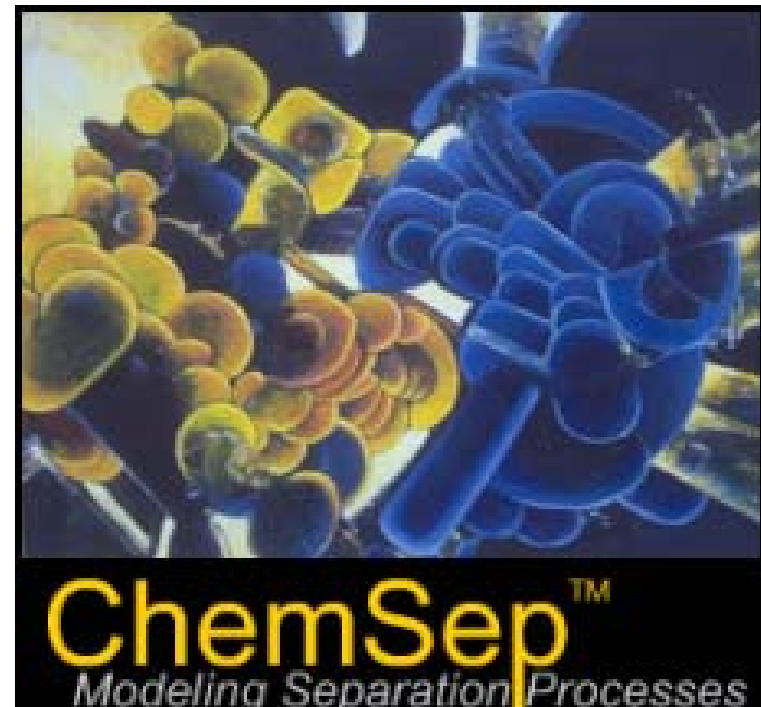


## Flowsheeting with



**Ross Taylor, Clarkson University**

**Jasper van Baten, AmsterCHEM**

**Rev5 – Apr 14 2010**

## Outline

- Introduction to COCO
- What is CAPE-OPEN?
- Setting up thermodynamic property packages with TEA
- Setting up flowsheets with COFE
- Using **ChemSep** in COFE
- Advanced flowsheeting features

## Introduction to COCO:



Simulation environment (COFE)



Thermodynamic property package (TEA)

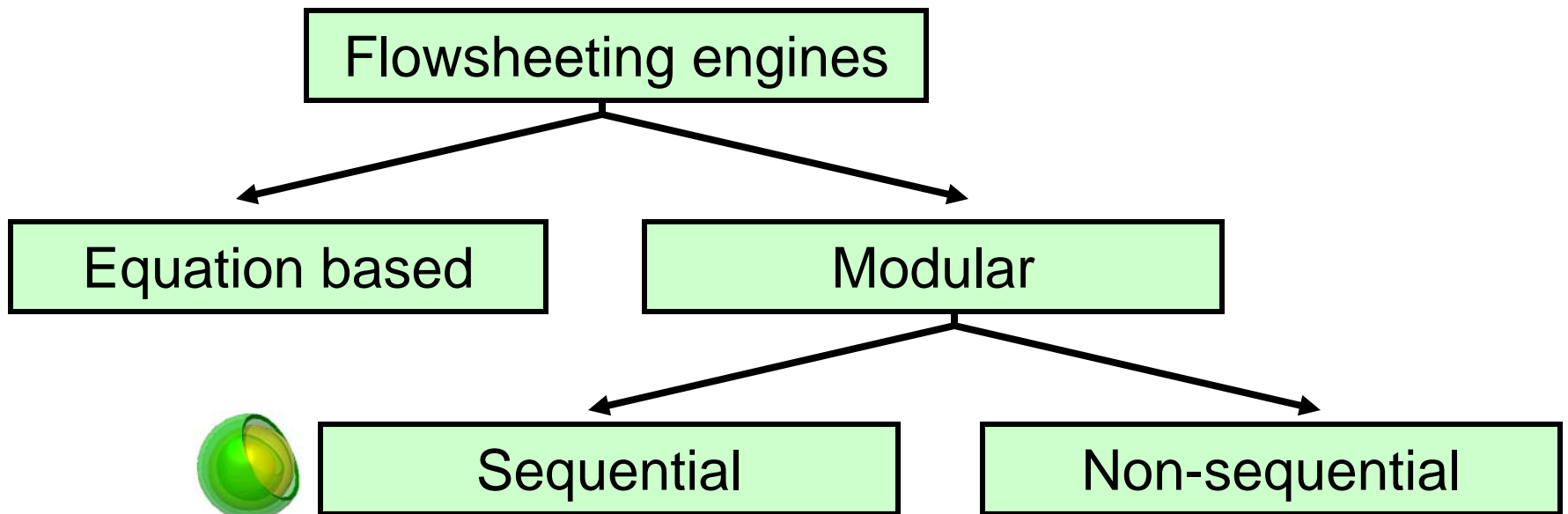
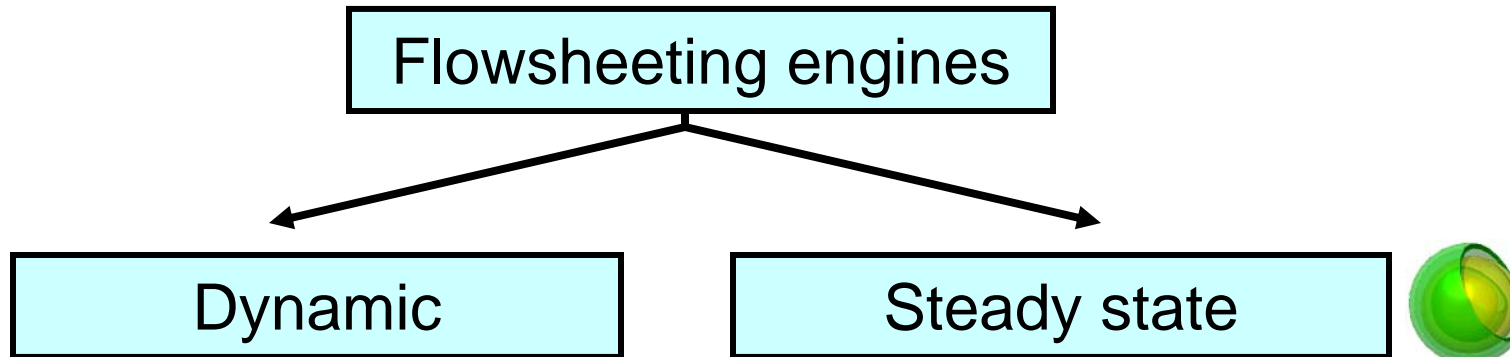


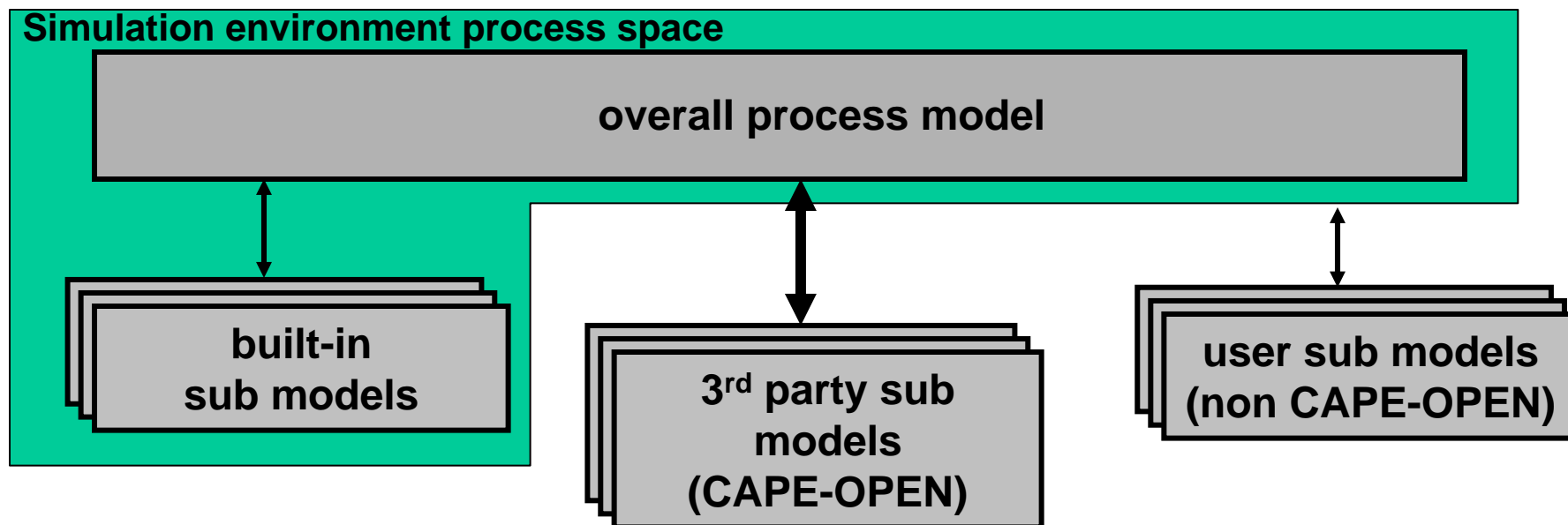
Collection of unit operations (COUSCOUS)

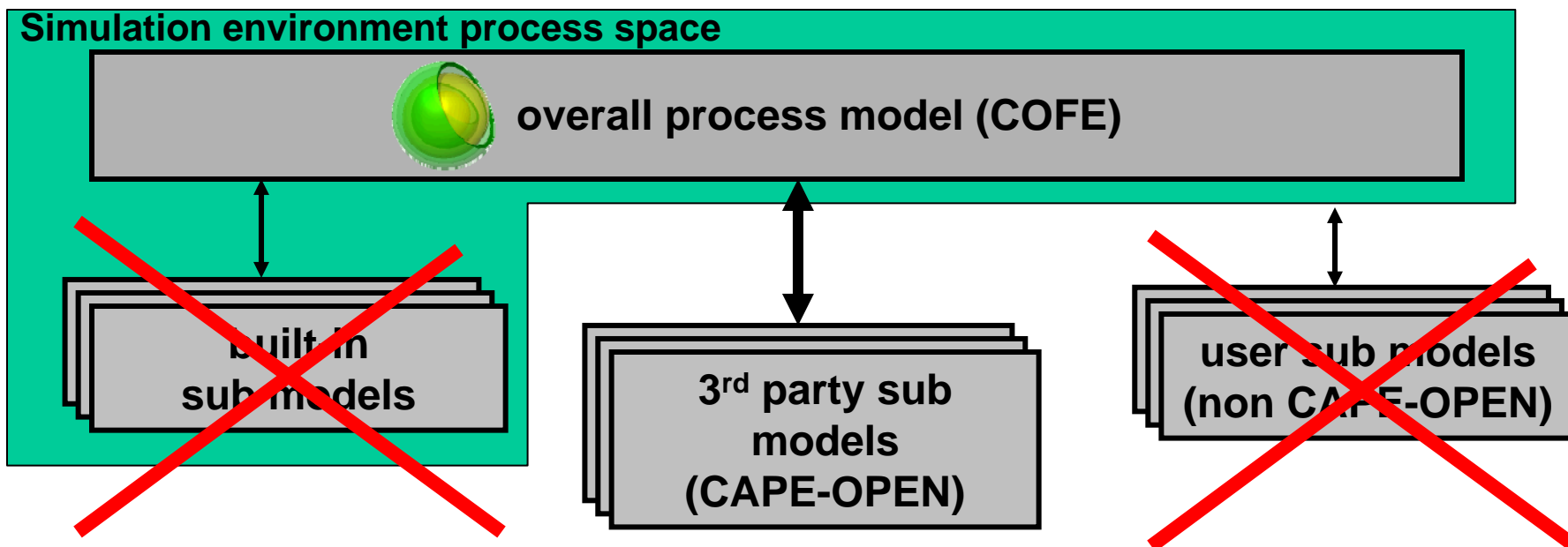


Reaction package (CORN)

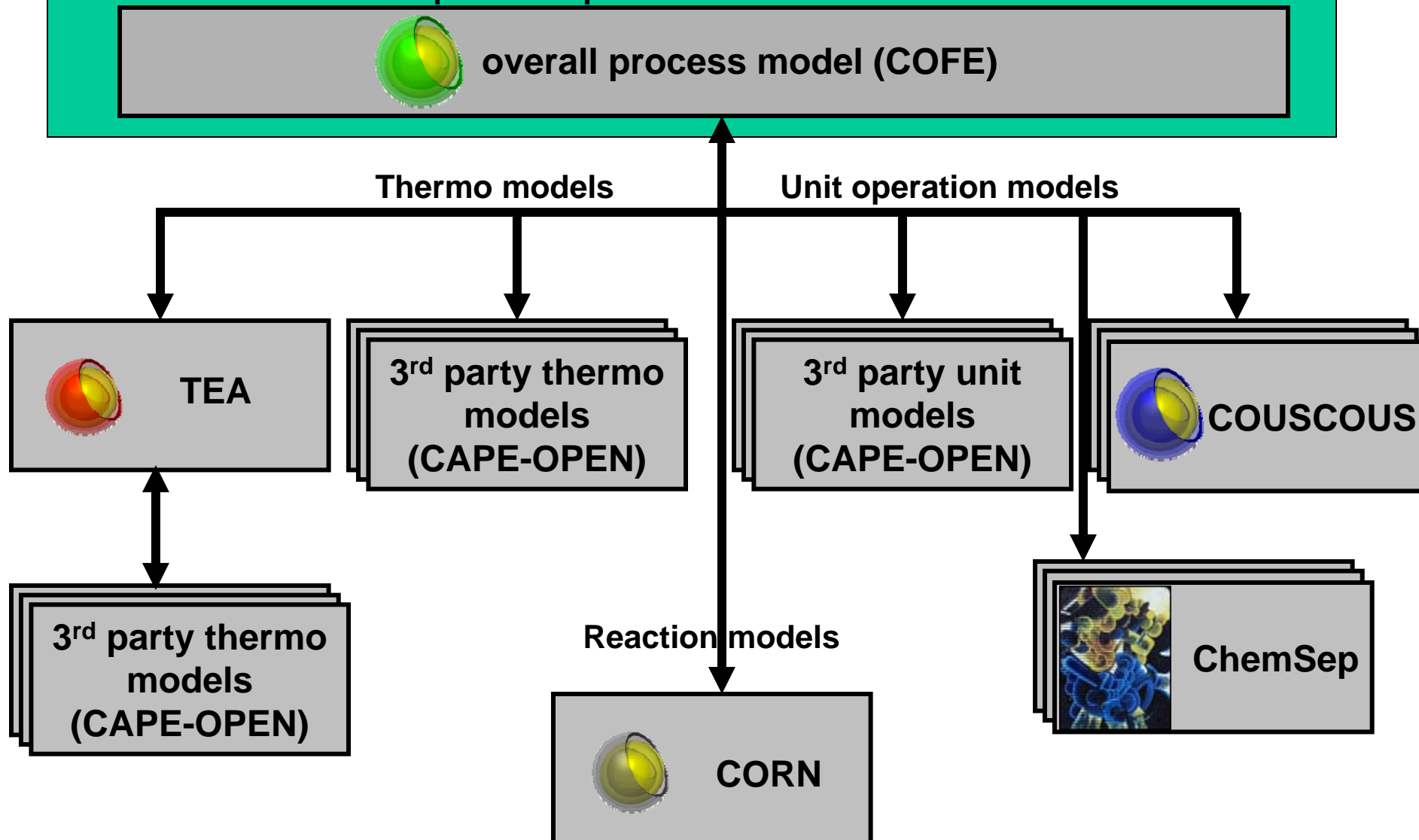
... and utilities







**Simulation environment process space**



# COFE: CAPE-OPEN Flowsheeting Environment

Multiple models

Document Explorer

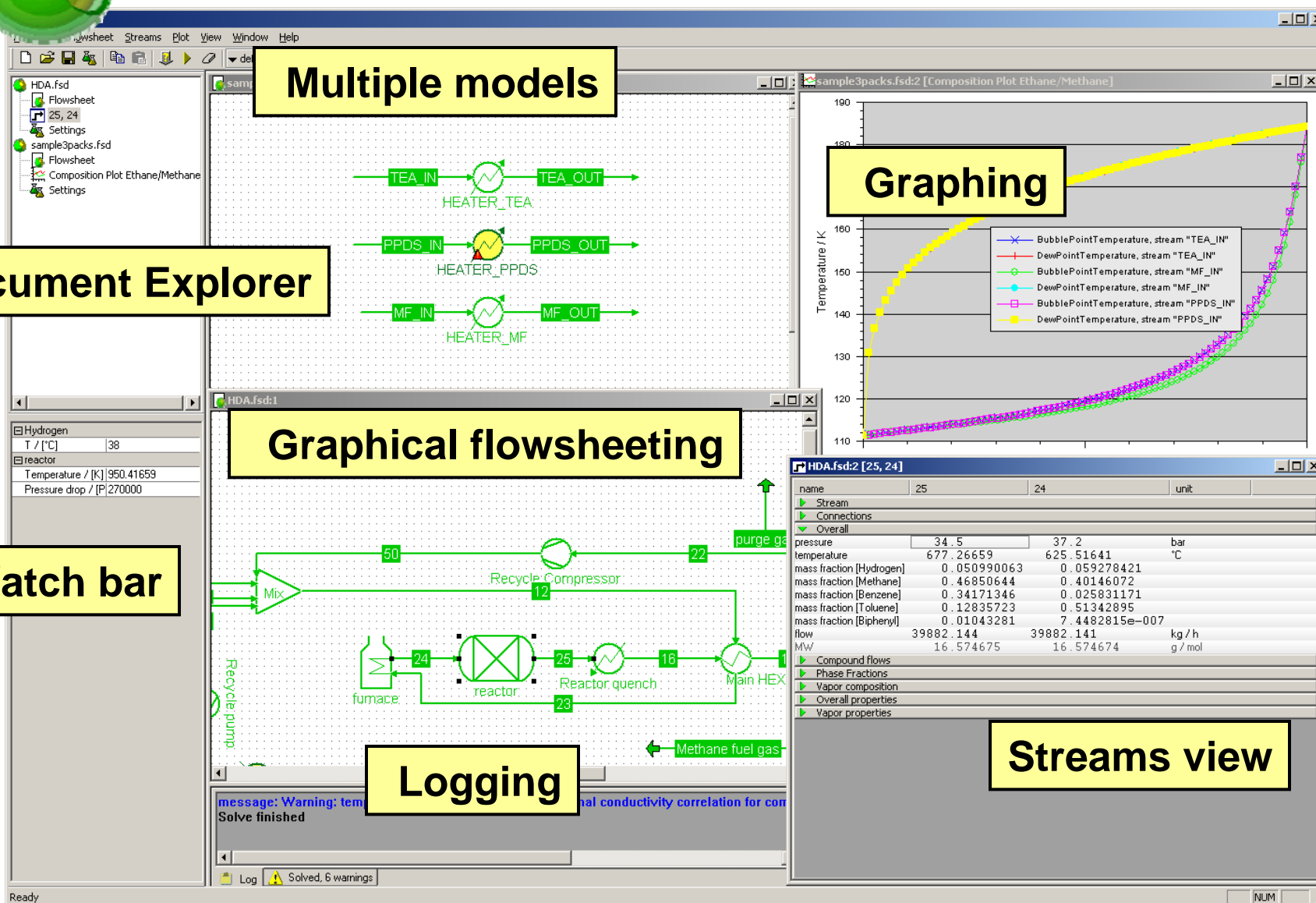
Graphing

Graphical flowsheeting

Watch bar

Logging

Streams view







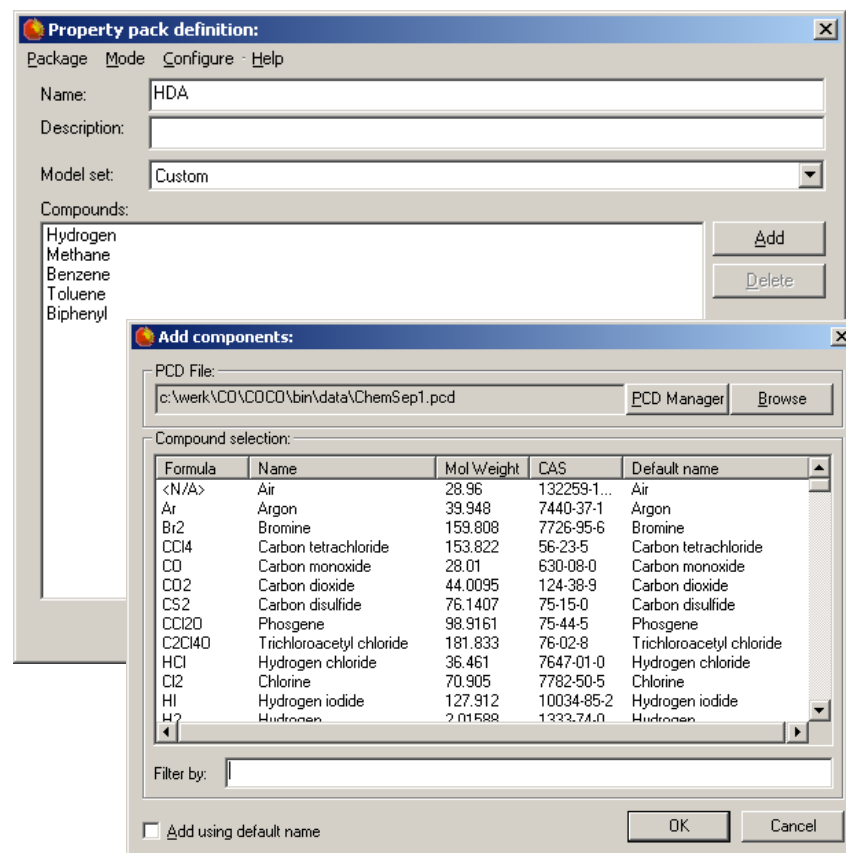
## **COFE: CAPE-OPEN Flowsheeting Environment**

- 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 Applications

- 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



Thermodynamic models and compounds from ChemSep



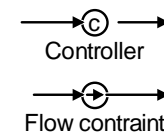
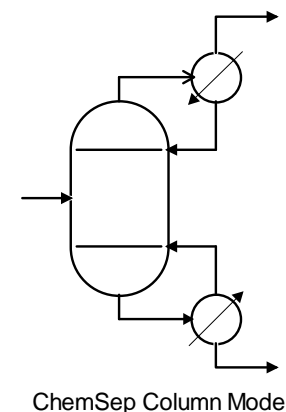
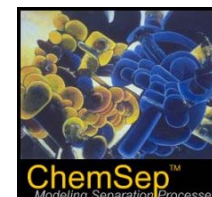
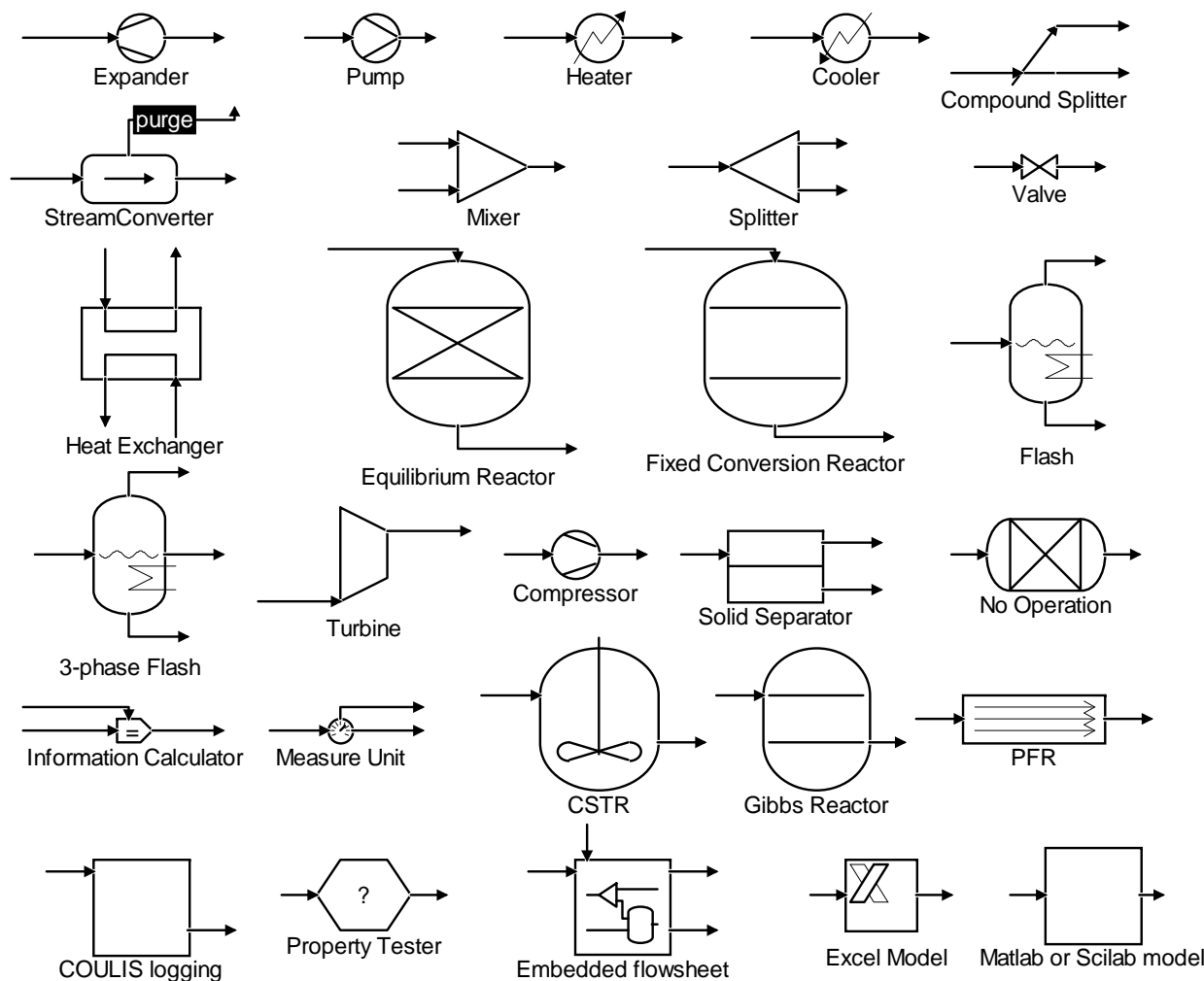
# TEA: Thermodynamics for Engineering Applications

## VLE equilibrium calculations

- Large diversity of supported flash specifications
- Inside-out approach
- Post-checking of solution
- Back-up full Newton approach



# COUSCOUS: Simple unit operations



- Download COCO: <http://www.cocosimulator.org/>  
(or ask for a copy during the workshop)
- Contact amster**CHEM** for CAPE-OPEN consulting
- Interoperability testing program:  
[http://www.cocosimulator.org/index\\_compliance.html](http://www.cocosimulator.org/index_compliance.html)

---

**Acknowledgements:**

- Richard Baur
- ChemSep: Ross Taylor, Harry Kooijman
- Cosmo*THERM*: Frank Eckert
- Testing: Michel Pons, Radovan Omorjan

## Presentation outline

- Introduction to COCO
- **What is CAPE-OPEN?**
- Setting up thermodynamic property packages with TEA
- Setting up flowsheets with COFE
- Using ChemSep in COFE
- Advanced flowsheeting features

## What is CAPE-OPEN?

**CAPE:**

**Computer Applications in Production and Engineering** (source: about.com)

**Computer-Aided Process Engineering**  
(source: CO-LaN leaflet)

**OPEN:**

**Freely available standard specification**

## What is CAPE-OPEN?

The CAPE-OPEN standard is the de facto standard for interfacing process modelling software components for use in the design and operation of chemical processes. It is based on universally recognised software technologies, such as COM and CORBA. The CO standard is open, multi-platform, uniform and available free of charge.

(Note: practical implementations restricted to COM at Windows platforms)



## What is CAPE-OPEN?

It is described in a formal documentation set covering areas such as unit operations, physical properties and numerical solvers, (...). In practice, it enables components supplied by third parties, such as niche physical property packages or unit operation models, to be used in “plug and play” mode in commercial process modelling software tools.

(Note: practical implementations limited to physical property packages and unit operations)

## What is CAPE-OPEN?

In reality this currently means:

- physical property package implementations
- unit operation implementations
- support for both of these in major simulation engines
- restricted to COM on Windows

## What is CAPE-OPEN?

CAPE-OPEN Laboratories Network



<http://www.colan.org/>

## What is CAPE-OPEN?



**Air Liquide**



**BASF AG**



**BP**



**DOW Chemical Company**



**IFP**



**Shell Global Solutions**



**TOTAL**



**AKZO-Nobel**

## What is CAPE-OPEN?



- 44 Software vendors**
- 24 Academic institutions**
- 2 Administrations**
- 7 Other members**

## Good reasons for going CAPE-OPEN:

- Wide support for process models in simulation engines
- Write your software once, run in multiple environments
- Validate your models by exchanging parts of your models with those of different vendors

## Presentation outline

- Introduction to COCO
- What is CAPE-OPEN?
- **Setting up thermo dynamic property packages with TEA**
- Setting up flowsheets with COFE
- Using ChemSep in COFE
- Advanced flowsheeting features

## Reasons to use TEA

- 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 routines



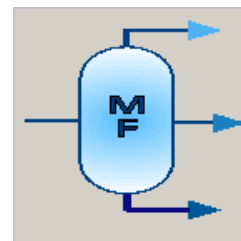
## Reasons not to use TEA

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

## Some other options



AspenProperties

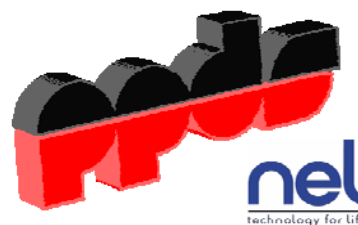


Infochem  
Multiflash



**ProSim**

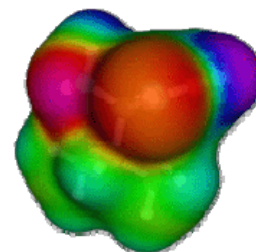
Simulis  
Thermodynamics



TUV/NEL  
PPDS



Virtual Materials  
Group



CosmoTherm



NIST REFPROP



AixCAPE

# Configuring TEA property packages

Windows Live Messenger

Programs

Documents

Settings

Search

Help and Support

Run...

Log Off jasper...

Undock Computer

Turn Off Computer...

Start

COCO

COCO Help

COFE

ConfigureCORN

ConfigureTEA

CORK

JUIcE

OATS

CUP

ConfigureTEA

on:

Flowsheet Options

Stream order

Unit Operation order

Reaction packs

Compounds

Properties

Phase Info

Property packages:

Add

Remove

Edit

Rename

Info

New

Packages

Info

Select

Cancel

alkanes

C1/C2 Amagat

C1/C2 PR

C1/C2 SRK

C1\_C2

C1\_C2 (EoS)

HDA

n-deopropanizer

water ethanol test

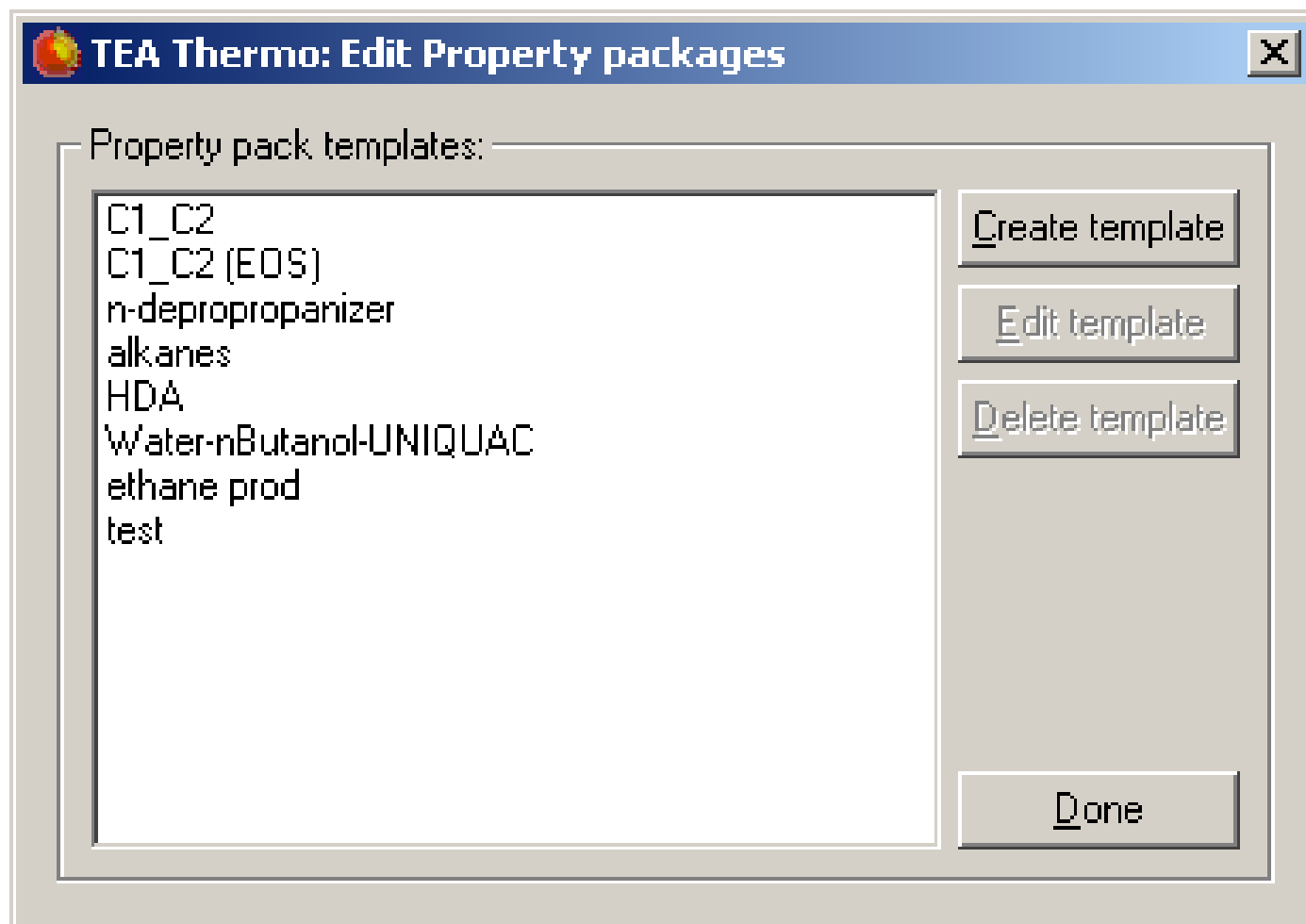
Water-nButanol-UNIQUAC

Description:

New package

Packages

## Configuring TEA property packages



# Configuring TEA property packages

The screenshot shows a Windows-style dialog box titled "Property pack definition:". It has a menu bar with "Package", "Mode", "Configure", and "Help". The dialog contains the following fields and controls:

- Name:** A text input field containing "MyPackage".
- Description:** A text input field containing "For use in my simulation".
- Model set:** A dropdown menu currently showing "Custom".
- Compounds:** A large empty rectangular list box.
- Buttons:** To the right of the "Compounds" list are "Add" and "Delete" buttons. At the bottom right of the dialog are "OK" and "Cancel" buttons.

## Configuring TEA property packages

**Property pack definition:**

Package Mode Configure - Help

Name: MyPackage

Description: For use in my simulation

Model set: UNIFAC VLE

Compounds:

Add

Delete

OK Cancel

# Configuring TEA property packages

**Add components:**

PCD File:

Compound selection:

Formula	Name	Mol Weight	CAS	Default name
CH4O	Methanol	32.042	67-56-1	Methanol
C2H6O	Ethanol	46.069	64-17-5	Ethanol
C2H6O2	2-Hydroxyethanol	62.0678	107-21-1	Ethylene glycol
C2H6S	Thioethanol	62.136	75-08-1	Ethyl mercaptan
C3H8O	1-methylethanol	60.096	67-63-0	Isopropanol
C4H10O	Propylmethanol	74.123	71-36-3	1-butanol
C4H10O	Trimethylmethanol	74.123	75-65-0	2-methyl-2-propanol
C4H10O3	2,2'-oxybis-ethanol	106.12	111-46-6	Diethylene glycol
C6H14O4	2,2'-[1,2-ethanediylbis(o...	150.173	112-27-6	Triethylene glycol
C8H18O5	2,2'-[oxybis(2,1-ethanedi...	194.226	112-60-7	Tetraethylene glycol

Filter by:

☐ Add using default name

# PCD Files

- PCD = **Pure Component Data** file for ChemSep
- Binary file that stores pure compound data
- ChemSep1.pcd – databank with nearly 200 compounds
- **PCDManager** – for editing and creating PCD files
- Import DIPPR source file (nearly 2000 compounds)
- Import data from NIST web site
- Can estimate many missing properties
- Fit temperature dependent properties



```

00002HC00CH2CH3
00002CH3C00CH3
00002CH3CH2C00H
00002HC0N(CH3)2
00002CH3CH2CH3
00002CH3CH(CH3)
00002CH3(CH2)2OH
00002(CH3)3N
00002CH2CHCCH
00002-S(CH)4-
00002CH2C(CH3)CN
00002CH3CCCH3
00002CH3CH2CCH
00002CH2CCHCH3
00002CH2CHCHCH2
00002CH2CHCH2CH3
00002CH3CHCHCH3
00002CH3CHCHCH3
00002CH2C(CH3)2
00002CH3CH(CH3)CH0
00002CH3C0CH2CH3
00002-CH2CH2CH2CH2O-
00002-0CH2CH20CH2CH2-
00002CH3CH2CH2C00H
00002CH3C00C2H5
00002CH3CH2C00CH3
00002HC00CH2CH2CH3
00002-(CH2)2S02(CH2)2-
00002(CH3)2NCOCH3
00002CH3(CH2)2CH3
00002CH3CH(CH3)CH3
00002CH3(CH2)3OH
00002(CH3)2CHCH2OH
00002CH3CH2CH(OH)CH3
00002C(CH3)3OH
00002CH3CH20CH2CH3
00002HOCH2CH20CH2CH2OH
00002C2H5NHCC2H5
00002(OC4H3)CH0
00002-CHCHCHCHCHN-
00002CH2C(CH3)CHCH2
00002-(CH2)5-
00002CH2C(CH3)CH2CH3
00002CH2CHCH(CH3)CH3
00002CH3CHC(CH3)CH3
00002CH2CH(CH2)2CH3
00002CH3CHCHCH2CH3
00002CH3CHCHCH2CH3
00002CH3CH2C0CH2CH3
00002CH3CH(CH3)C0CH3
00002CH3C00(CH2)2CH3
00002CH3CH(CH3)CH2CH3
00002CH3(CH2)3CH3
00002C(CH3)4
00002(C6H3)Cl3
00002(C6H4)Cl2
00002(C6H4)Cl2
00002(C6H5)Br
00002C6H5Cl
00002C6H5I
00002C6H5NO2
00002-CHCHCHCHCHCH-
W<C 00000. A30jW',A70000000000Ef>X#004M CD
1'5c00p000jAL WNA,A,00000000.00-0A+0z<

```

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

Key	Value
Name	Benzene
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 bicarburetofhydrogen carbonoil coalnaphtha cyclohexatriene mineralnaphtha motorbenzol  
phenylhydride pyrobenzole

Critical	Molecular	T Correlations	Group Data	EOS	Miscellaneous	Log	Units	Paths
				Value				
				Benzene				
				501				
				71-43-2				
				c1cccc1				
				-CHCHCHCHCHCH-				
				78.11				
				Inorganic bases				
				C6H6				

A large, stylized graphic of a computer keyboard with the text "PCD File" overlaid in a large, bold, black font. The keyboard is shown from a slightly elevated angle, with keys like "Benzen", "Comp", "Key", "Criti", "Non", "Mel", "Trip", and "Click" visible. The background is a light blue gradient.

☒ Order by property      ☐ Order by method

**Table 1: Thermodynamic Properties of 1,3,5-Trisubstituted Benzene Derivatives**

Property	Value
Molar volume at normal boiling point (m <sup>3</sup> /kmol)	0.08941
Compressibility factor (-)	0.2090
Diffusion coefficient (m)	3.004E-10
Diffusion parameter (sqrt(J/m <sup>3</sup> ))	1.870E+04
Dielectric constant (Coulomb.m)	0.0000
Partial molar volume (m <sup>3</sup> /kmol)	0.04840
Partial molar area (m <sup>2</sup> /kmol)	6.000E+08
Enthalpy of formation (J/kmol)	8.288E+07
Enthalpy of formation (J/kmol)	1.296E+08
Entropy (J/kmol.K)	2.693E+05
Enthalpy at melting point (J/kmol)	9.866E+06
Enthalpy of vaporization at normal boiling point (J/kmol)	*
Enthalpy of combustion (J/kmol)	-3.136E+09

Order by property ☒ Order by method

Apply

## PCD Files

**ChemSep PCDmanager - chemsep1.pcd**

File Edit Help

Information: ChemSep v6 pure component data - adapted from Properties of Gases and Liquids 5th Ed.

Components (194):

- Isopentane
- N-pentane
- Neopentane
- 1,2,4-trichlorobenzene
- M-dichlorobenzene
- O-dichlorobenzene
- P-dichlorobenzene
- Bromobenzene
- Monochlorobenzene
- Iodobenzene
- Nitrobenzene
- Benzene**
- Phenol

Up Down Remove Add New

Search:

- not matched - Find Next

No data checking

**Benzene**

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

Table Plot

Copy Data Copy Plot Mass densities Ln

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

Data: ds=1831.

Fit

**Ideal gas heat capacity (J/kmol/K)**

C:\ChemSep\pcd\chemsep1.pcd

# Configuring TEA property packages

The screenshot shows a Windows-style dialog box titled "Property pack definition:". It has a menu bar with "Package", "Mode", "Configure", and "Help". The "Configure" menu is active. Below the menu bar, there are three text input fields: "Name:" with the value "MyPackage", "Description:" with the value "For use in my simulation", and "Model set:" with a dropdown menu showing "UNIFAC VLE". Below these fields is a list box labeled "Compounds:". The list box contains a list of compounds: "Ethanol", "Diethyl ether", "Water", "Custom", "Peng Robinson", "Soave Redlich Kwong", "Wilson", "NRTL", "UNIFAC VLE", and "UNIQUAC". The "UNIFAC VLE" option is currently selected and highlighted. At the bottom right of the dialog box are two buttons: "OK" and "Cancel".

Compounds:
Ethanol
Diethyl ether
Water
Custom
Peng Robinson
Soave Redlich Kwong
Wilson
NRTL
<b>UNIFAC VLE</b>
UNIQUAC

# Configuring TEA property packages

**Property pack definition:**

Package Mode Configure Help

General		Options		Compounds		Equilibrium		External Routines	
Property Calculations			Interaction Parameters			Group Contributions			
Property	Overall	Vapor	Liquid	VaporLiquid					
Equation of state		Ideal gas law	N/A						
activity	N/A	N/A	UNIFAC-VL	N/A					
activityCoefficient	N/A	N/A	UNIFAC-VL	N/A					
density	N/A	EOS	COSTALD / Hankins...	N/A					
enthalpy	SumOfP...	EOS	Ideal+Excess	N/A					
enthalpyF	SumOfP...	EOS	Ideal+Excess	N/A					
entropy	SumOfP...	EOS	From fugacity coeffi...	N/A					
entropyF	SumOfP...	EOS	From fugacity coeffi...	N/A					
excessEnthalpy	N/A	N/A	From activity coefficient	N/A					
fugacity	N/A	EOS	Dechema	N/A					
fugacityCoefficient	N/A	EOS	Dechema	N/A					
gibbsEnergy	N/A	From enthalpy and en...	From enthalpy and en...	N/A					
heatCapacityCp	N/A	From Enthalpy	From Enthalpy	N/A					
heatOfVaporization	Compound defined								
idealGasEnthalpy	IdealGas								
logFugacityCoefficient	N/A	EOS	Dechema	N/A					
molecularWeight	MolWt	MolWt	MolWt	N/A					
surfaceTension	N/A	N/A	N/A	Ideal					

☒ Only show equilibrium phases

Add property Delete property

OK Cancel

# Configuring TEA property packages

**Property pack definition:**

Package Mode Configure Help

Property Calculations				Interaction Parameters		Group Contributions			
General		Options		Compounds		Equilibrium		External Routines	
Name	Formula	MW	CAS	Ideal gas Cp	Vapor pressure	Heat of va			
Ethanol	C2H6O	46.069	64-17-5	T Correlation	T Correlation	T Correlat	Add		
Diethyl ether	C4H10O	74.123	60-29-7	T Correlation	T Correlation	T Correlat	Delete		
Water	H2O	18.015	7732-18-5	T Correlation	T Correlation	T Correlat	Edit		
							Up		
							Down		

OK Cancel

# Configuring TEA property packages

**Property pack definition:**

Package Mode Configure Help

General Options Compounds Equilibrium External Routines

Property Calculations Interaction Parameters Group Contributions

Group contribution model: UNIFAC-VL

Compound: Ethanol

Sub-group	Count
CH3	1
CH2	1
OH	1

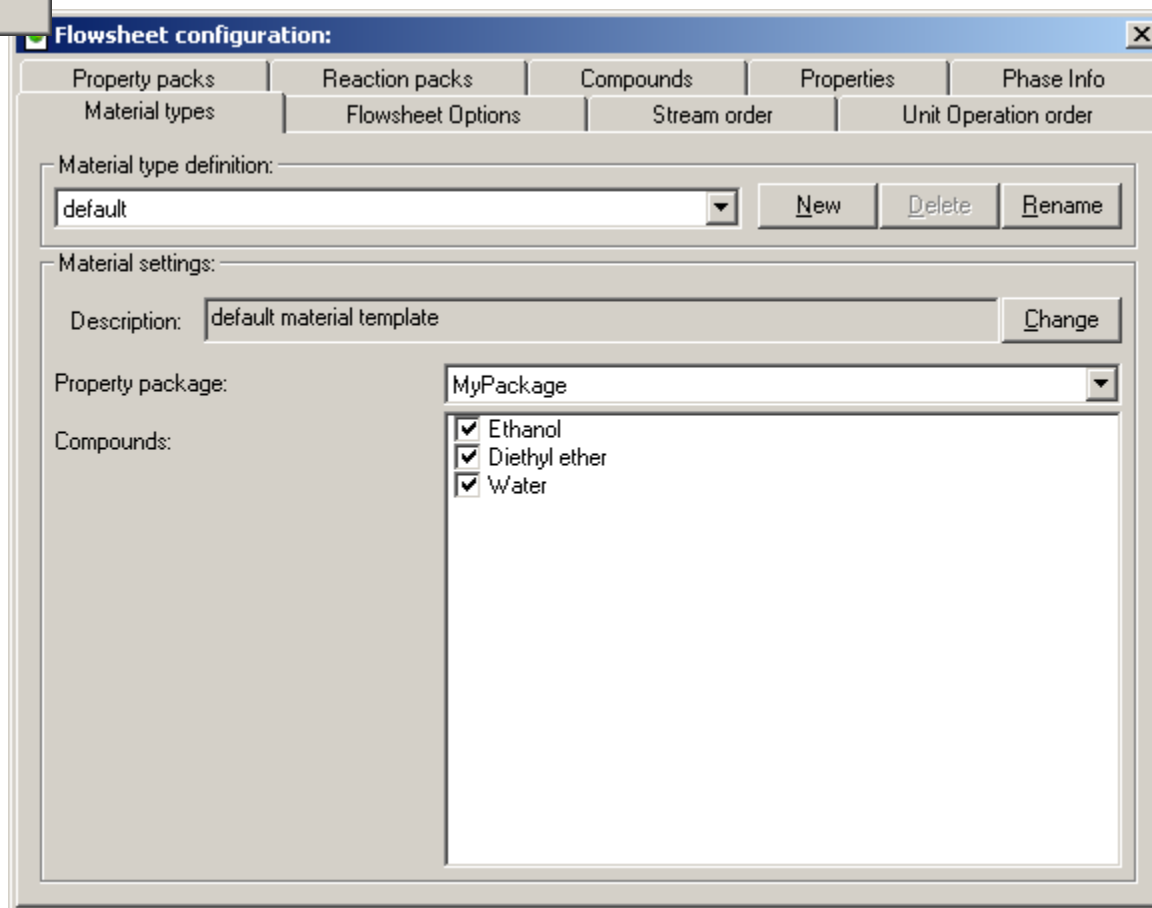
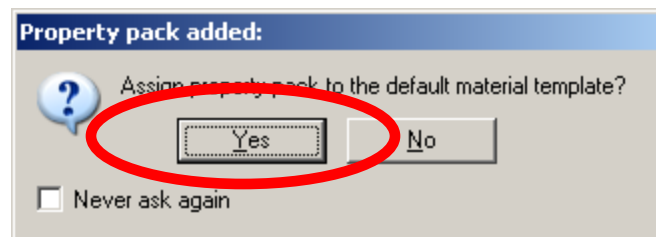
Molar weight: 46.068 of 46.069

Add sub-group Delete sub-group Edit groups Edit sub-groups

OK Cancel



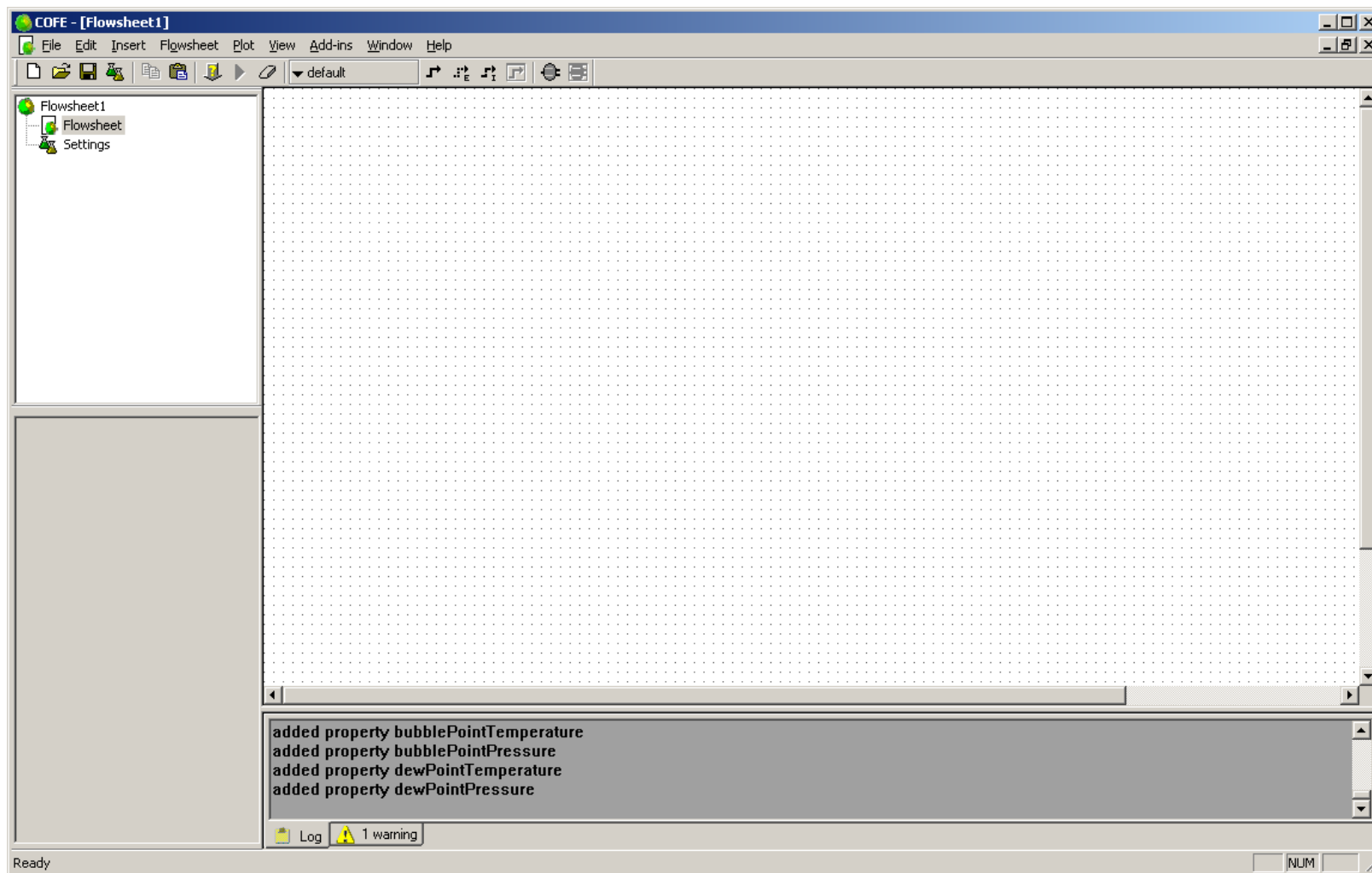
# Finally:



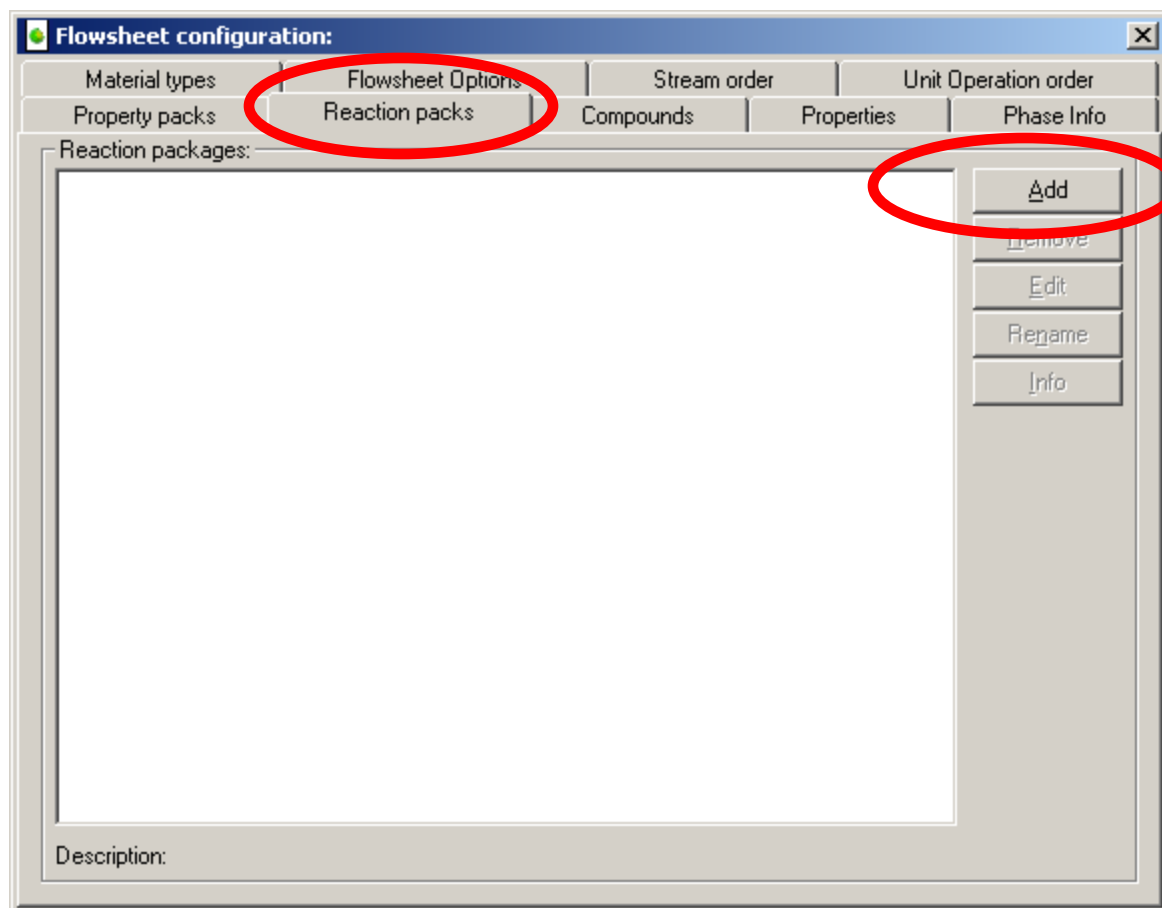
## Presentation outline

- Introduction to COCO
- What is CAPE-OPEN?
- Setting up thermo dynamic property packages with TEA
- **Setting up flowsheets with COFE**
- Using ChemSep in COFE
- Advanced flowsheeting features

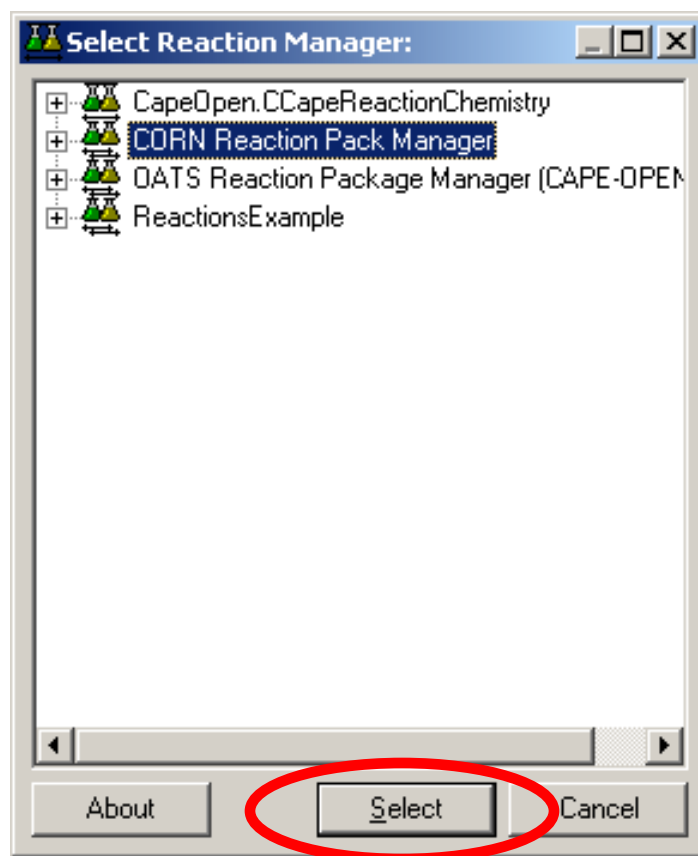
# Empty COFE document



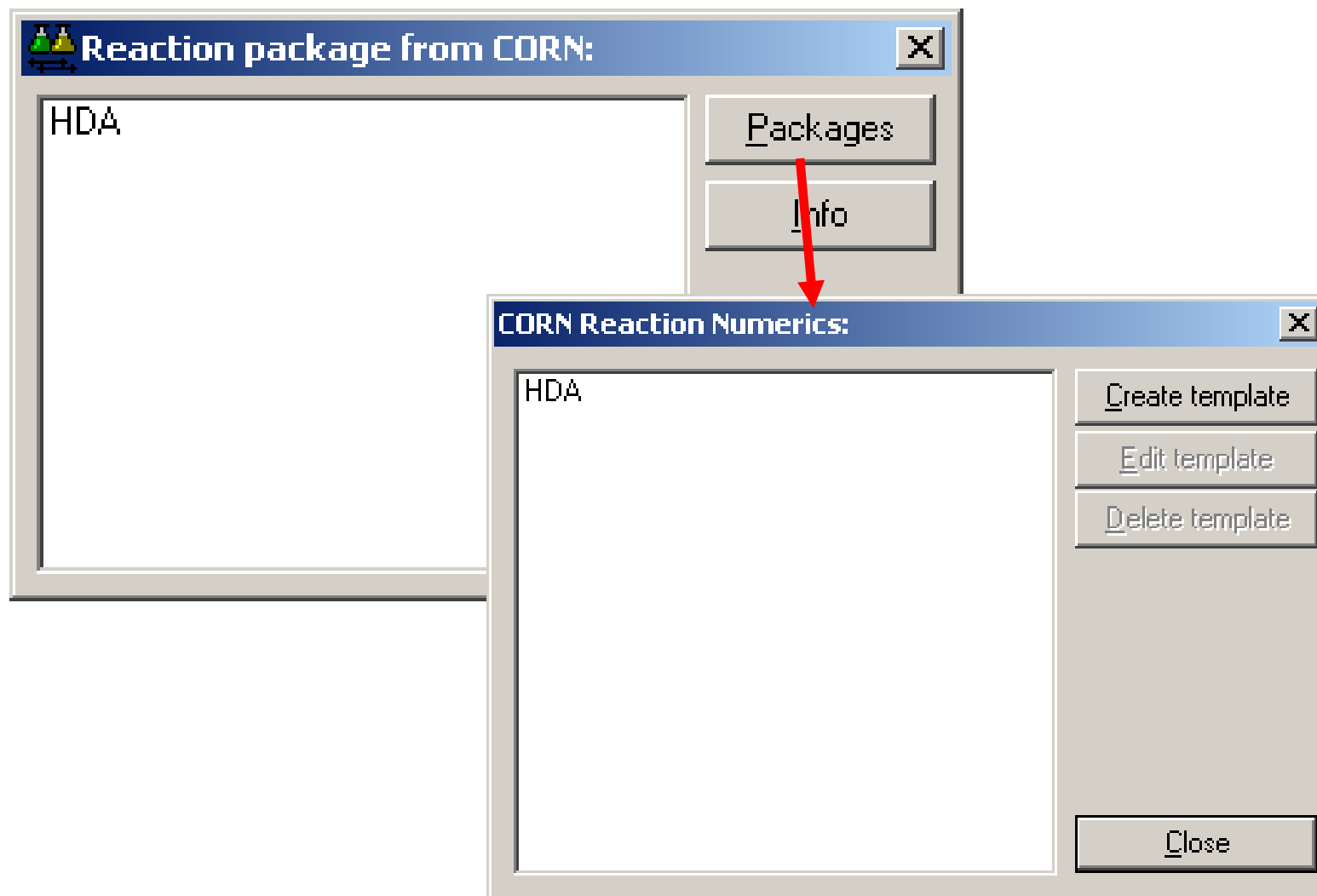
# Setting up reactions



## CORN: CAPE-OPEN Reaction Numerics



## Setting up CORN



## Editing a reaction package (1/4):

The screenshot shows a Windows-style dialog box titled "Edit:". It has three tabs: "General", "Compounds", and "Reactions". The "General" tab is selected. Inside the dialog, there are three labeled text input fields: "Name:" with the value "Ethanol2Ethyl", "Description:" with the value "Reaction definitions for the ethanol conversion reaction", and "Standard:" with the value "Version 1.1". Below these fields is a large empty text area. At the bottom of the dialog, there are four buttons: "Help", "Load", "OK", and "Cancel".

**Edit:**

General | Compounds | Reactions

General:

Name: Ethanol2Ethyl

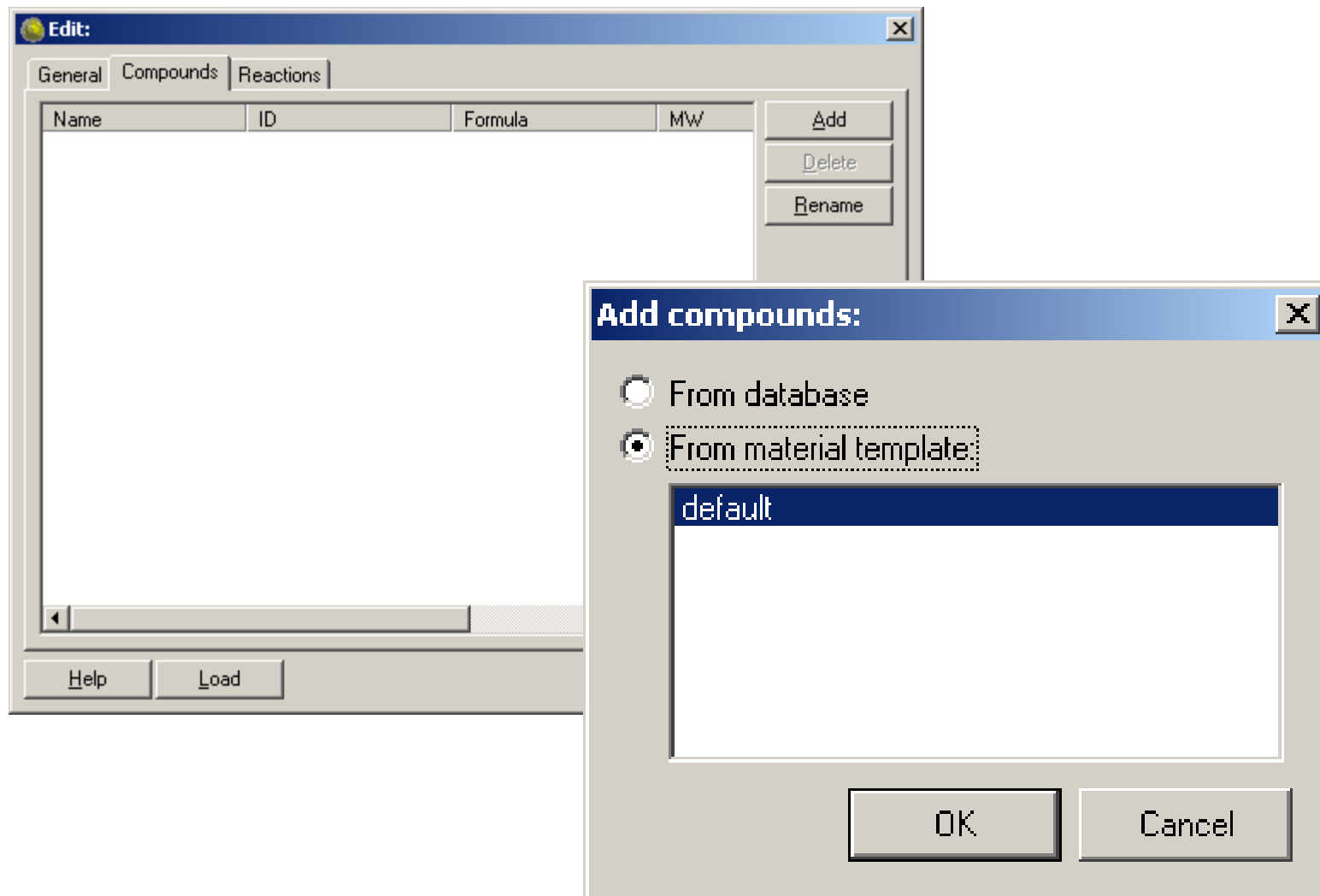
Description: Reaction definitions for the ethanol conversion reaction

Standard:

CAPE-OPEN thermo version: Version 1.1

Help Load OK Cancel

## Editing a reaction package (2/4):





## Editing a reaction package (3/4):

**Add compounds:** [X]

Name	Formula	Mol Weight	CAS
<input checked="" type="checkbox"/> Ethanol	C <sub>2</sub> H <sub>6</sub> O	46.069	64-17-5
<input checked="" type="checkbox"/> Diethyl ether	C <sub>4</sub> H <sub>10</sub> O	74.123	60-29-7
<input checked="" type="checkbox"/> Water	H <sub>2</sub> O	18.015	7732-18-5

OK Cancel

## Editing a reaction package (4/4):

**Edit:**


General | Compounds | Reactions


Reaction: conversion

Reaction properties:


Stoichiometry	Compound
-2	Ethanol
1	Diethyl ether
1	Water

☐ Equilibrium Reaction ☐ Heterogeneous

Rate:   mol/s/m<sup>3</sup>

Equilibrium constant:  

Equilibrium basis: Molarity

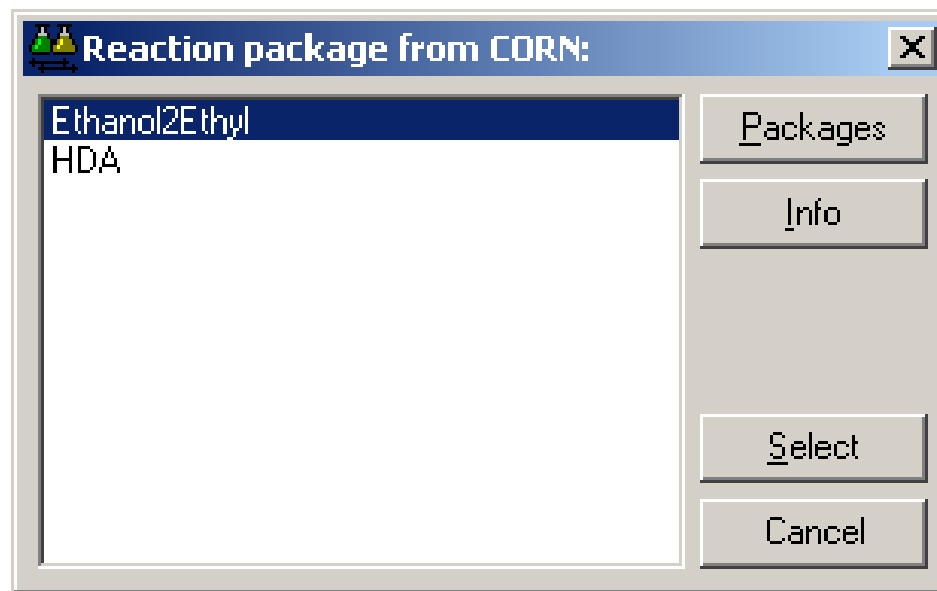
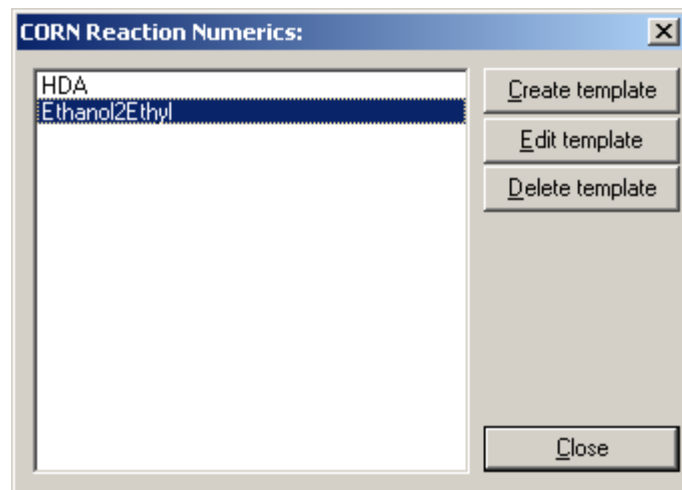
Heat of reaction:   J / mol

Phase: Liquid

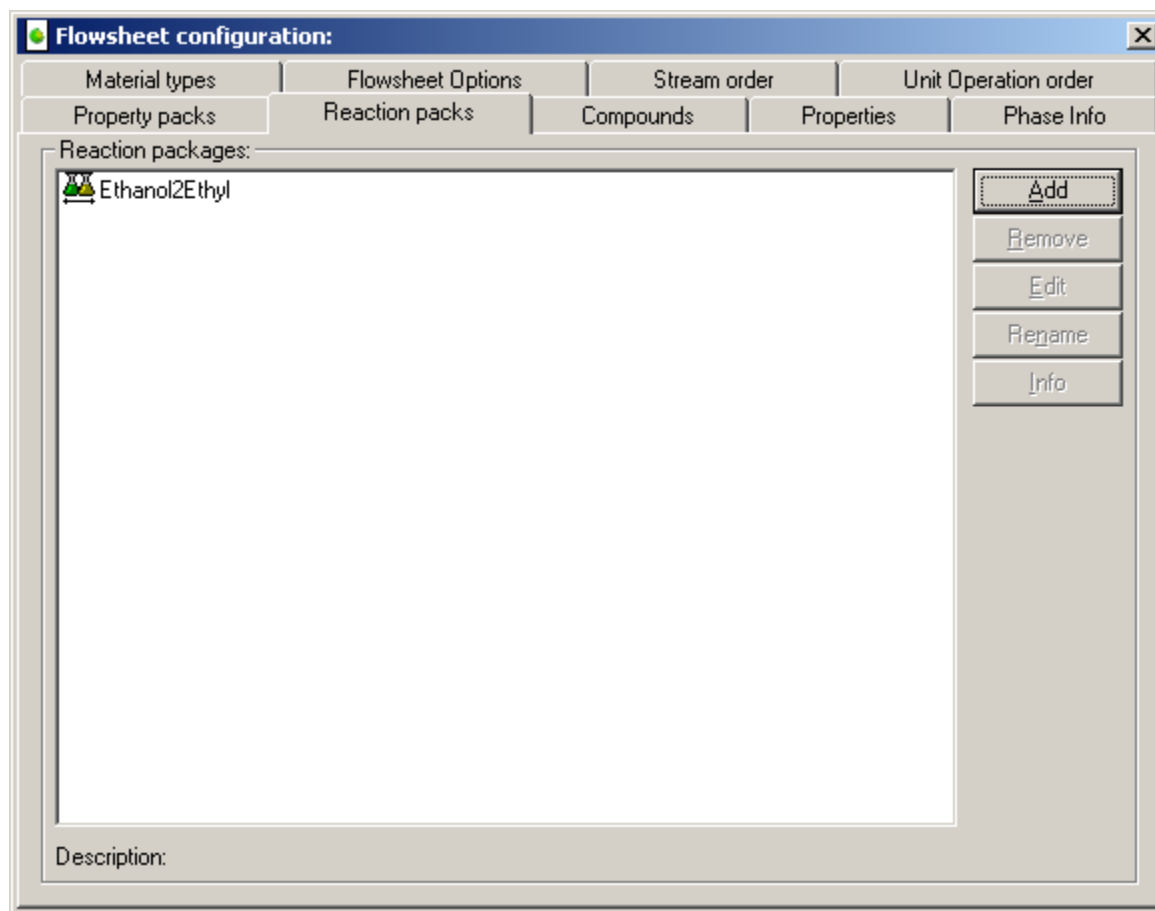
Create Rename Delete

Help Load OK Cancel

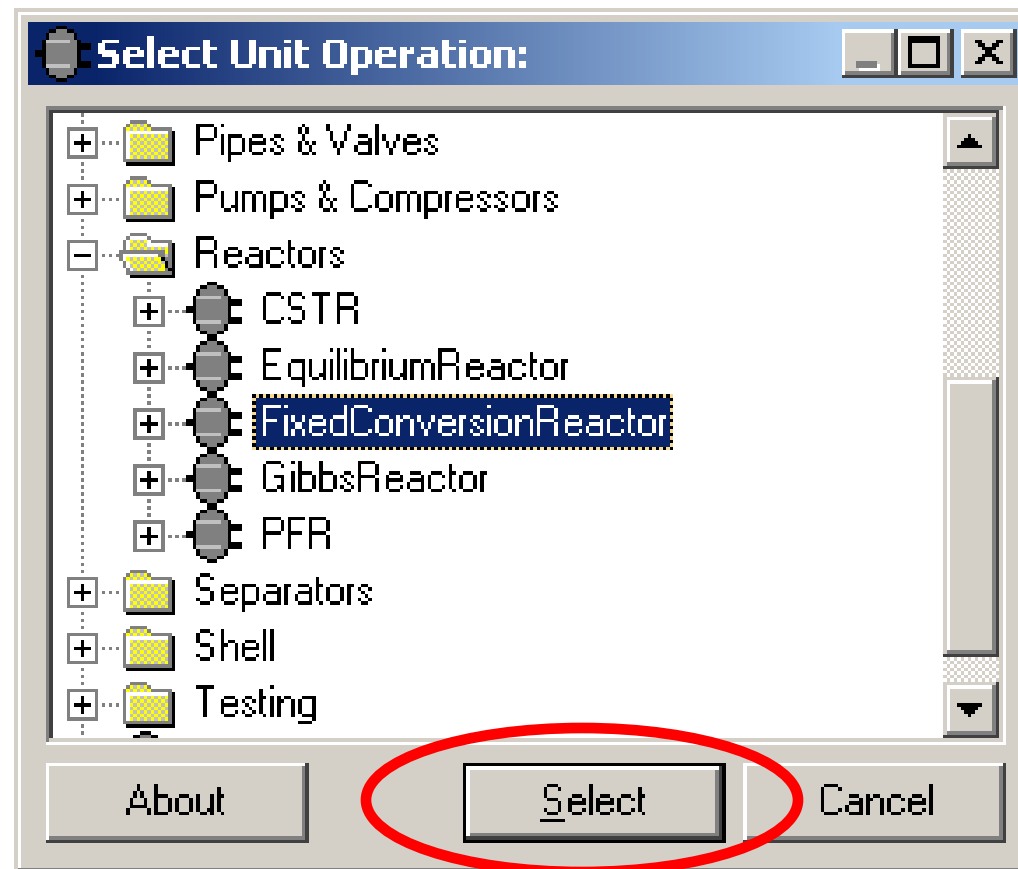
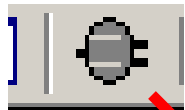
## Add it to the simulation



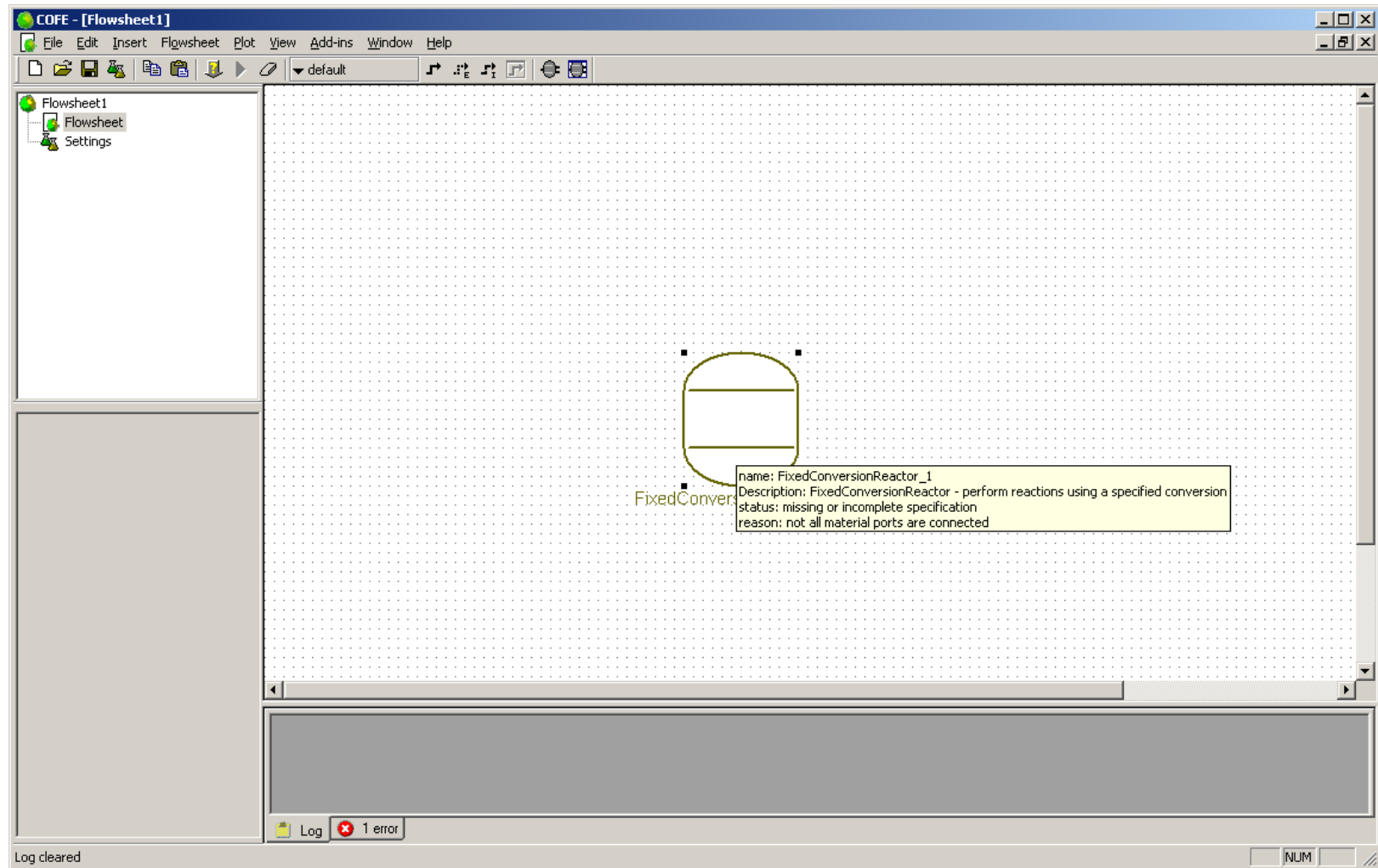
## We have a reaction package:



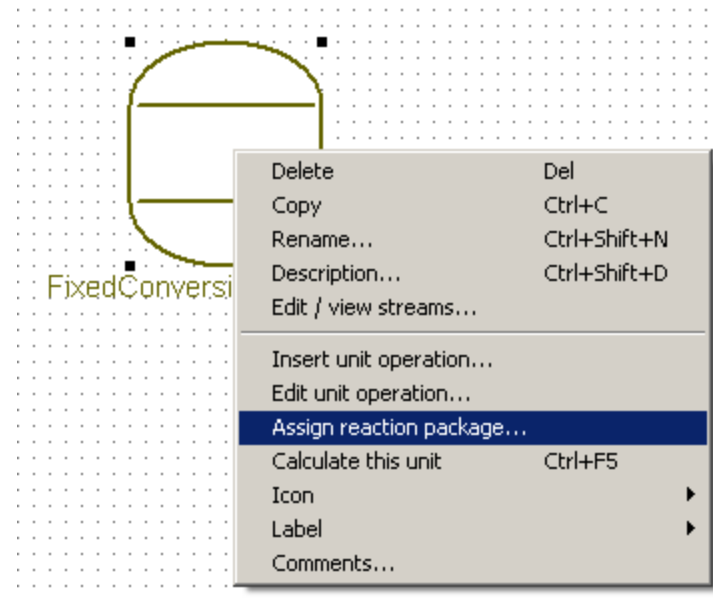
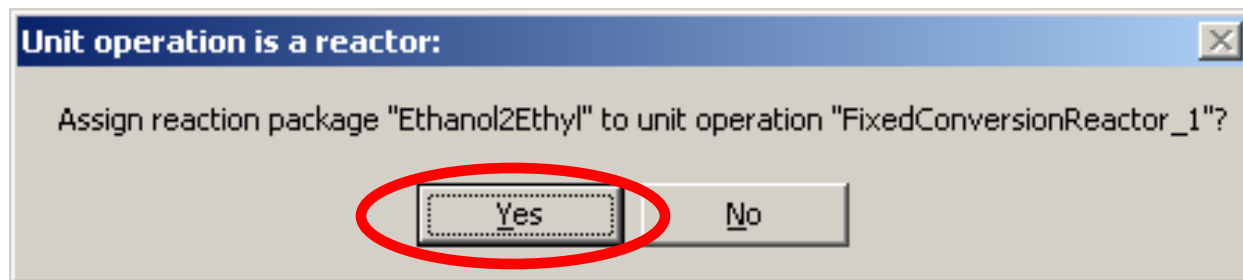
## Inserting our reactor:



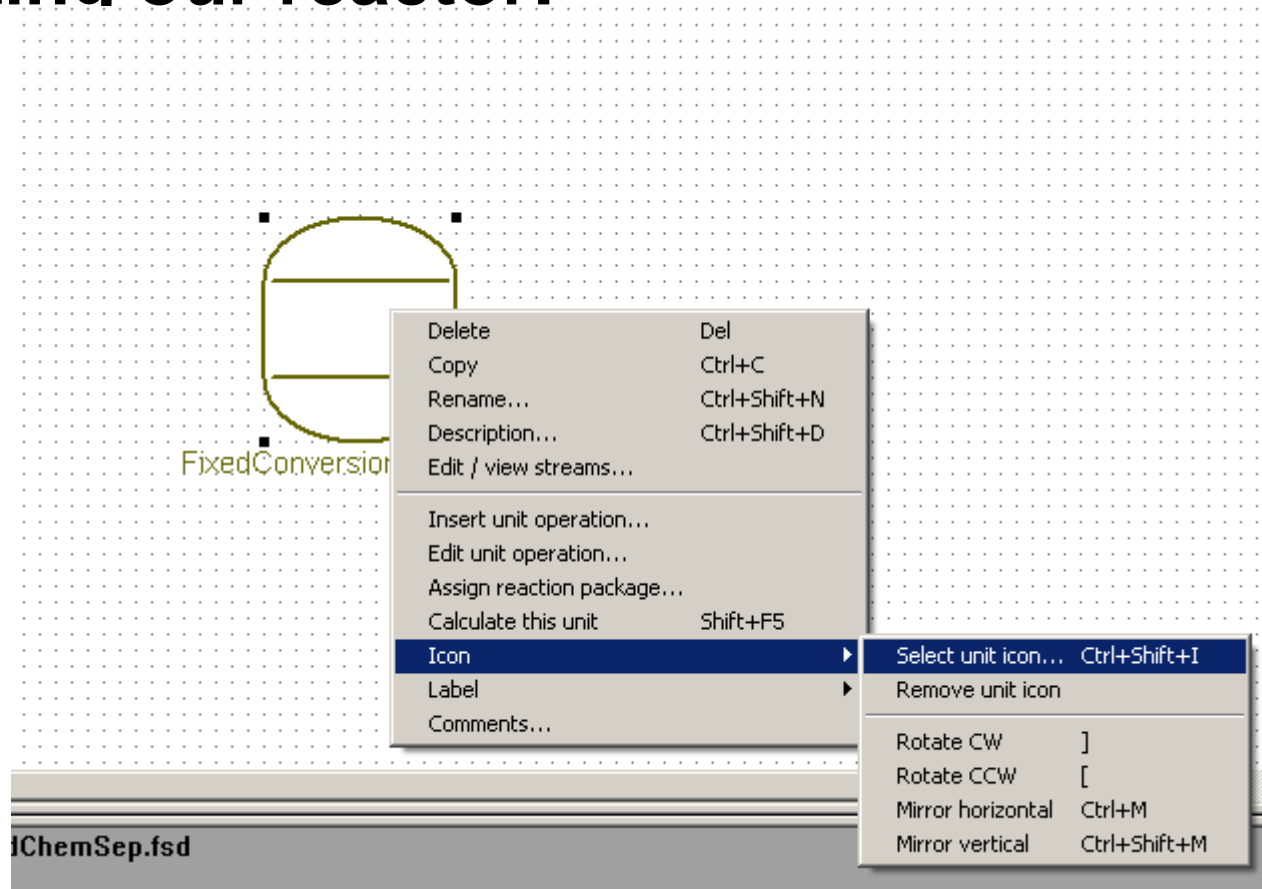
# Inserting our reactor:



## Inserting our reactor:

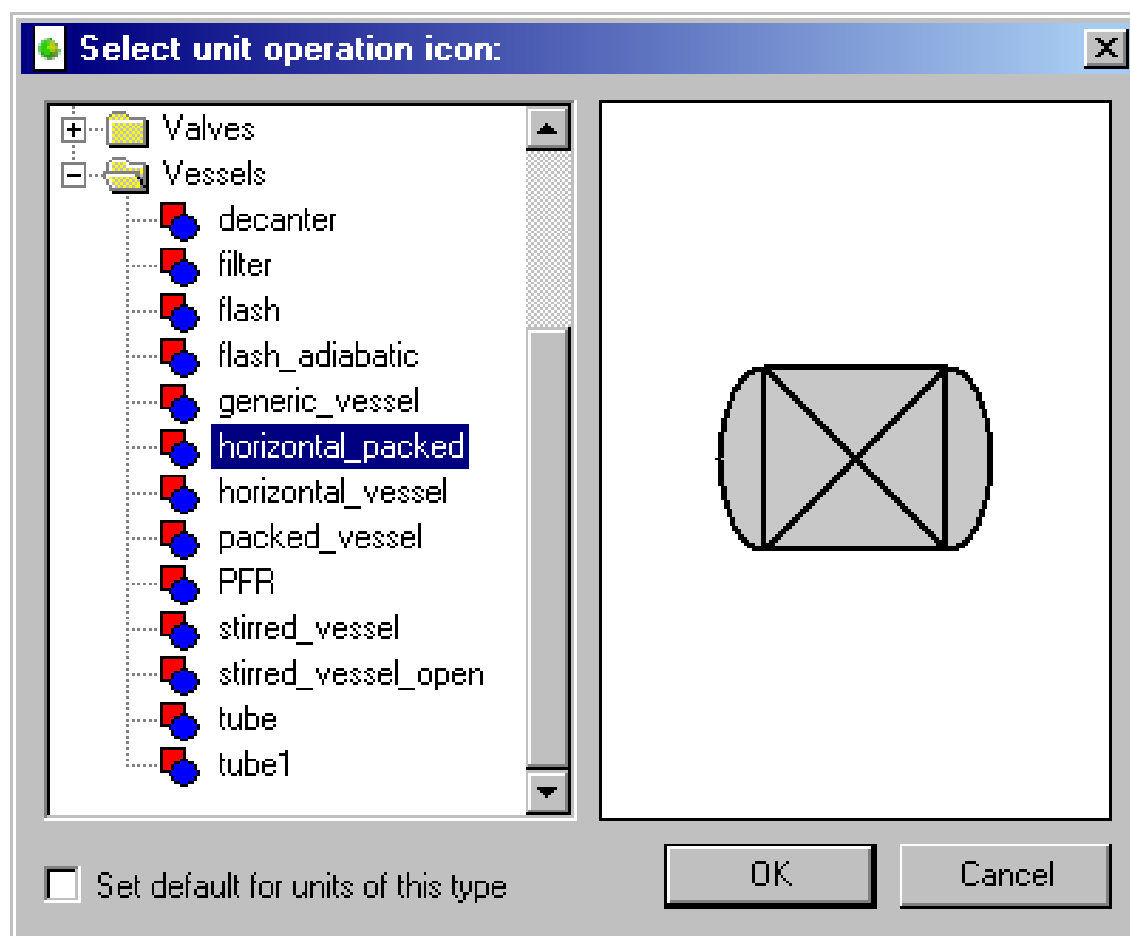


## Inserting our reactor:

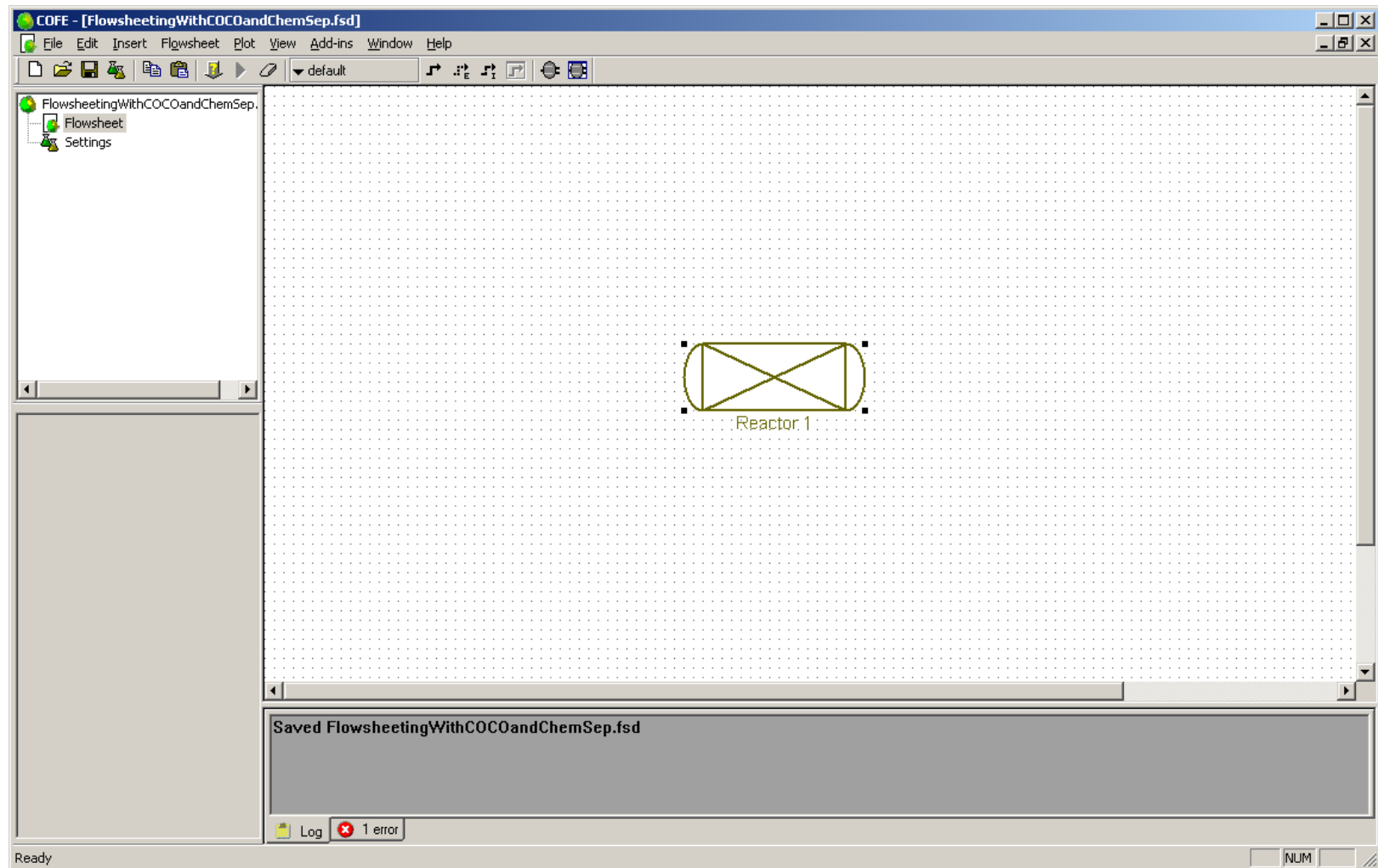




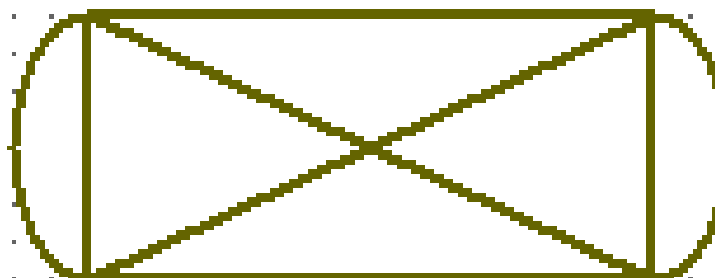
## Inserting our reactor:



# Inserting our reactor:

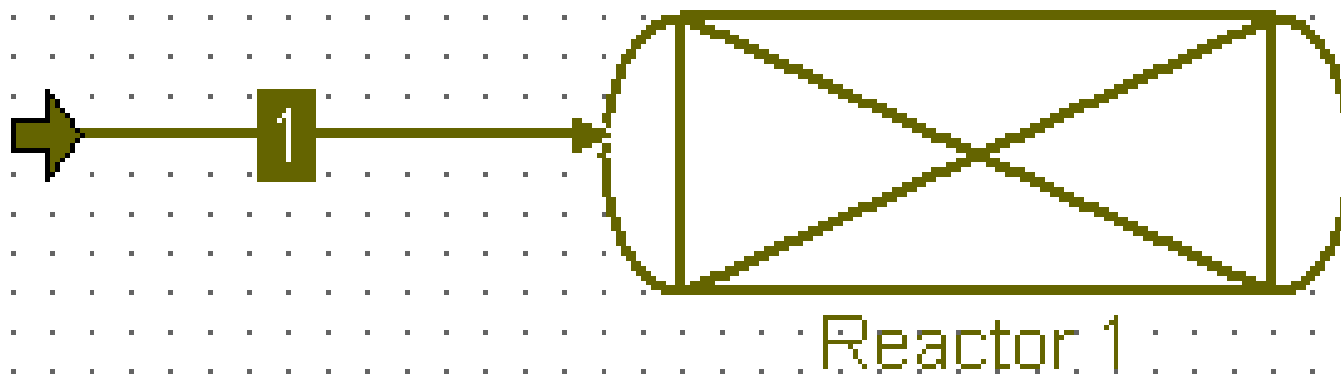


## Inserting the reactor feed:

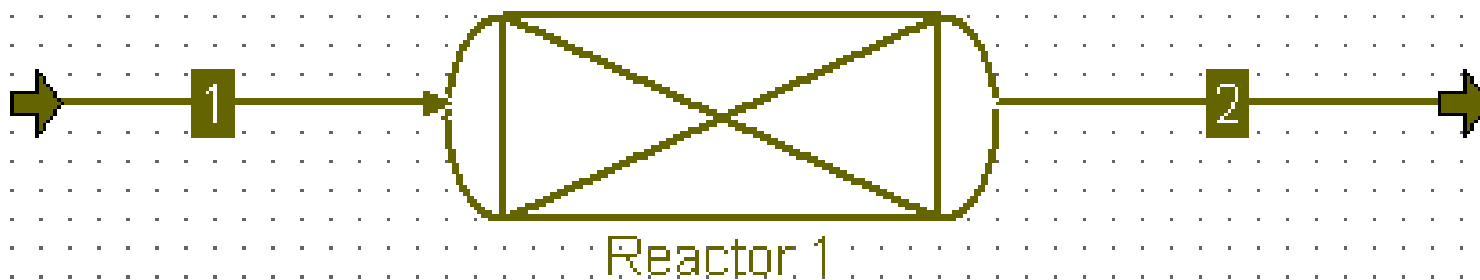


Reactor 1

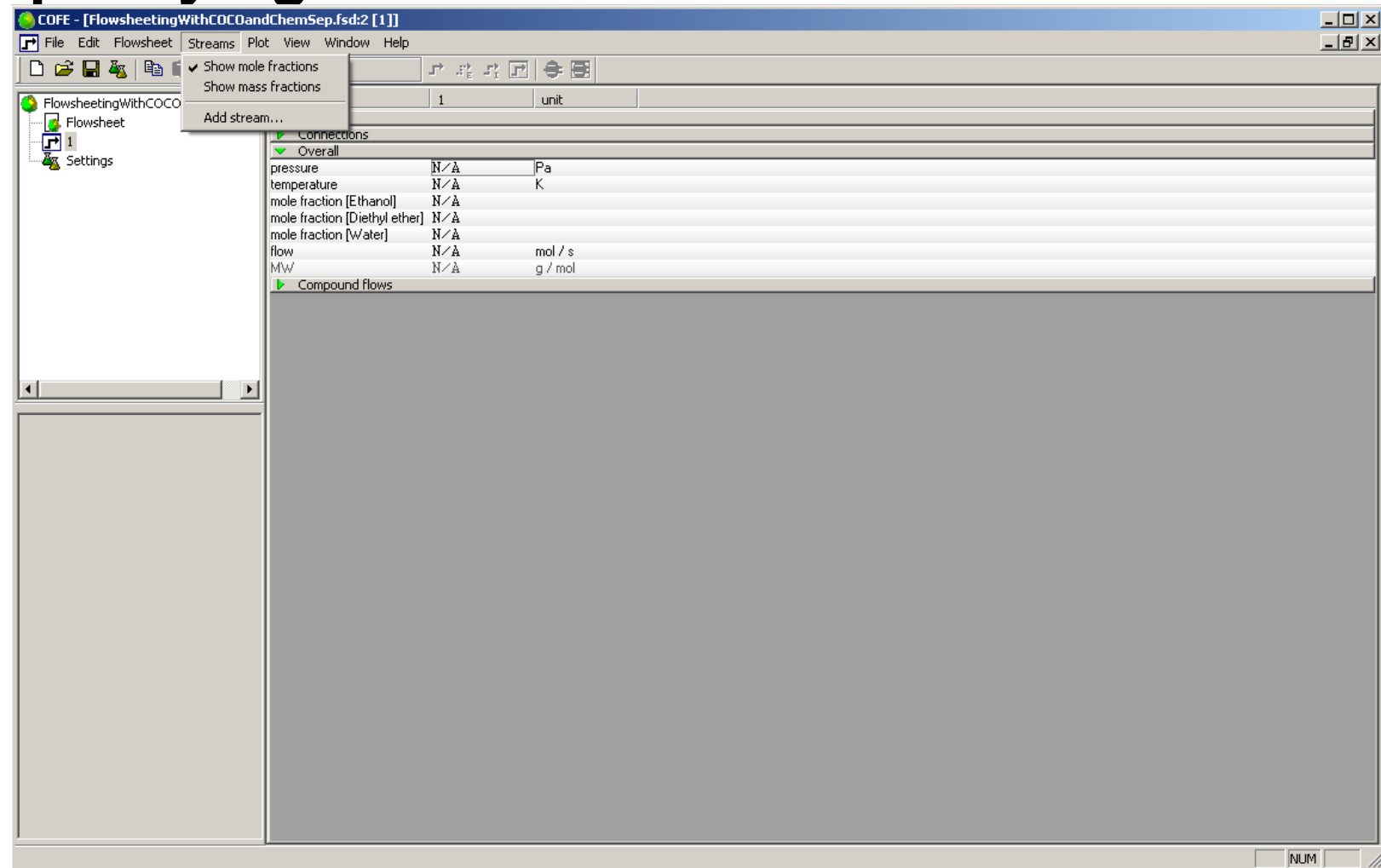
## Connecting the feed:



## The product stream:



# Specifying the feed stream:



## Specifying 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 specifications:

**Unit operation Reactor 1:**

Status Edit Balance Ports Info

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	

Show GUI



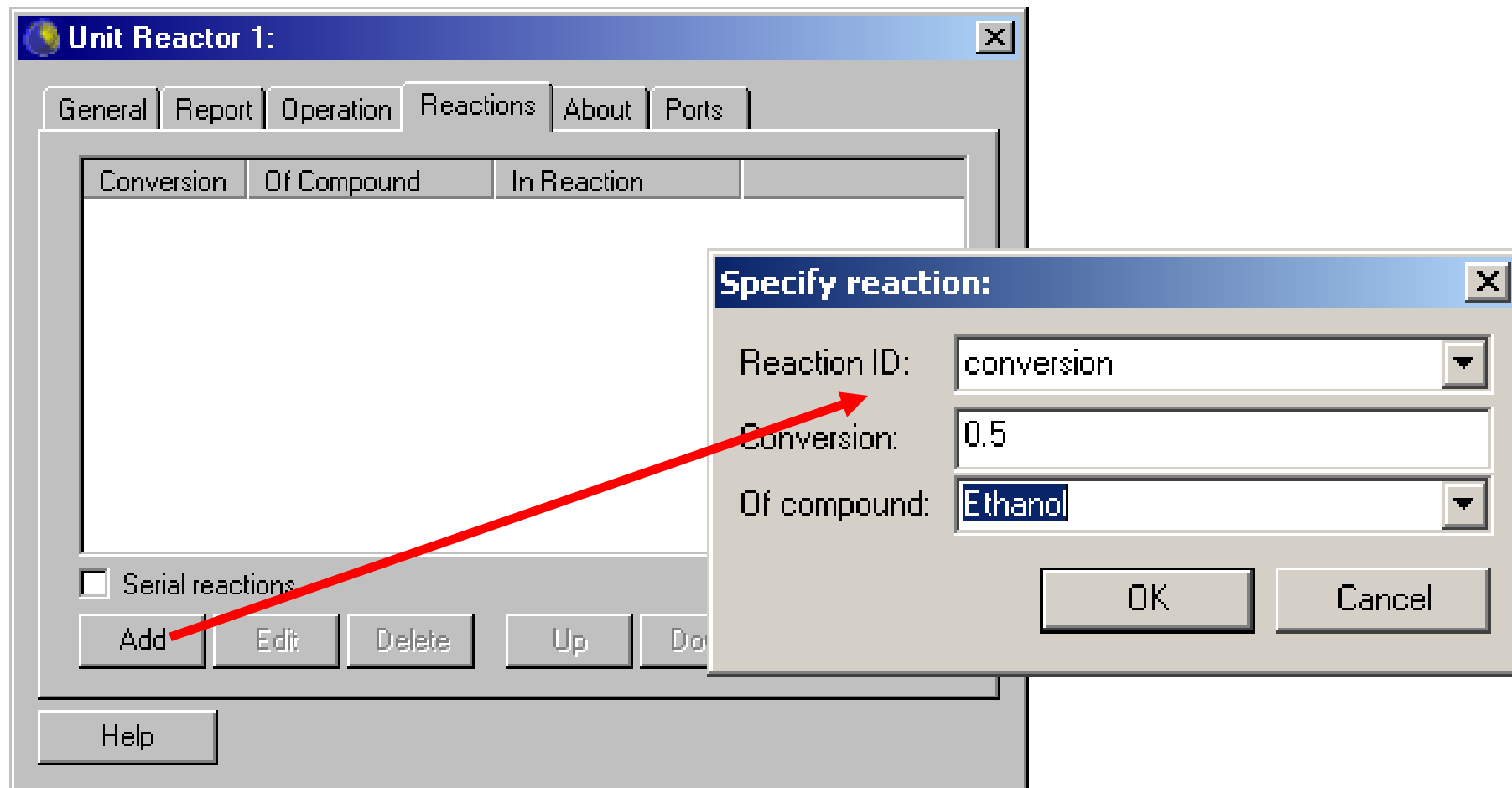
## Reactor specifications:

The screenshot shows a software window titled "Unit Reactor 1:". It contains several tabs: "General", "Report", "Operation" (which is selected), "Reactions", "About", and "Ports". The "Operation" tab displays the following settings:

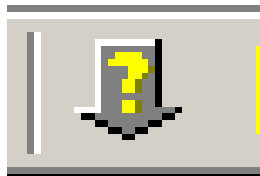
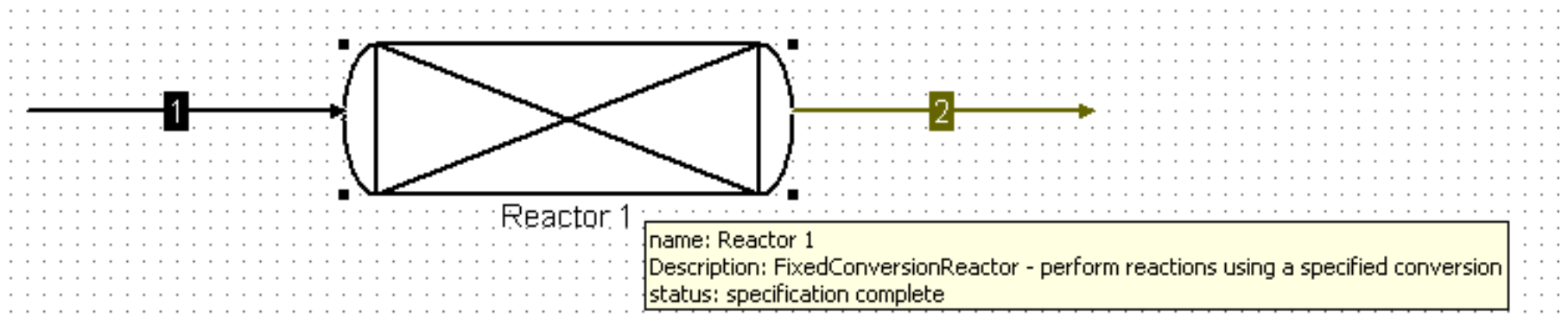
- Pressure drop: 0 Pa
- ☒ Isothermal: 313.15 K
- ☐ Heat duty: 0 J/s
- ☐ Heat duty from inlet stream
- Enthalpy balance: Use EnthalpyF
- Reaction phase: (empty dropdown menu)

A "Help" button is located at the bottom left of the window.

## Reactor specifications:

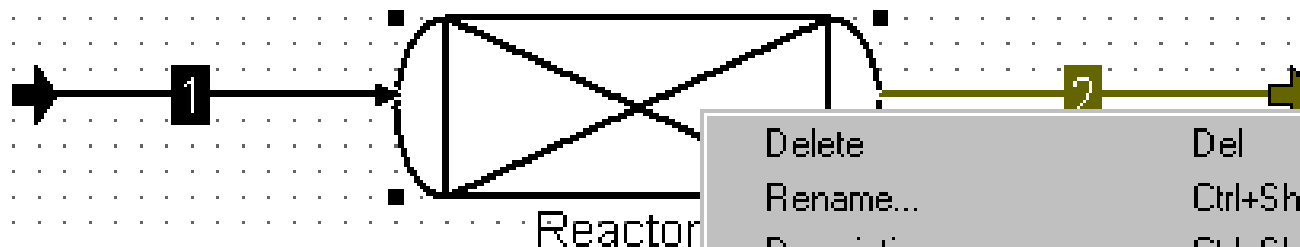


## Reactor specifications:




Validate

## 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...	
<b>Calculate this unit</b>	<b>Ctrl+F5</b>
Icon	▶
Label	▶
Comments...	

**Calculate unit:**

 Finished calculating unit Reactor 1

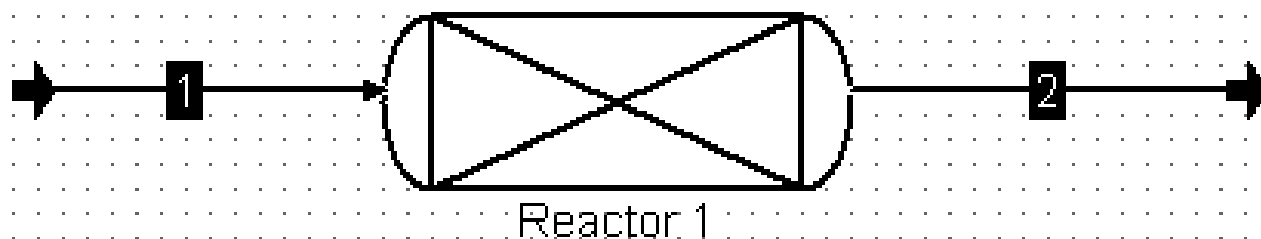
☐ Never show this message again

## Reactor 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			

## Reactor results:

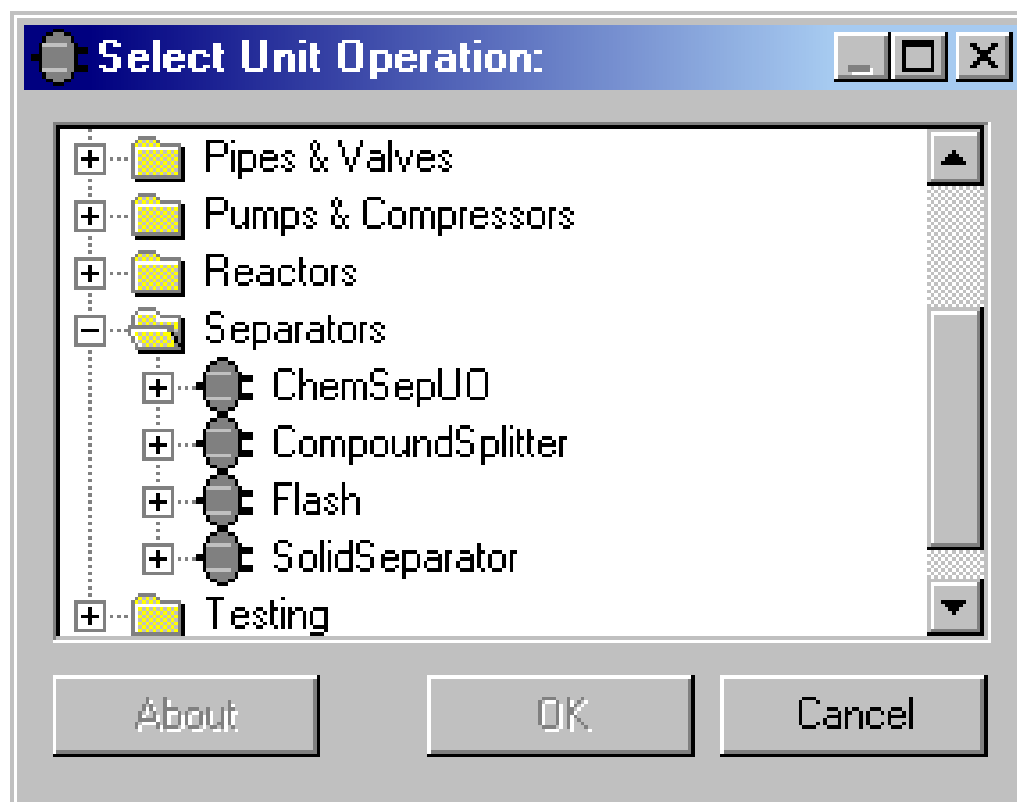


Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

## Presentation outline

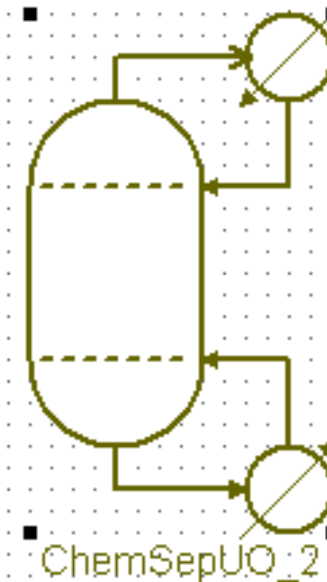
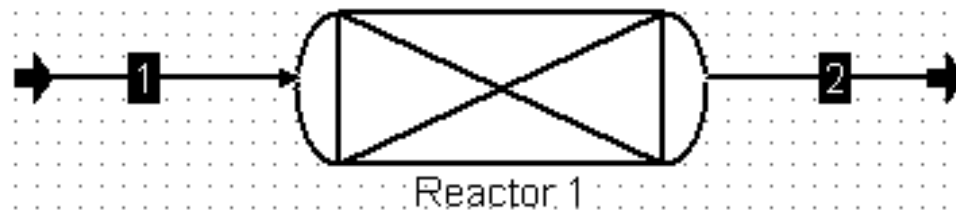
- Introduction to COCO
- What is CAPE-OPEN?
- Setting up thermo dynamic property packages with TEA
- Setting up flowsheets with COFE
- **Using ChemSep in COFE**
- Advanced flowsheeting features

## Inserting a ChemSep column:



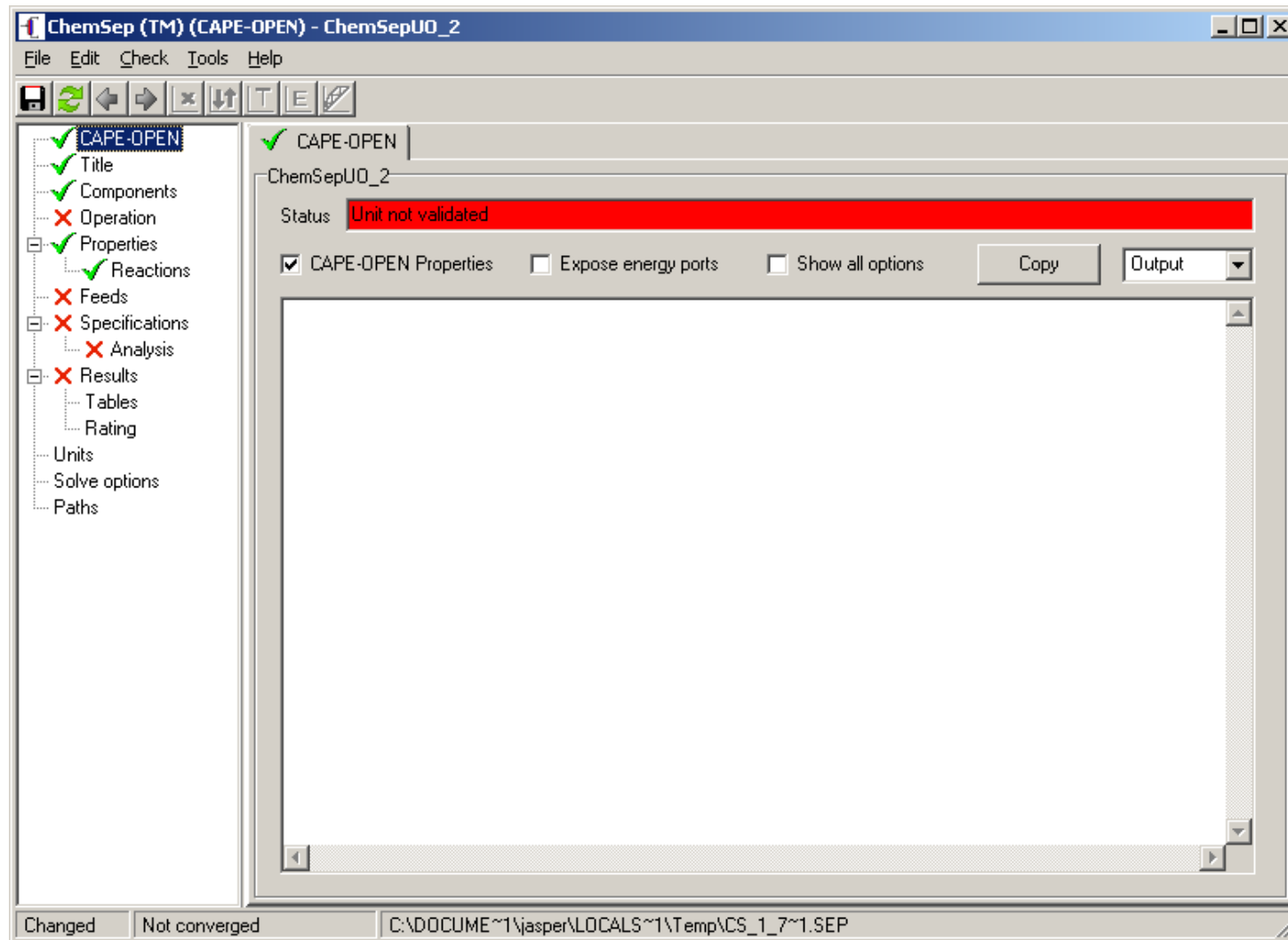


## Inserting a ChemSep column:

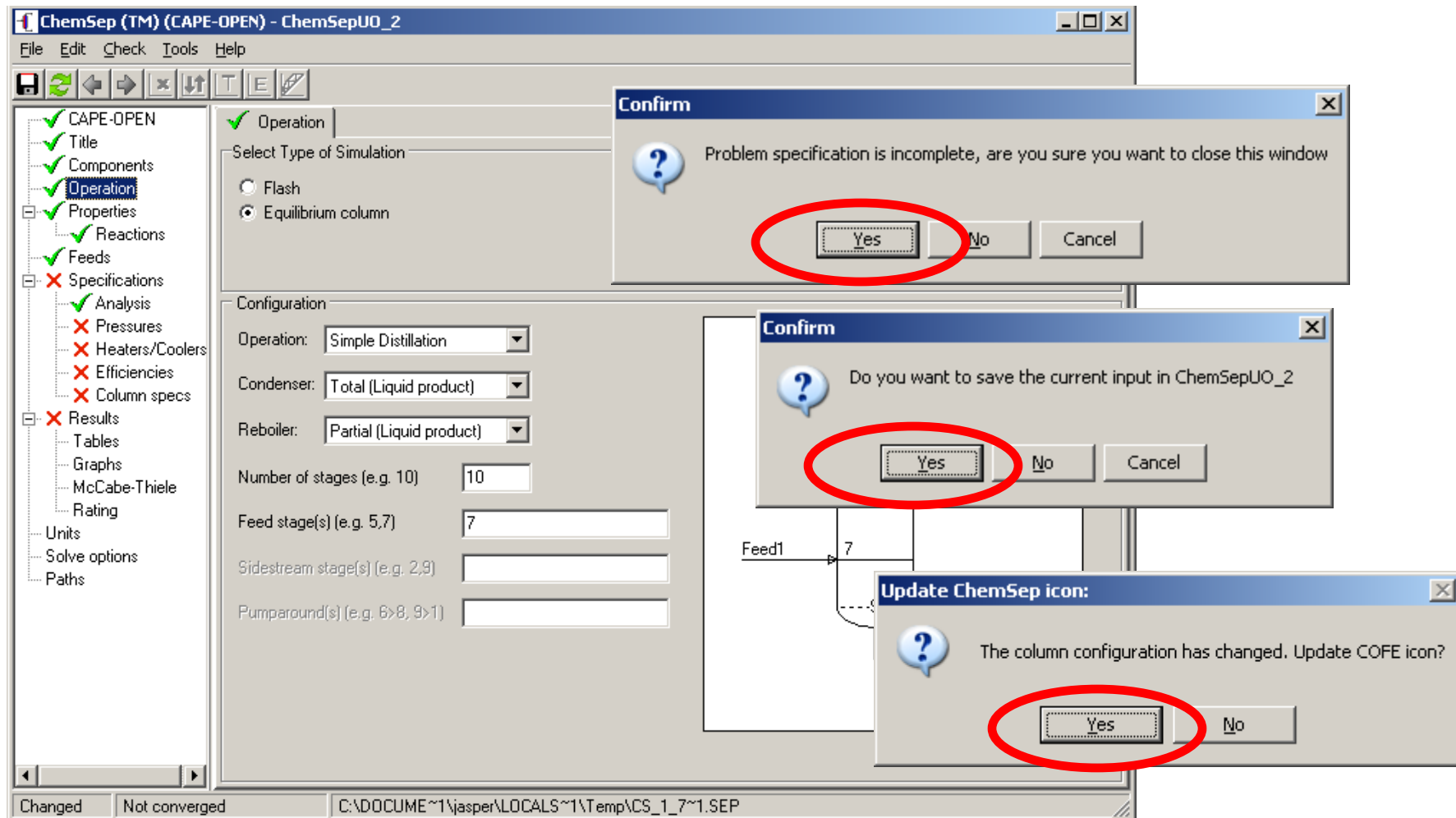


Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

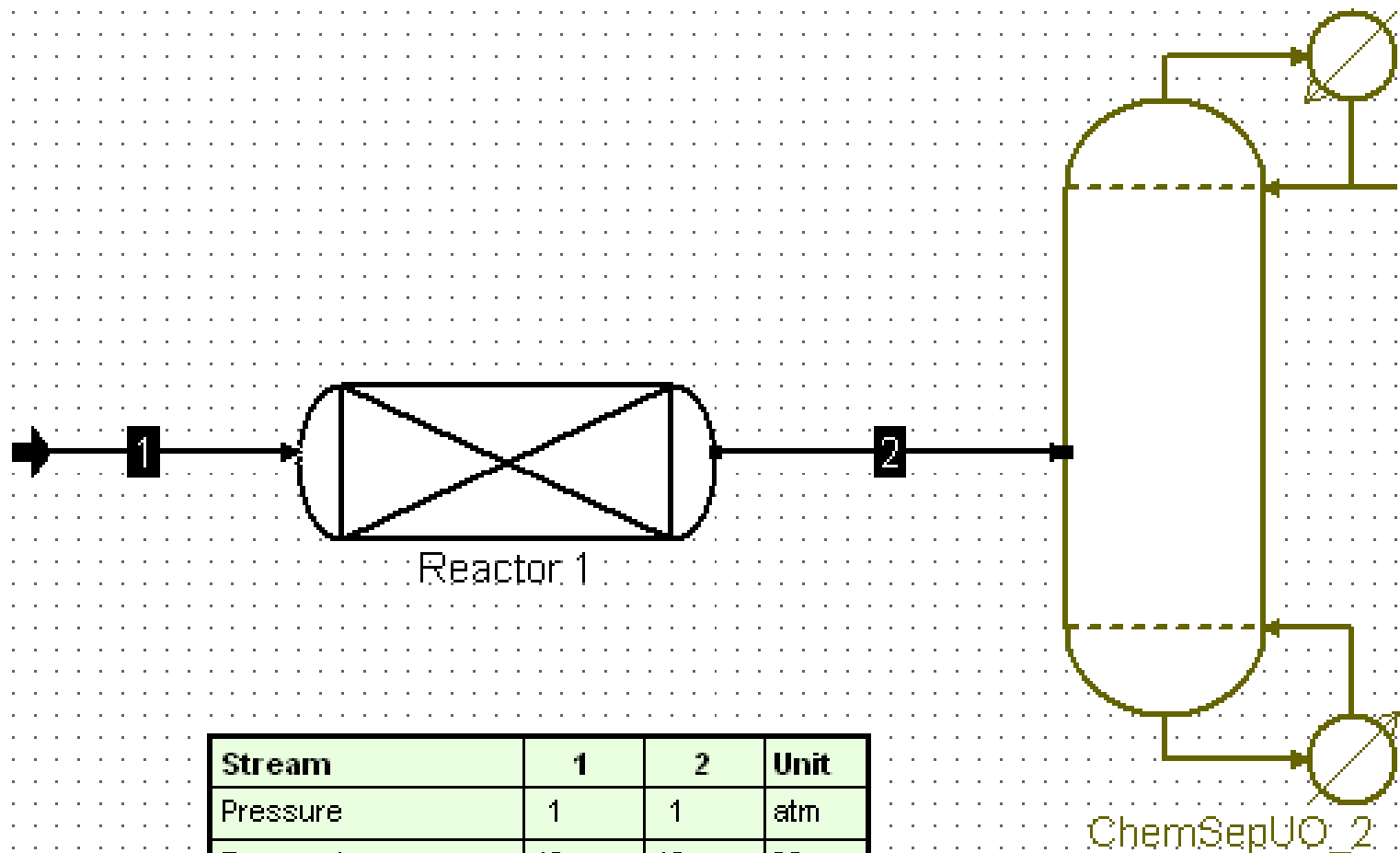
## Inserting a ChemSep column:



# Configuring the ChemSep column:

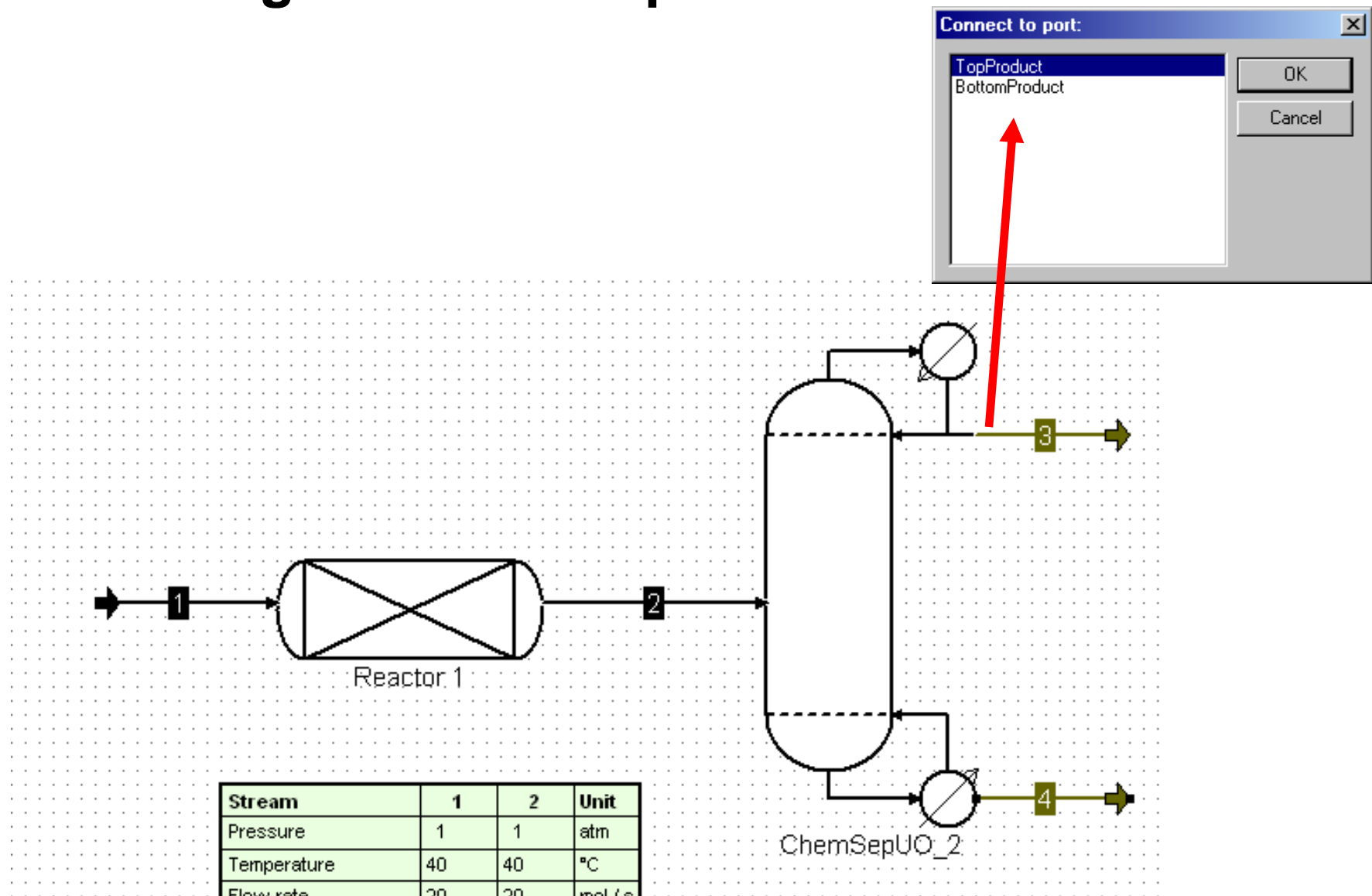


## Connecting the ChemSep column:



Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Molar composition	0.95	0.95	

# Connecting the ChemSep column:



## Configuring the ChemSep column:

✓ Pressures

Column Pressure Specifications

Condenser pressure  (N/m<sup>2</sup>)

Column pressure

Top pressure  (N/m<sup>2</sup>)

Pressure drop / stage  (N/m<sup>2</sup>)

Bottom pressure  (N/m<sup>2</sup>)

✓ Heaters/Coolers

Column and Stage Heat Duties

Column heat loss  (J/s)

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

✓ Efficiencies

Specify Stage Efficiencies

Default stage efficiency  (-)

## Configuring the ChemSep column:

✓ Column specs

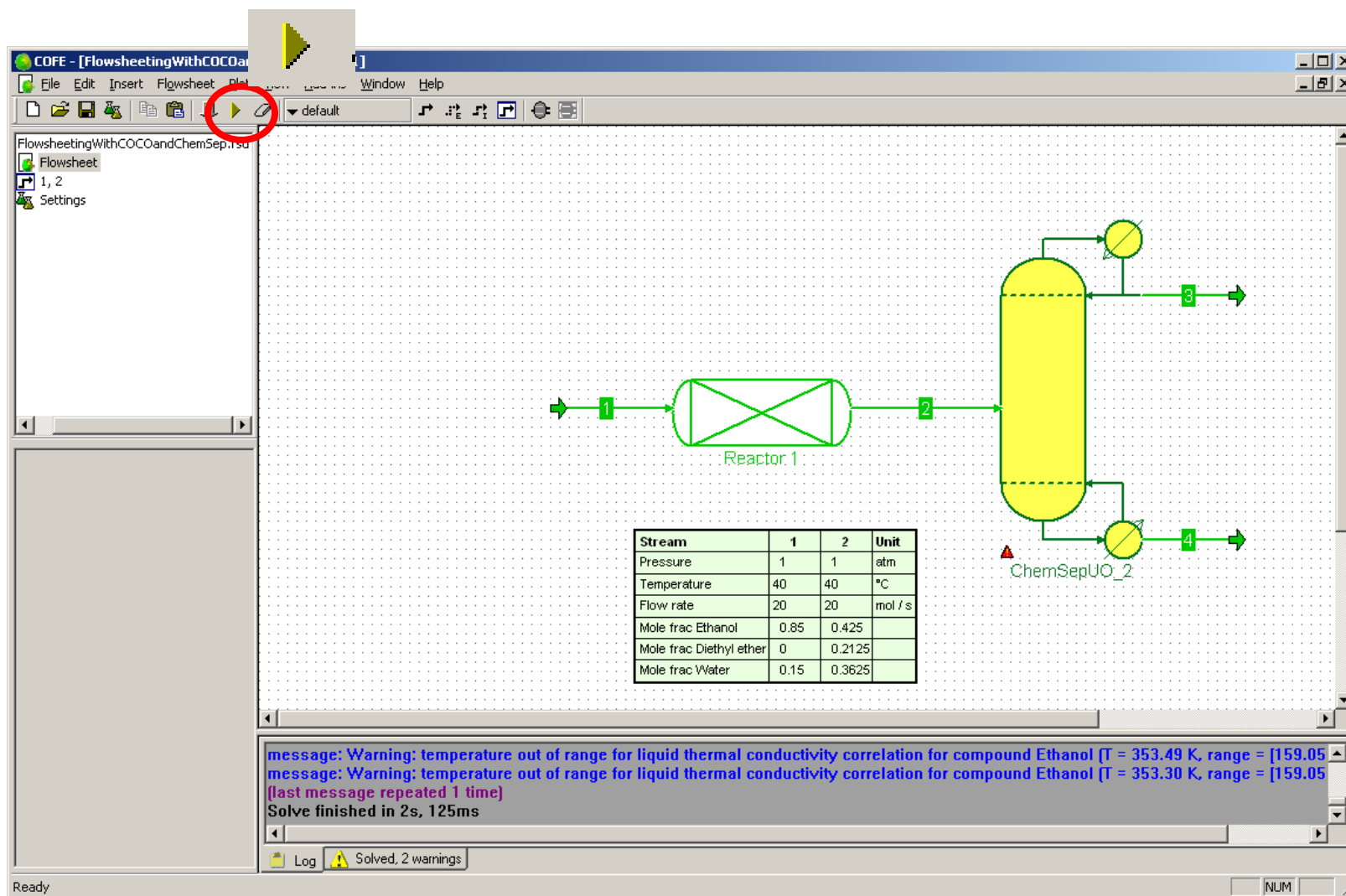
### Column Product Specifications

Top product name	<input type="text" value="Top"/>	Condenser duty name	<input type="text" value="Qcondenser"/>
Top specification	<input type="text" value="Reflux ratio"/> <input type="button" value="v"/>	=	<input type="text" value="10.0000"/> (-)
Bottom product name	<input type="text" value="Bottom"/>	Reboiler duty name	<input type="text" value="Qreboiler"/>
Bottom specification	<input type="text" value="Bottom product flow rate"/> <input type="button" value="v"/>	=	<input type="text" value="0.0150000"/> (kmol/s)

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

15 mol/s

## We can now run the column:



The screenshot shows the amsterCHEM software interface. The main window displays a process flow diagram with a reactor (Reactor 1) and a distillation column (ChemSepUO\_2). The reactor output (Stream 2) feeds into the distillation column. The column has two product streams (Stream 3 and Stream 4). The interface includes a menu bar (File, Edit, Insert, Flowsheet, Plot, Window, Help) and a toolbar. A red circle highlights the 'Run' button (a green play icon) in the toolbar. A data table is displayed below the reactor, showing the composition and flow rate of the streams. The status bar at the bottom indicates 'Solved, 2 warnings'.

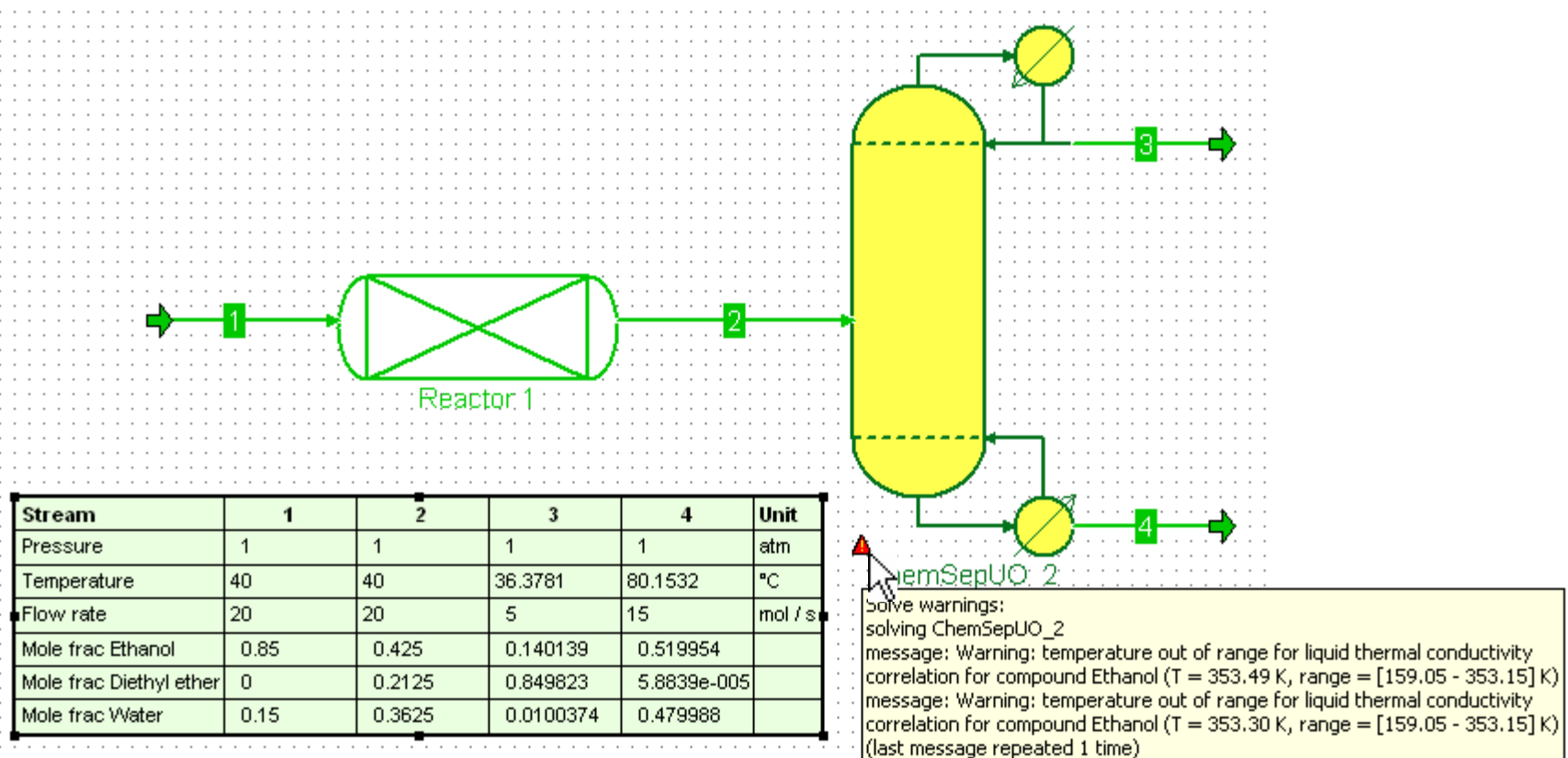
Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

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 the column results:



## Inserting the second column:

COFE - [FlowsheetingWithCOCOandChemSep.fsd:1]

File Edit Insert Flowsheet Plot View Add-ins Window Help

FlowsheetingWithCOCOandChemSep.fsd

Flowsheet

1, 2

Settings

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
				0.519954	
				5.8839e-005	
				0.479988	

Reactor.1

ChemSepUO\_2

ChemSepUO\_3

Select Unit Operation:

- Pumps & Compressors
- Reactors
- Separators
  - ChemSepUO
  - CompoundSplitter
  - Flash
  - SolidSeparator
- Shell

About OK Cancel

## Configuring the second column:

The screenshot displays the ChemSep (TM) - ChemSepU0\_3 software window. The left sidebar shows a tree view of the simulation setup, with 'Operation' selected. The main panel is divided into two sections: 'Select Type of Simulation' and 'Column Configuration'.

**Select Type of Simulation:**

- ☐ Flash
- ☒ Equilibrium column

**Column Configuration:**

- Operation: Simple Distillation
- Condenser: Total (Liquid product)
- Reboiler: Partial (Liquid product)
- Number of stages (e.g. 10): 15
- Feed stage(s) (e.g. 5,7): 4
- Sidestream stage(s) (e.g. 2,9):
- Pumparound(s) (e.g. 6>8, 9>1):

On the right, a process flow diagram illustrates the column configuration. It shows a vertical distillation column with 15 stages. Feed1 enters at stage 4. The top product is labeled 'Top' and exits from stage 1. The bottom product is labeled 'Bottom' and exits from stage 15. The column is equipped with a total condenser at the top and a partial reboiler at the bottom.

At the bottom of the window, the status bar indicates 'Changed' and 'Not converged', and the file path is 'C:\DOCUME~1\jasper\LOCALS~1\Temp\CS1773.sep'.

## Configuring the second column:

✓ Pressures

Column Pressure Specifications

Condenser pressure  (N/m<sup>2</sup>)

Column pressure

Top pressure  (N/m<sup>2</sup>)

Pressure drop / stage  (N/m<sup>2</sup>)

Bottom pressure  (N/m<sup>2</sup>)

✓ Heaters/Coolers

Column and Stage Heat Duties

Column heat loss  (J/s)

✓ Efficiencies

Specify Stage Efficiencies

Default stage efficiency  (-)

## Configuring the second column:

ChemSep (TM) - ChemSepU0\_3

File Edit Check Tools Help

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

Analysis Pressures Heaters/Coolers Efficiencies Column specifications

Column Product Specifications

Top product name: Top Condenser duty name: Qcondenser

Top specification: Reflux ratio = 3.00000 (-)

Bottom product name: Bottom Reboiler duty name: Qreboiler

Bottom specification: Mole fraction of a component = 0.990000 (-)

Water

Product Guesses (optional)

☐ Use guesses for initialization Reset

Saved Converged 7 iterations C:\DOCUME~1\jasper\LOCALS~1\Temp\CS176E.sep

# Connecting the streams:

COFE - [FlowsheetingWithCOCOandChemSep.fsd:1]

File Edit Insert Flowsheet Plot View Add-ins Window Help

default

FlowsheetingWithCOCOandChemSep.fsd

- Flowsheet
- 1, 2
- Settings

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

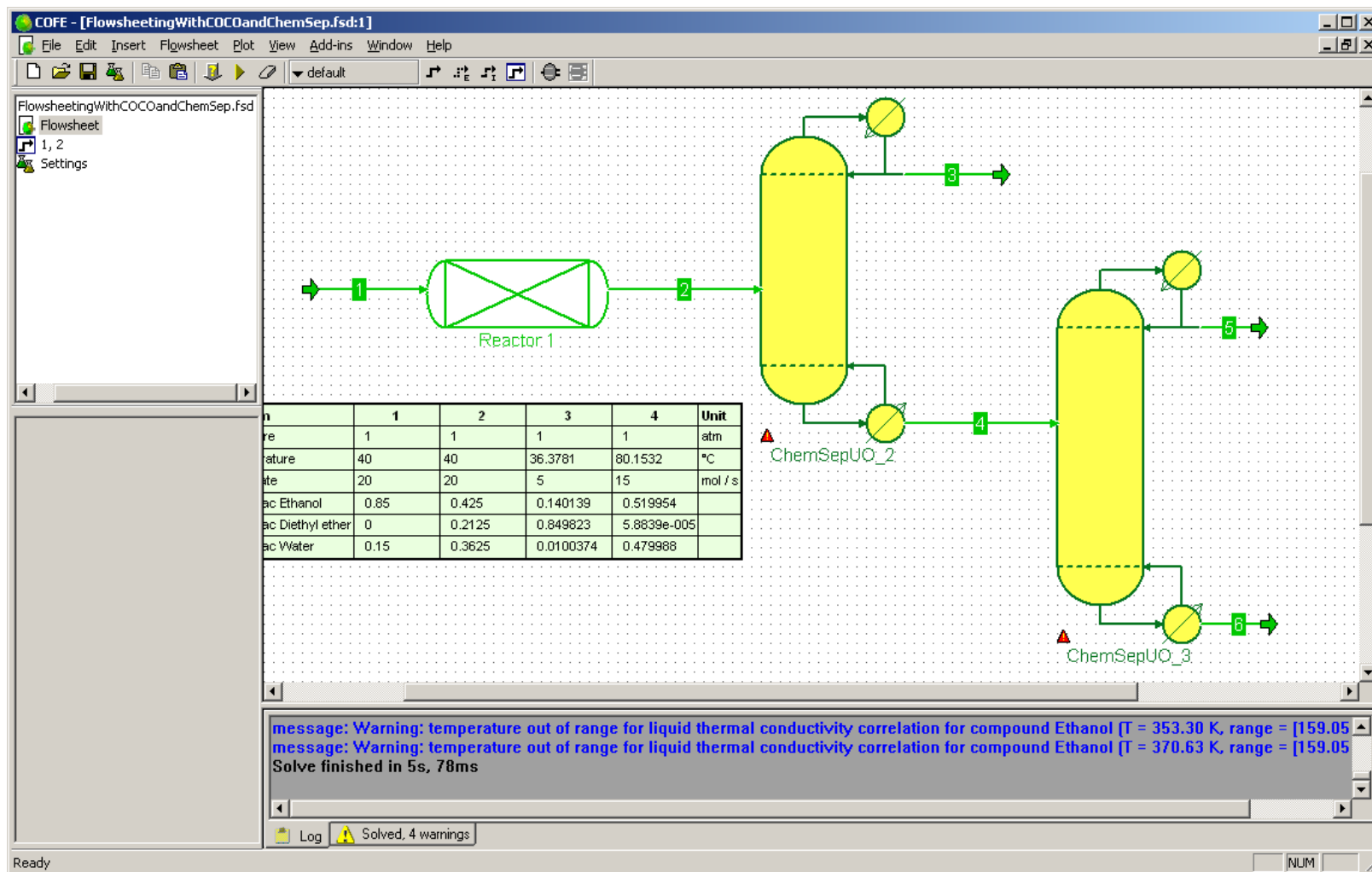
connected stream 5 to unit ChemSepUO\_3 as OUTLET at port TopProduct  
inserted stream 6  
connected stream 6 to unit ChemSepUO\_3 as OUTLET at port BottomProduct

Log 2 warnings

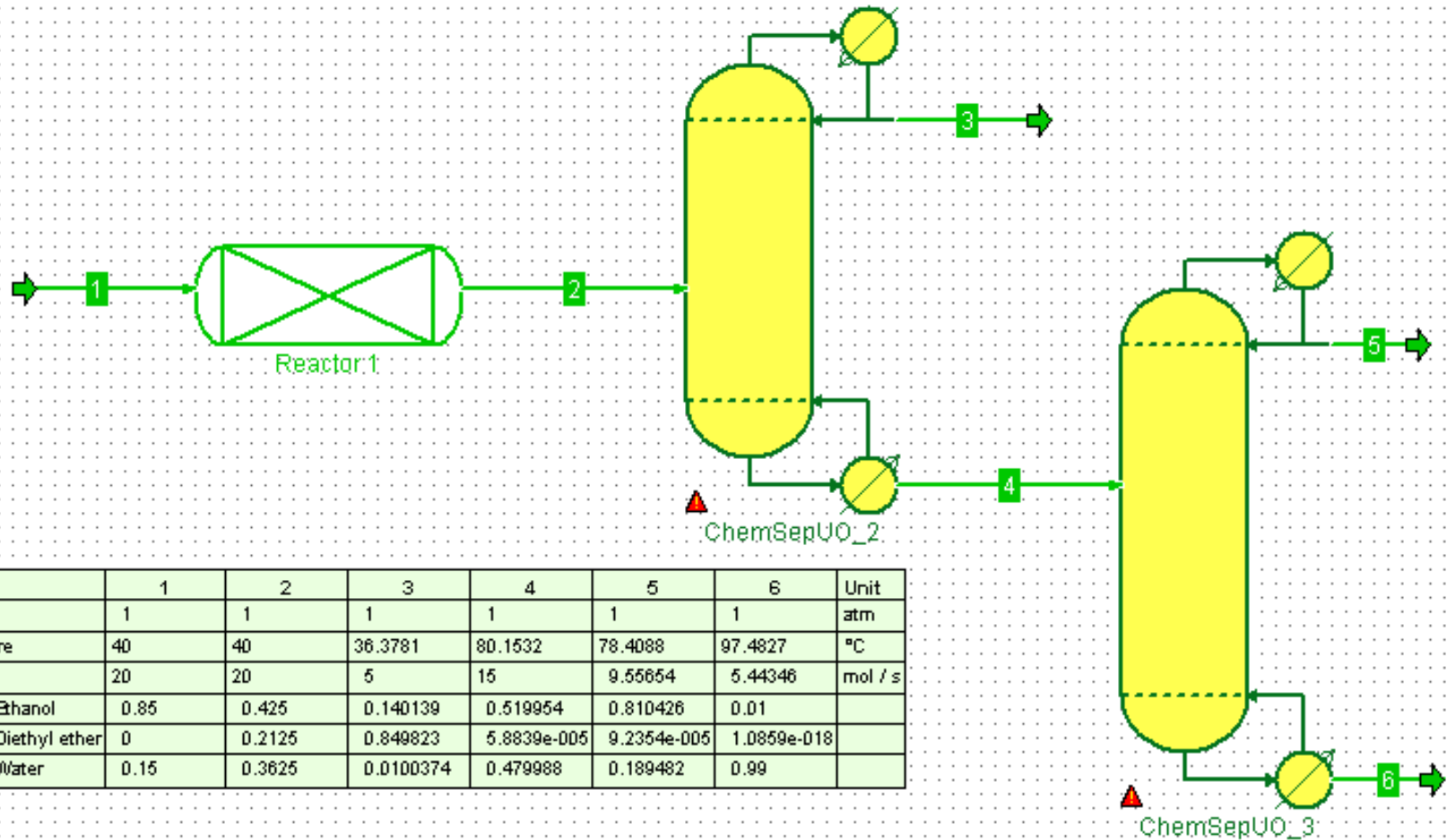
Ready

NUM

# Solving the second column:

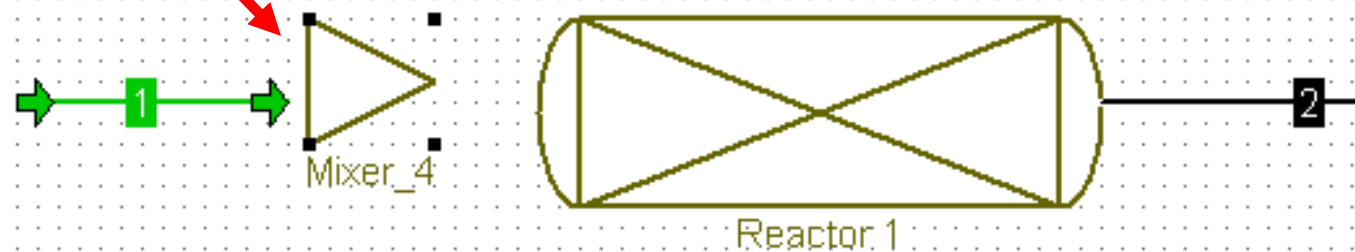
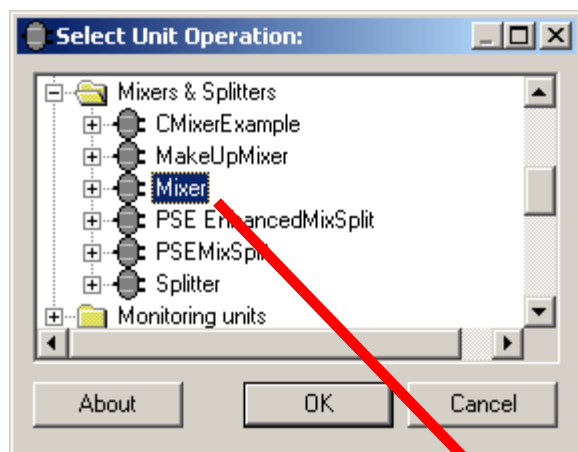


## Let's see what we get:

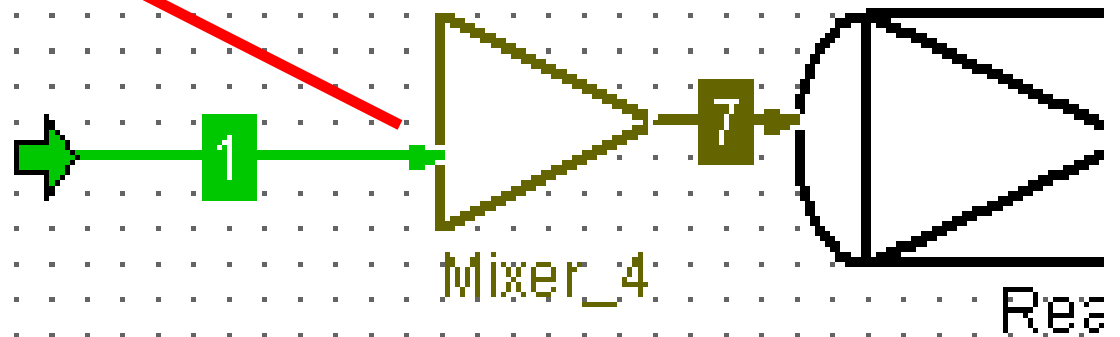
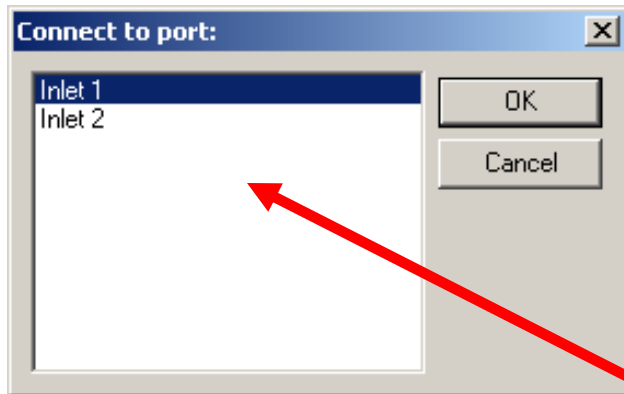




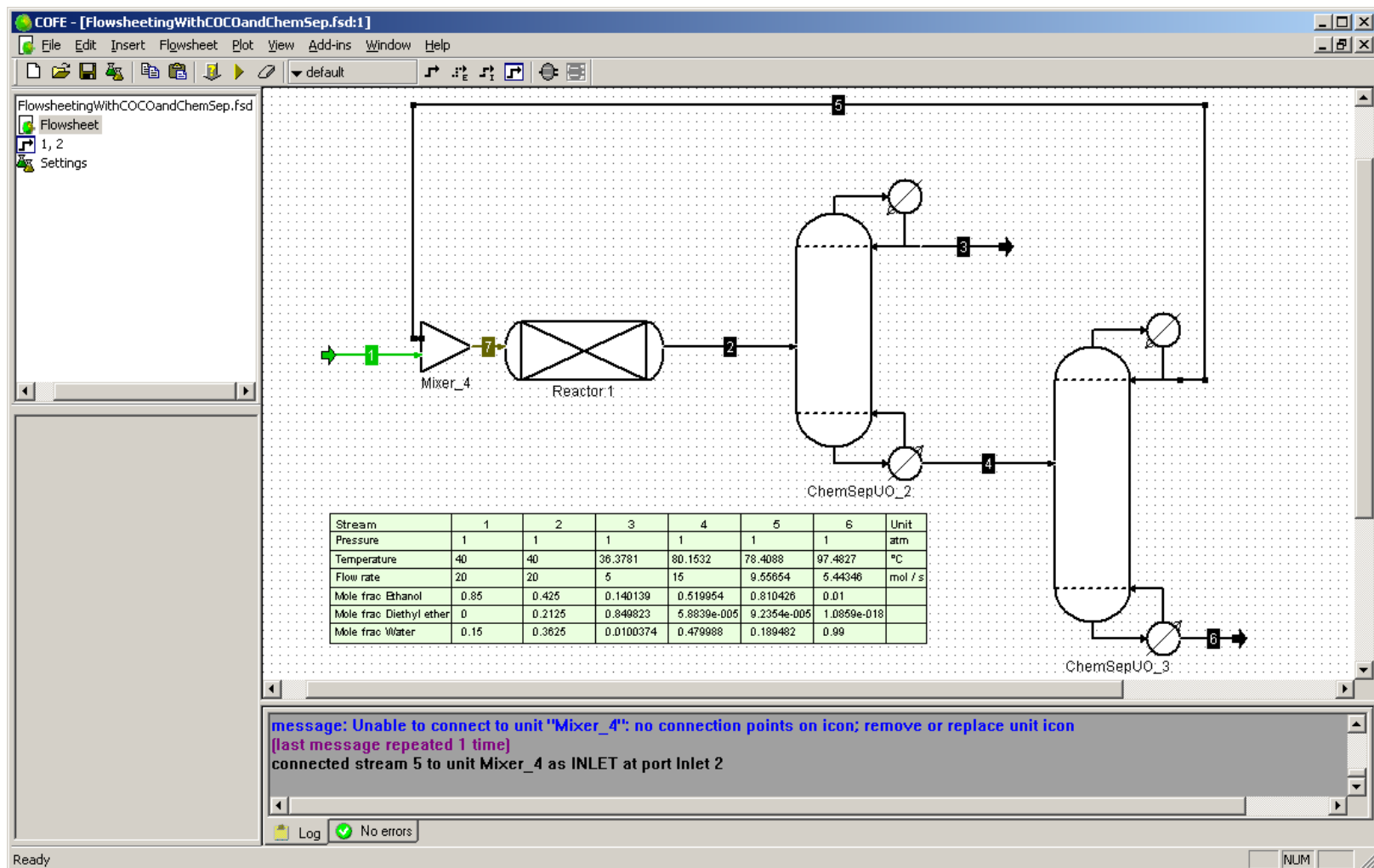
## Setting up the recycle:



## Setting up the recycle:



# Closing the recycle:



# Redoing the specifications for Column 1:

The screenshot displays the amsterCHEM software interface. The main window shows a process flowsheet with units: Mixer\_4, Reactor\_1, and ChemSepUO\_2. A stream table is visible at the bottom left of the flowsheet area:

Stream	1	2	3	4	5	6
Pressure	1					
Temperature	40					
Flow rate	20					
Mole frac Ethanol	0.85					
Mole frac Diethyl ether	0					
Mole frac Water	0.15					

The 'ChemSep (TM) (CAPE-OPEN) - ChemSepUO\_2' window is open, showing the 'Column specs' tab. The 'Column Product Specifications' section is visible, with the following settings:

- Top product name: Top
- Condenser duty name: Qcondenser
- Top specification: Reflux ratio = 10.0000 (-)
- Bottom product name: Bottom
- Reboiler duty name: Qreboiler
- Bottom specification: Mole fraction of a component = 1.0000E-05 (-)

A red circle highlights the 'Bottom specification' section, and a red arrow points to it from the text 'Note new specification'.

message: Unable to connect (last message repeated 1 ti connected stream 5 to unit)

Log No errors

Ready

# Redoing the specifications for Column 1:

The screenshot shows the ChemSep (TM) (CAPE-OPEN) - ChemSepUO\_2 interface. The 'Specifications' tab is selected in the left-hand tree view. The 'Number of stages (e.g. 10)' field is set to 20, and the 'Feed stage(s) (e.g. 5,7)' field is set to 8. A red circle highlights the 'Number of stages' field, and a red arrow points to it from the text 'Note new specification'.

The 'Configuration' section on the right shows the following settings:

- Operation: Simple Distillation
- Condenser: Total (Liquid product)
- Reboiler: Partial (Liquid product)
- Number of stages (e.g. 10): 20
- Feed stage(s) (e.g. 5,7): 8
- Side stream stage(s) (e.g. 2,9):
- Pumparound(s) (e.g. 6>8, 9>1):

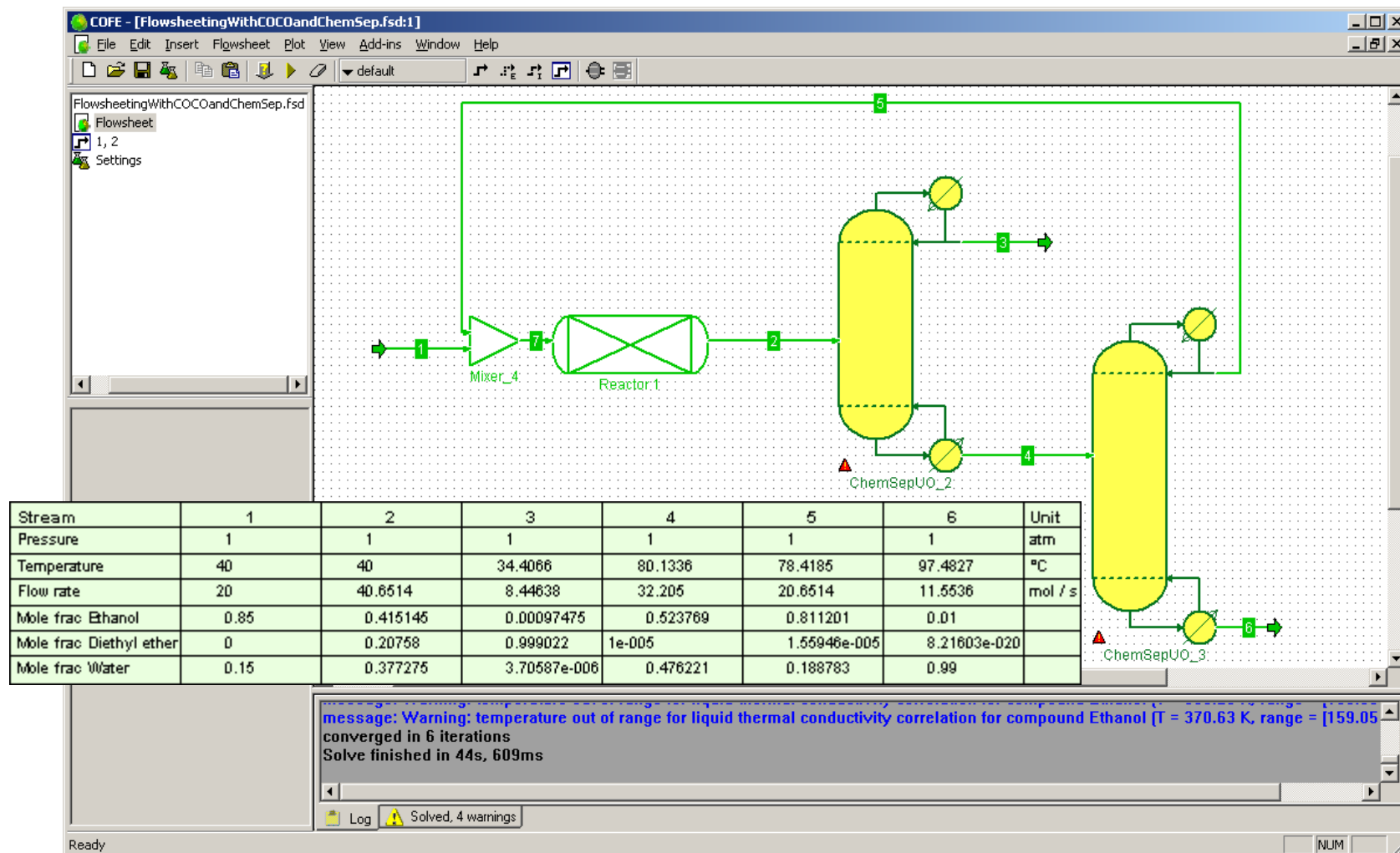
The 'Results' section on the left shows the following data:

Stream	Pressure	Temperature	Flow rate	Mole frac Ethanol	Mole frac Diethyl ether	Mole frac Water
1						
2						

The status bar at the bottom indicates 'Changed', 'Converged 1 iterations', and the file path 'C:\DOCUME~1\jasper\LOCALS~1\Temp\CS\_5\_8~1.SEP'.

Note new specification

# The solution:



## Presentation outline

- Introduction to COCO
- What is CAPE-OPEN?
- Setting up thermo dynamic property packages with TEA
- Setting up flowsheets with COFE
- Using ChemSep in COFE
- **Advanced flowsheeting features**

## Stream types (1/3): material streams

- Multiple material types (Flowsheet Configuration)
- Each material type associated with Property Package
- Each material type associated with list of compounds
- You can connect different material types to a unit operation
- StreamConverter unit



## Stream types (2/3): energy streams

- Heat integration
- Connect to energy ports
- Many COUSCOUS units have energy ports
- ChemSep has energy ports for column heat duty, stage heat duty, the condensor and reboiler
- Energy streams have a direction, like material streams

## Stream types (3/3): information streams

- Typically one double precision number
- Numbers have a unit of measure
- Can be used for measured data (MeasureUnit)
- Can be manipulated (InformationCalculator)
- Can be used for controllers
- COFE allows exposing a parameter as information port

# Graphs

- Temperature or pressure dependent property calculations
- Phase envelopes
- Binary property calculations
- Parameter plots of unit operations
- ...

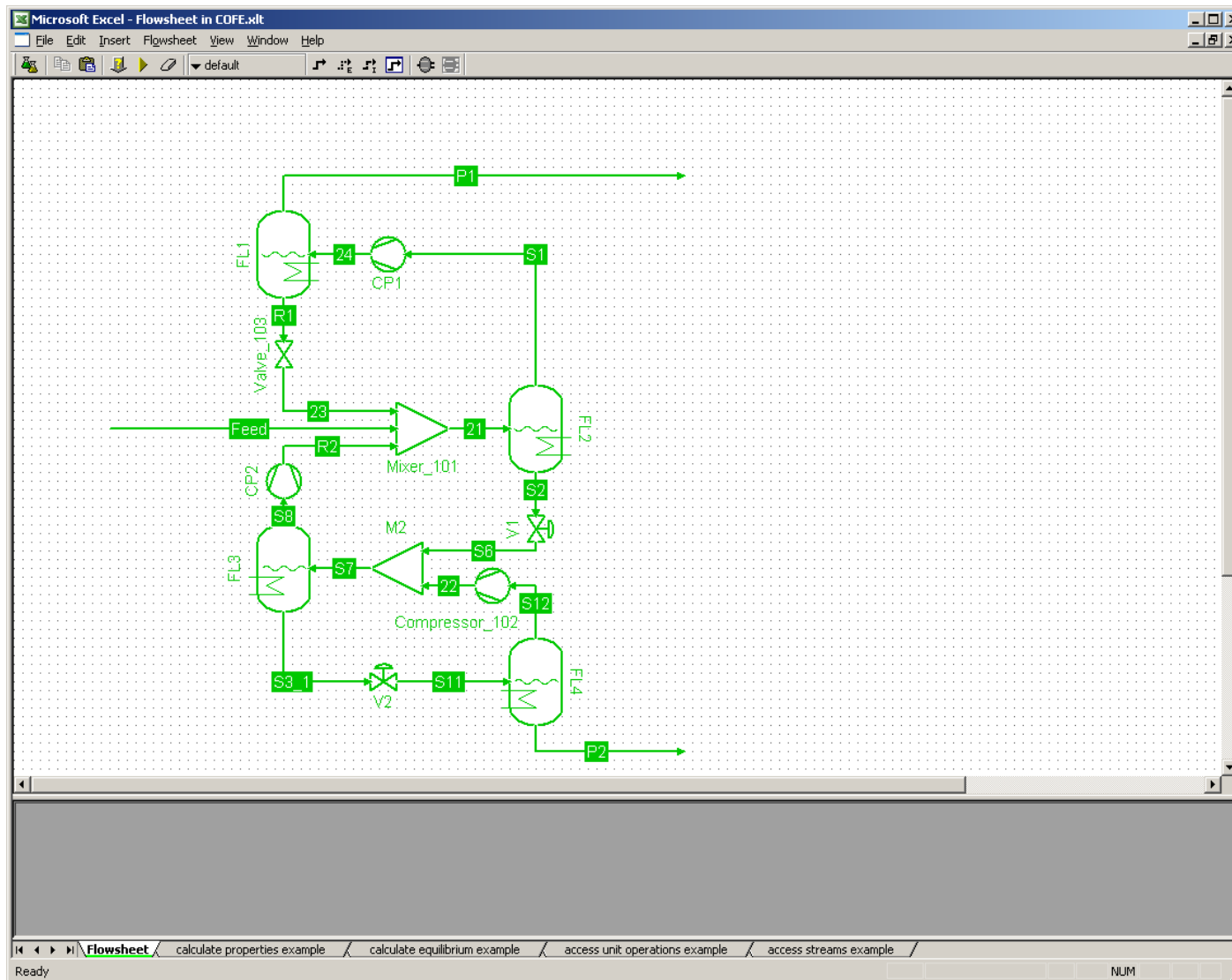
# Reports and graphical elements

- Stream reports
- Unit operation reports
- Basic shapes and text
- Embed OLE objects
- Stream and unit operation comments
- ...

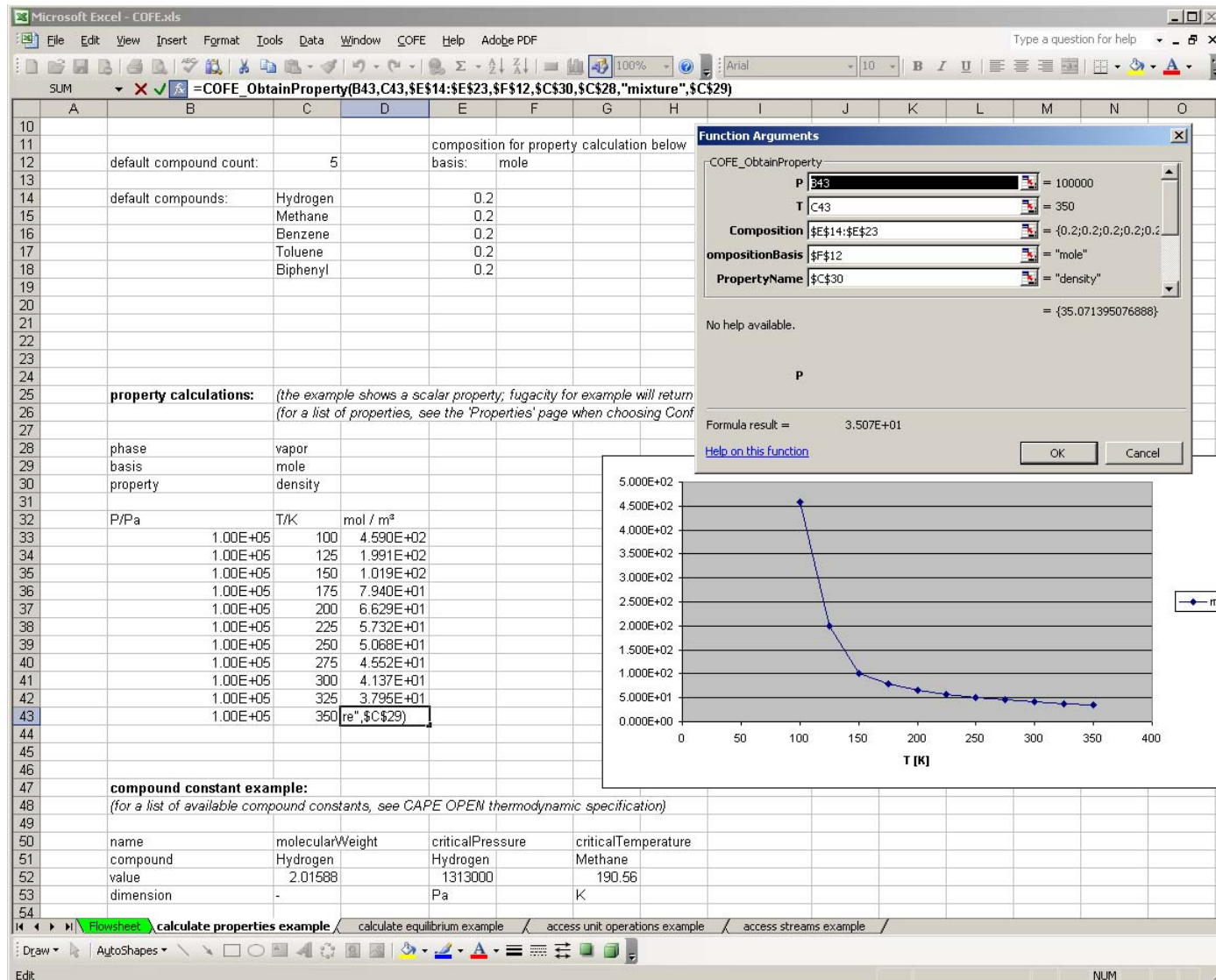
## Parametric studies

- Solve the flowsheet
- Choose Parametric Study from the flowsheet menu
- Define inputs and their ranges
- Define outputs
- Solve
- ...

# Embedding flowsheets in Excel



# Embedding flowsheets in Excel



## Presentation outline

- Introduction to COCO
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- Advanced flowsheeting features