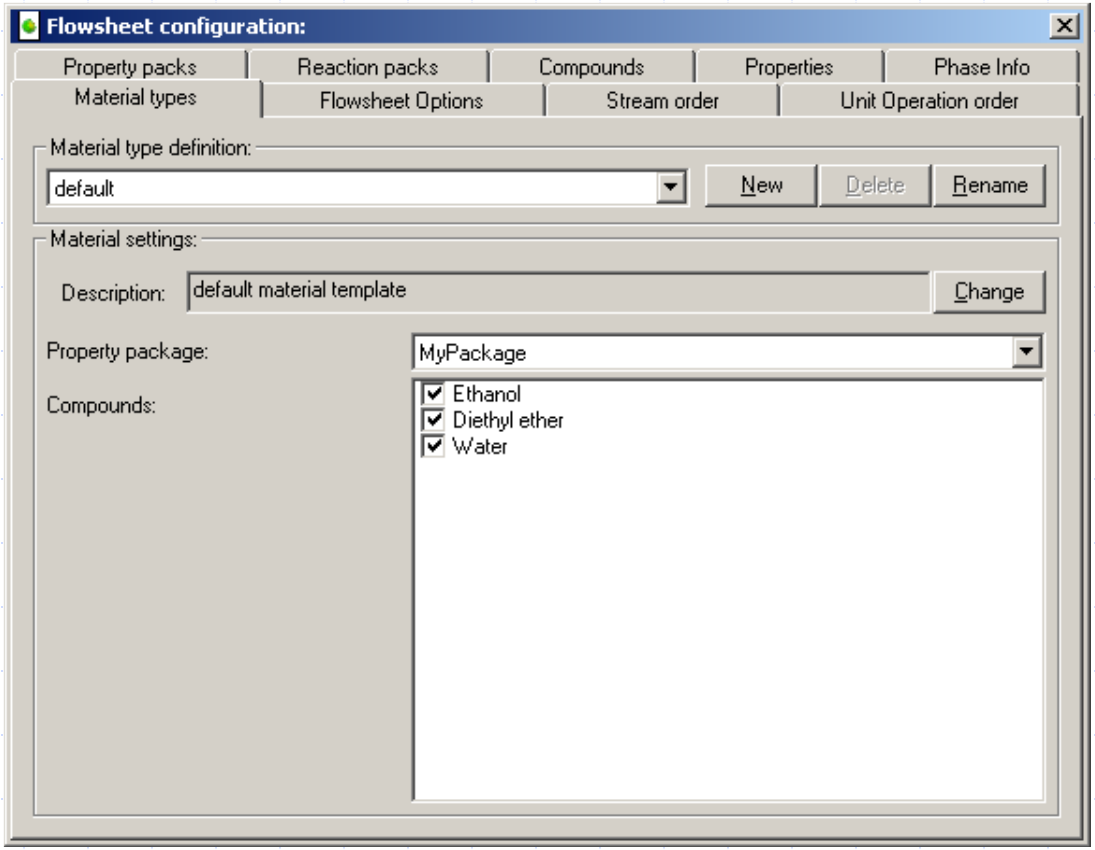
- Parameters of models can also be inspected.
  - Here, we see the UNIFAC groups that define ethanol.
  - Group and sub-group parameters are available via the buttons.



Configuring TEA property packages

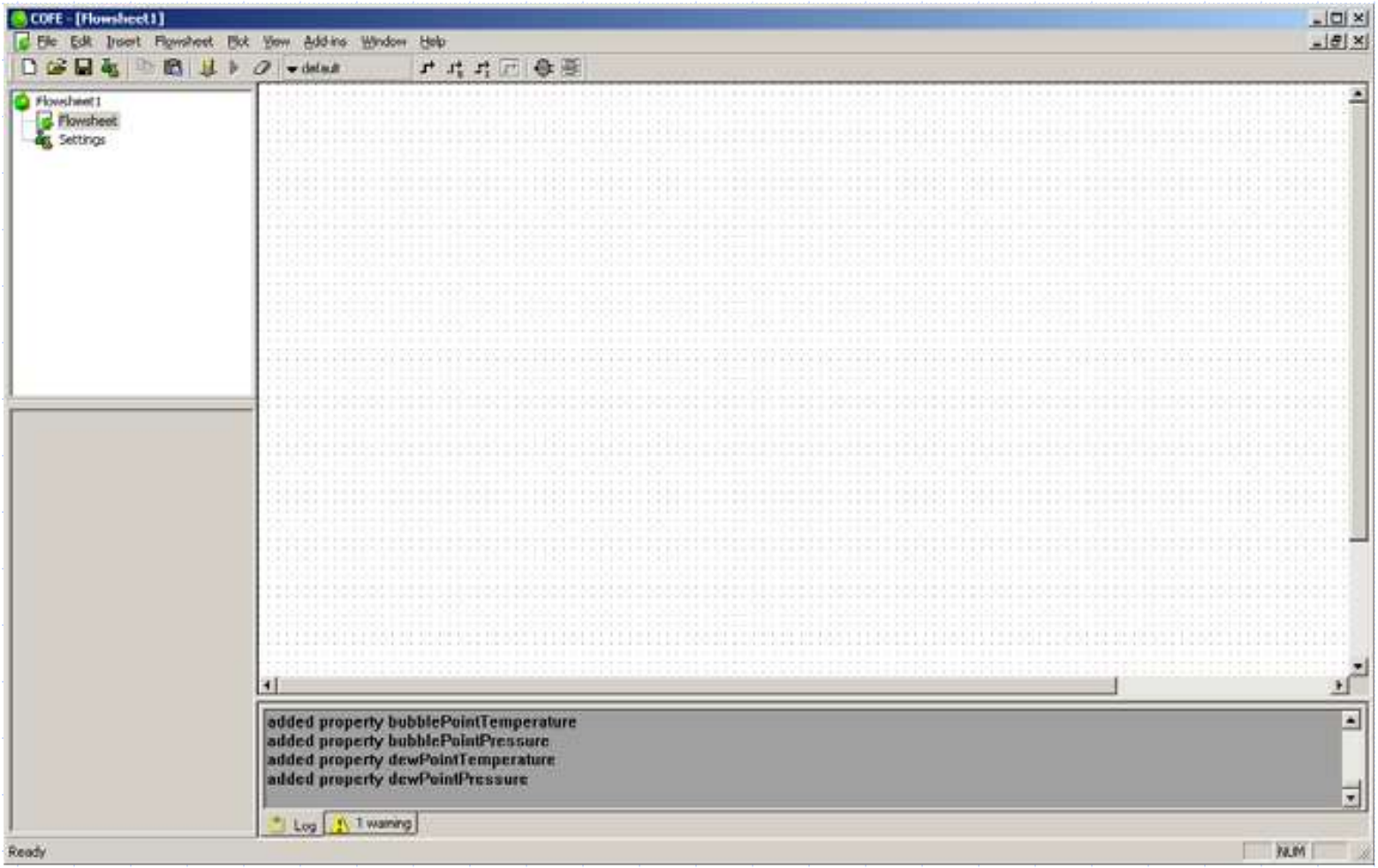
- Finally we click OK to accept the Property Package configuration.
  - After it is inserted into COFE, we are asked whether we want to couple this to the default material template. We do.



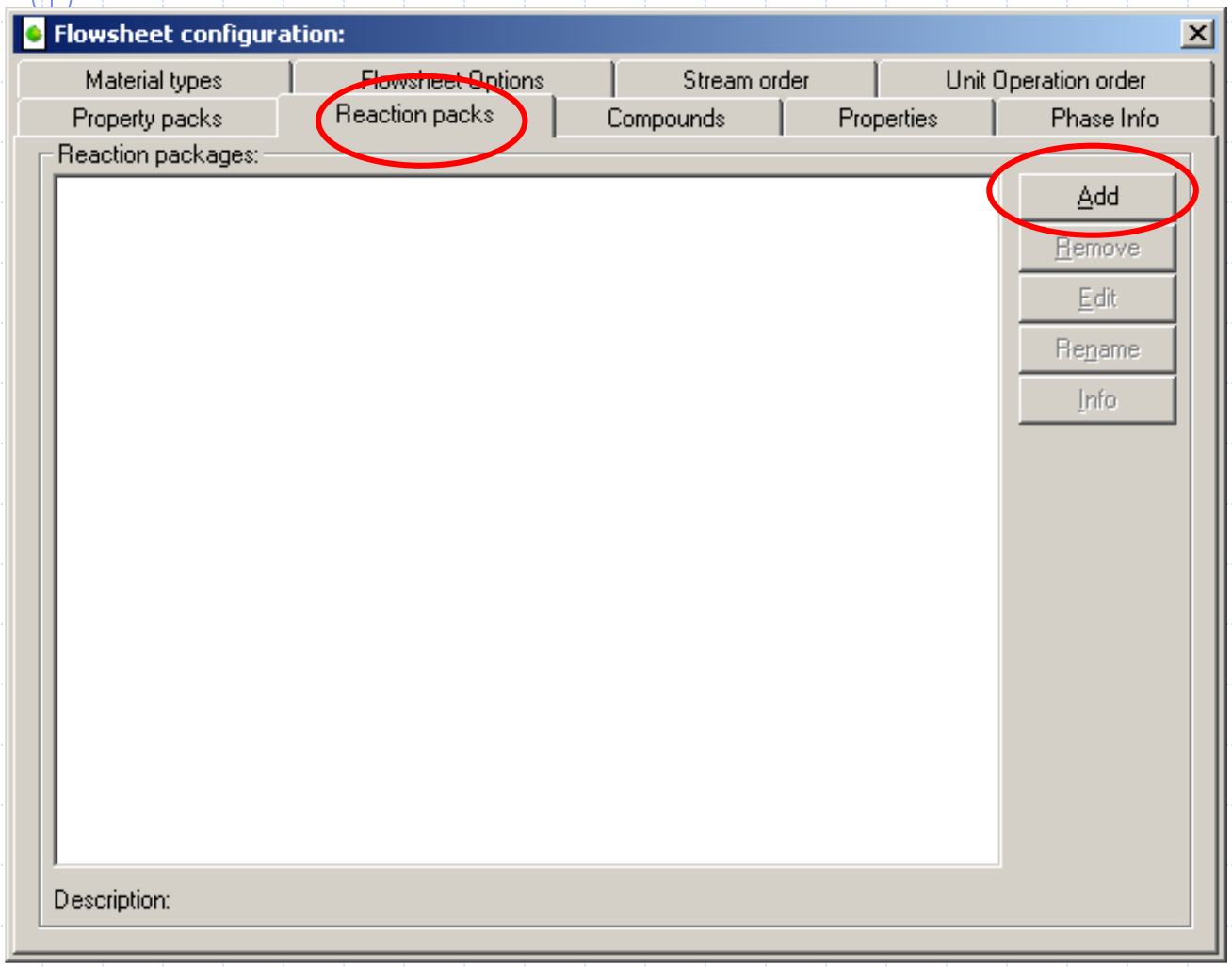


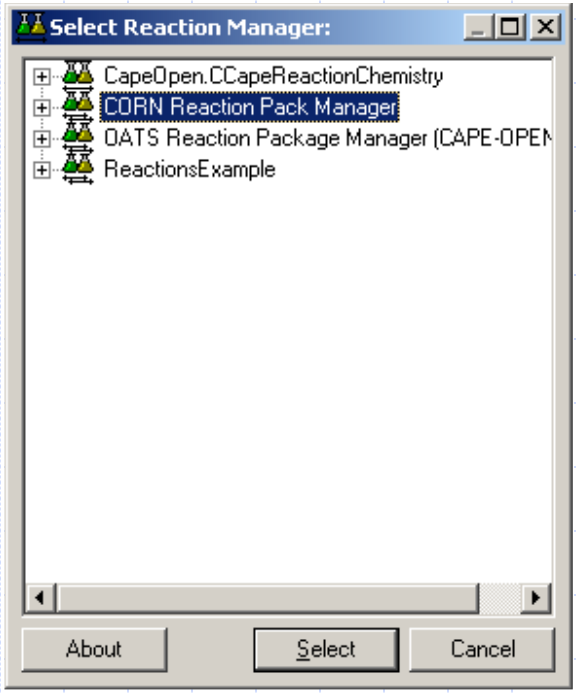
Setting up flowsheet with COFE

- Empty COFE document

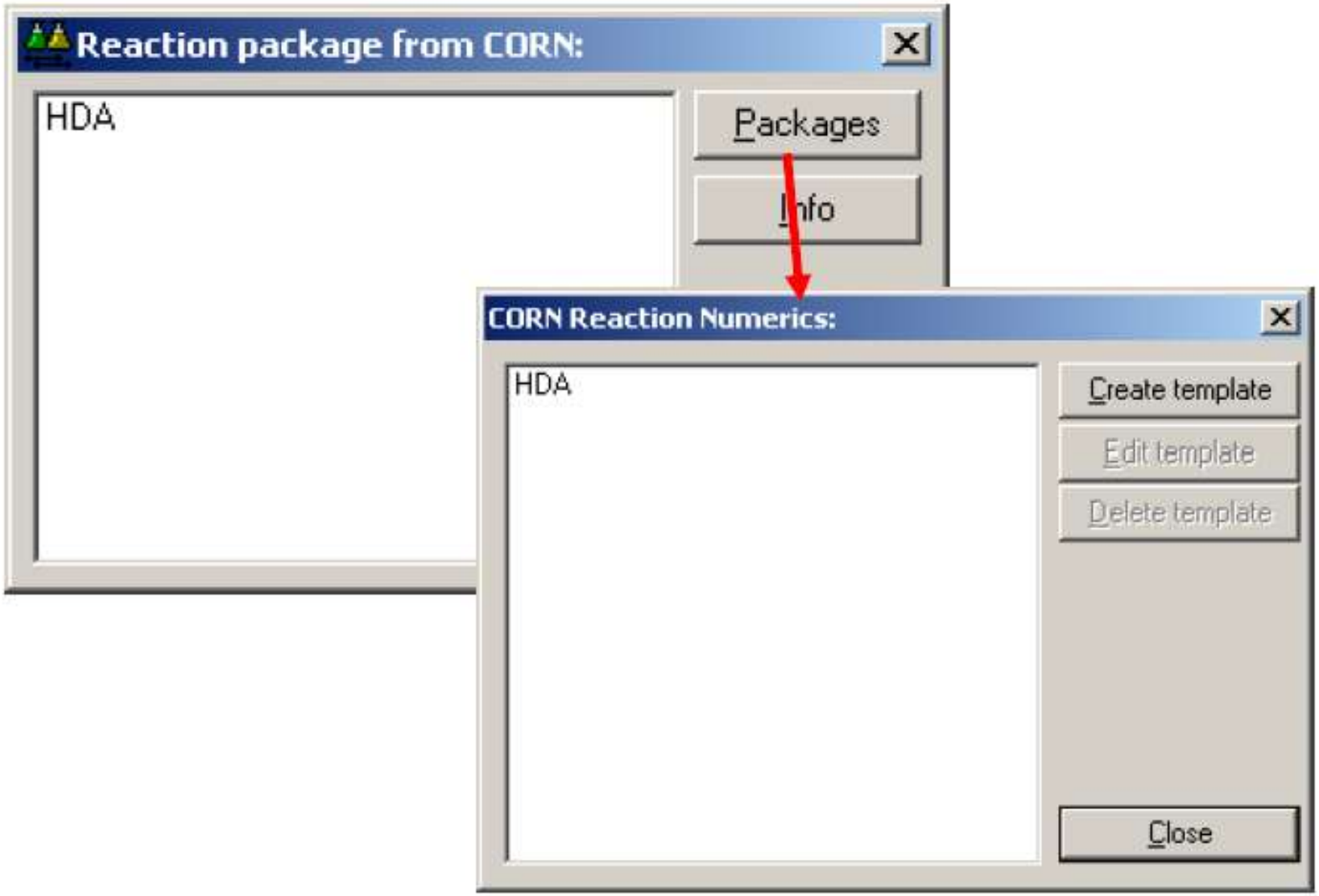


Setting up reactions



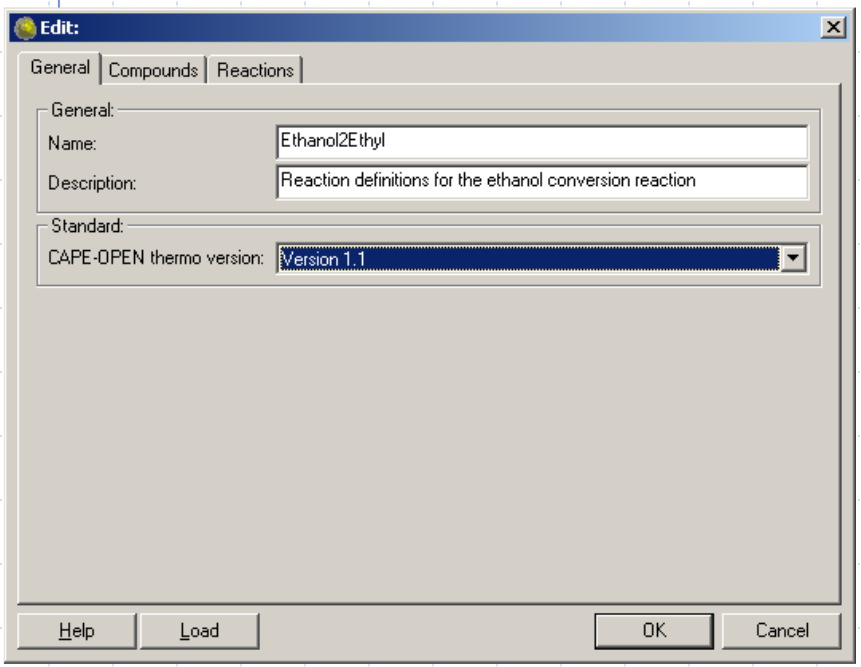


Setting up CORN

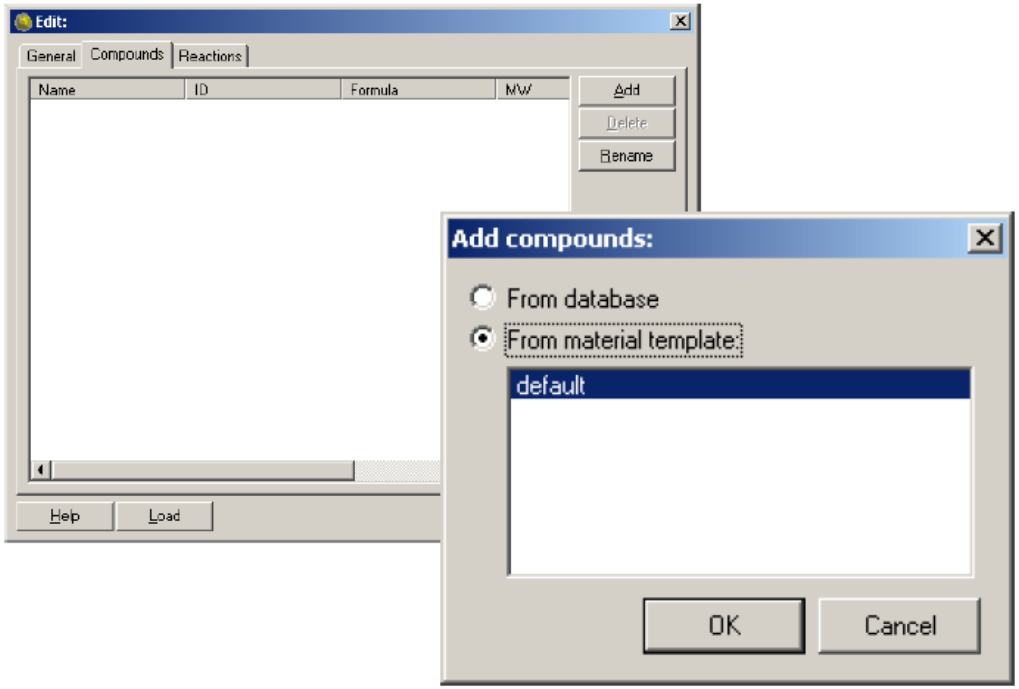


Editing a reaction package

- Create a name and description for the reaction package template

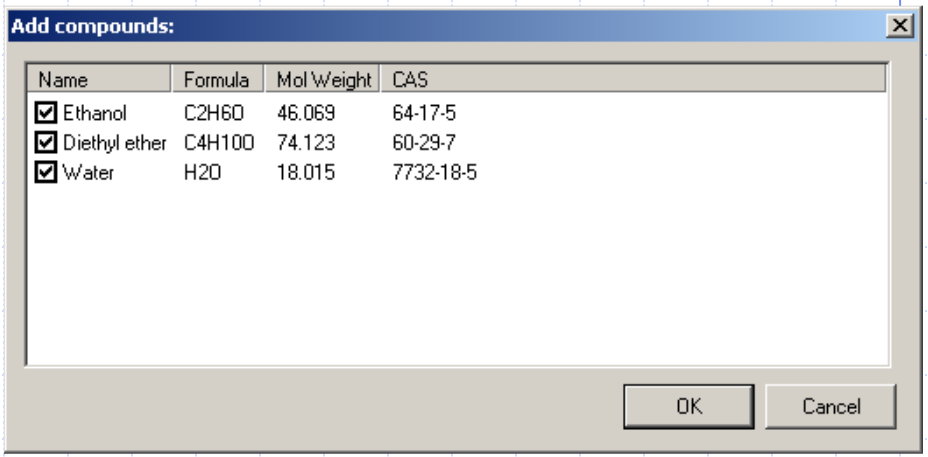


- add the compounds.
  - Hit Add on the Compounds page.
  - To use compounds defined in the simulation, choose a material template as the source for compounds and hit OK

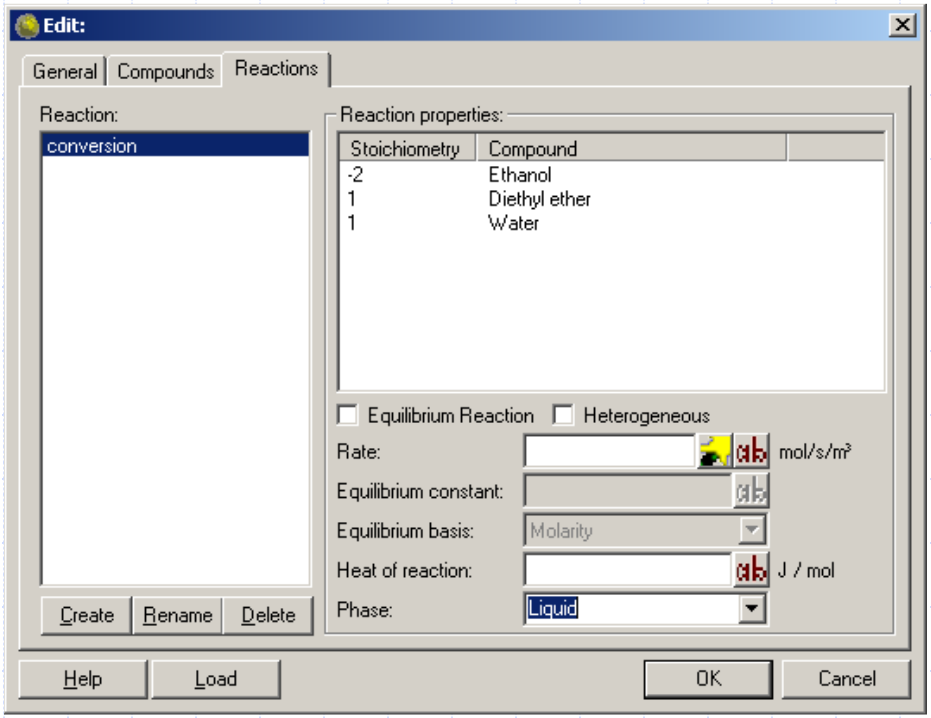


Editing a reaction package

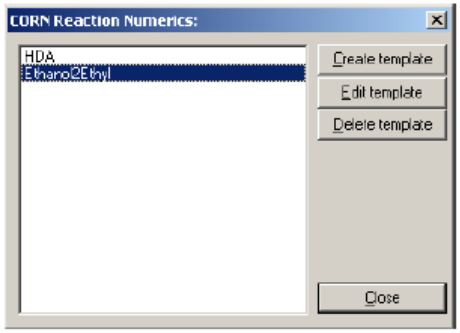
- Add all the components needed

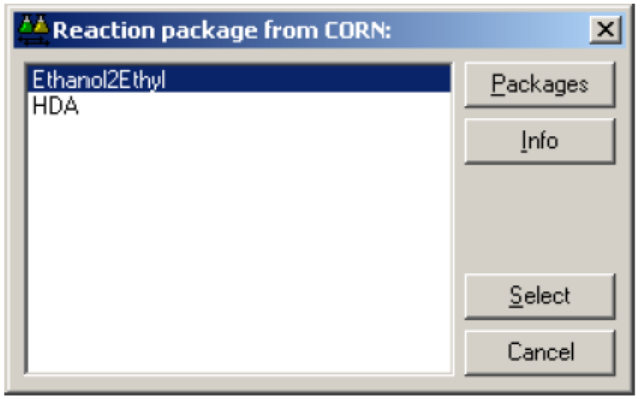


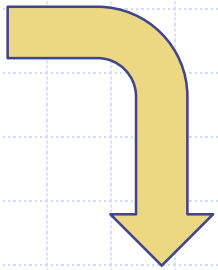
- Define the reaction.
  - On the reaction page, click Create and give a name.
  - Define sto stoichiometry
  - Select the reaction phase
  - Define a reaction rate, equilibrium constant or heat of reaction.
  - For conversion reactions no specification are needed



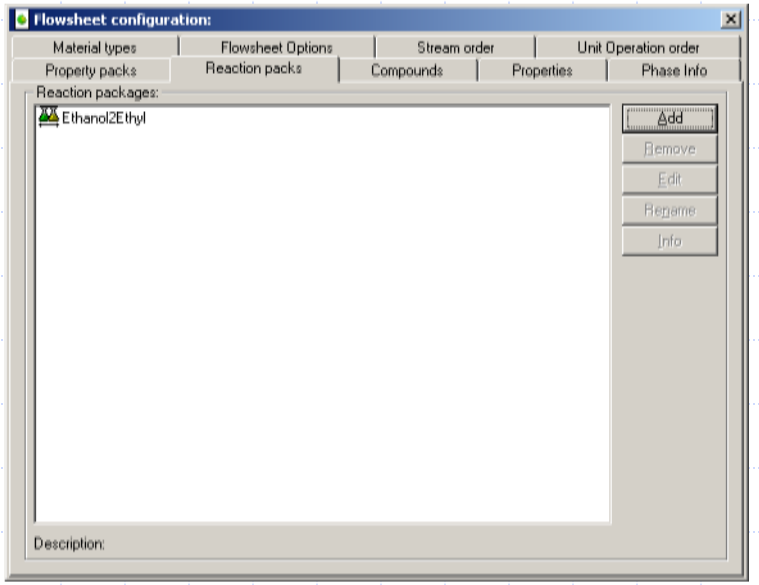
Add the reaction package to the simulation



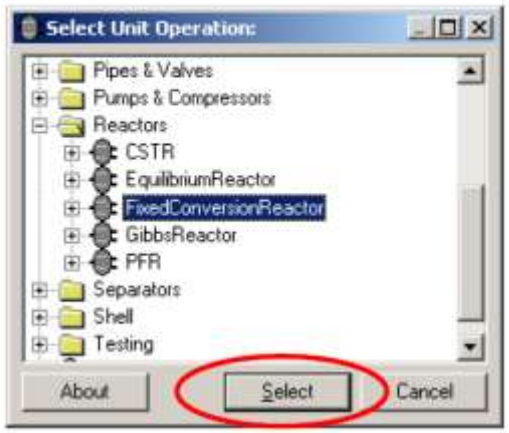


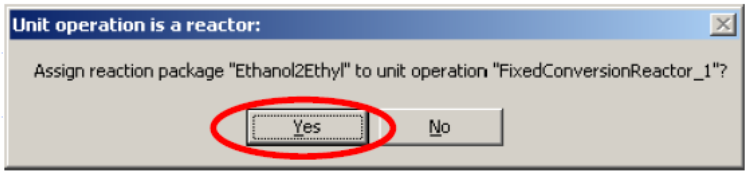


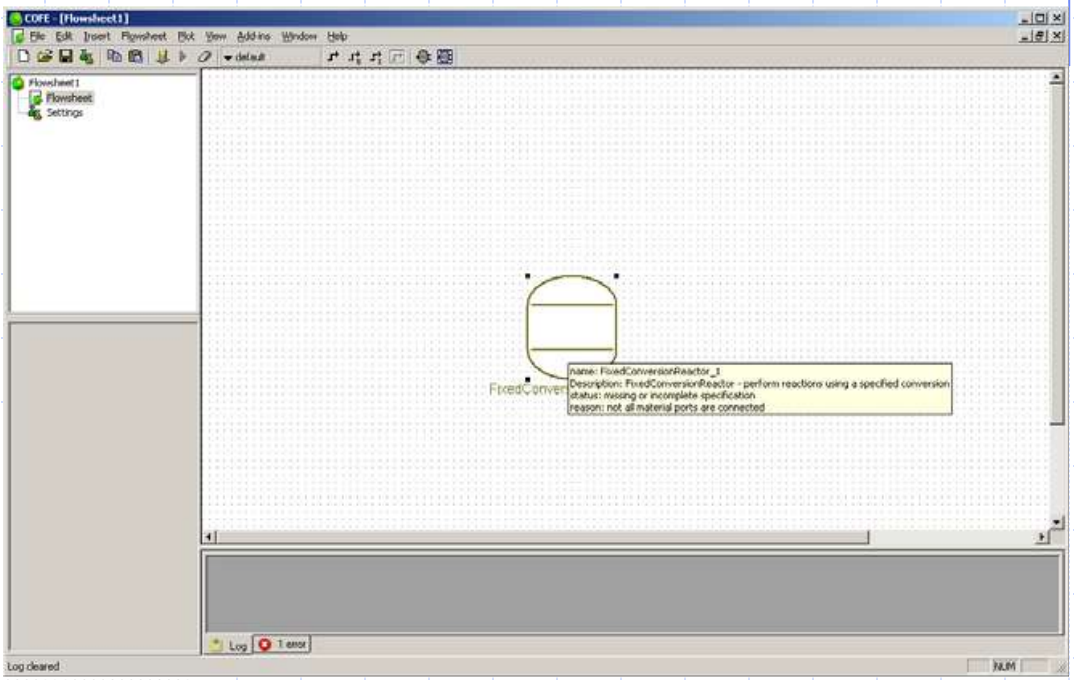
Back to COFE

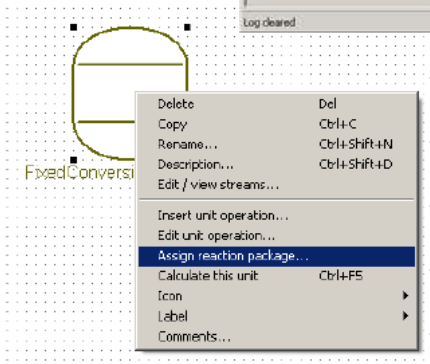


Inserting the reactor into COFE



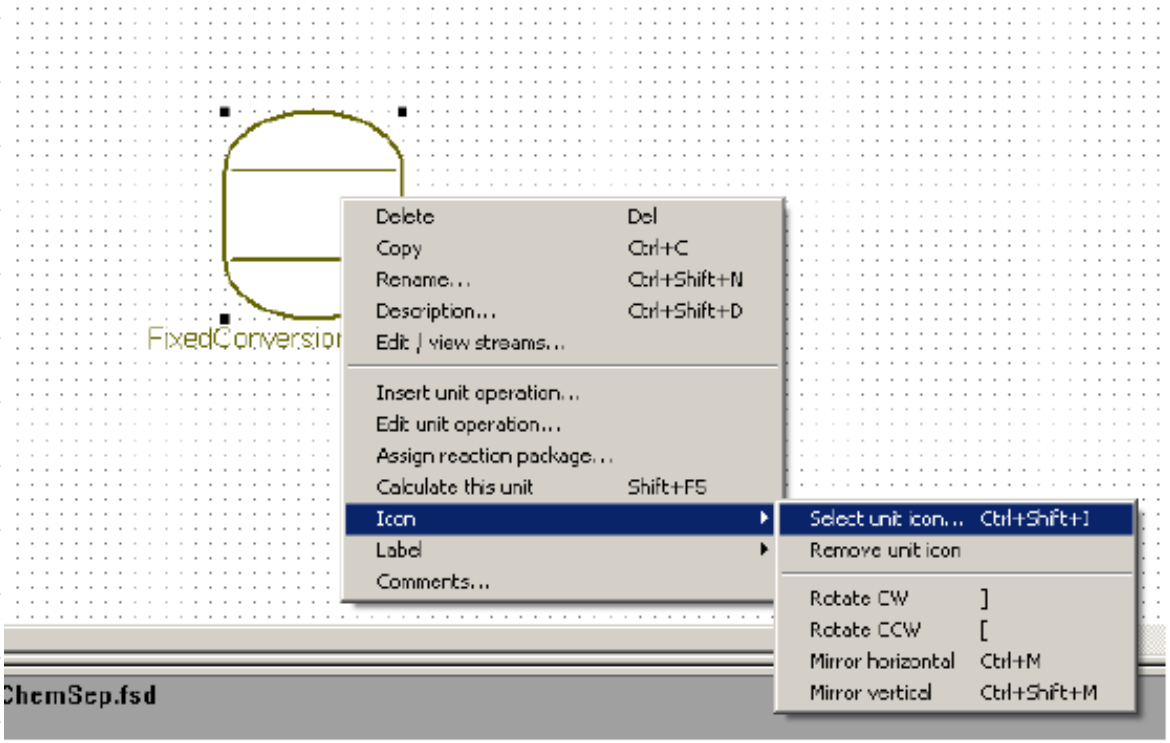


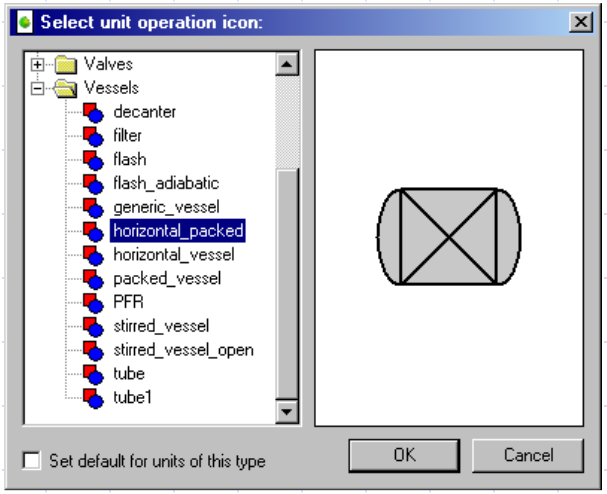




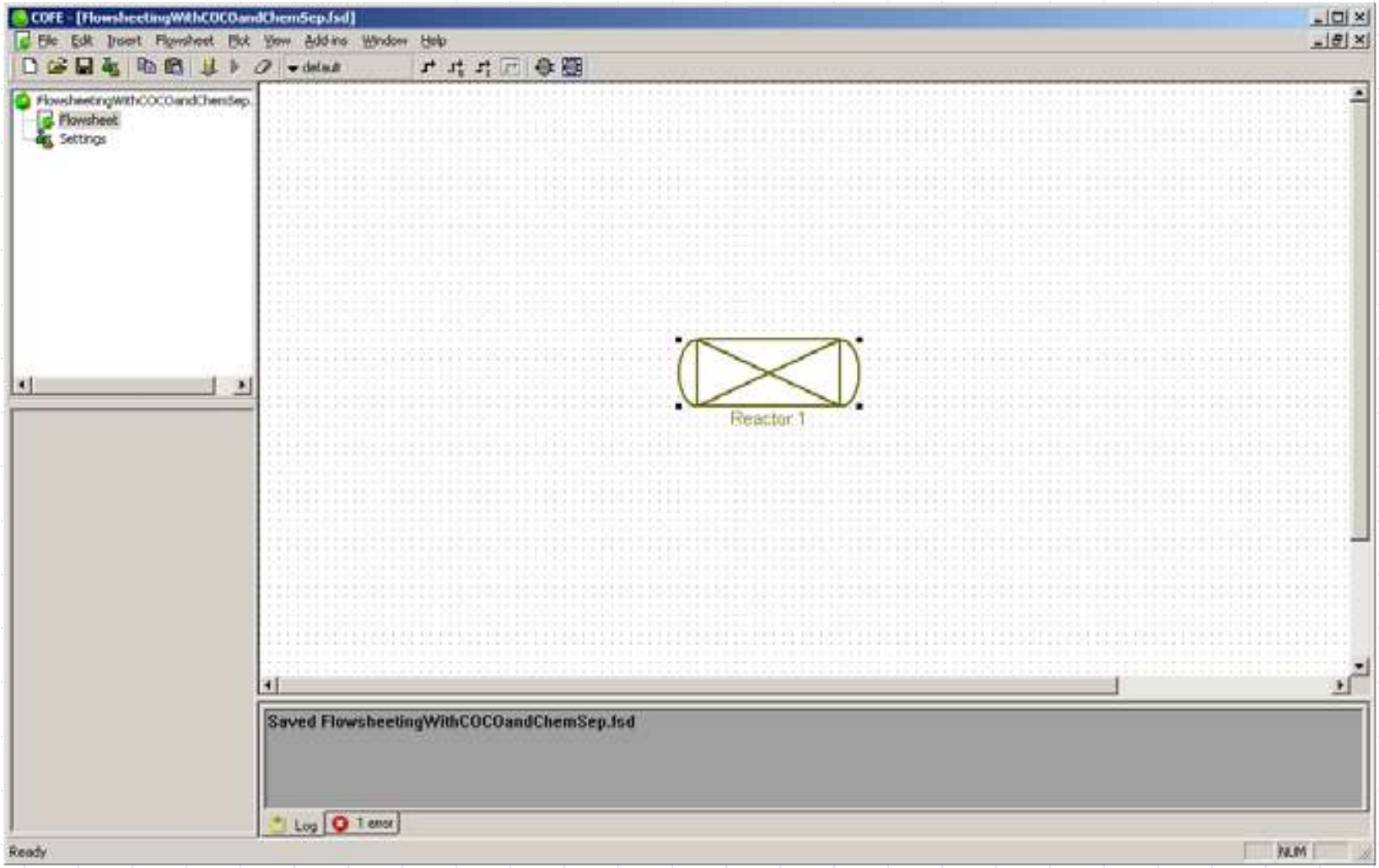
Changing the appearance of the reactor

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



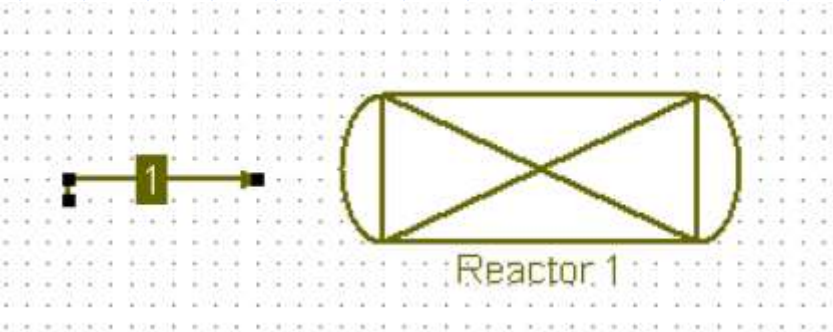


Inserting the reactor

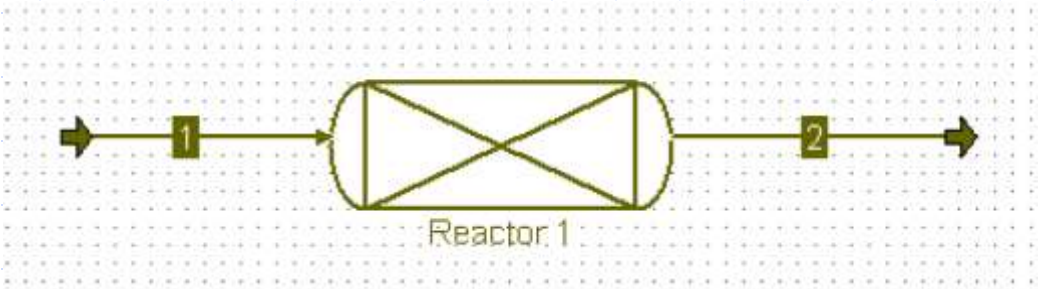


Inserting reactor feed and product stream

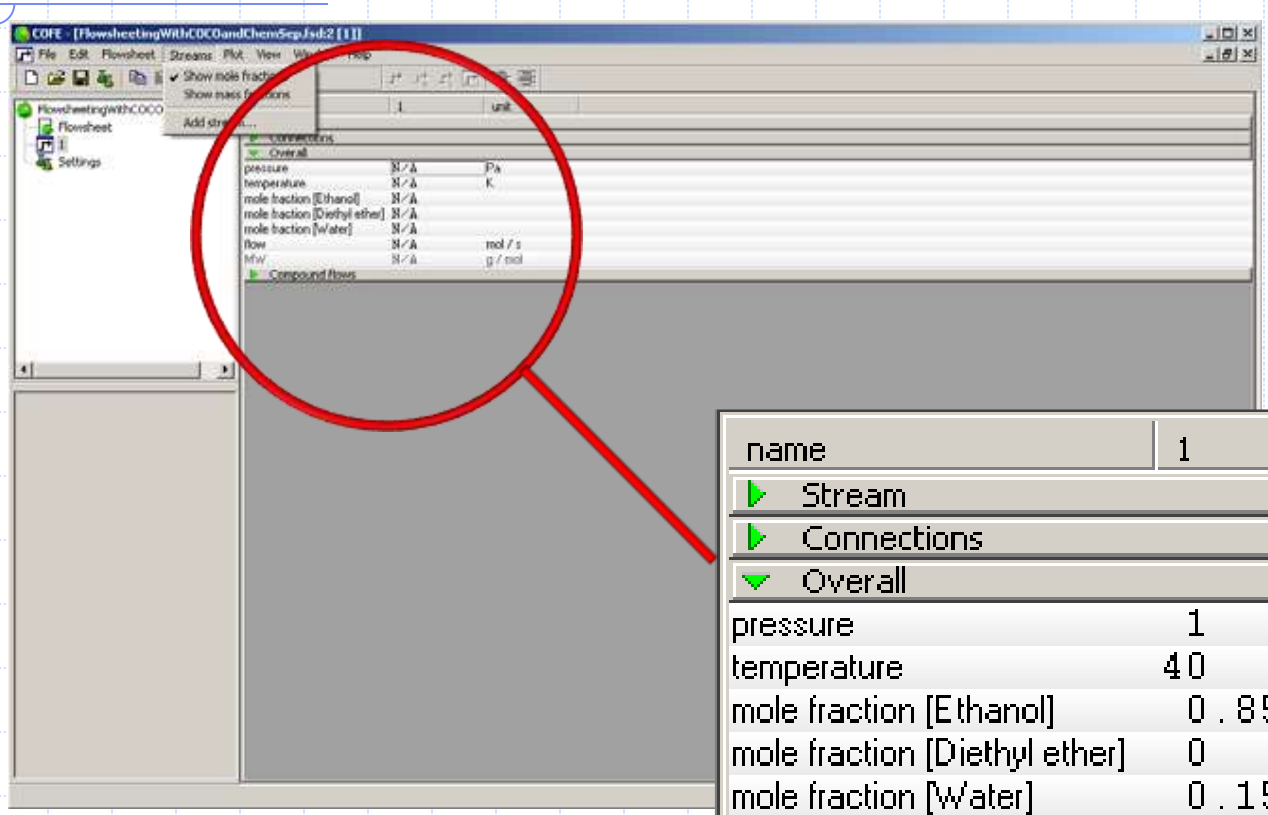
- Reactor feed stream



- Product stream

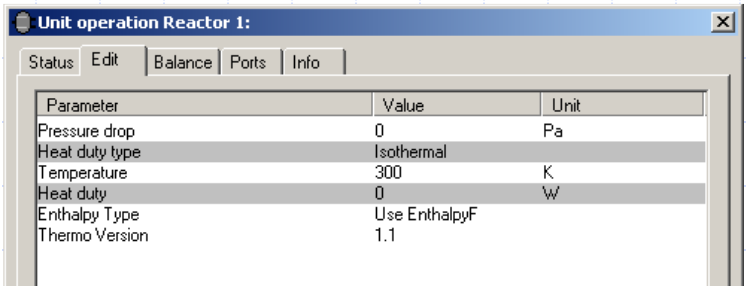


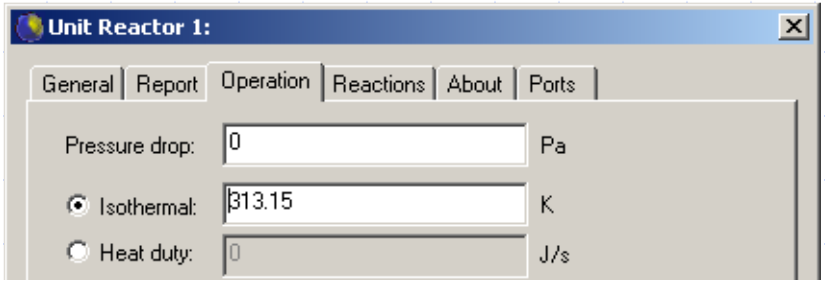
Specify the feed stream

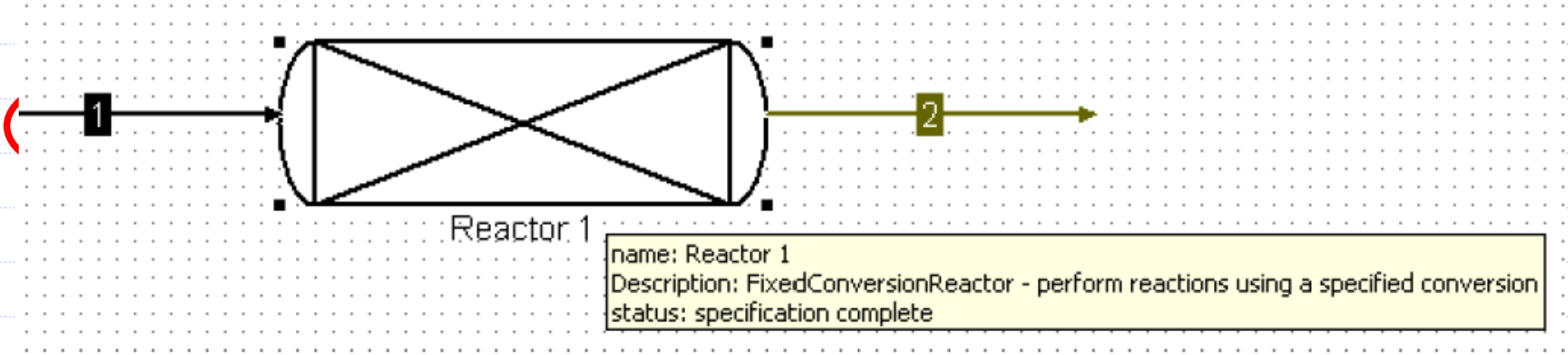


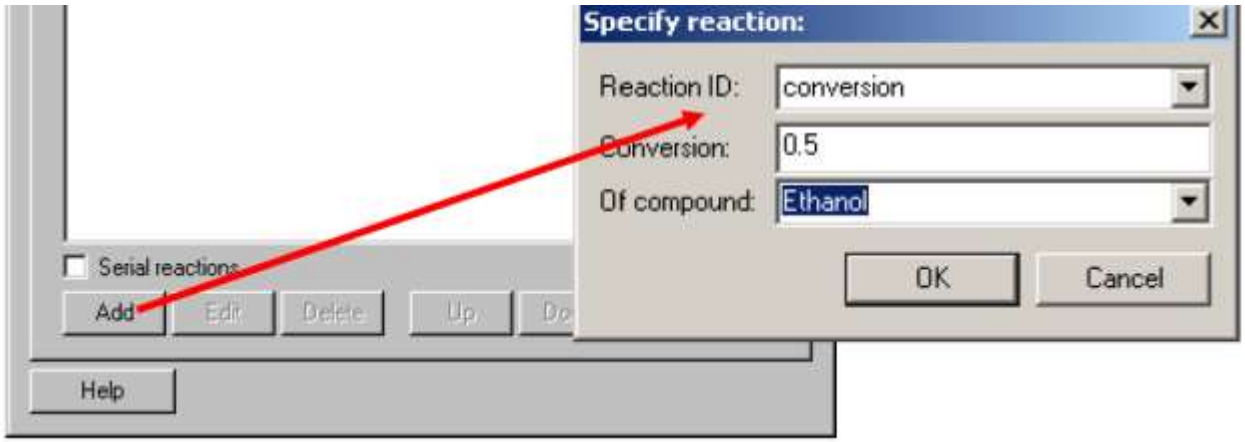
name	1	unit
Stream		
Connections		
Overall		
pressure	1	atm
temperature	40	°C
mole fraction [Ethanol]	0.85	
mole fraction [Diethyl ether]	0	
mole fraction [Water]	0.15	
flow	20	mol / s
MW	41.8609	g / mol
Compound flows		
Phase Fractions		
molar phaseFraction [Liquid]	1	
Liquid composition		
Overall properties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

Reactor's specification

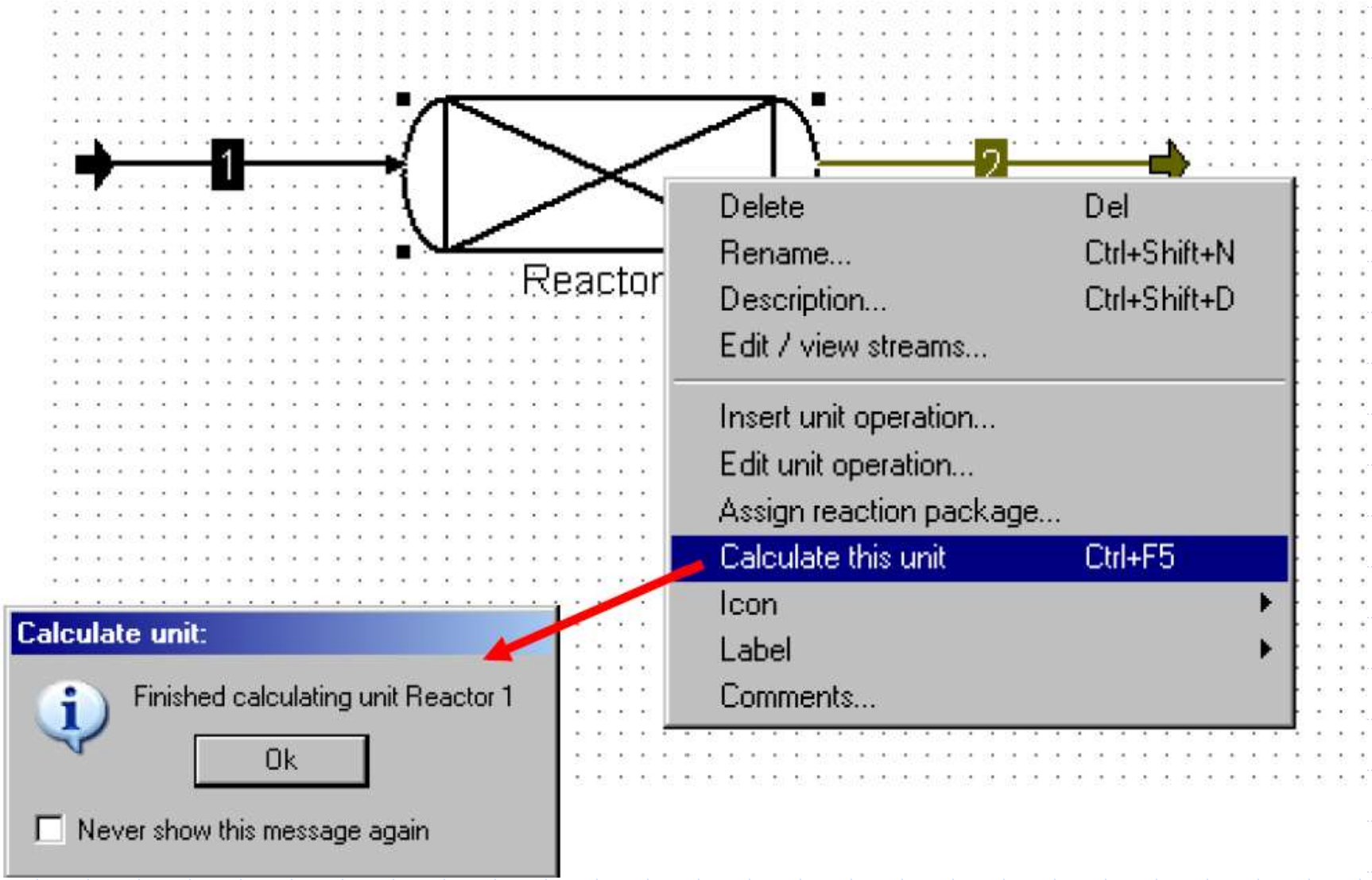




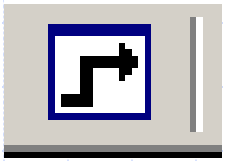




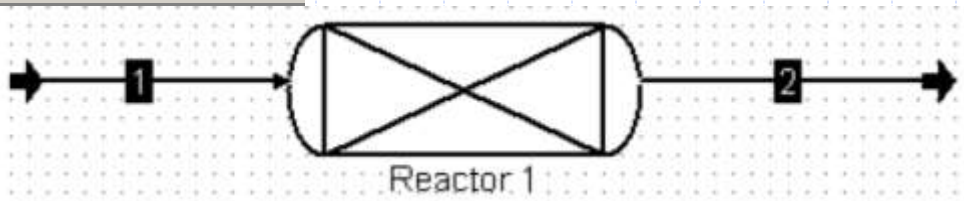
Calculate the reactor



Reactor's results



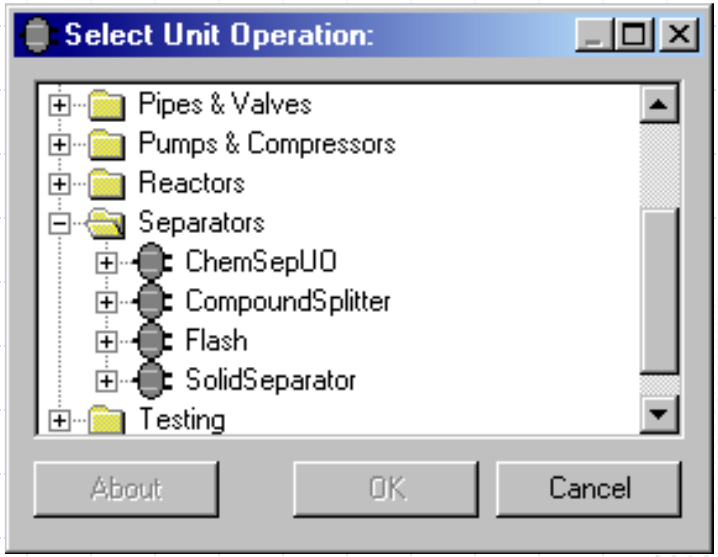
name	1	2	unit
Stream			
Connections			
Overall			
pressure	1	1	atm
temperature	40	40	°C
mole fraction [Ethanol]	0.85	0.425	
mole fraction [Diethyl ether]	0	0.2125	
mole fraction [Water]	0.15	0.3625	
flow	20	20	mol / s
MW	41.8609	41.8609	g / mol
Compound flows			
Phase Fractions			
molar phaseFraction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

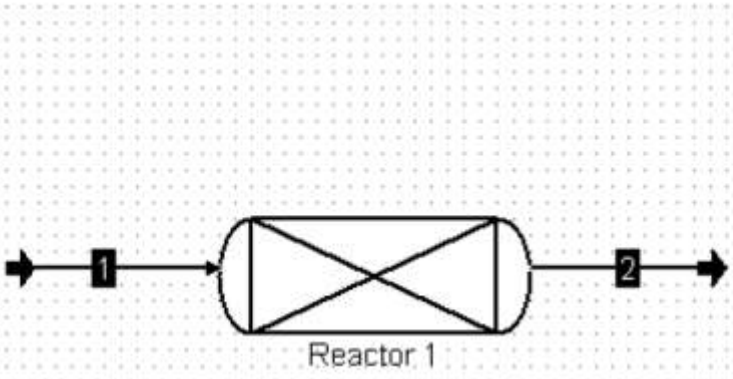


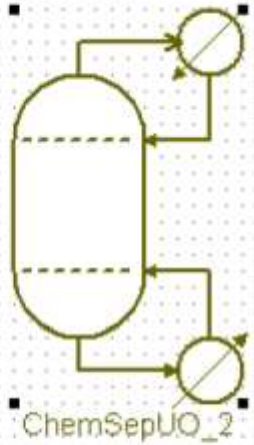
Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

Using ChemSep in COFE

- Inserting ChemSep in COFE

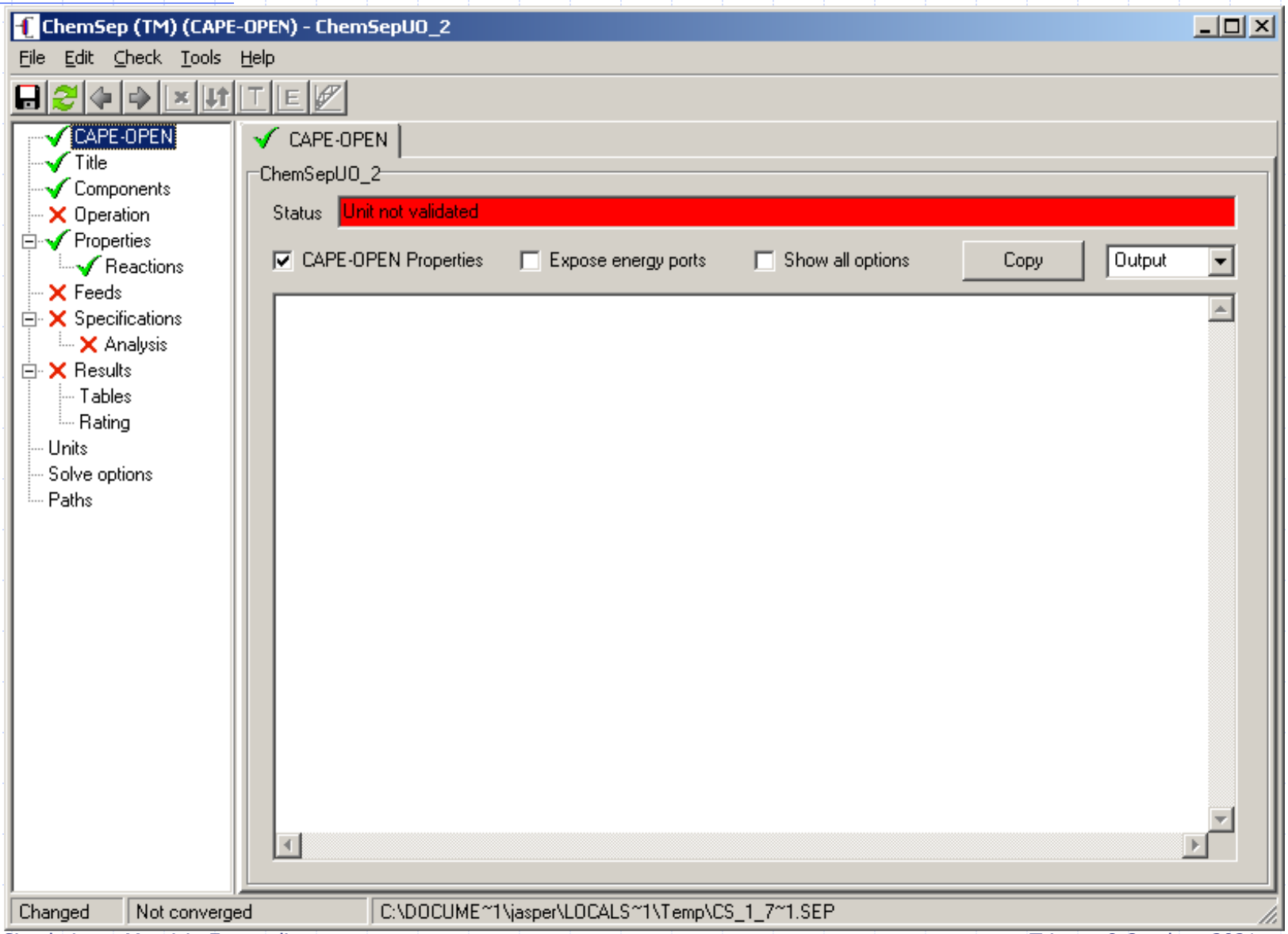




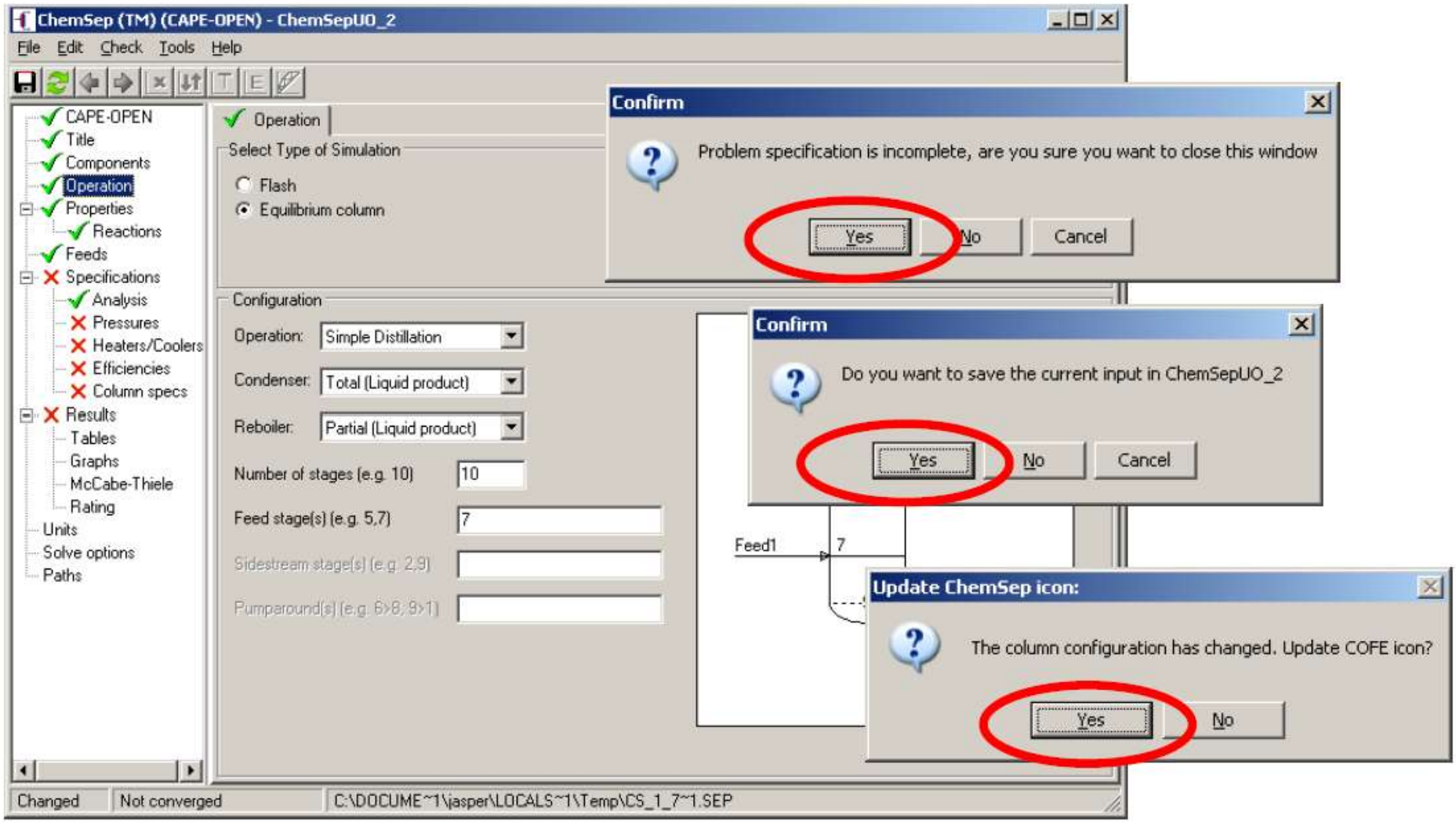


Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

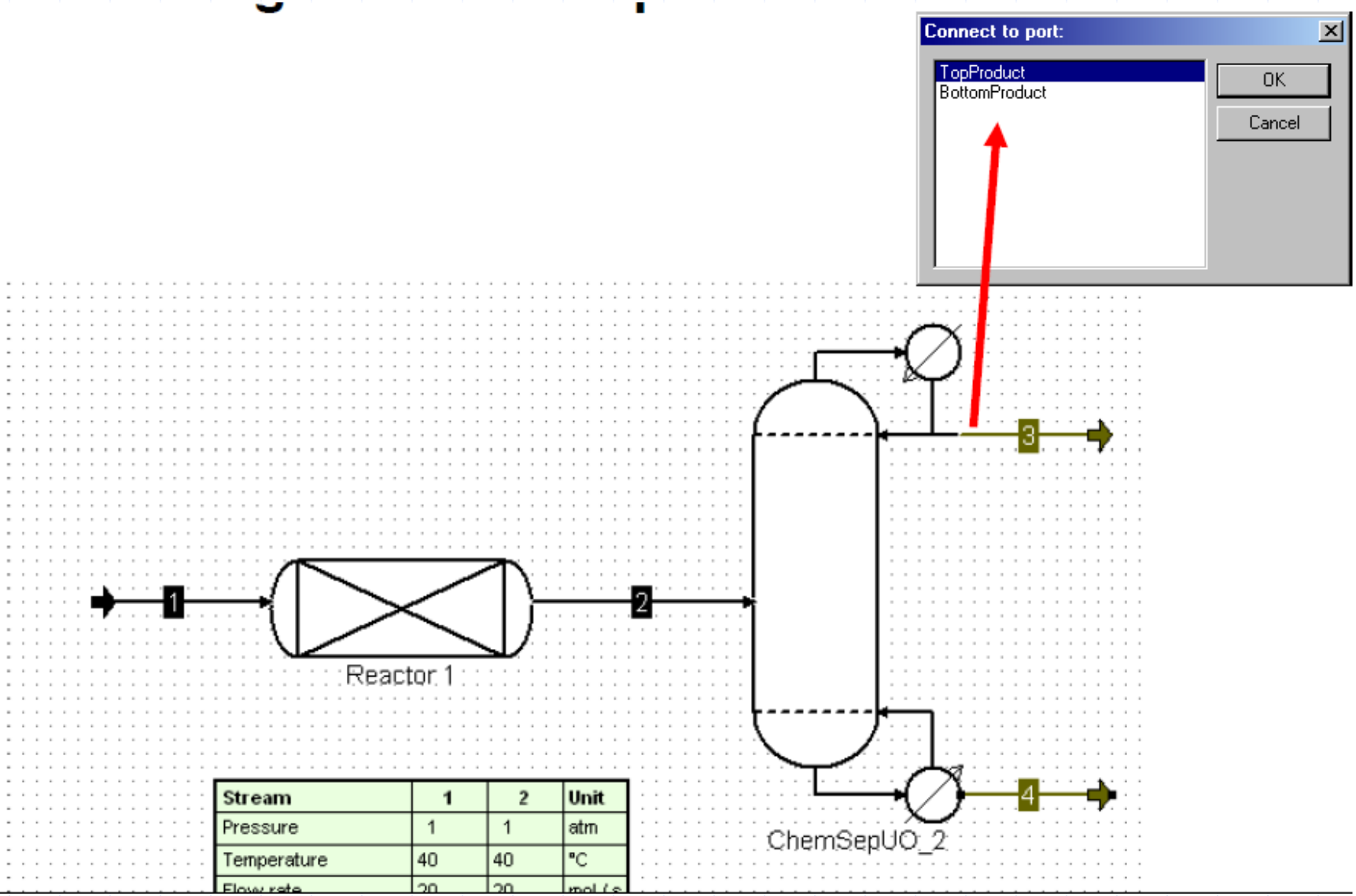
Inserting ChemSep column



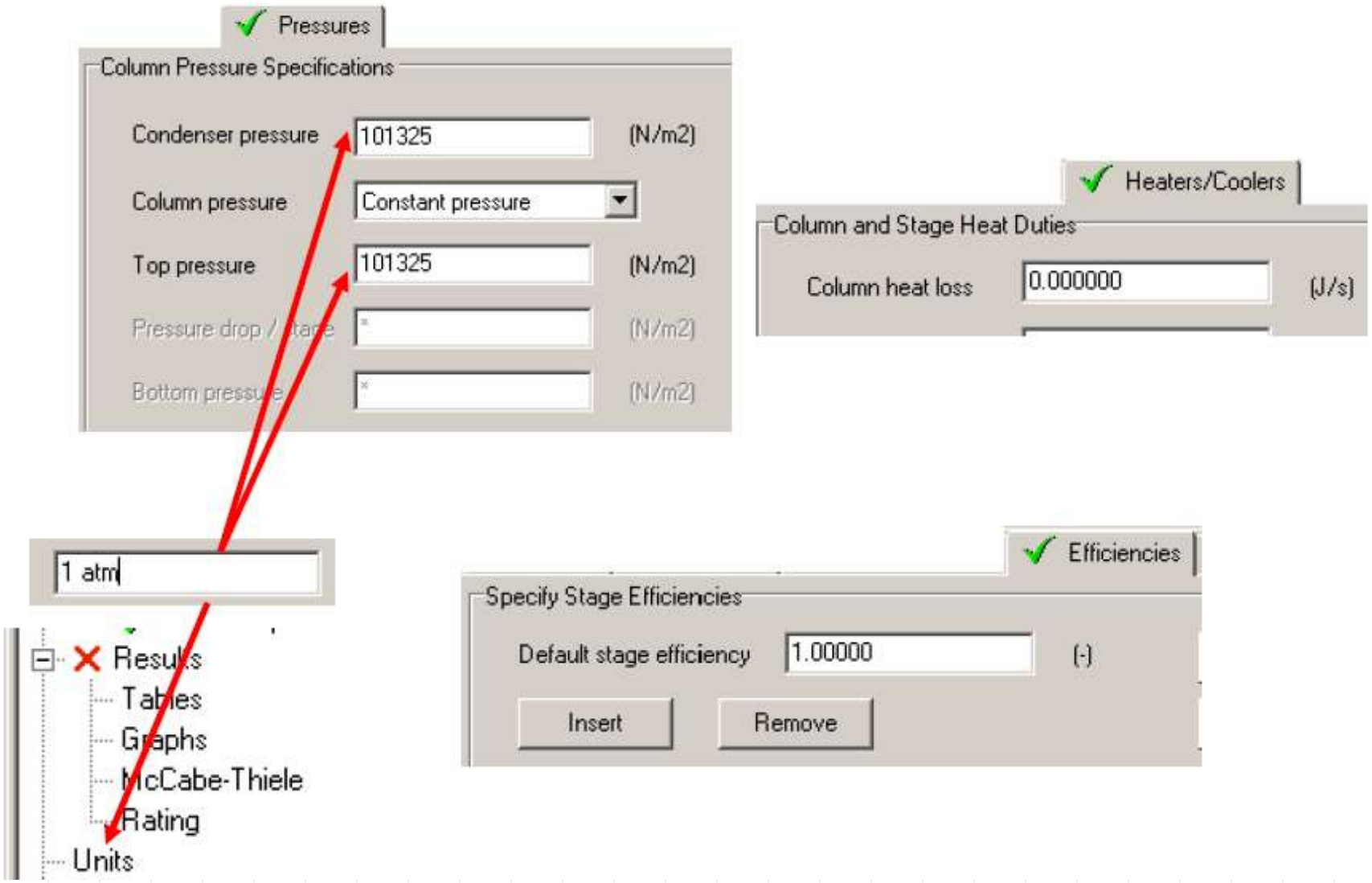
Configuring ChemSep column



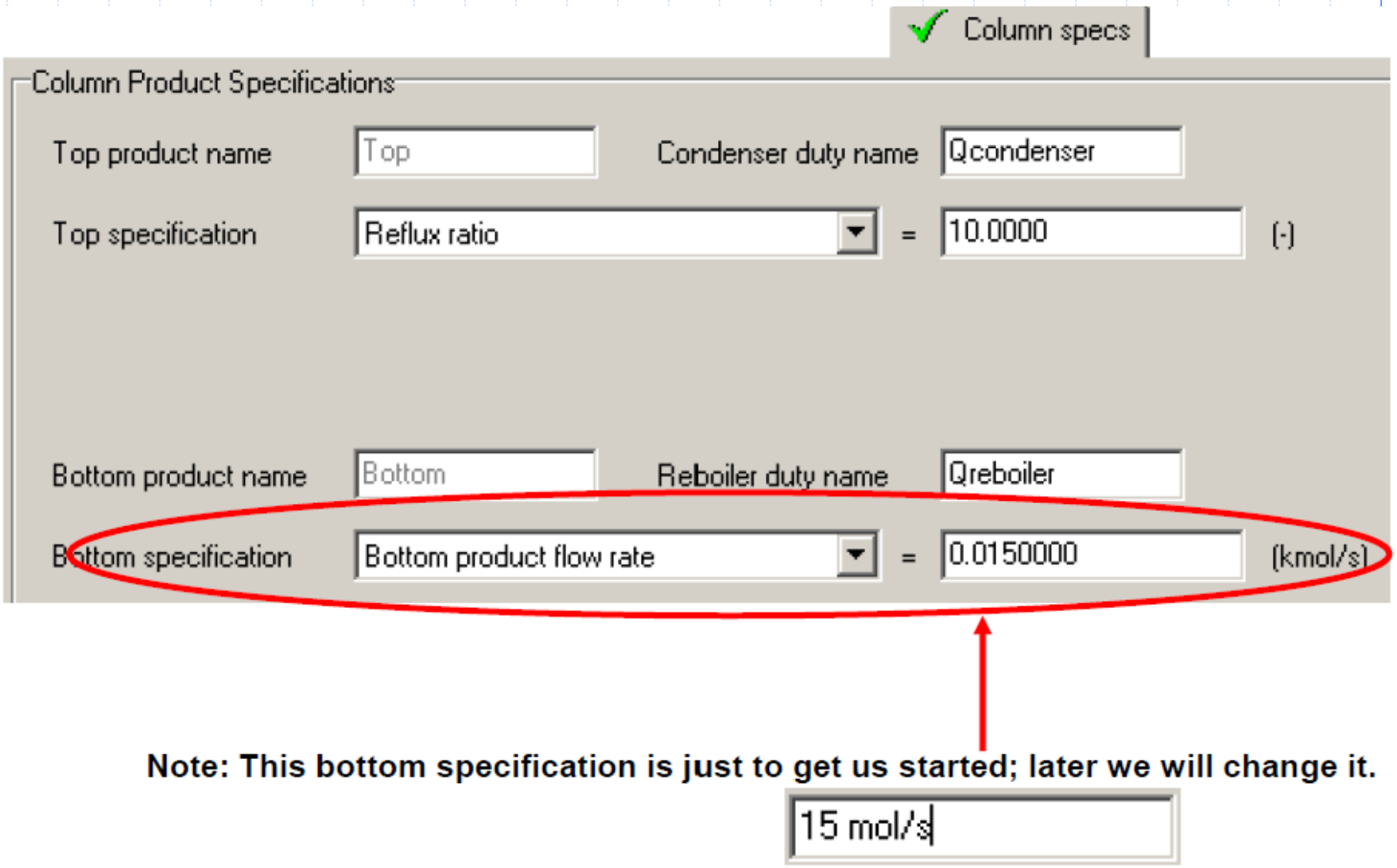
Connecting the ChemSep column



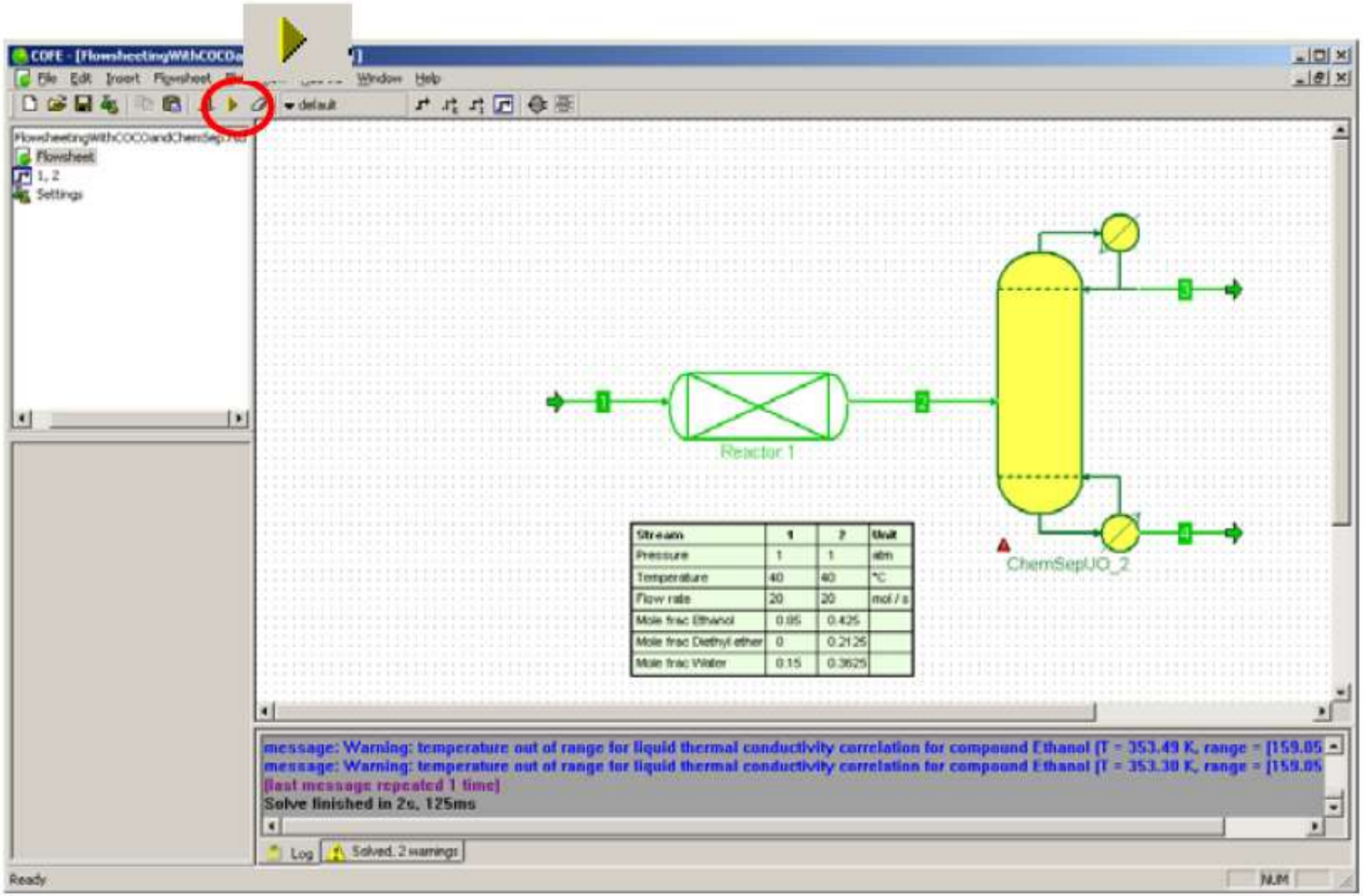
Configuring ChemSep column



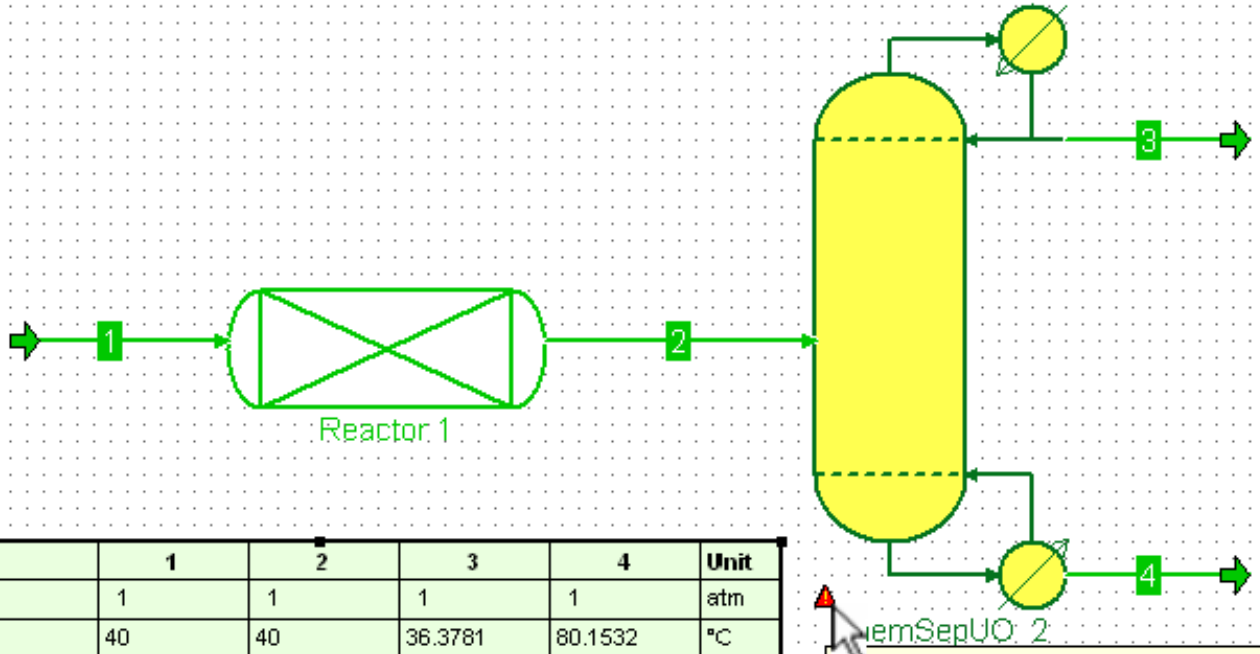
Configuring ChemSep column



Run the column



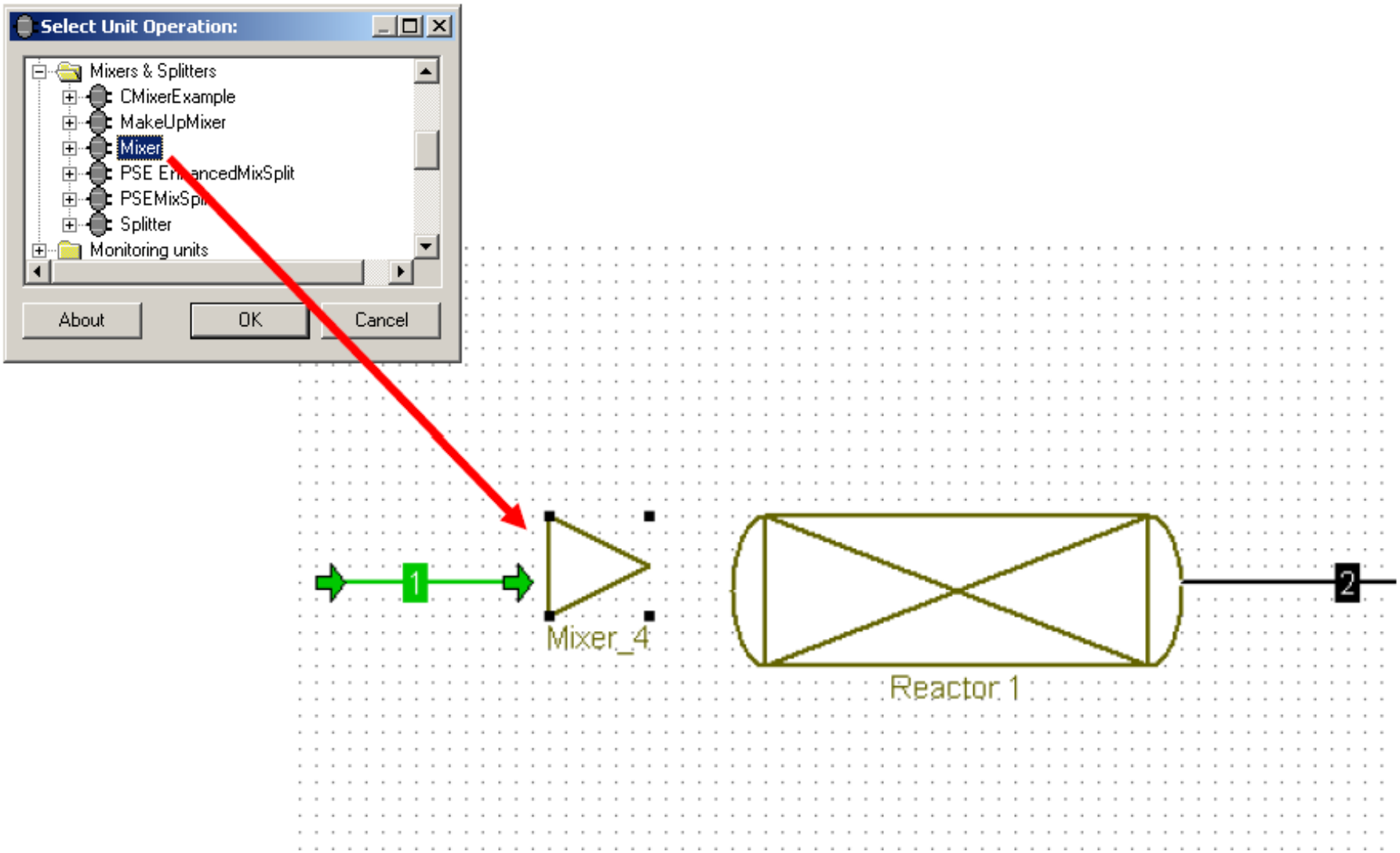
Checking column results



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	

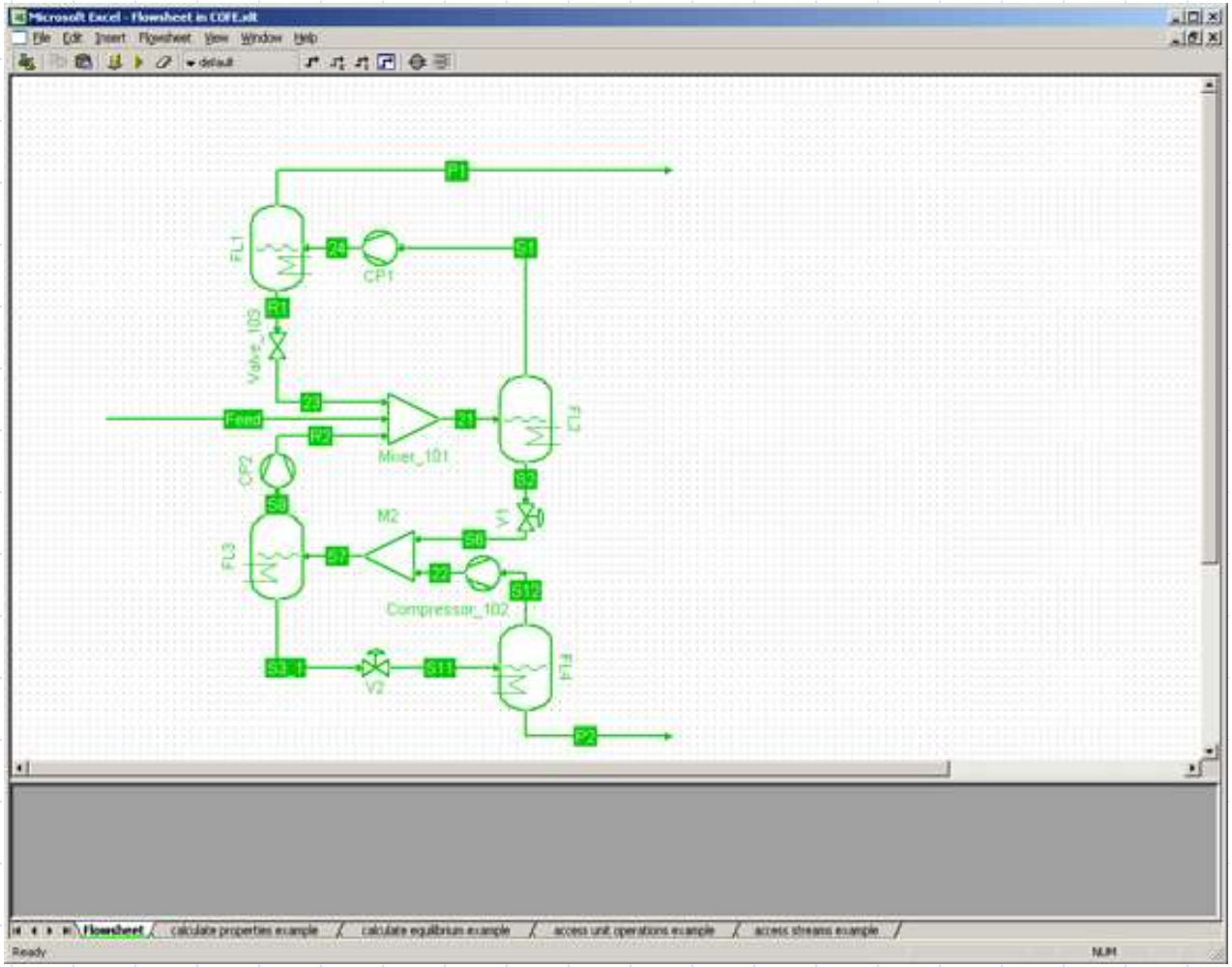
olve warnings:
solving ChemSepUO_2
message: Warning: temperature out of range for liquid thermal conductivity correlation for compound Ethanol (T = 353.49 K, range = [159.05 - 353.15] K)
message: Warning: temperature out of range for liquid thermal conductivity correlation for compound Ethanol (T = 353.30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

Setting up the recycle



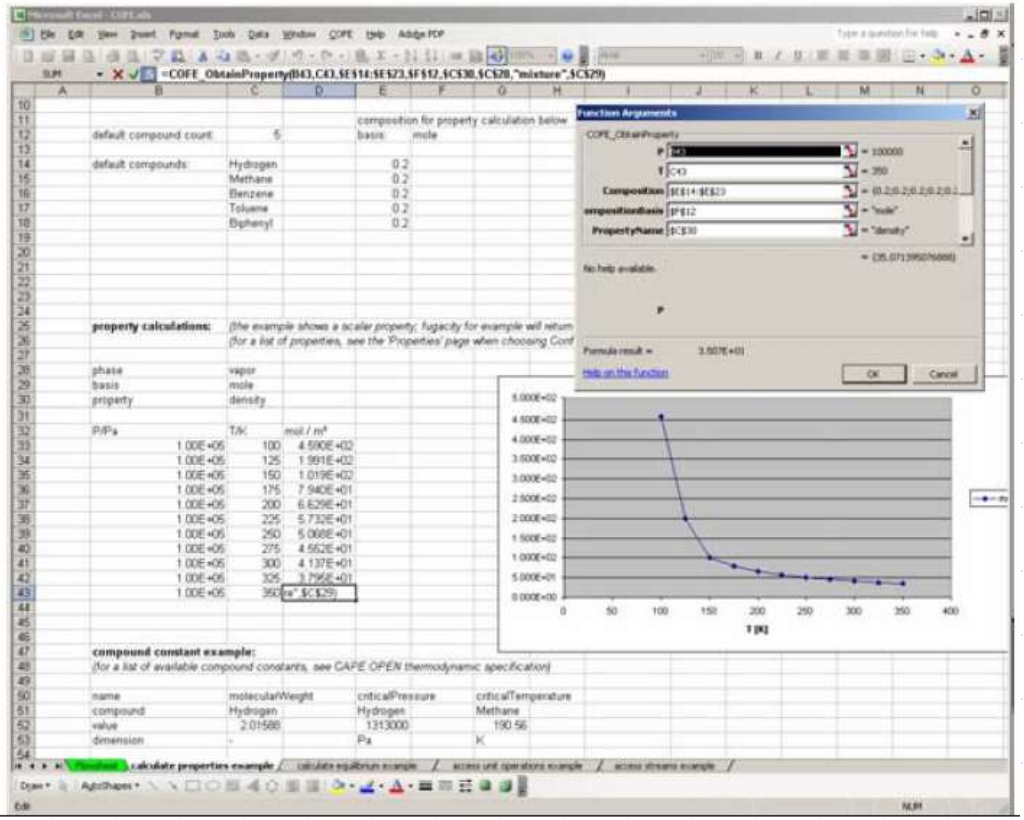
Embedding flowsheets in EXCEL

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



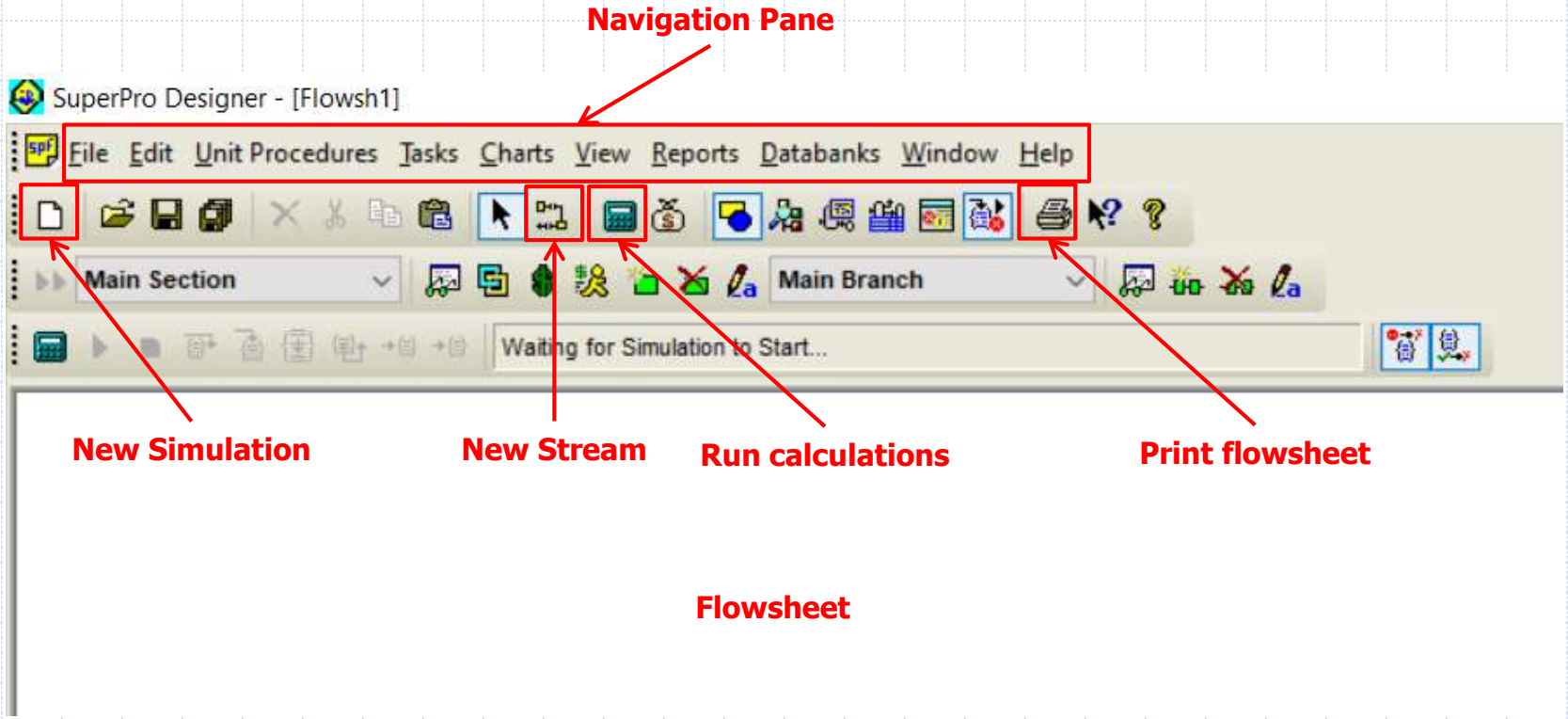
Embedding flowsheets in EXCEL

- Once the flowsheet is embedded a 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

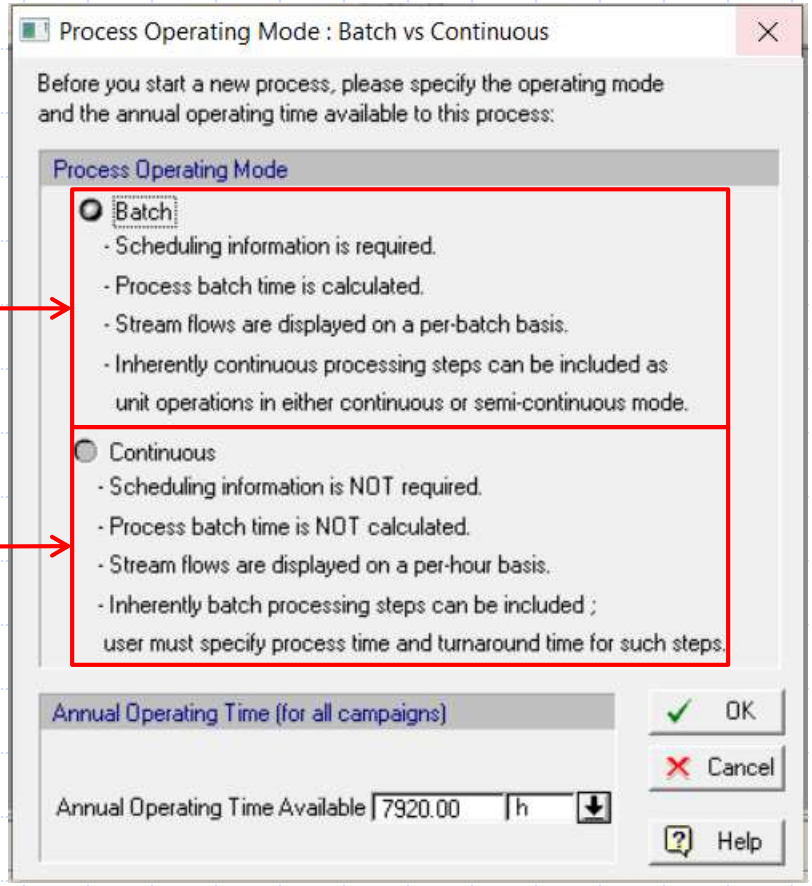
User interface



SuperPro Start Page

Batch Operating Mode

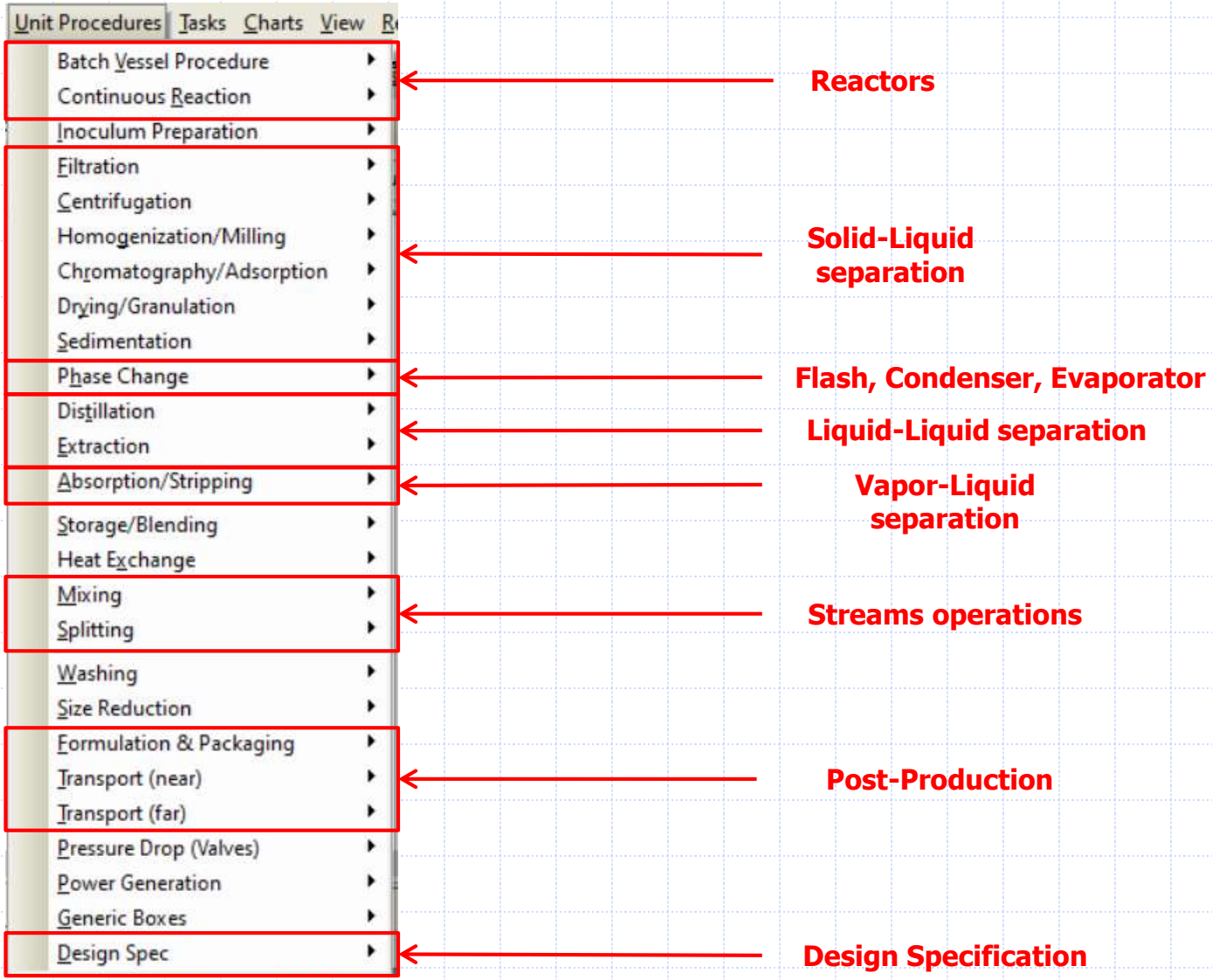
Continuous Operating Mode



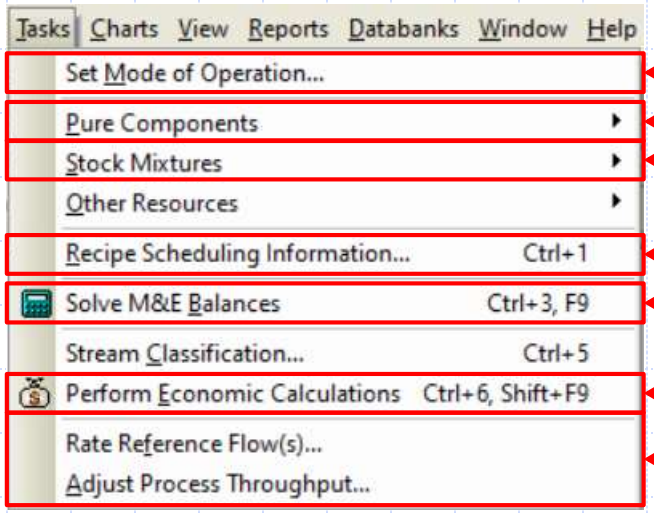
SuperPro Procedure

- 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



SuperPro Tasks



Batch/Continuous mode

Add components to simulation

Add mixtures to simulation

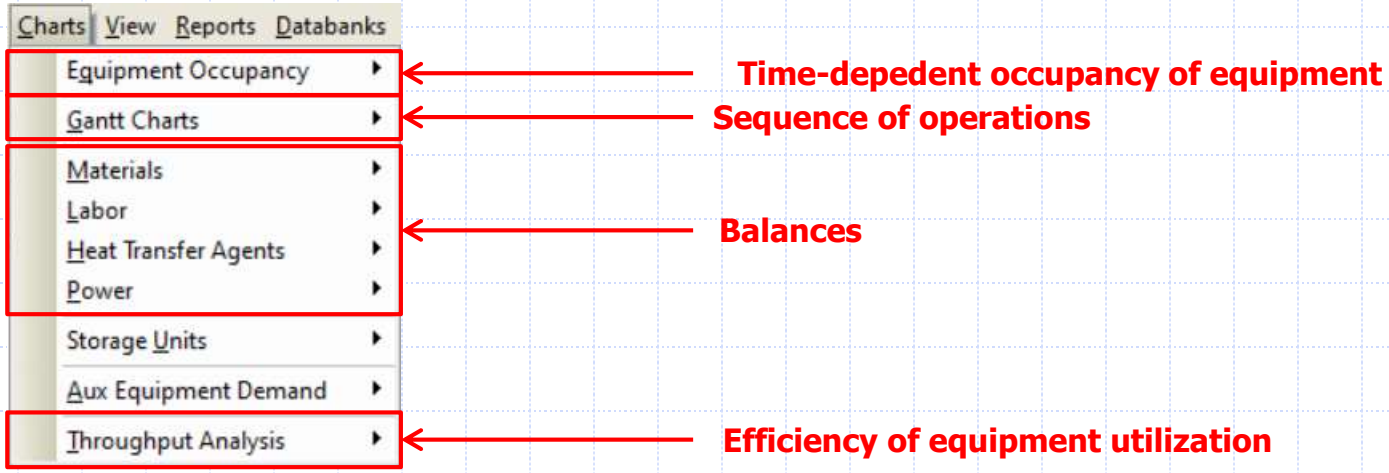
 # Batches, Time, bottlenecks

Run command

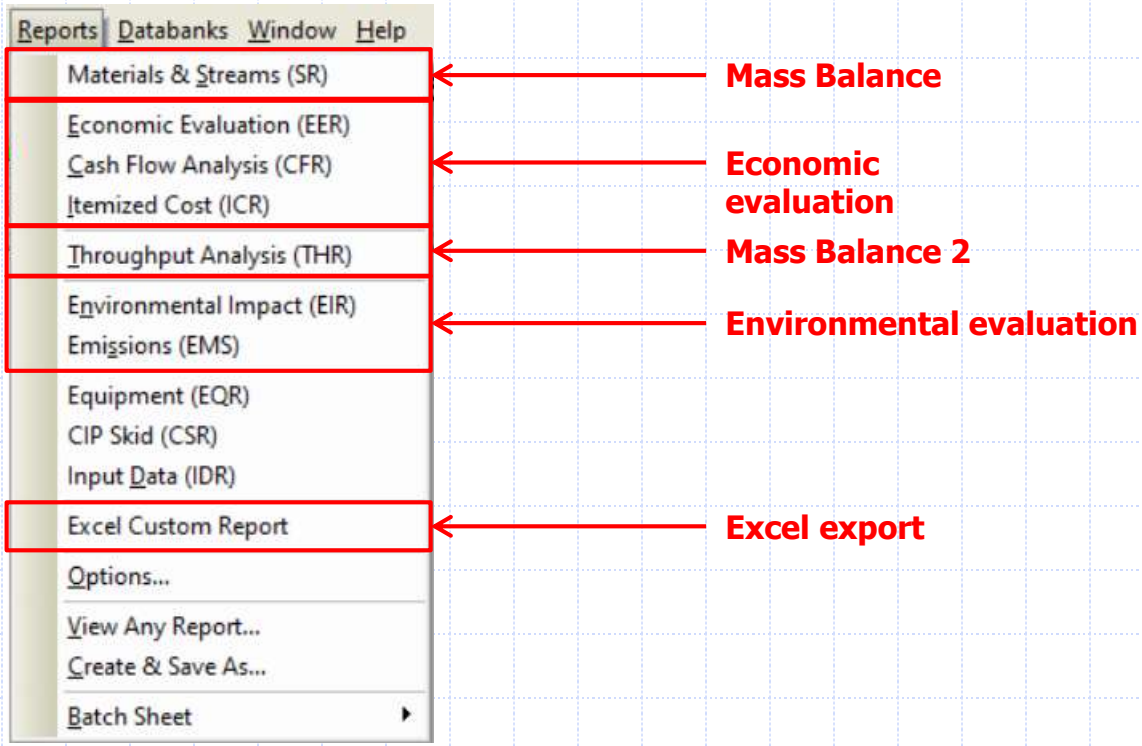
Perform economic calculations

Production potentiality

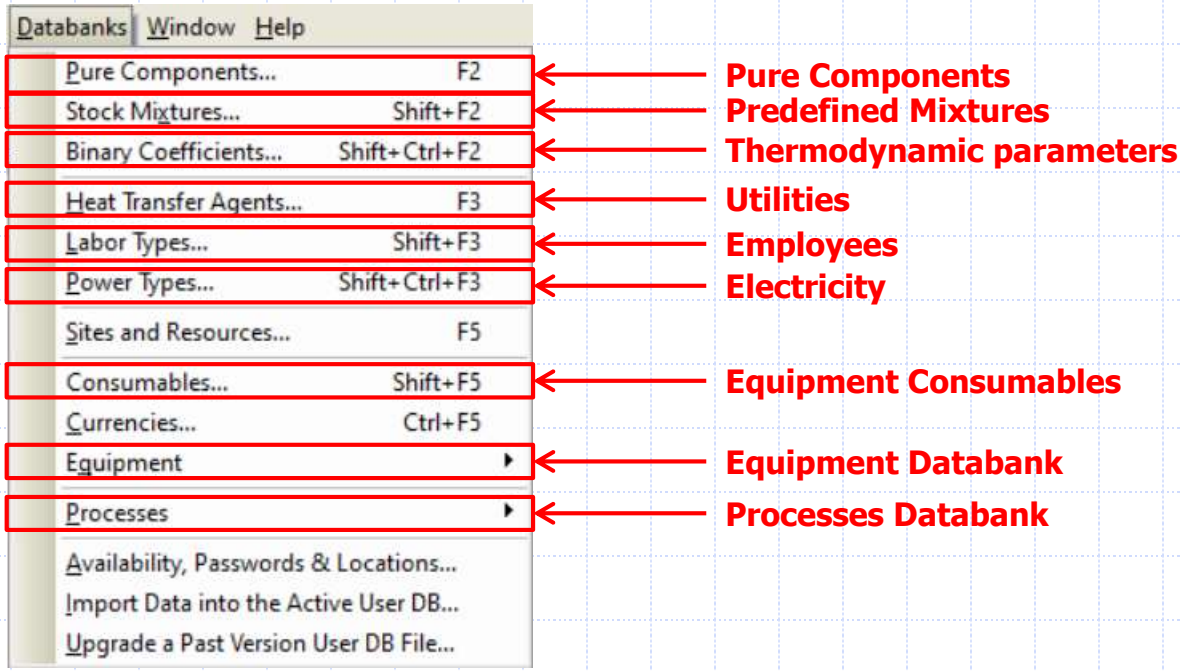
SuperPro Charts



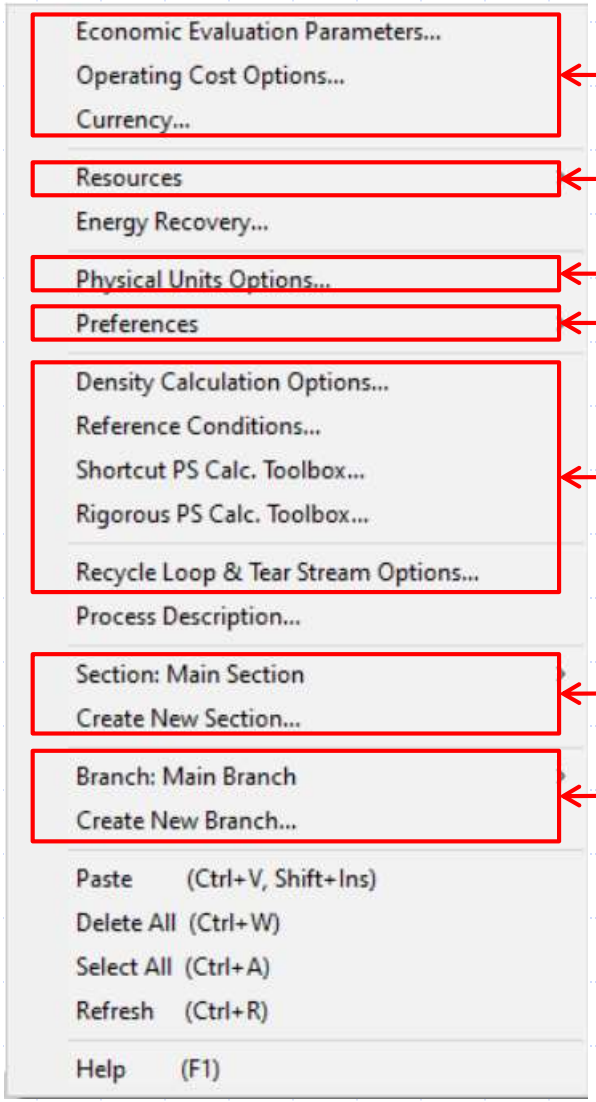
SuperPro Reports



SuperPro Databanks



SuperPro Flowsheet Right-Click



Financial aspects

Strams info

Definition of physical units

Report information

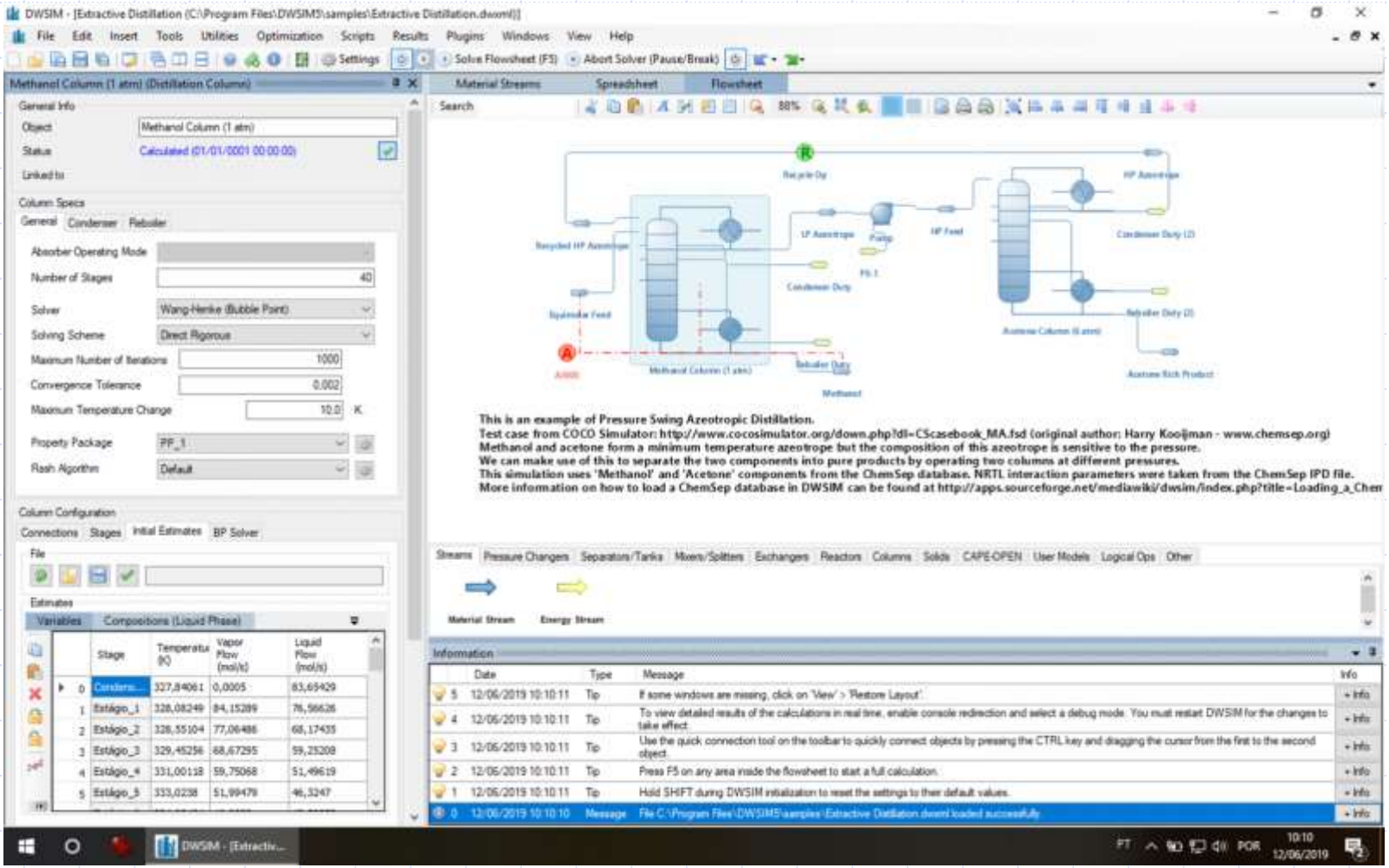
Calculation methods and parameters

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



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)
- .....