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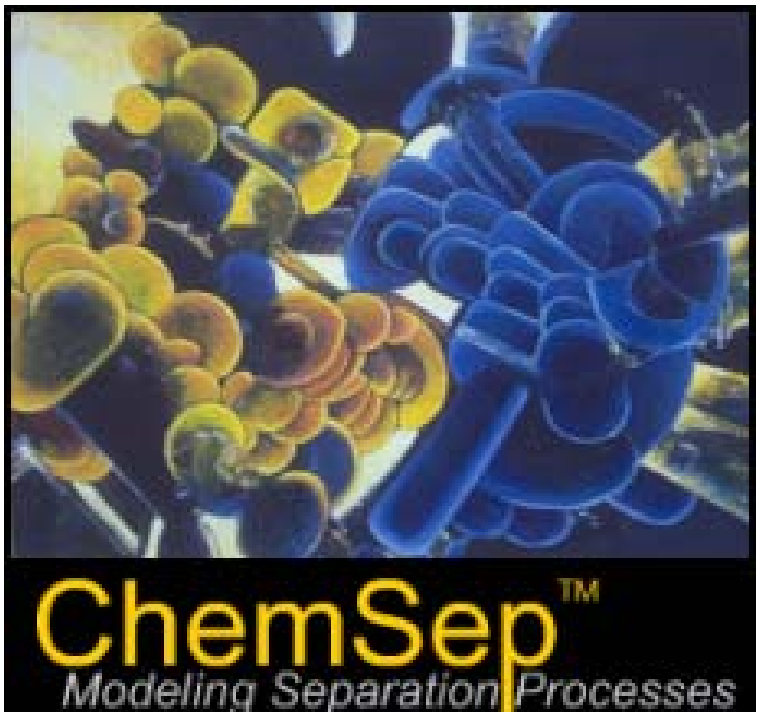
ChemSep
Modeling Separation Processes

Flowsheeting with

COCO and



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:

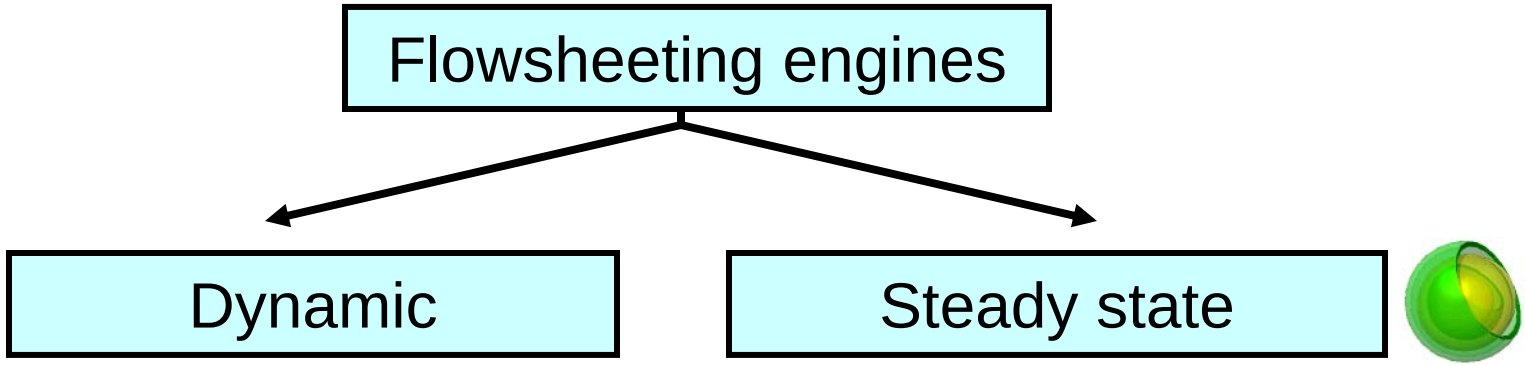
Simulation environment (COFE)

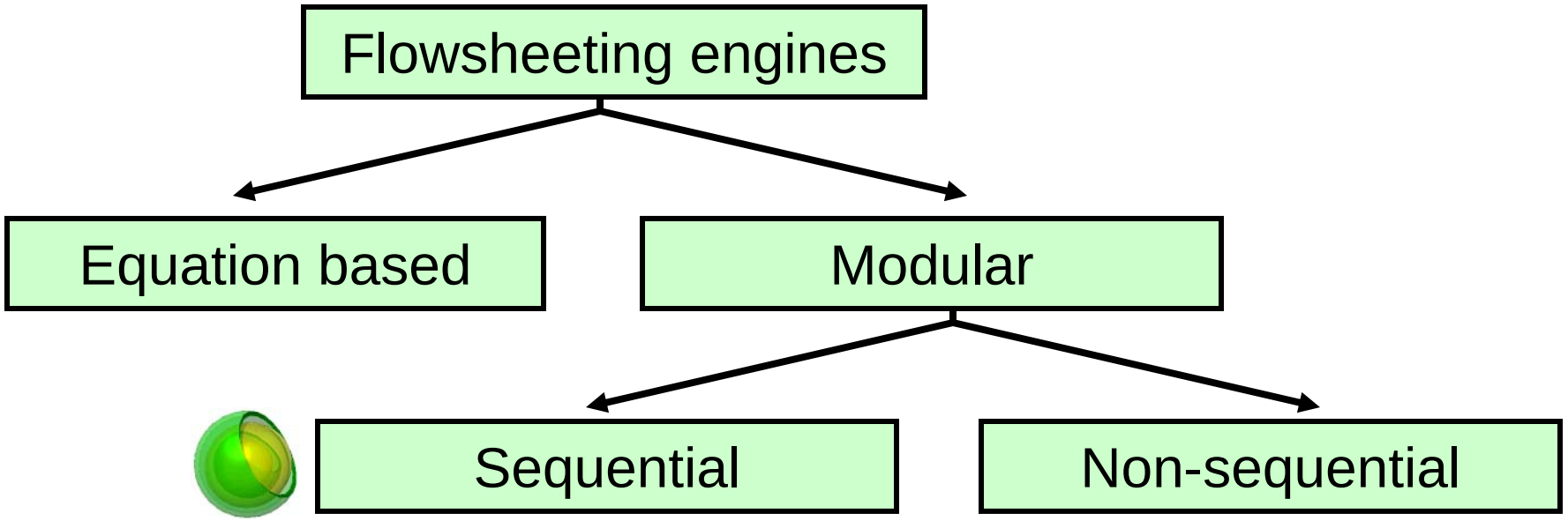
Thermodynamic property package (TEA)

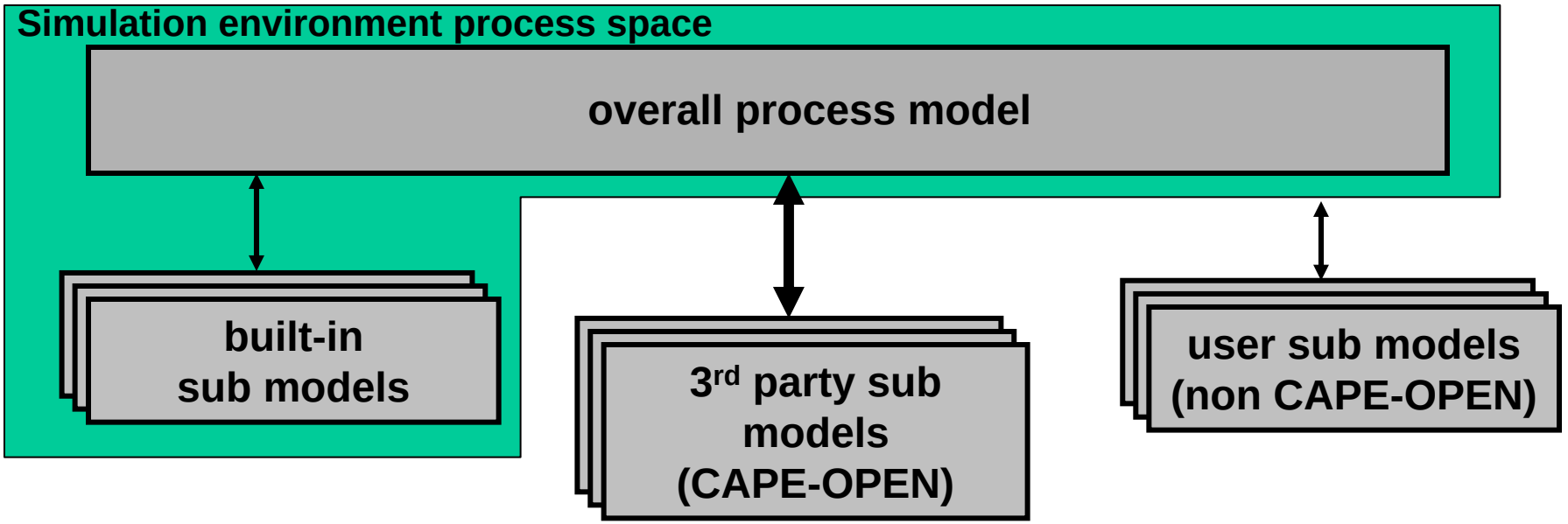
Collection of unit operations (COUSCOUS)

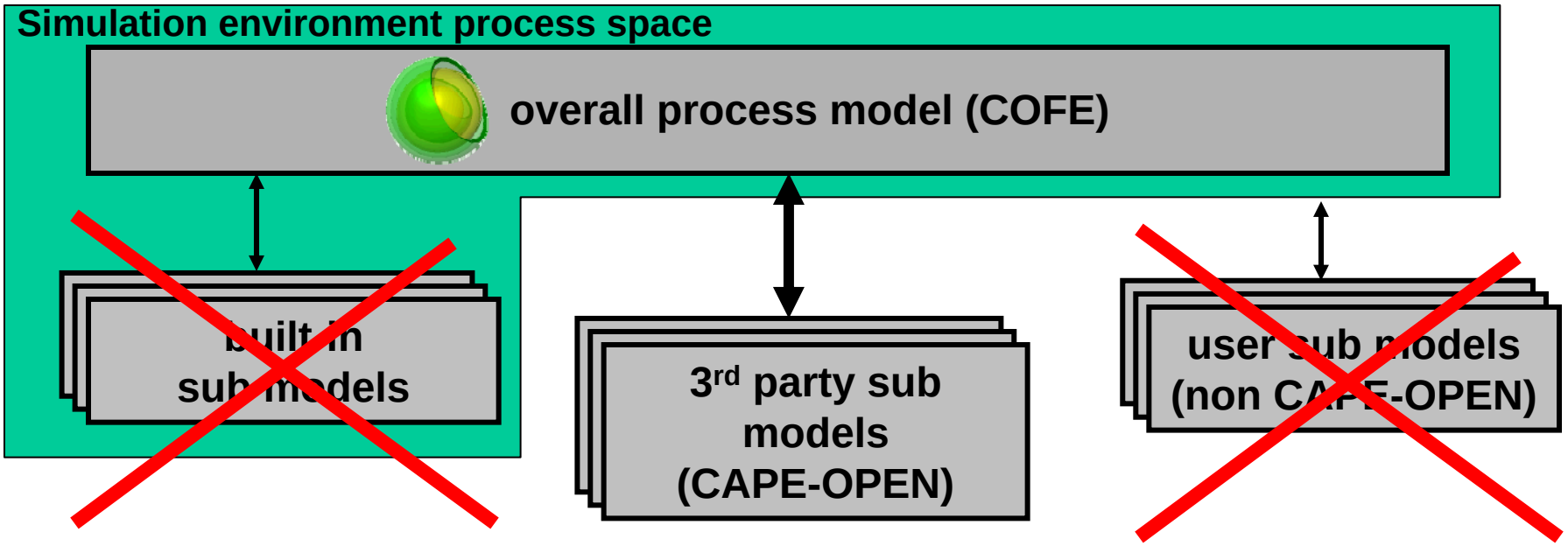
Reaction package (CORN)

… and utilities


Flowsheeting engines
Dynamic
Steady state


Flowsheeting engines
Equation based
Modular
Sequential
Non-sequential


Simulation environment process space
overall process model
built-in
sub models
3rd party sub
models
(CAPE-OPEN)
user sub models
(non CAPE-OPEN)


Simulation environment process space
overall process model (COFE)
built in sub models
3rd party sub models (CAPE-OPEN)
user sub models (non CAPE-OPEN)

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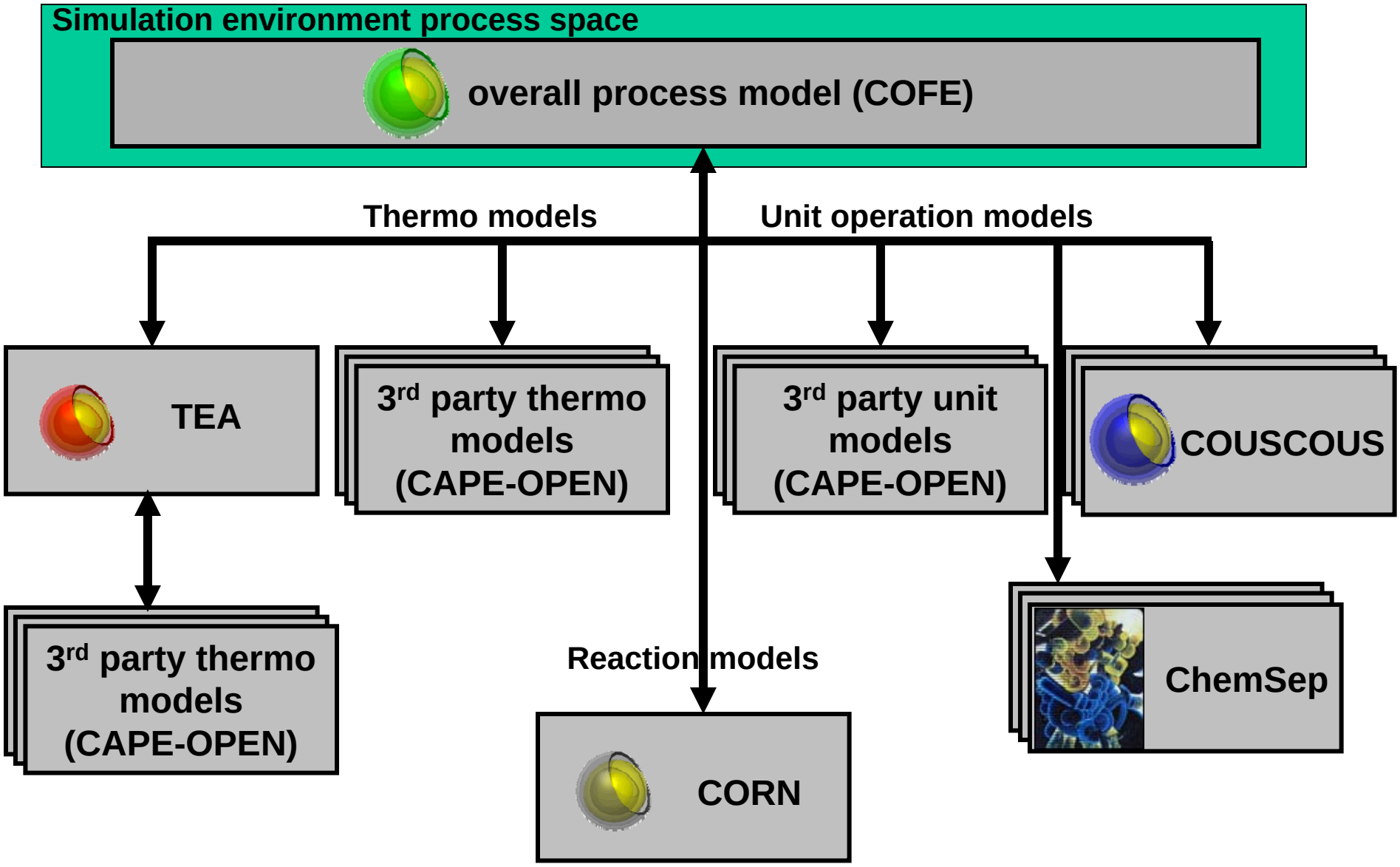
ChemSep
Modeling Separation Processes



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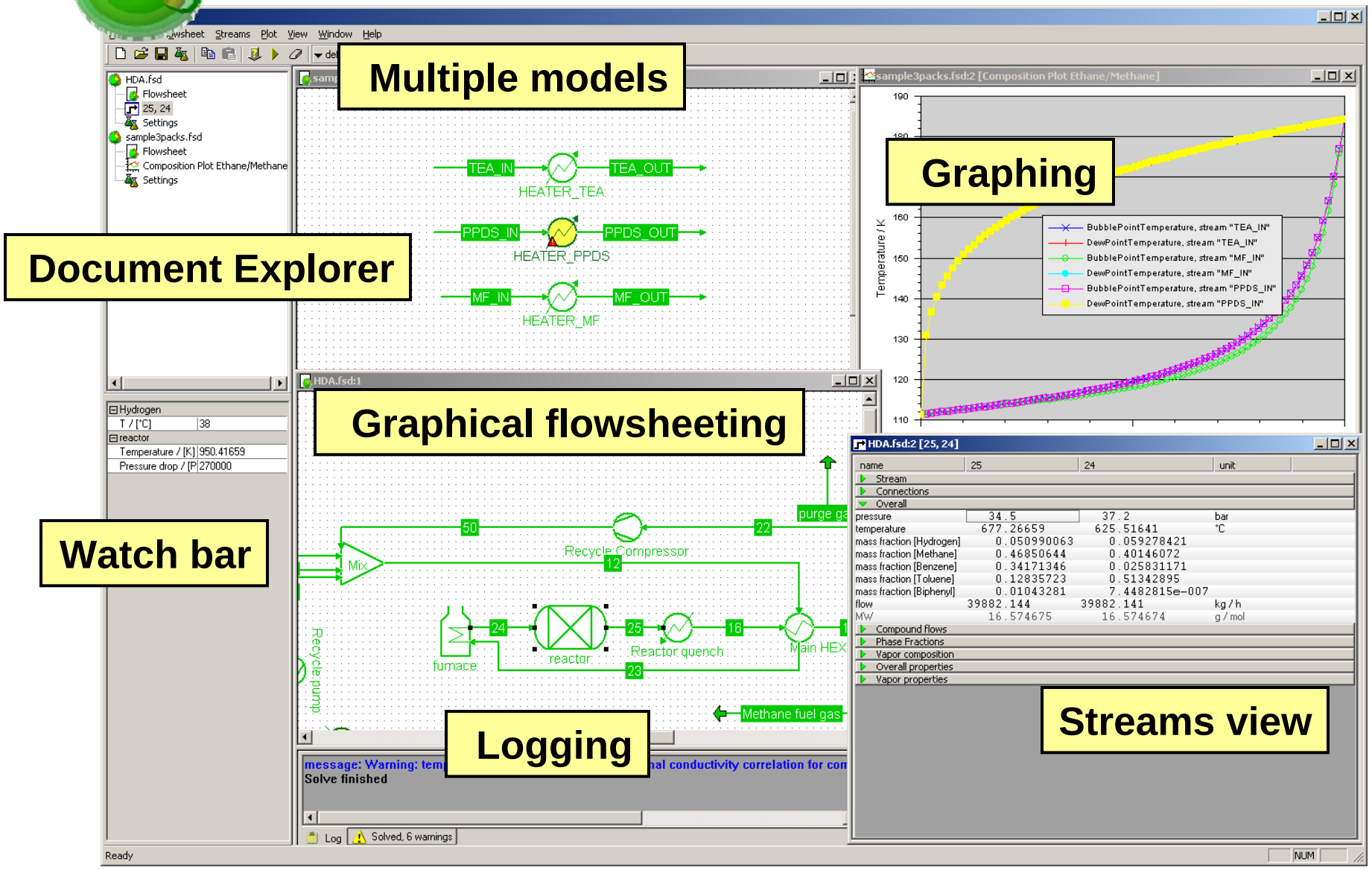
ChemSep
Modeling Separation Processes

COFE: CAPE-OPEN Flowsheeting Environment



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

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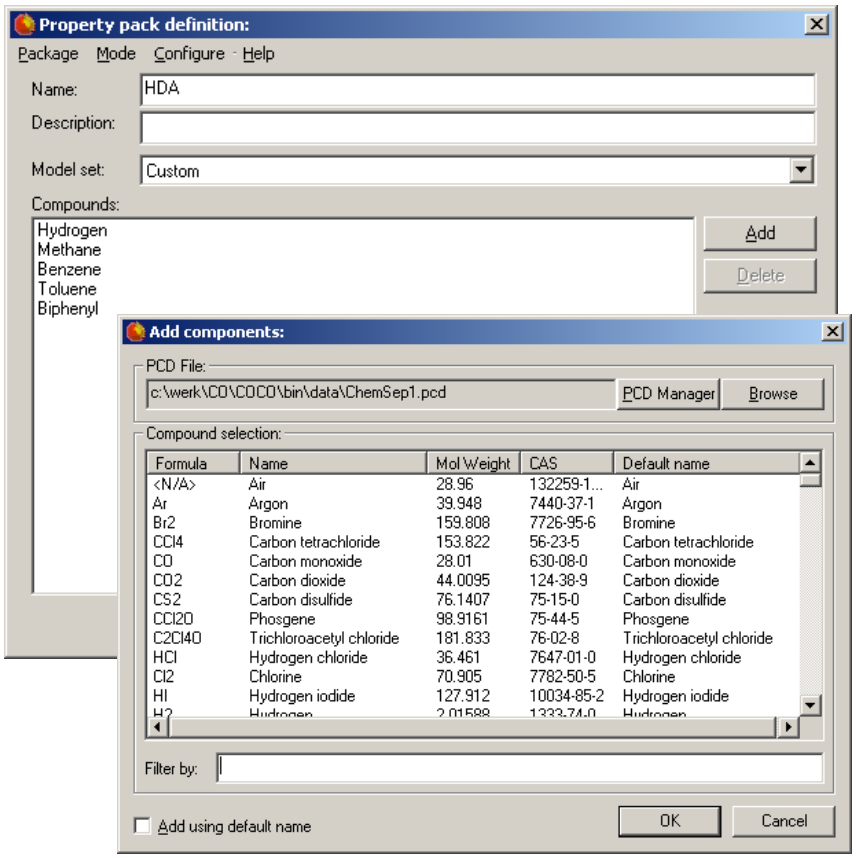
TEA: Thermodynamics for Engineering Applications

- **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

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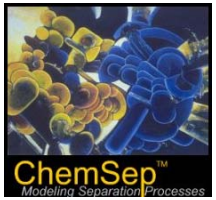
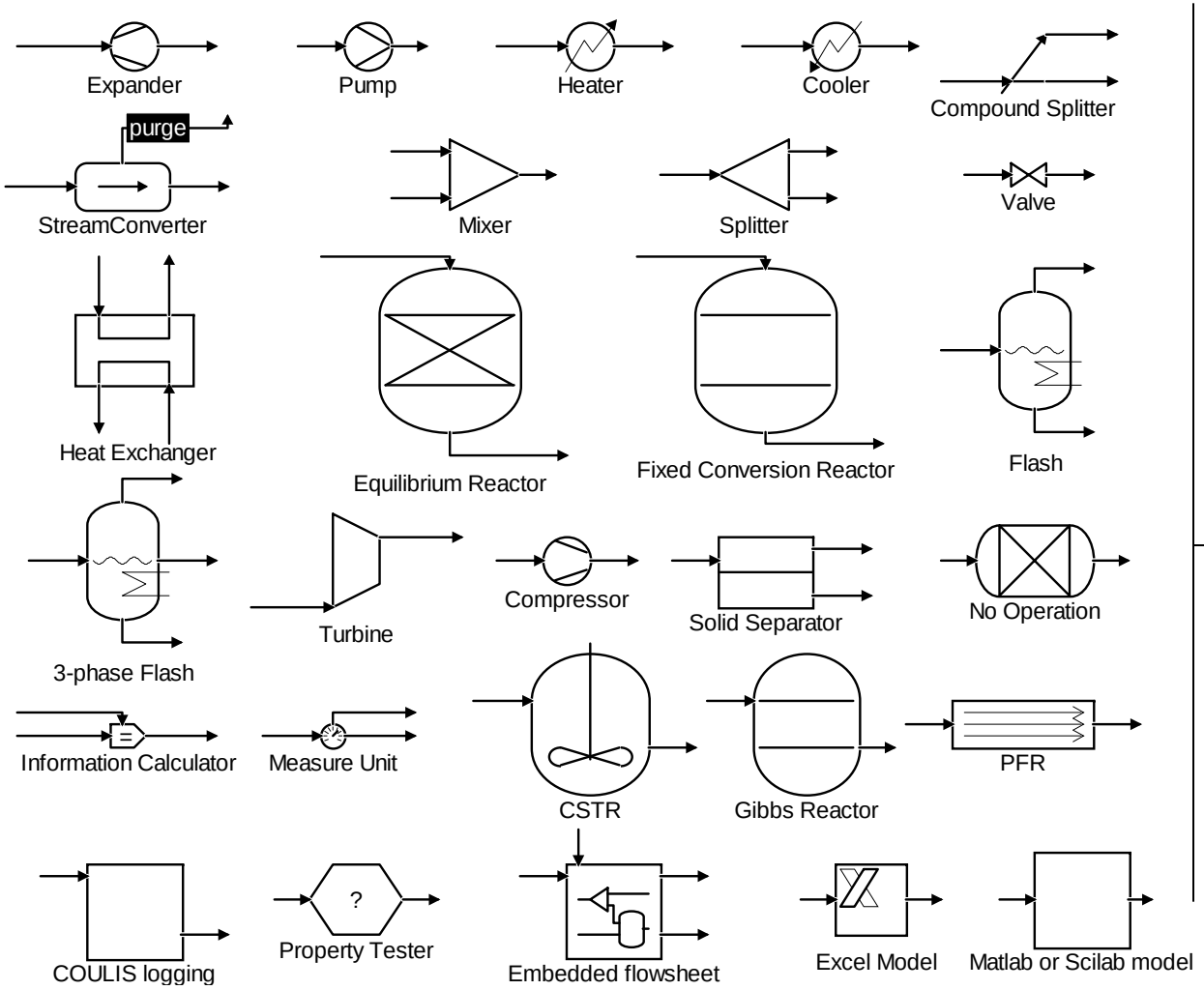
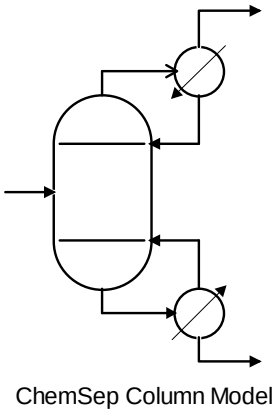
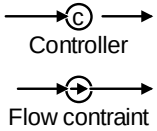
COUSCOUS: Simple unit operations









- 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_compliancy.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:

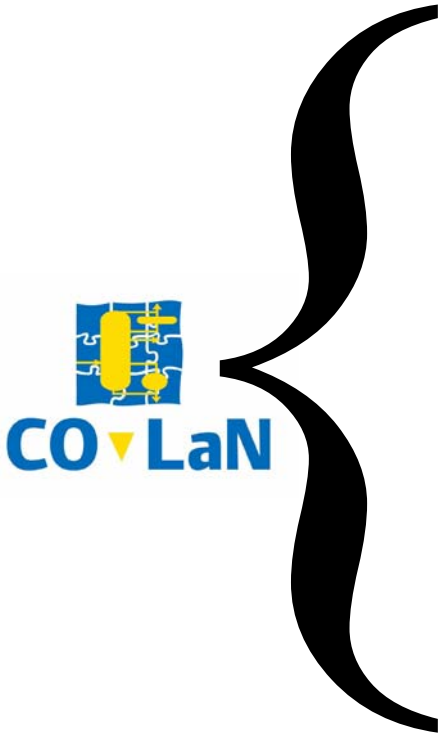
- physical property package implementations
- unit operation implementations
- support for both of these in major simulation engines
- restricted to COM on Windows

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
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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

Simulis
Thermodynamics

TUV/NEL
PPDS

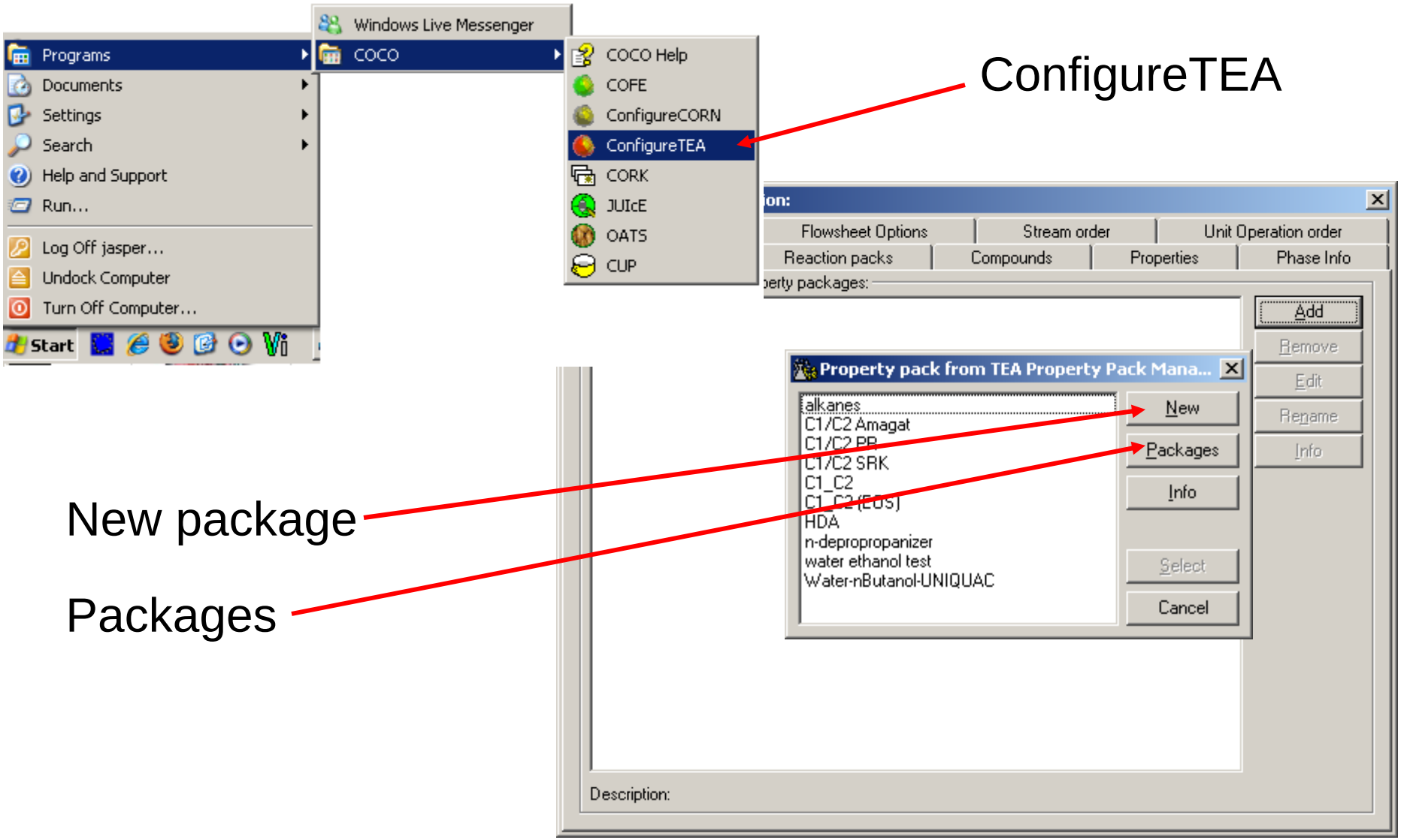
Virtual Materials
Group

CosmoTherm

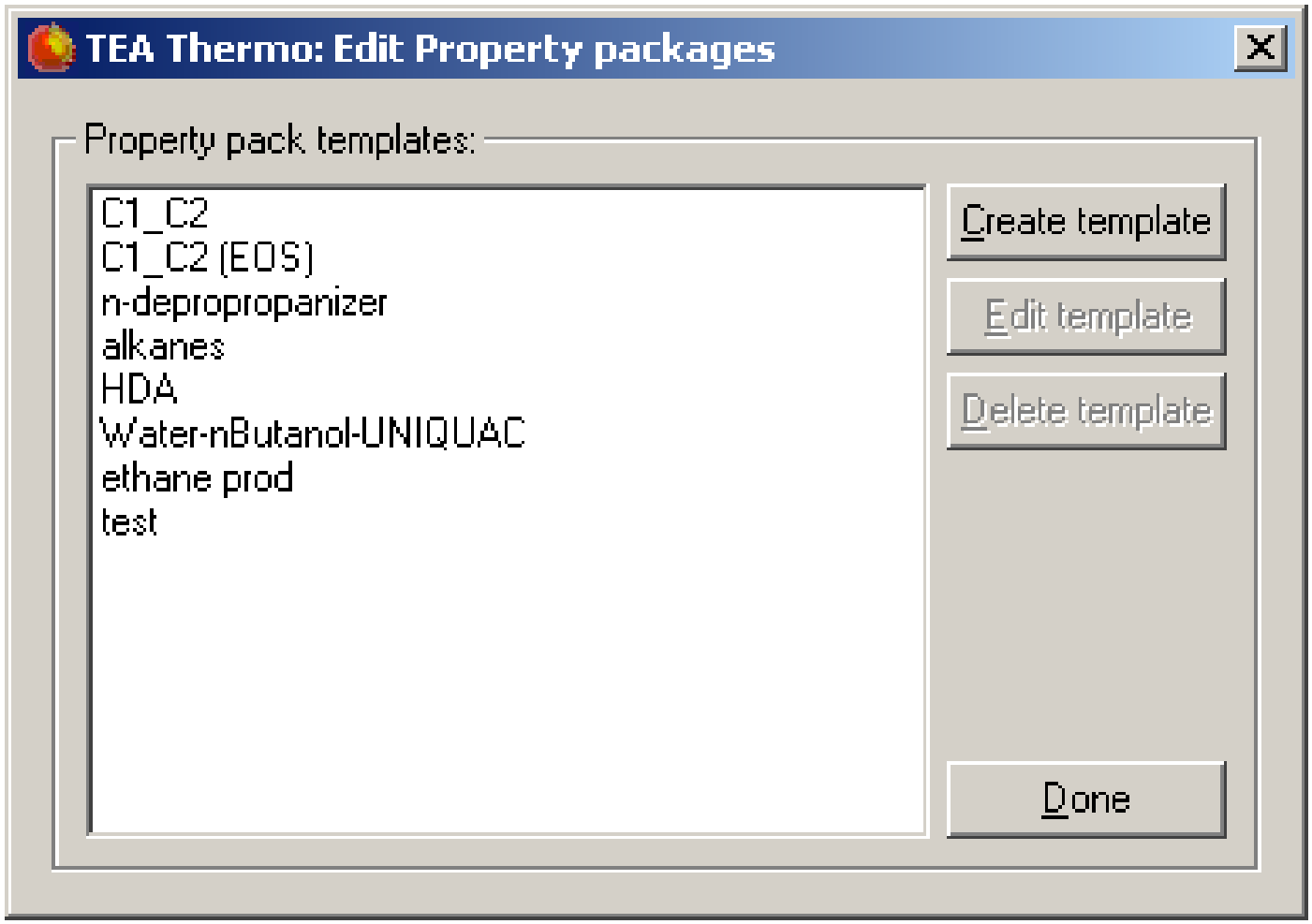
NIST REFPROP

AixCAPE

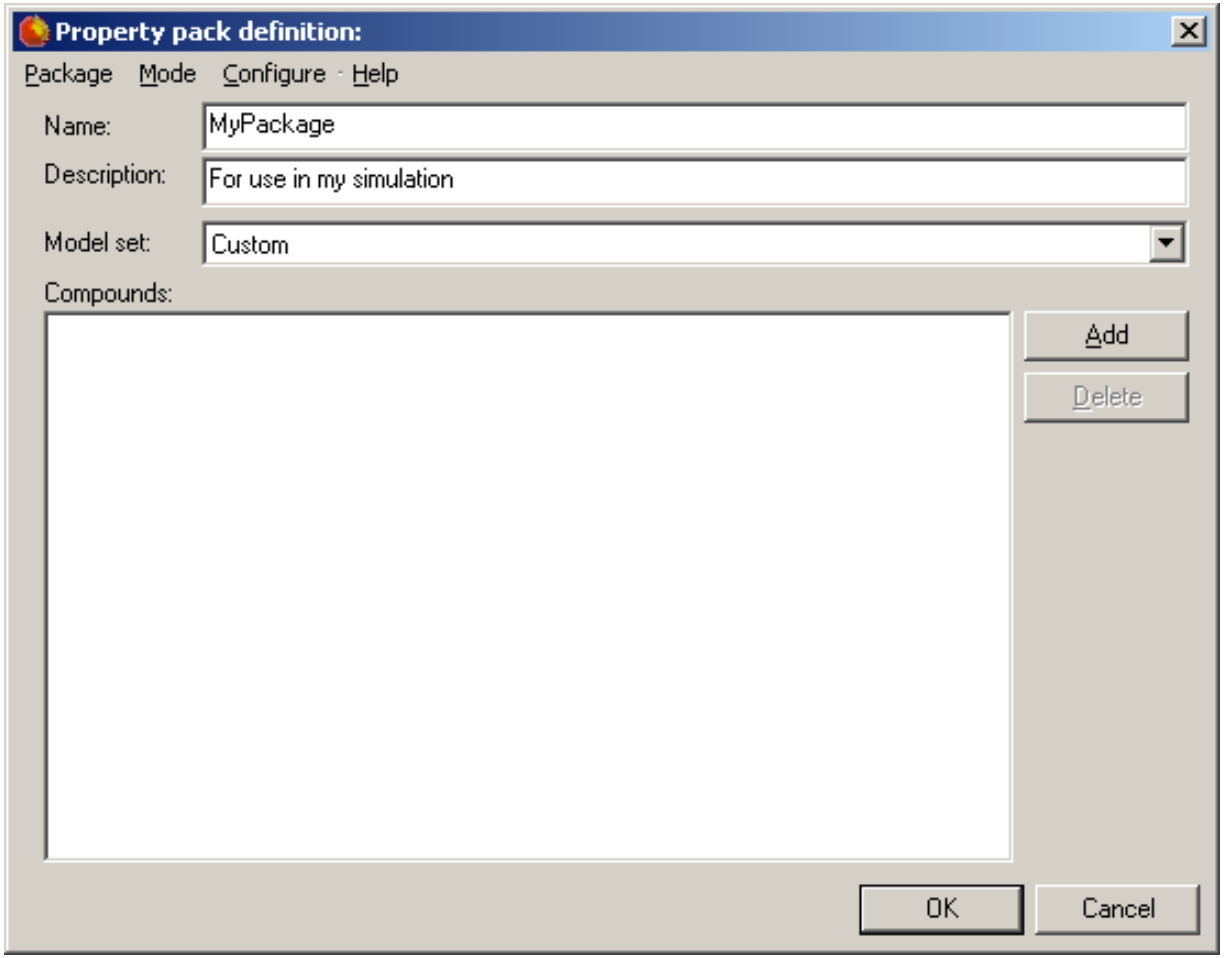
Configuring TEA property packages



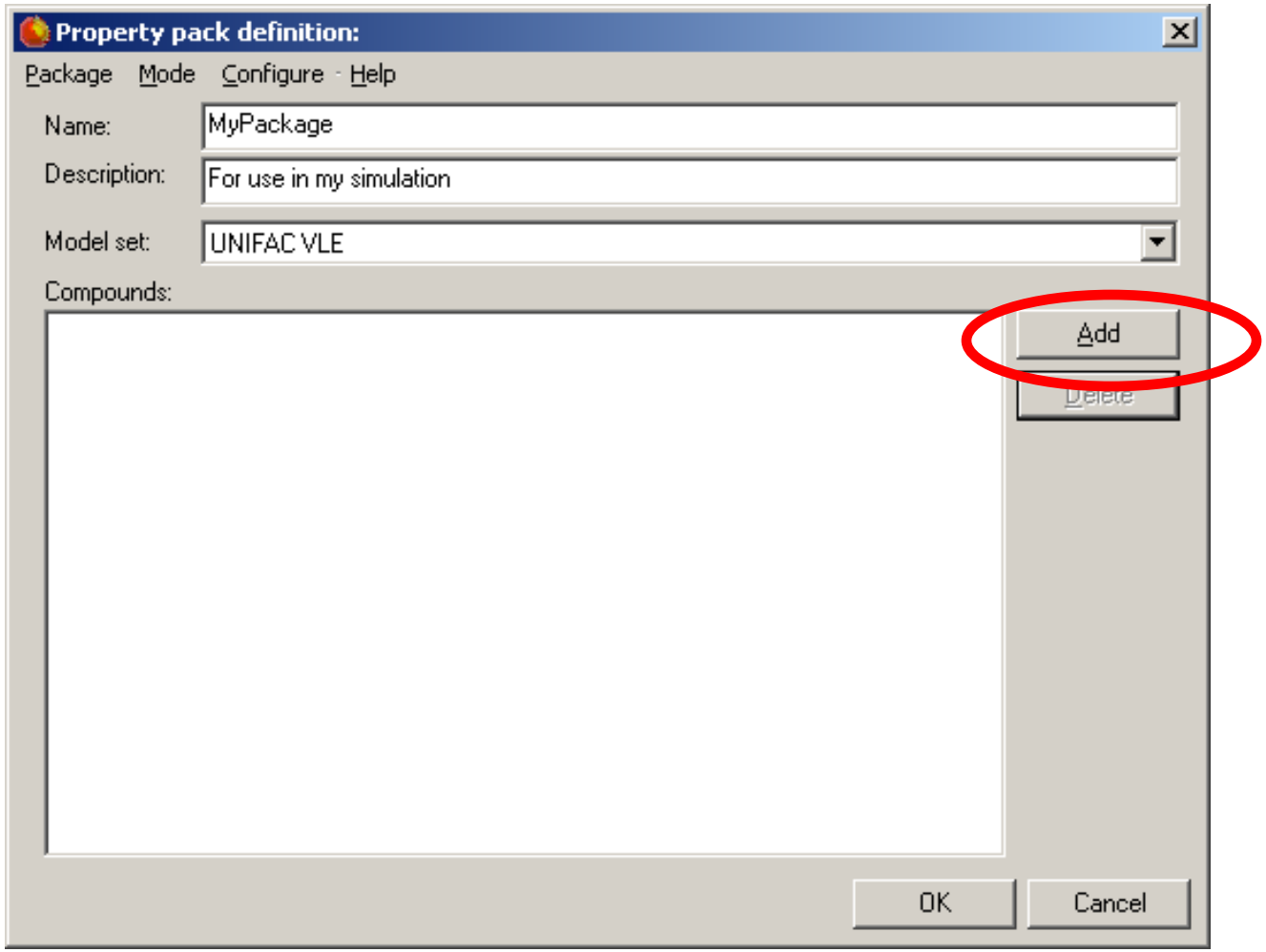
Configuring TEA property packages



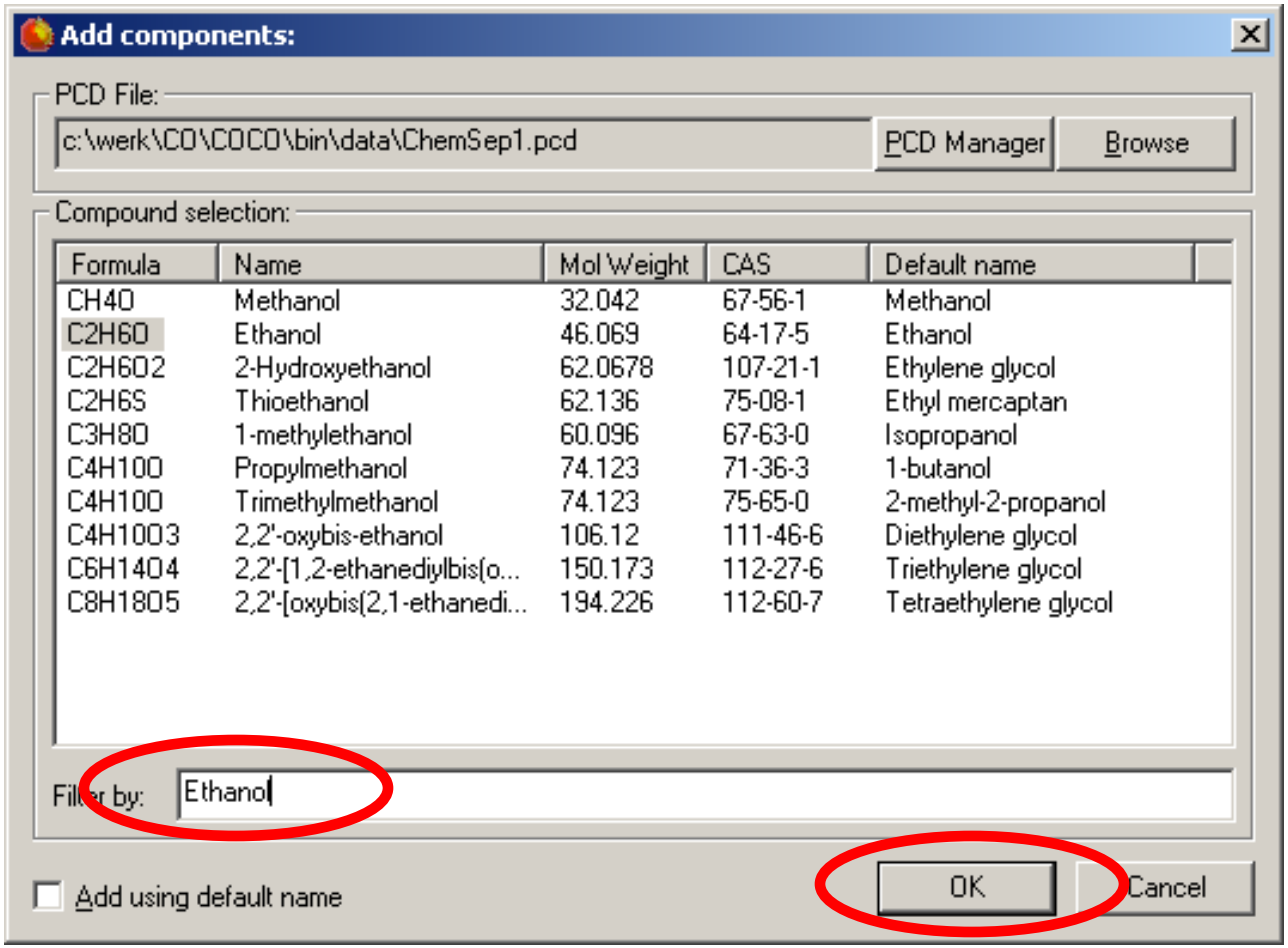
Configuring TEA property packages



Configuring TEA property packages



Configuring TEA property packages



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PCD Files

- PCD = **P**ure **C**omponent **D**ata 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

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ChemSep
Modeling Separation Processes

PCD Files

Benzene

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

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ChemSep
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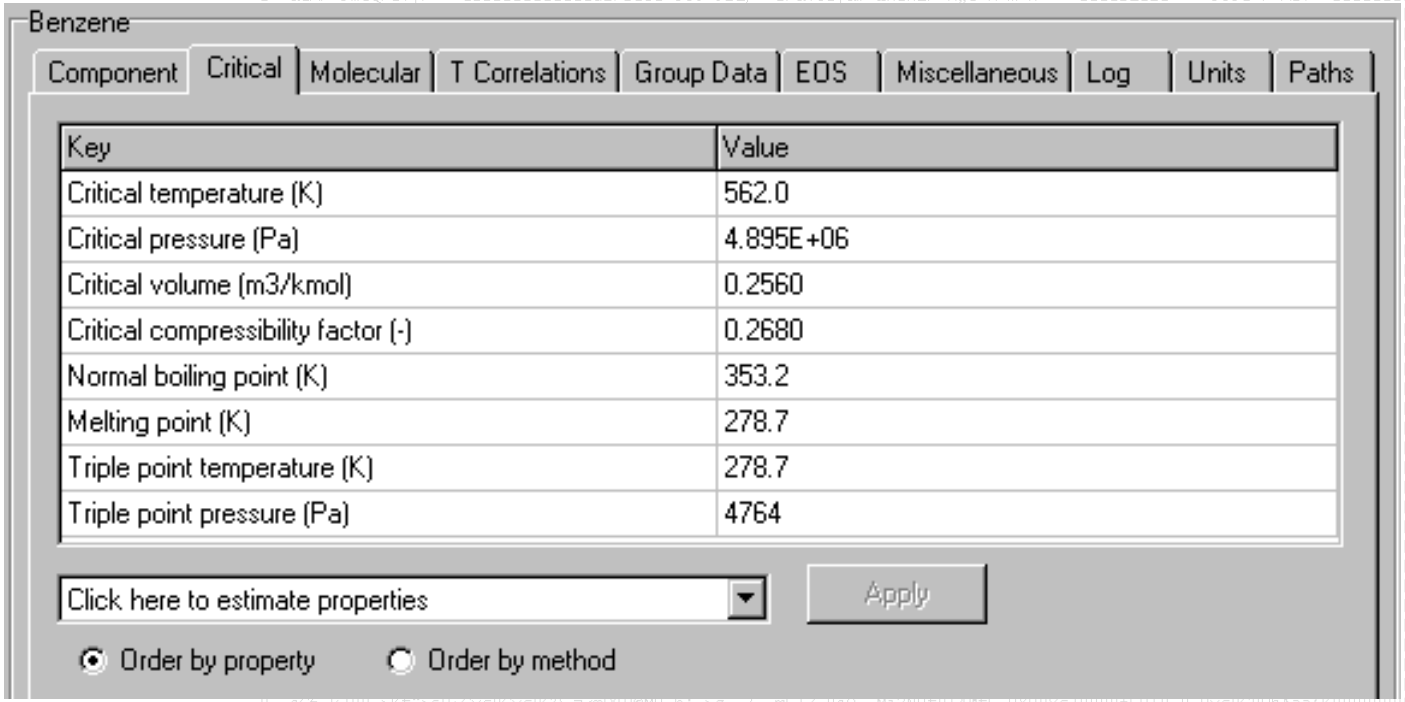
PCD Files



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ChemSep
Modeling Separation Processes

PCD Files

Benzene

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

Key	Value
Liquid molar volume at normal boiling point (m3/kmol)	0.08941
Acentric factor (-)	0.2090
Radius of gyration (m)	3.004E-10
Solubility parameter (sqrt(J/m3))	1.870E+04
Dipole moment (Coulomb.m)	0.0000
Van der Waals volume (m3/kmol)	0.04840
Van der Waals area (m2/kmol)	6.000E+08
IG heat of formation (J/kmol)	8.288E+07
IG Gibbs energy of formation (J/kmol)	1.296E+08
IG 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)	-3.136E+09

Apply

Order by property Order by method

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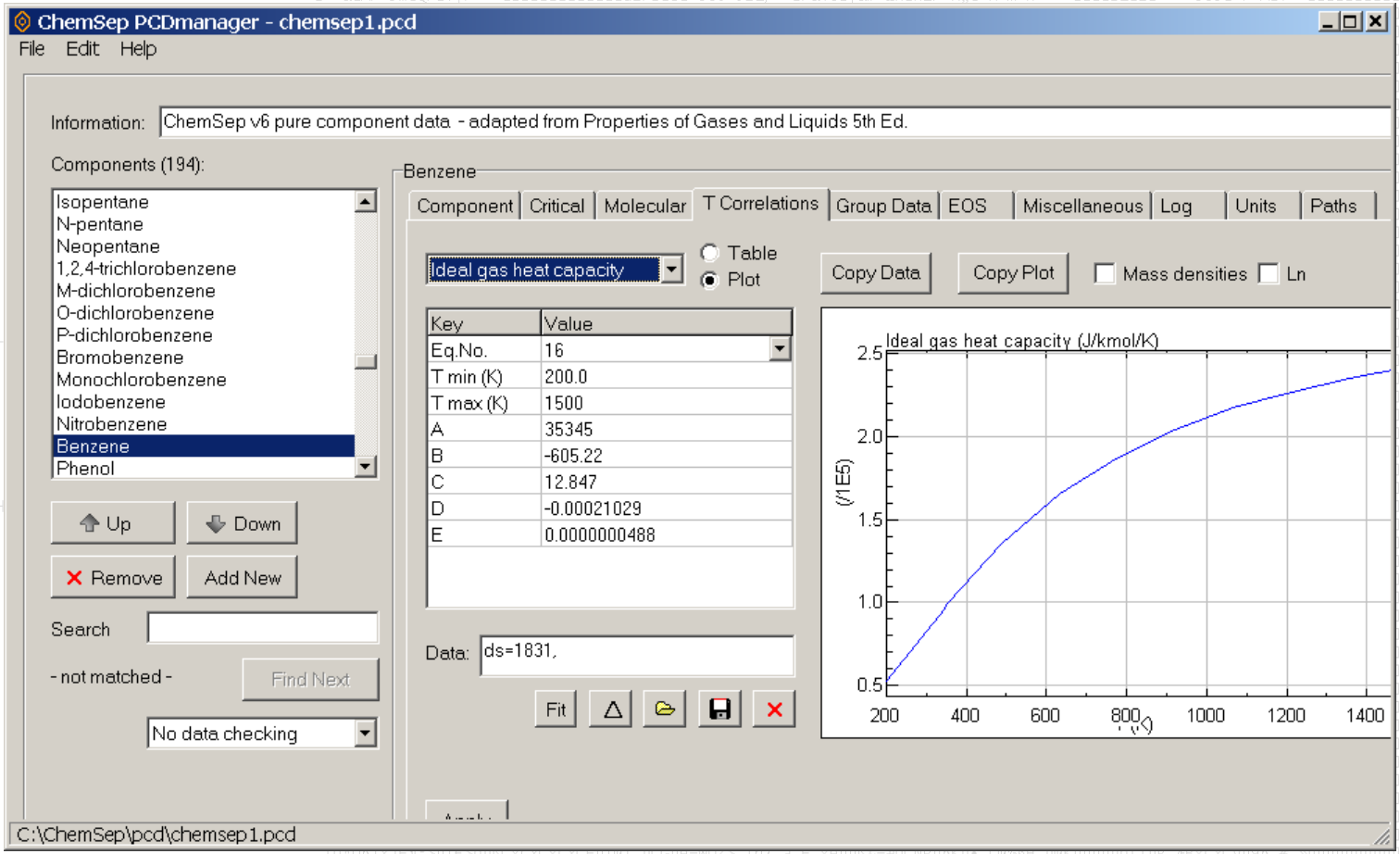
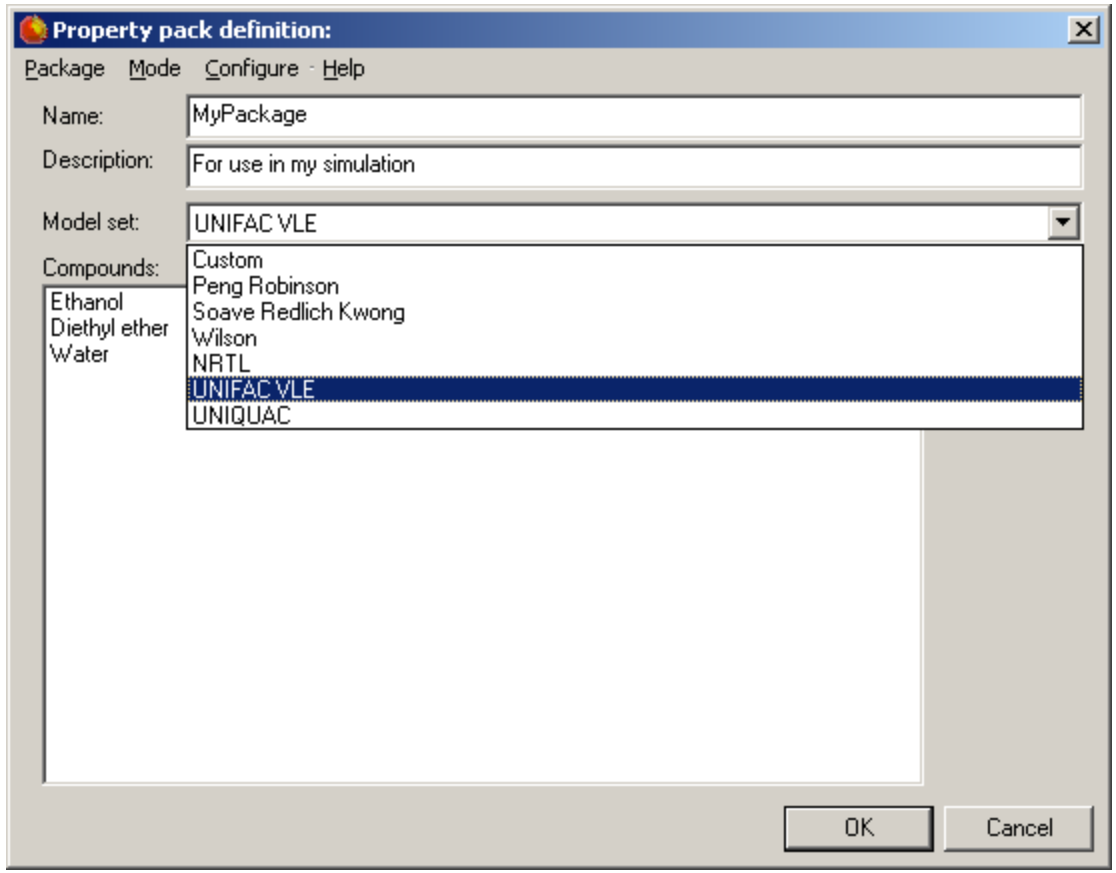
ChemSep
Modeling Separation Processes

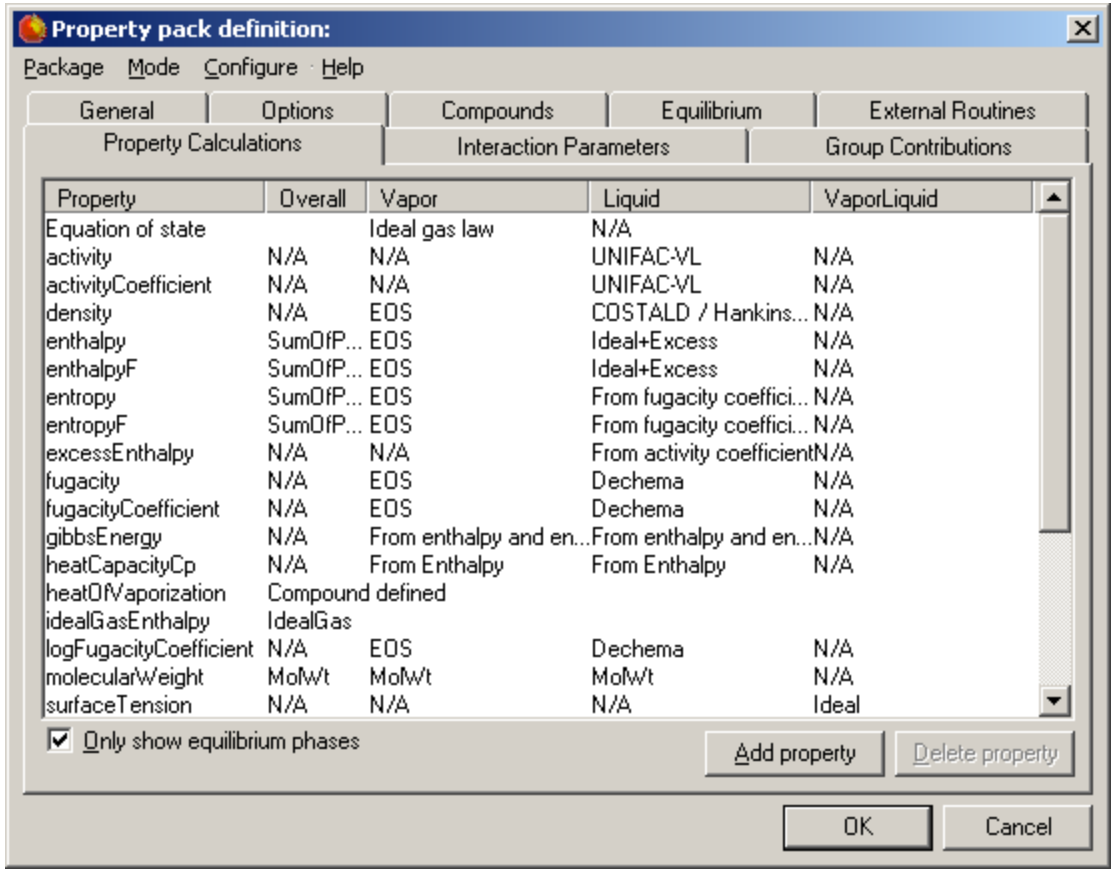
PCD Files



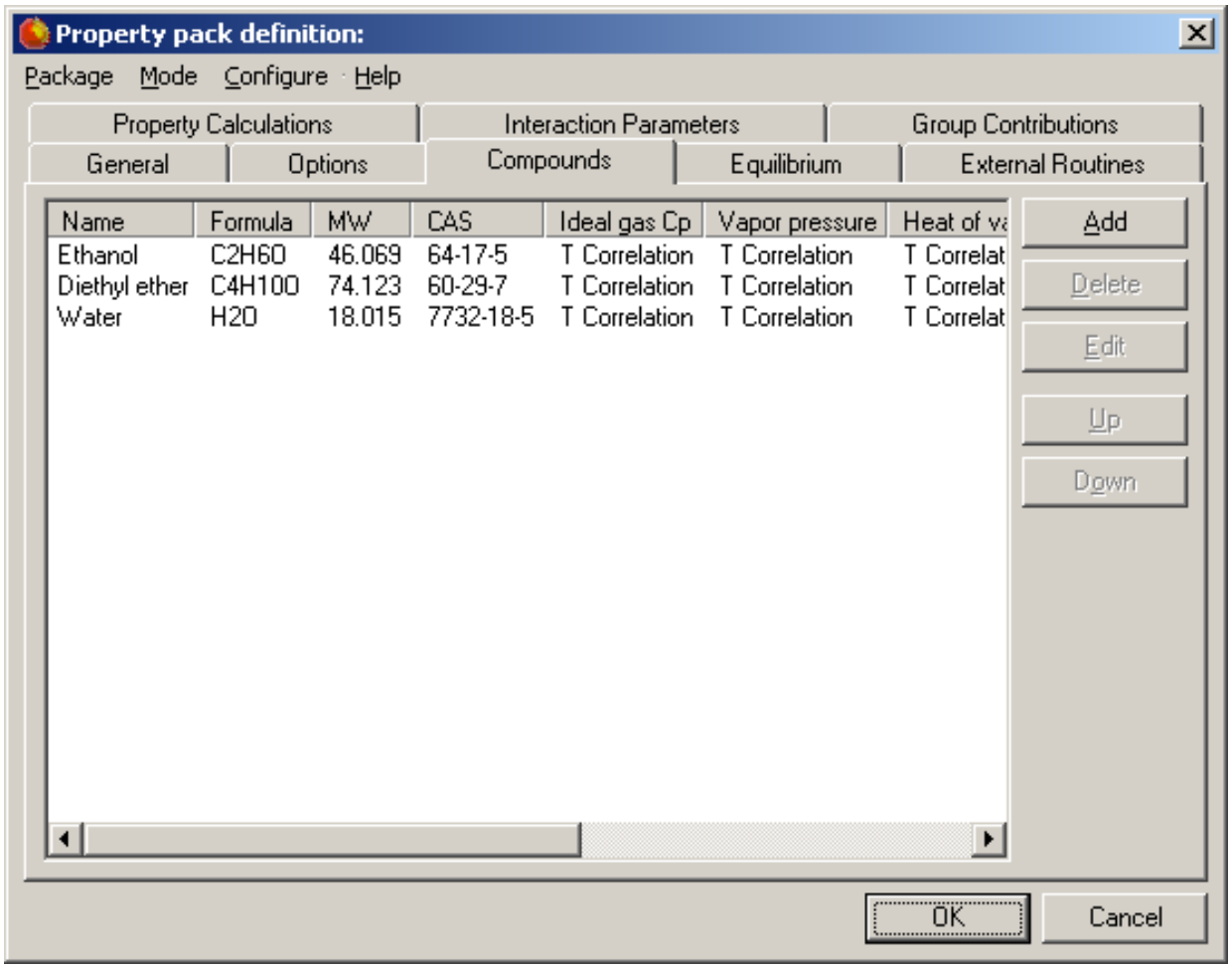
Configuring TEA property packages



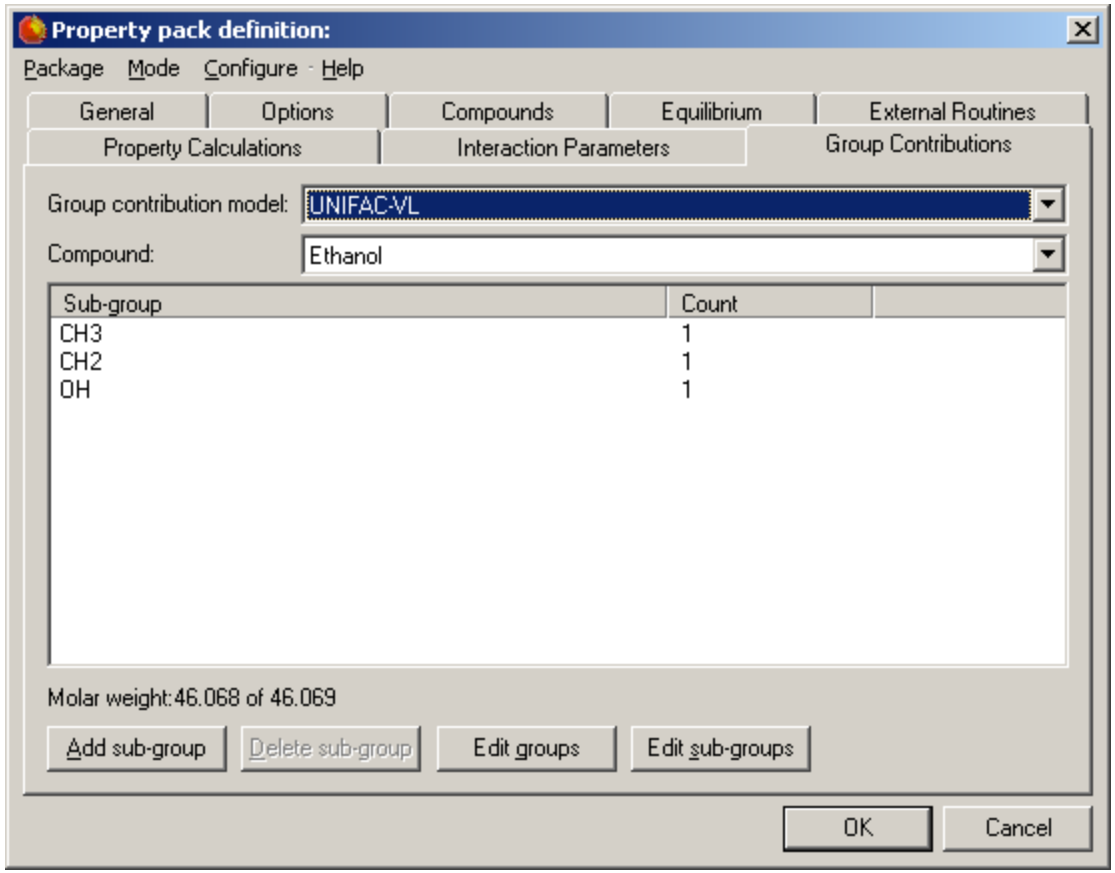
Configuring TEA property packages



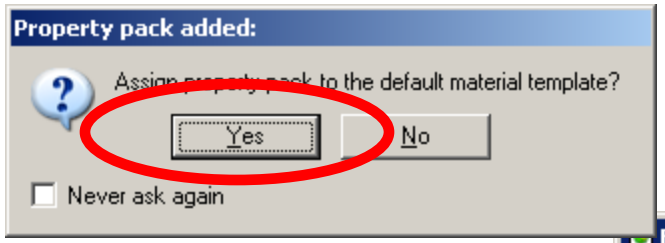
Configuring TEA property packages

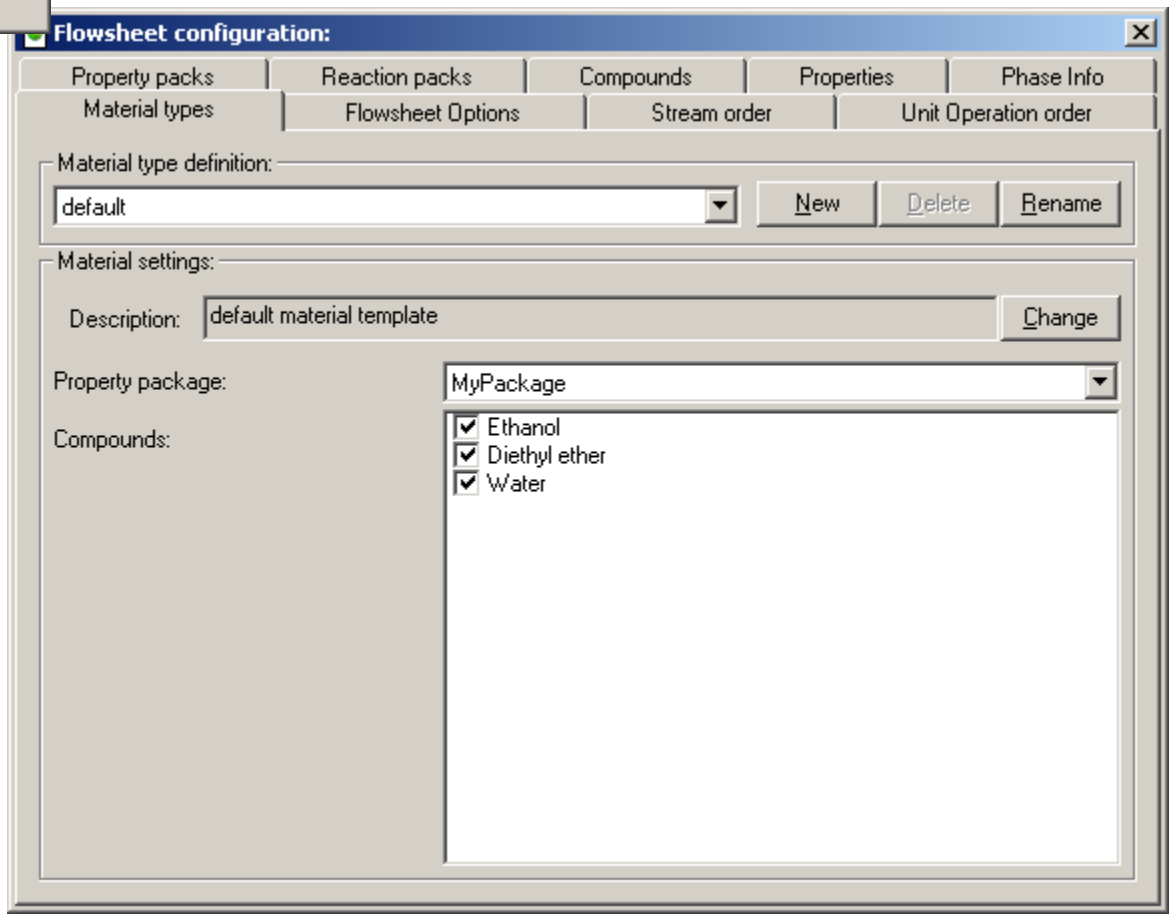


Configuring TEA property packages



Finally:


Property pack added:
Assign property pack to the default material template?
Yes
No
Never ask again


Flowsheet configuration:
Property packs
Reaction packs
Compounds
Properties
Phase Info
Material types
Flowsheet Options
Stream order
Unit Operation order
Material type definition:
default
New
Delete
Rename
Material settings:
Description:
default material template
Change
Property package:
MyPackage
Compounds:
Ethanol
Diethyl ether
Water

Presentation outline

- Introduction to COCO
- What is CAPE-OPEN?
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- **Setting up flowsheets with COFE**
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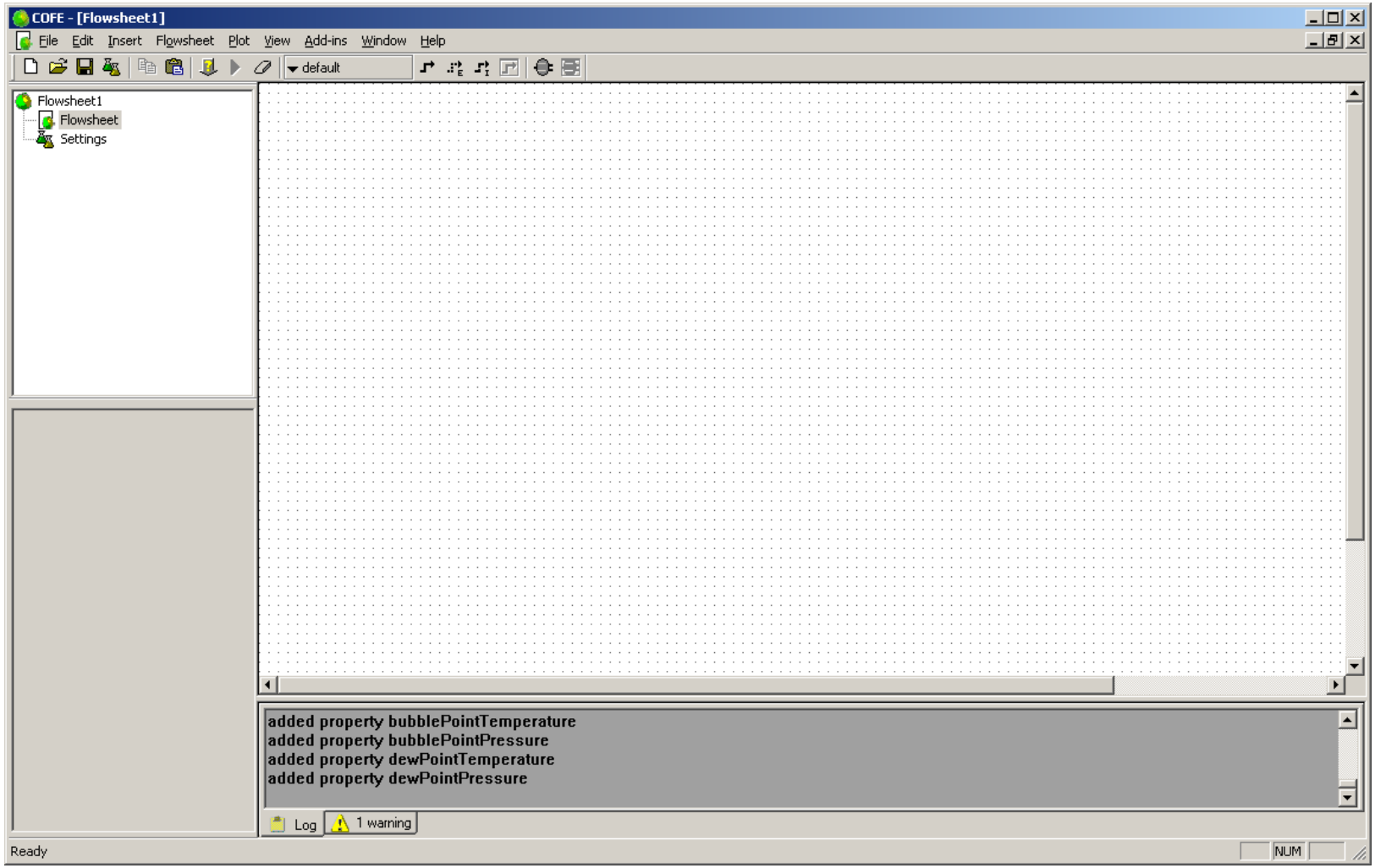
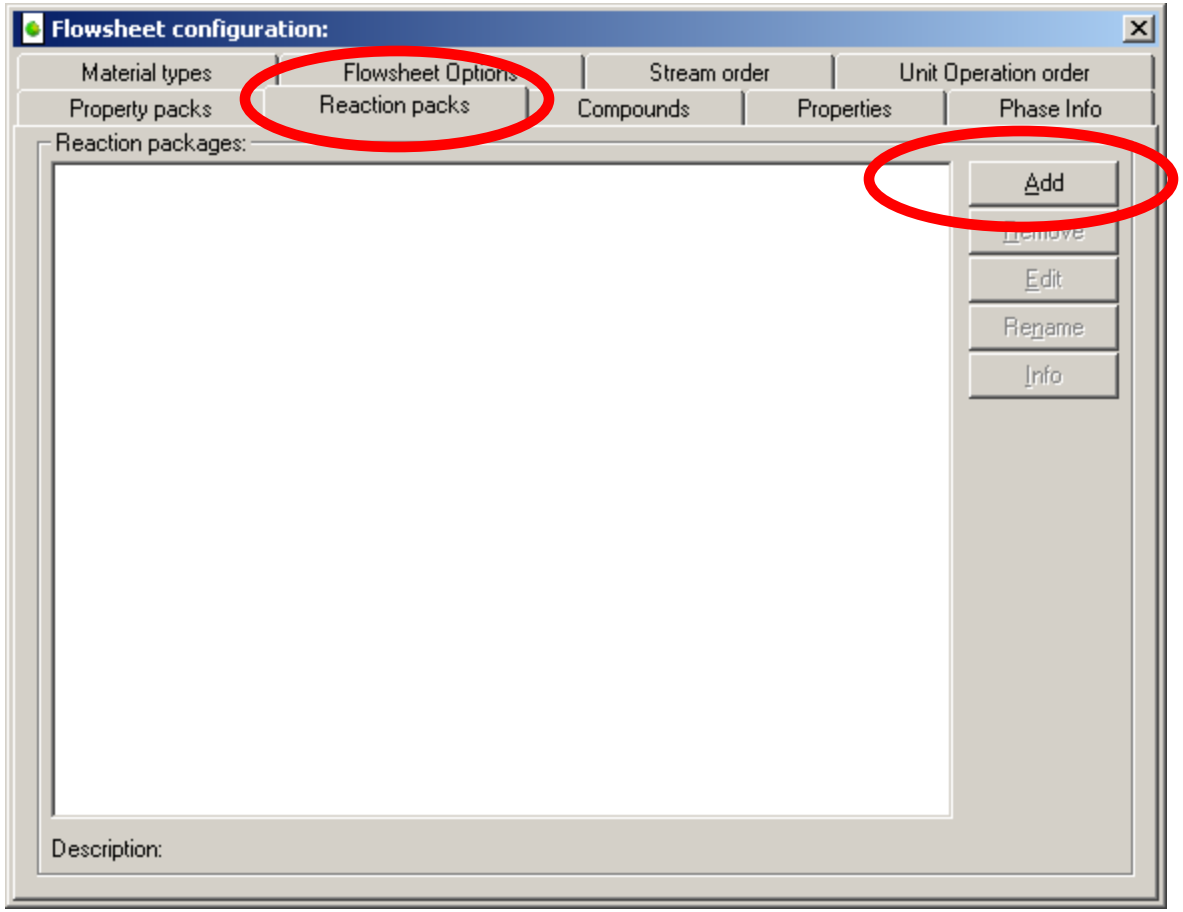
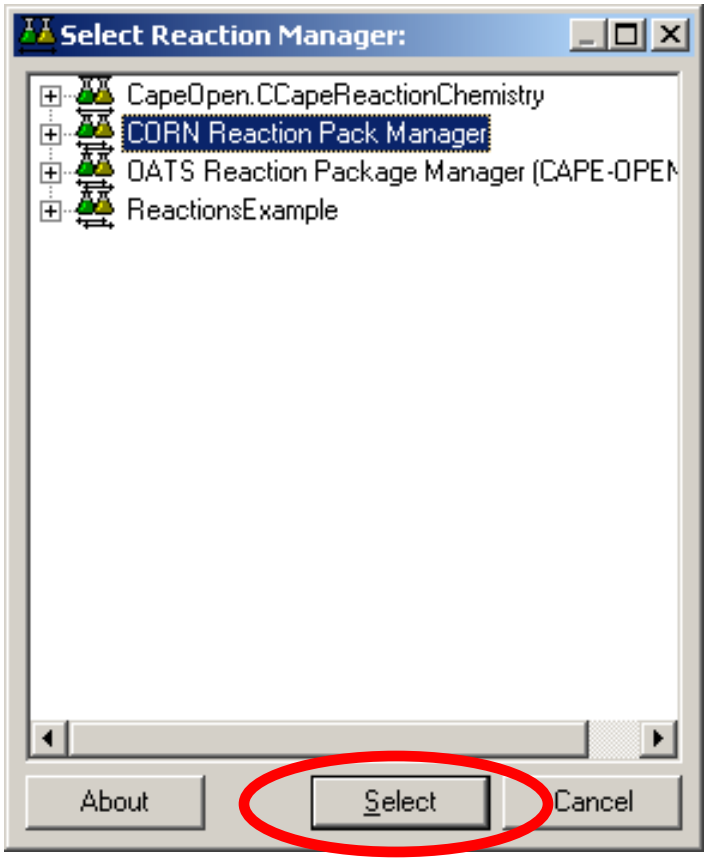
Empty COFE document



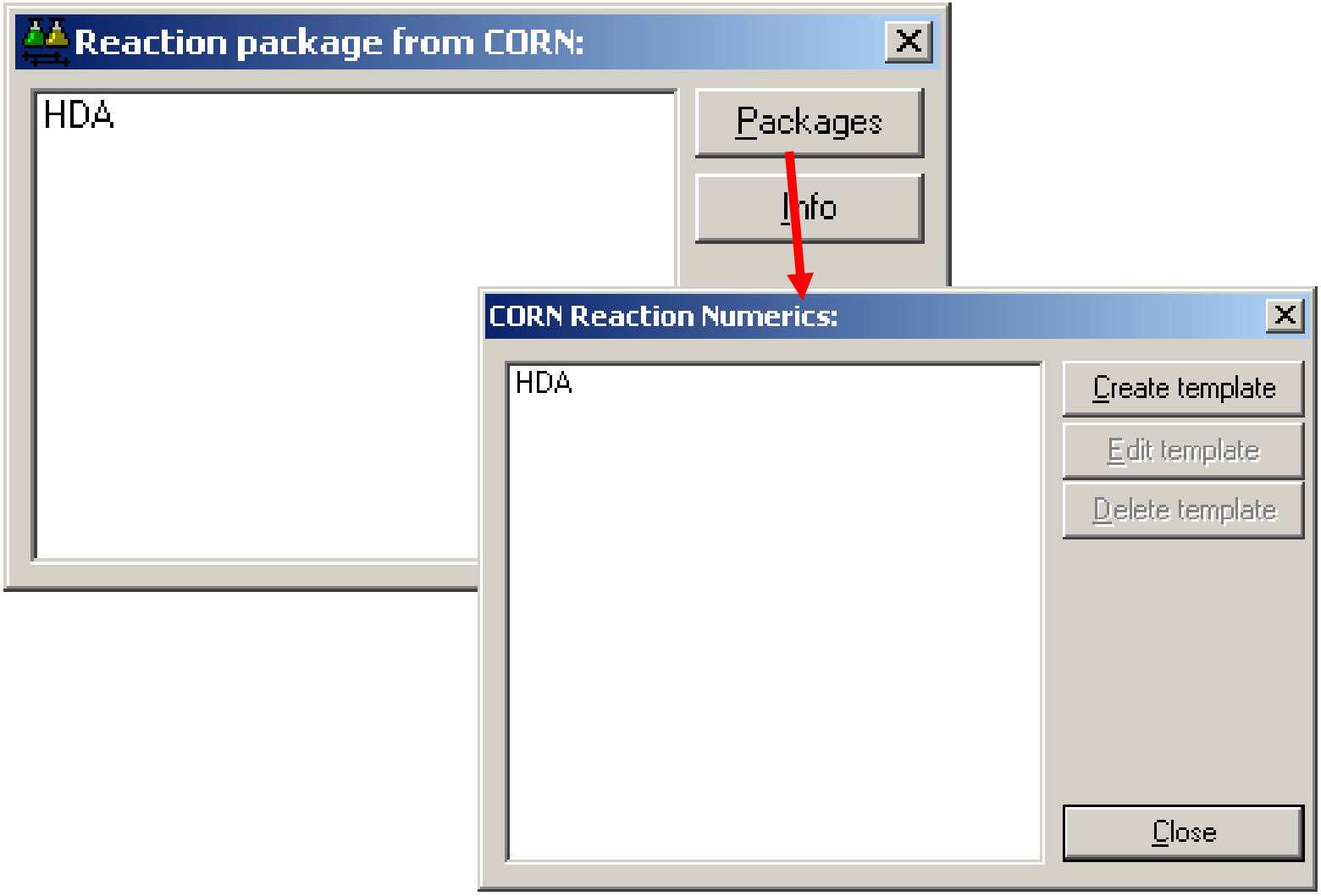
Setting up reactions



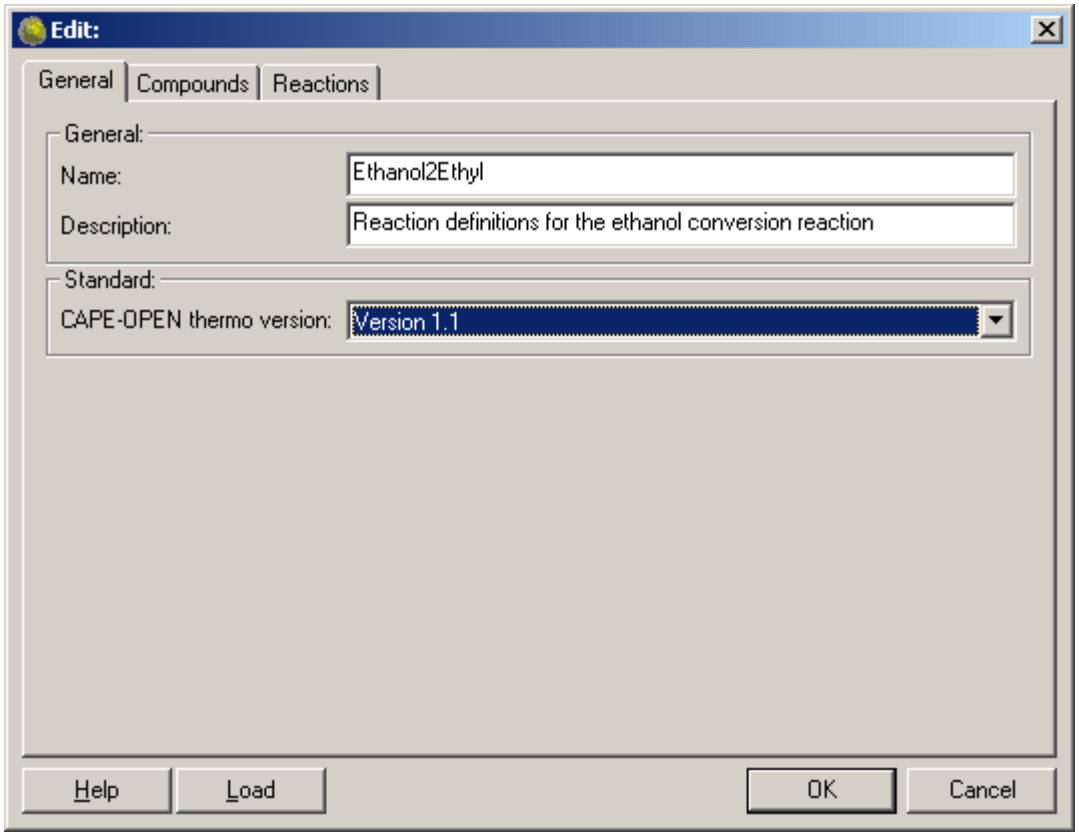
CORN: CAPE-OPEN Reaction Numerics



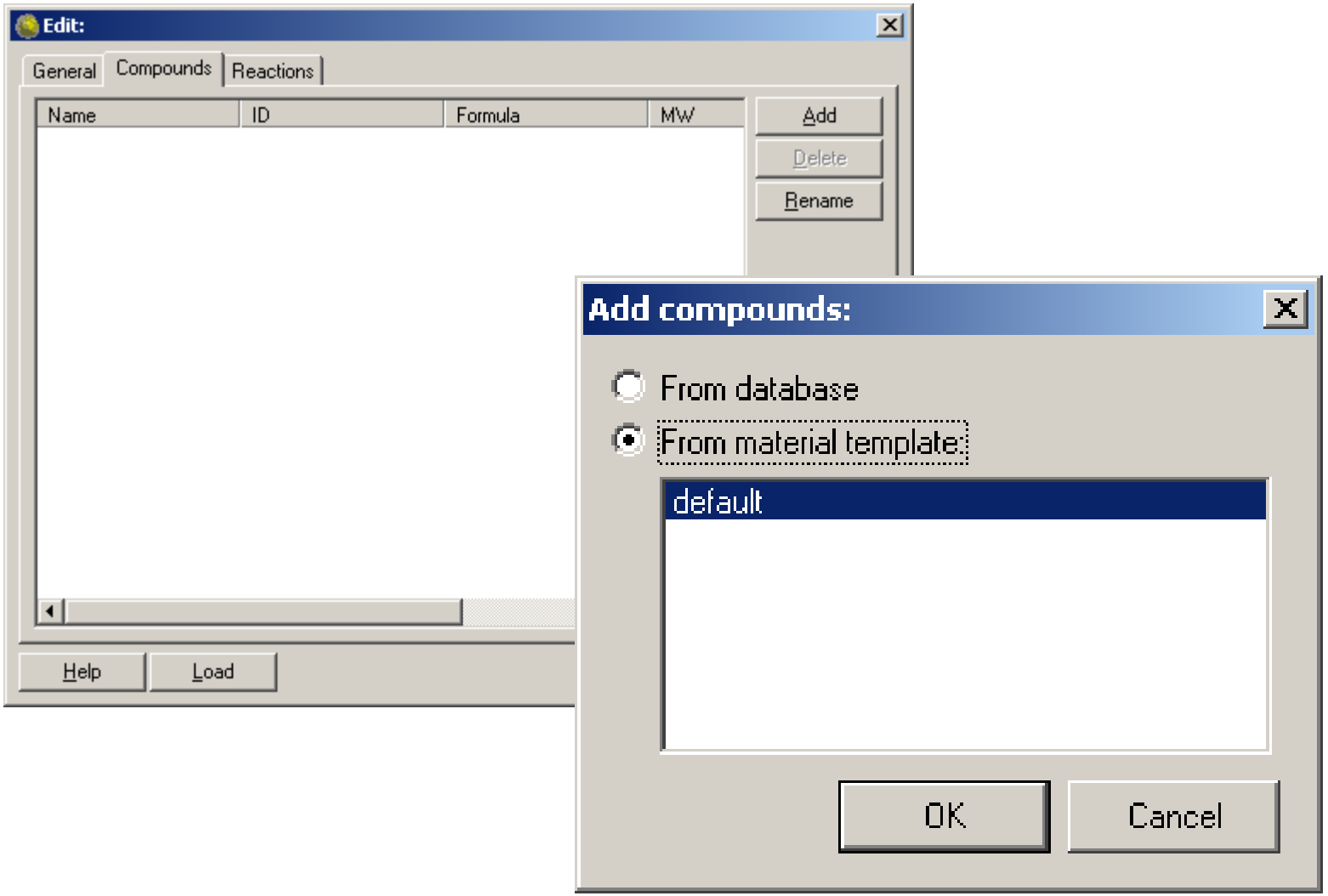
Setting up CORN



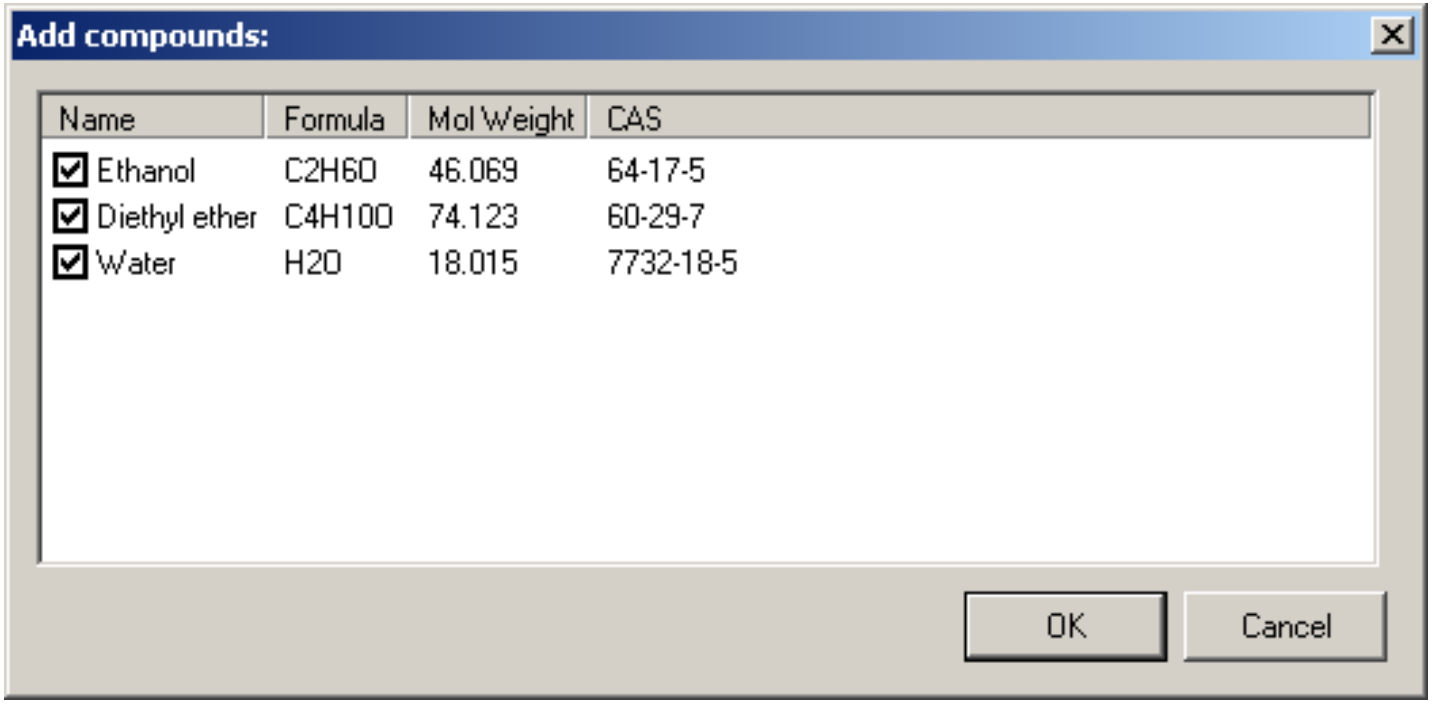
Editing a reaction package (1/4):



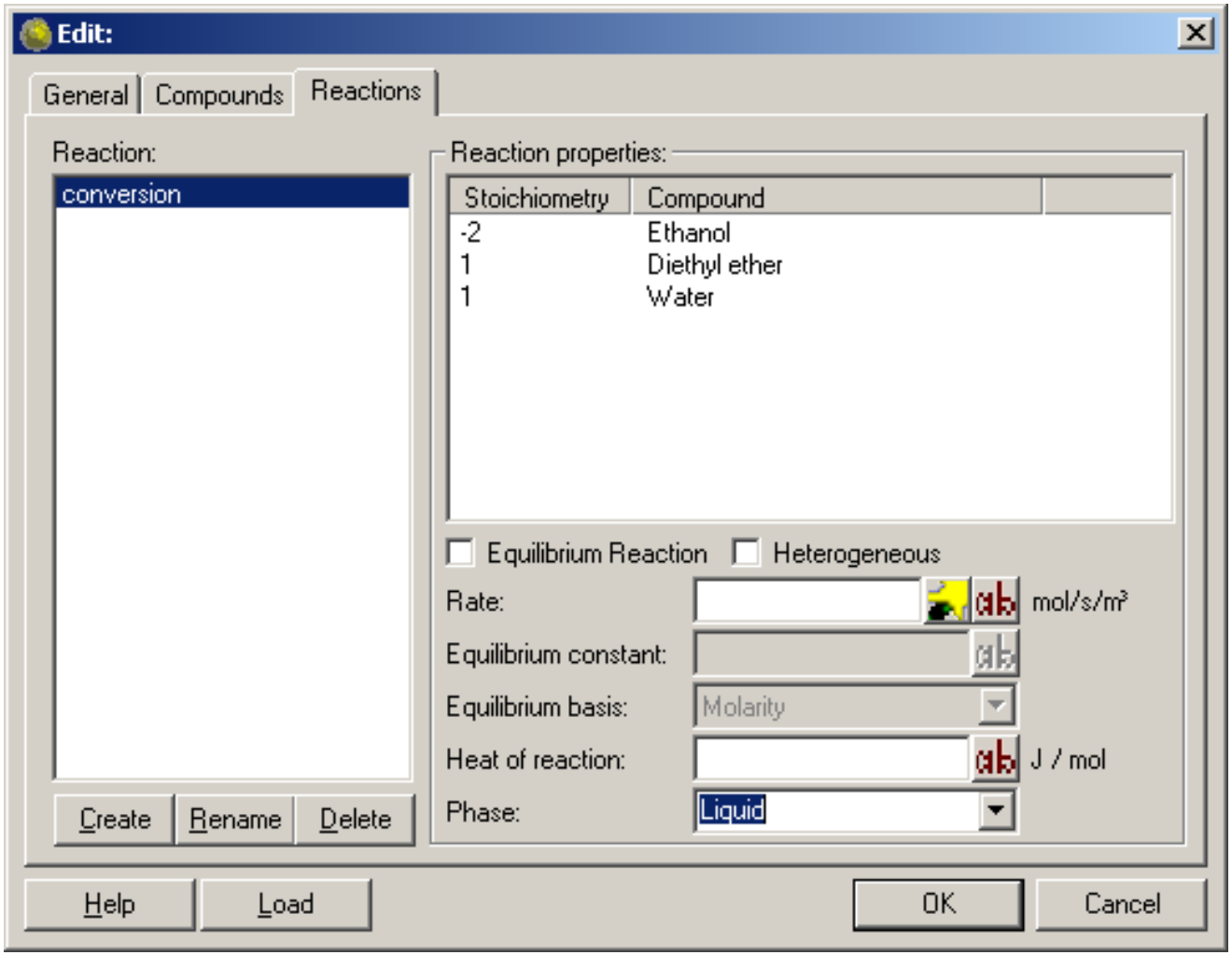
Editing a reaction package (2/4):



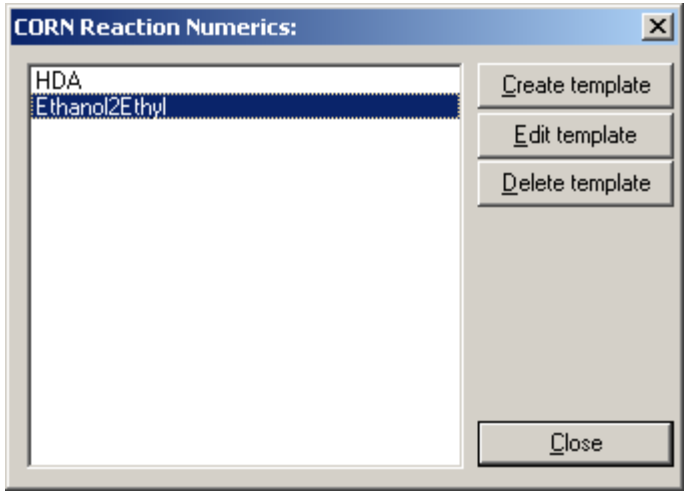
Editing a reaction package (3/4):

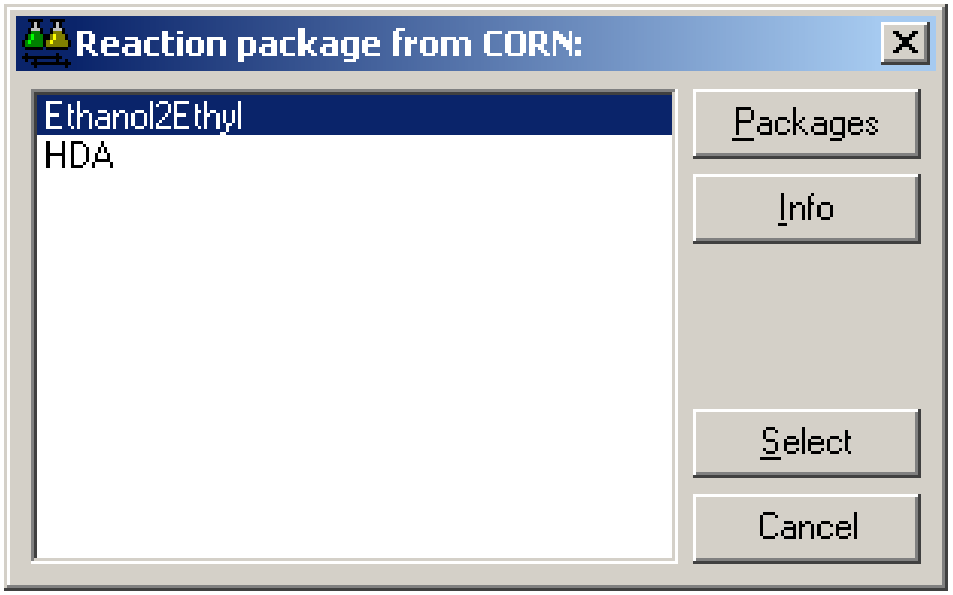


Editing a reaction package (4/4):

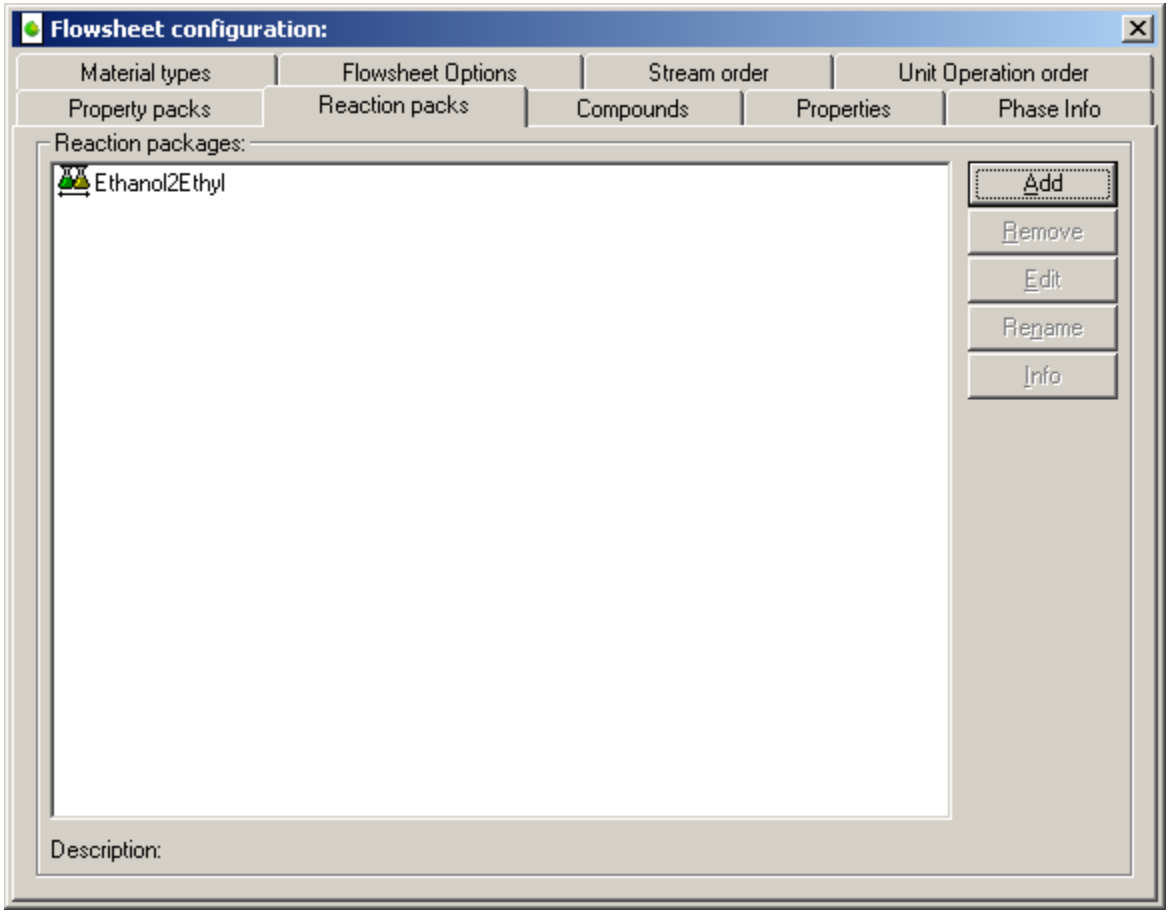


Add it to the simulation

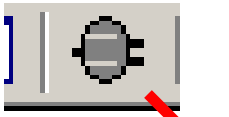


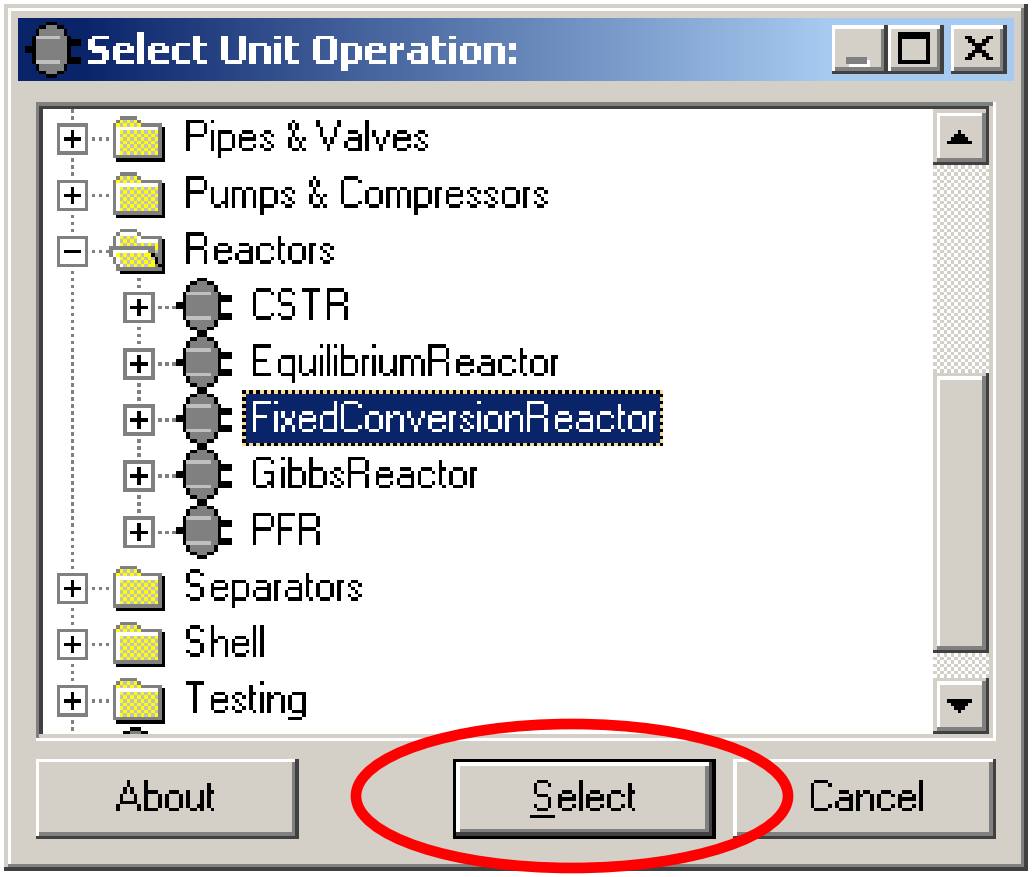


We have a reaction package:



Inserting our reactor:





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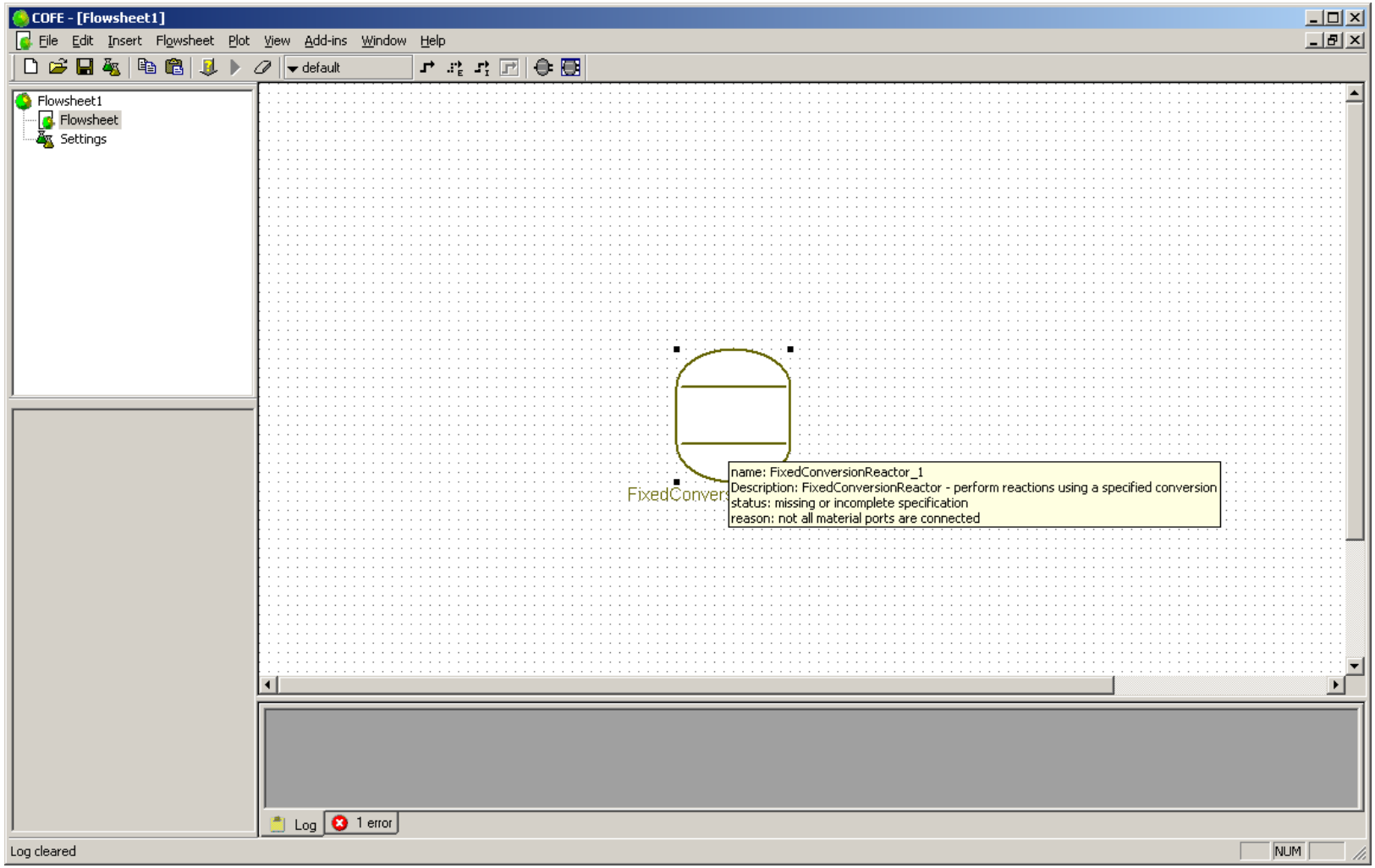
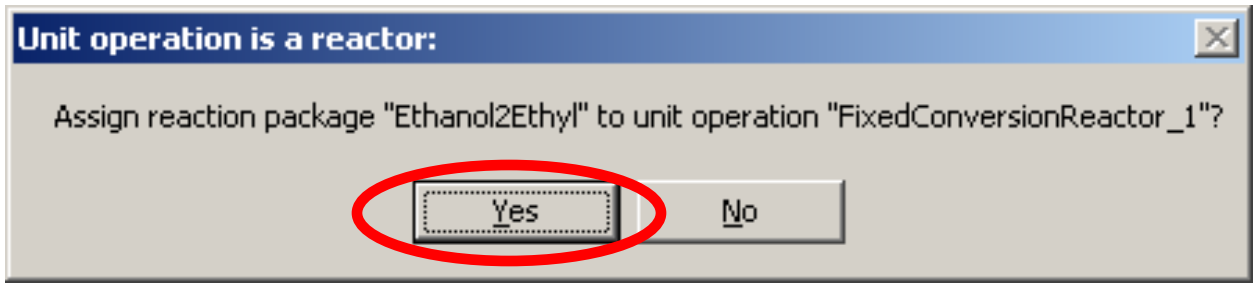
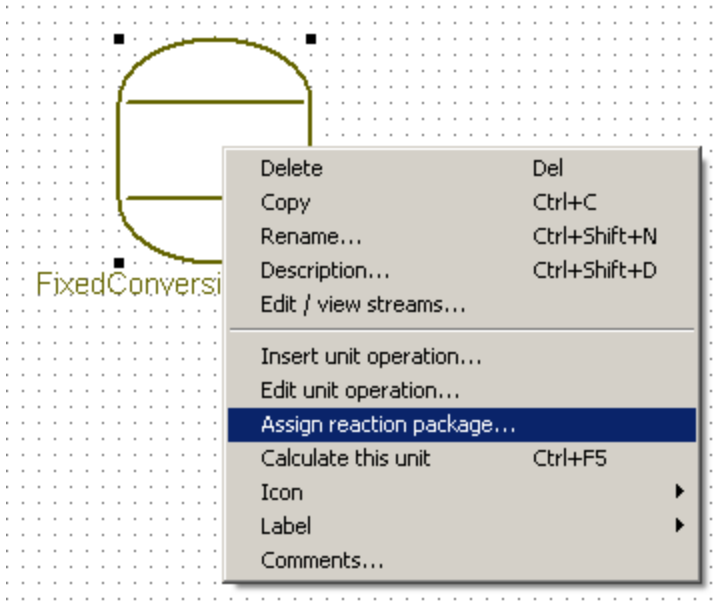
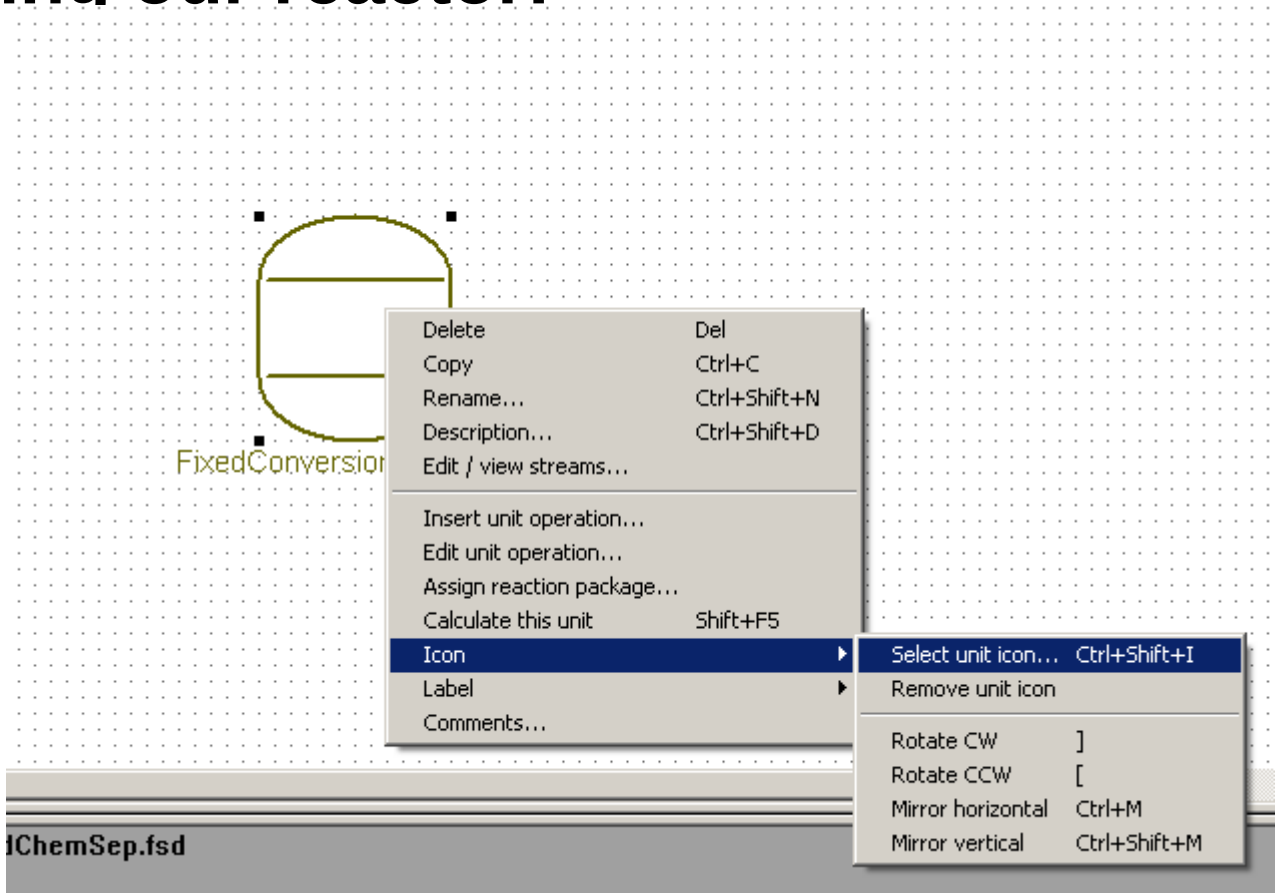


Inserting our reactor:

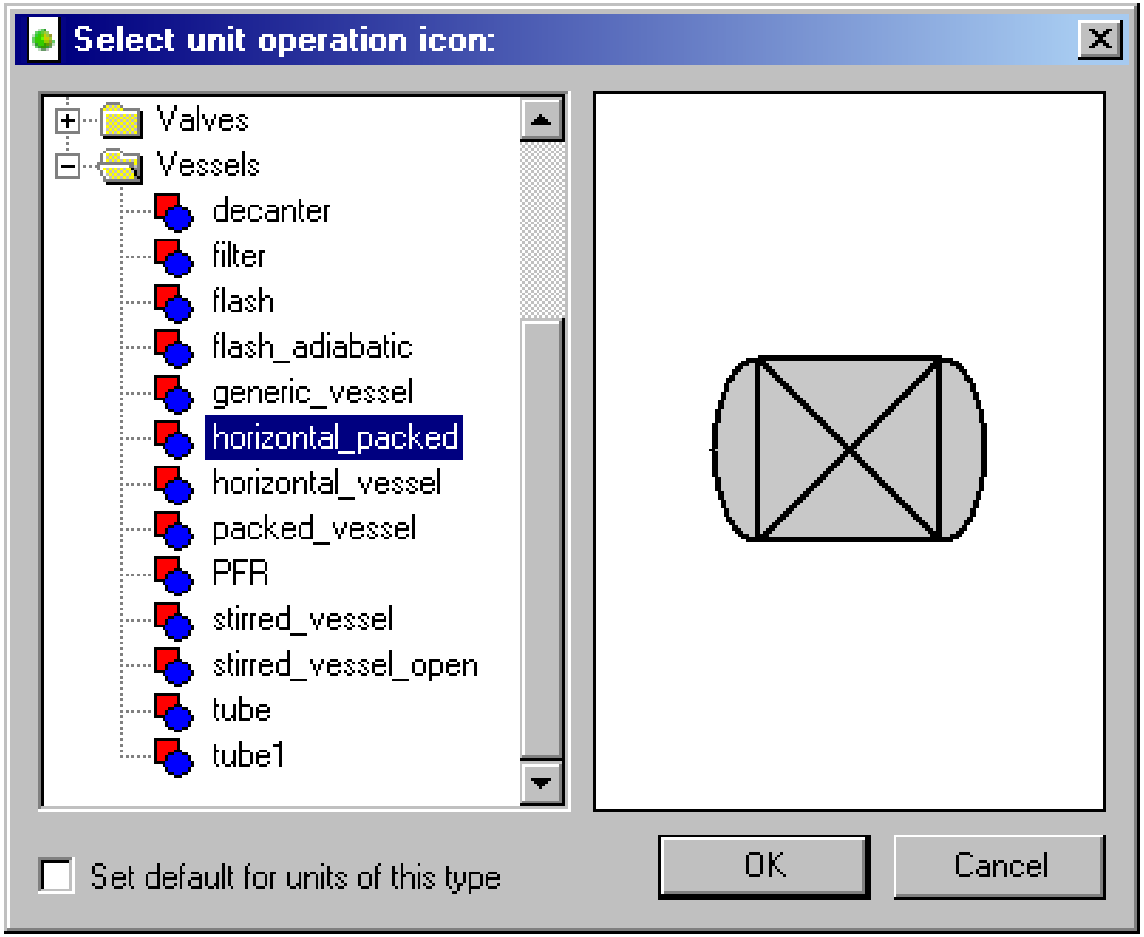




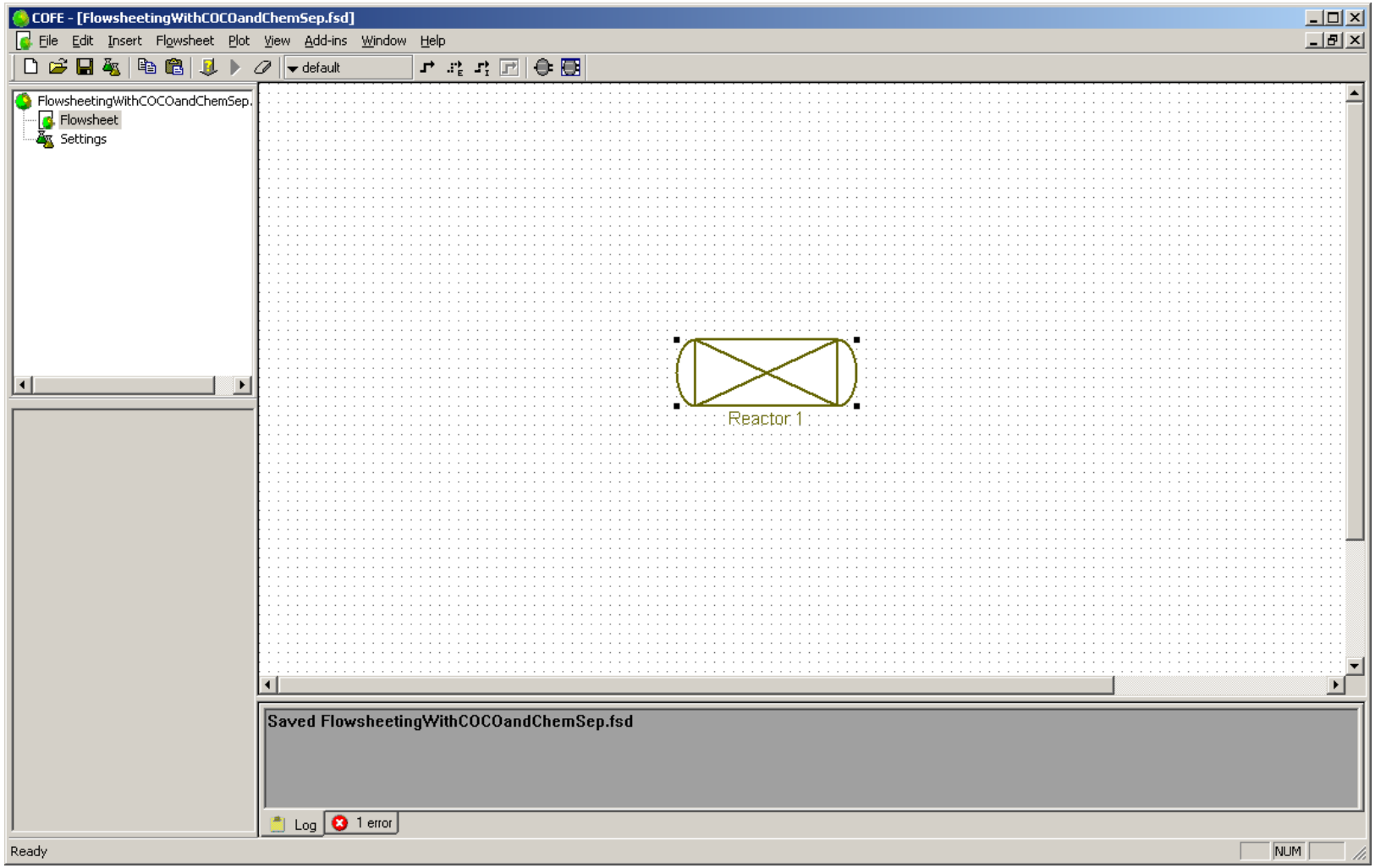
Inserting our reactor:



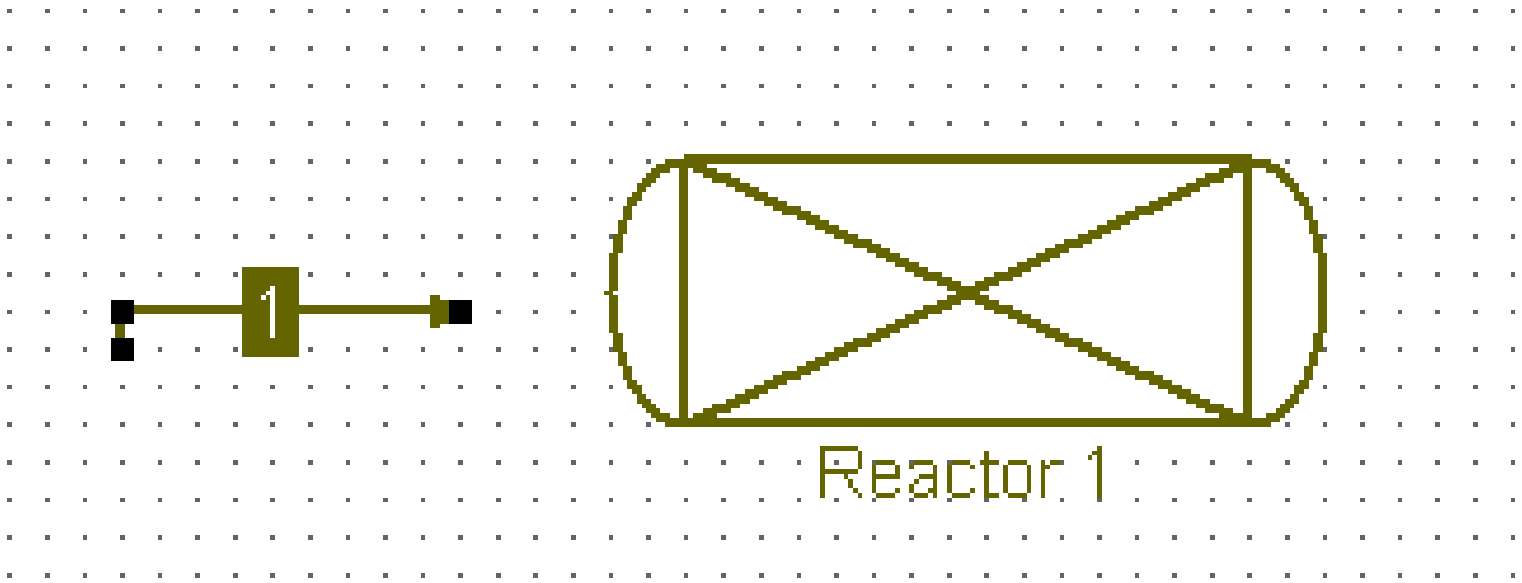
Inserting our reactor:



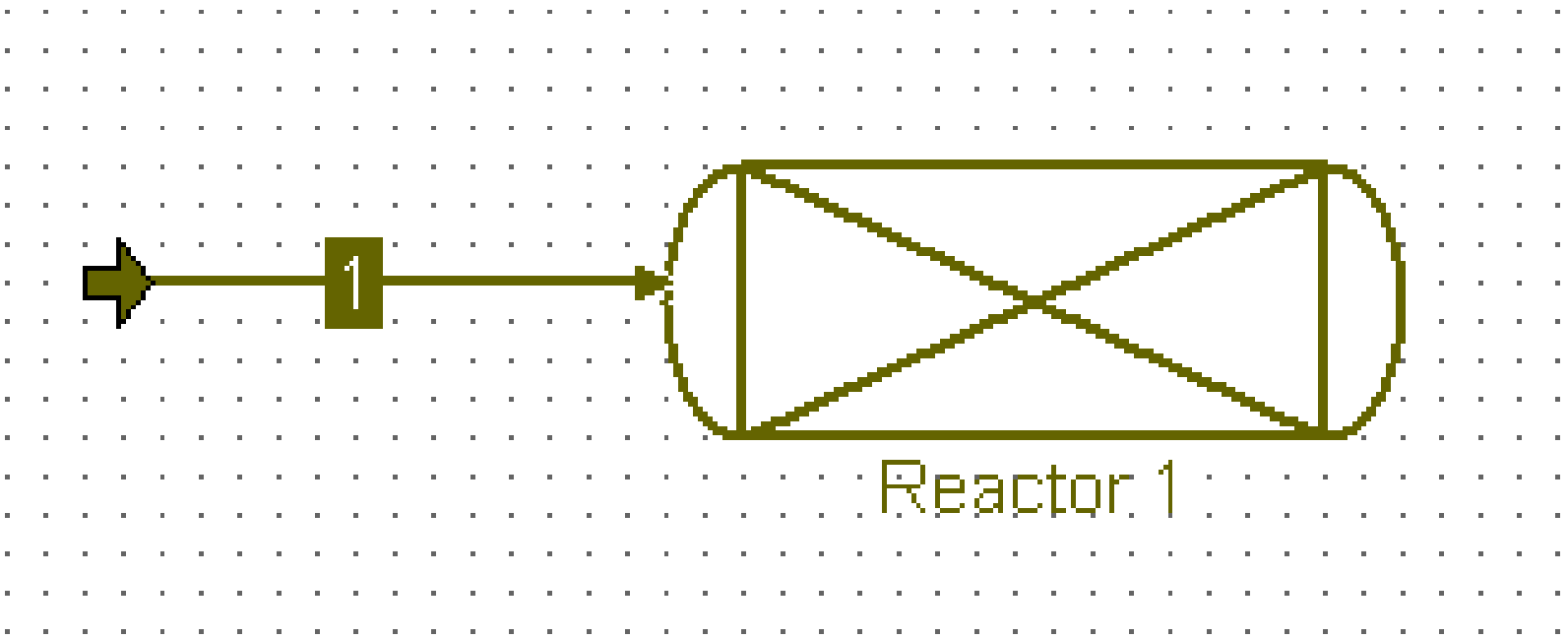
Inserting our reactor:



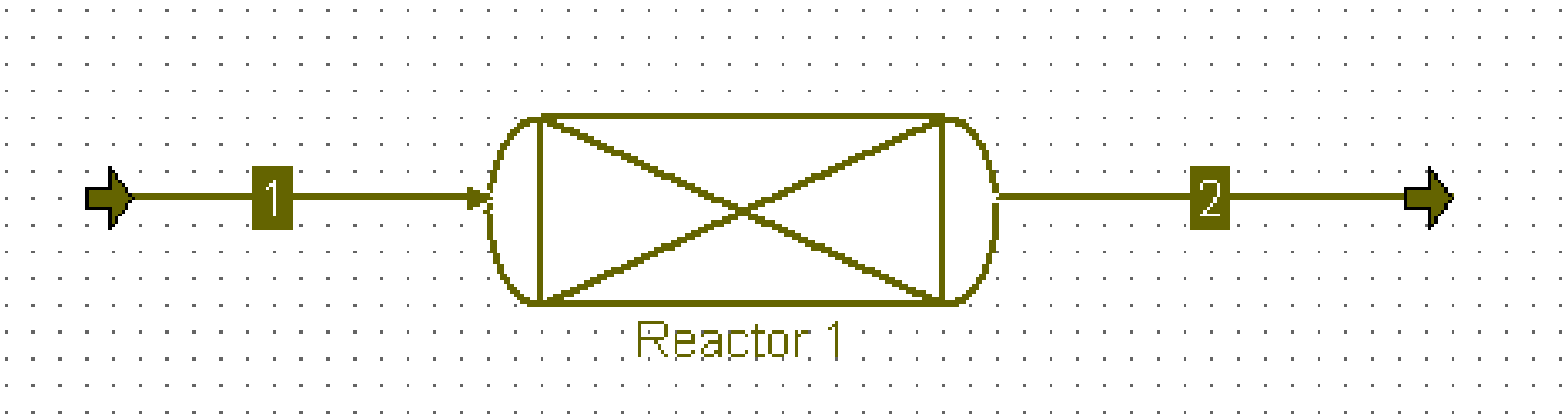
Inserting the reactor feed:



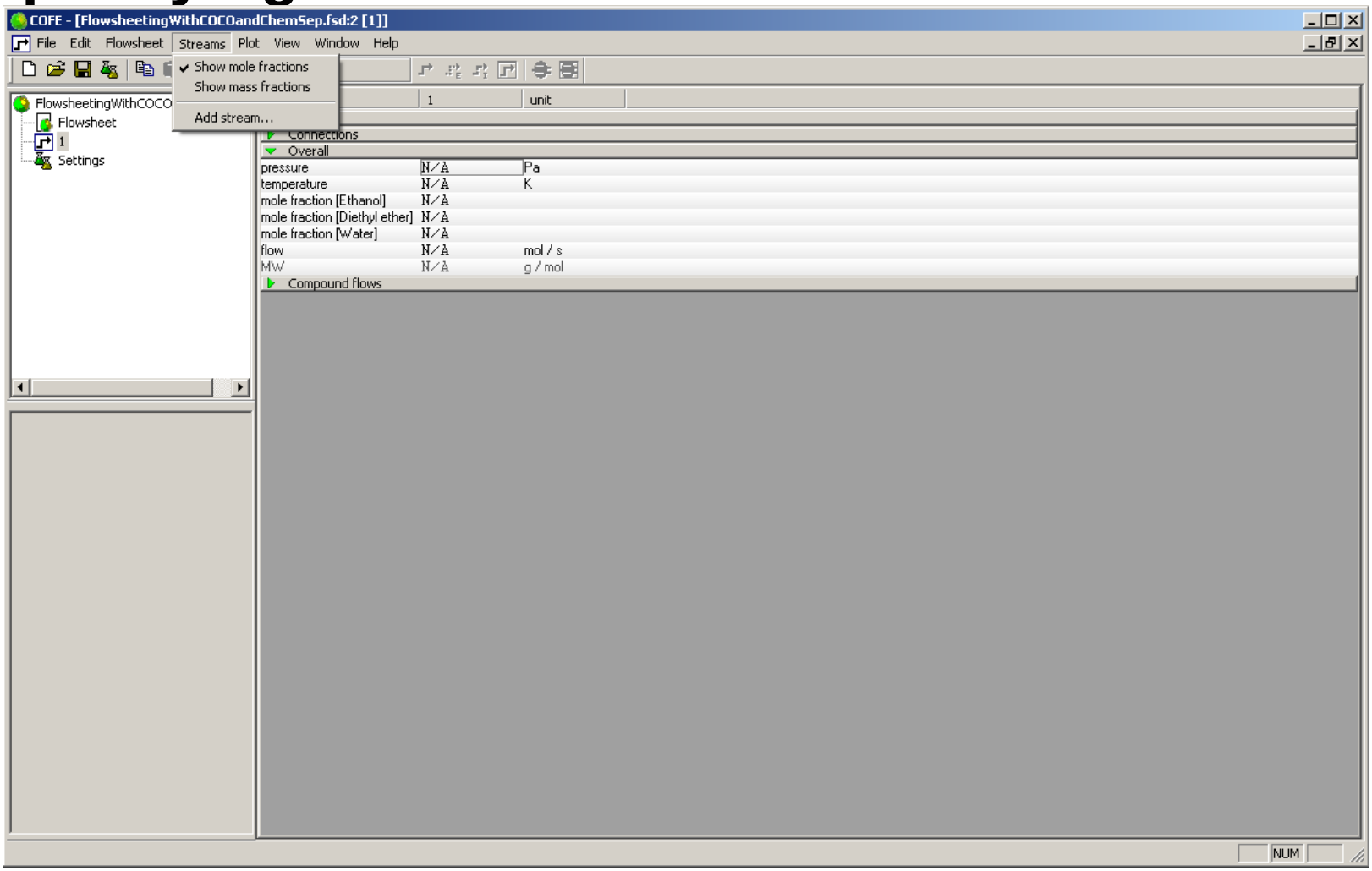
Connecting the feed:



The product stream:



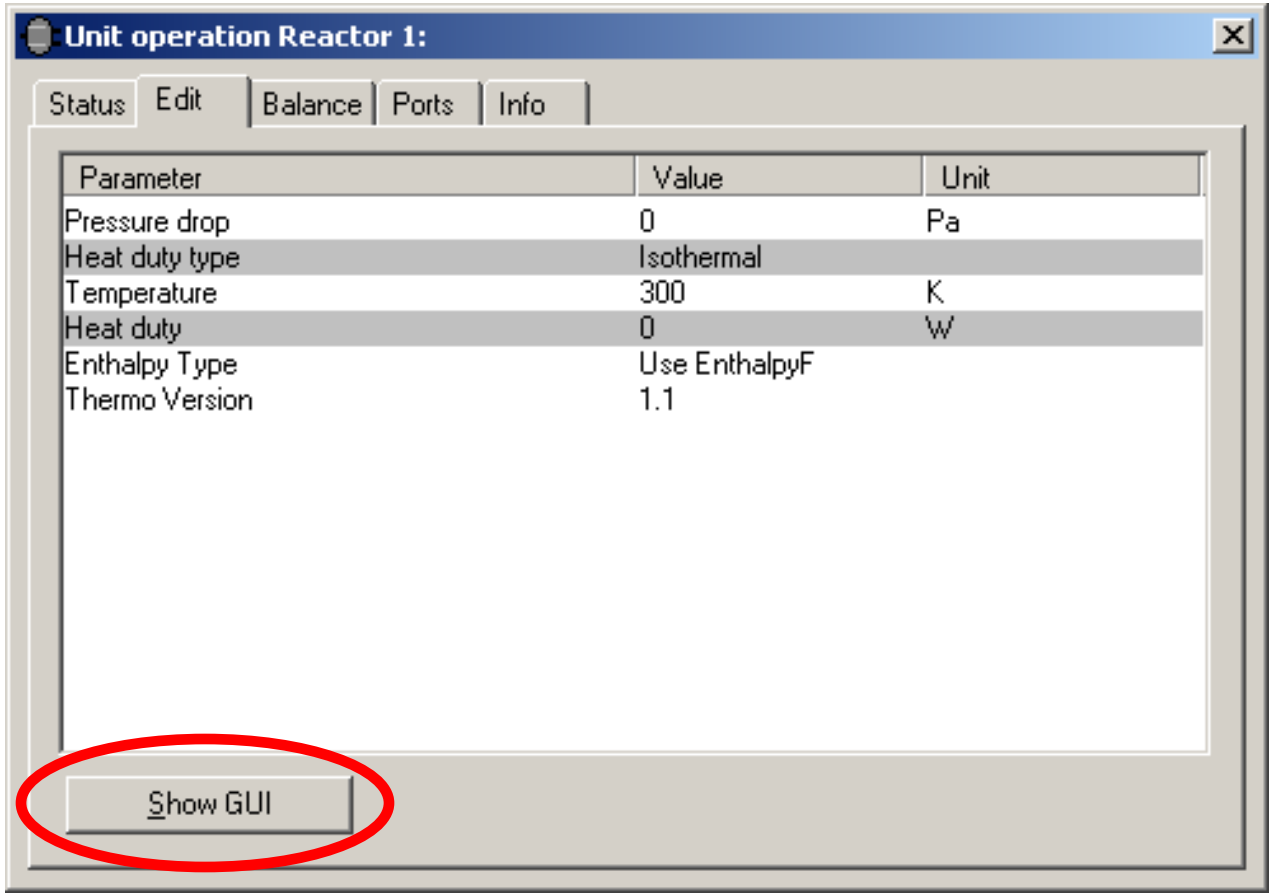
Specifying the feed stream:



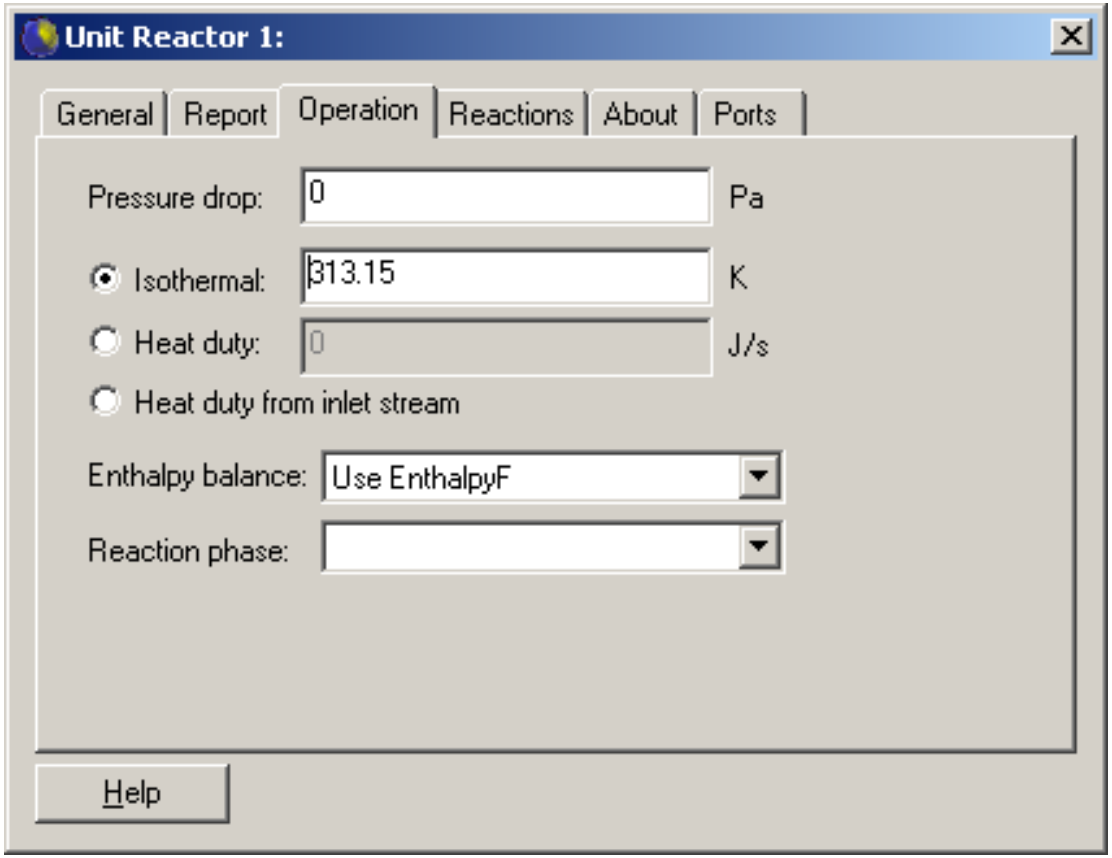
Specifying the feed stream:

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
MW	41.8609	g / mol
▶ Compound flows		
▼ Phase Fractions		
molar phaseFraction [Liquid]	1	
▶ Liquid composition		
▶ Overall properties		
▶ Liquid properties		

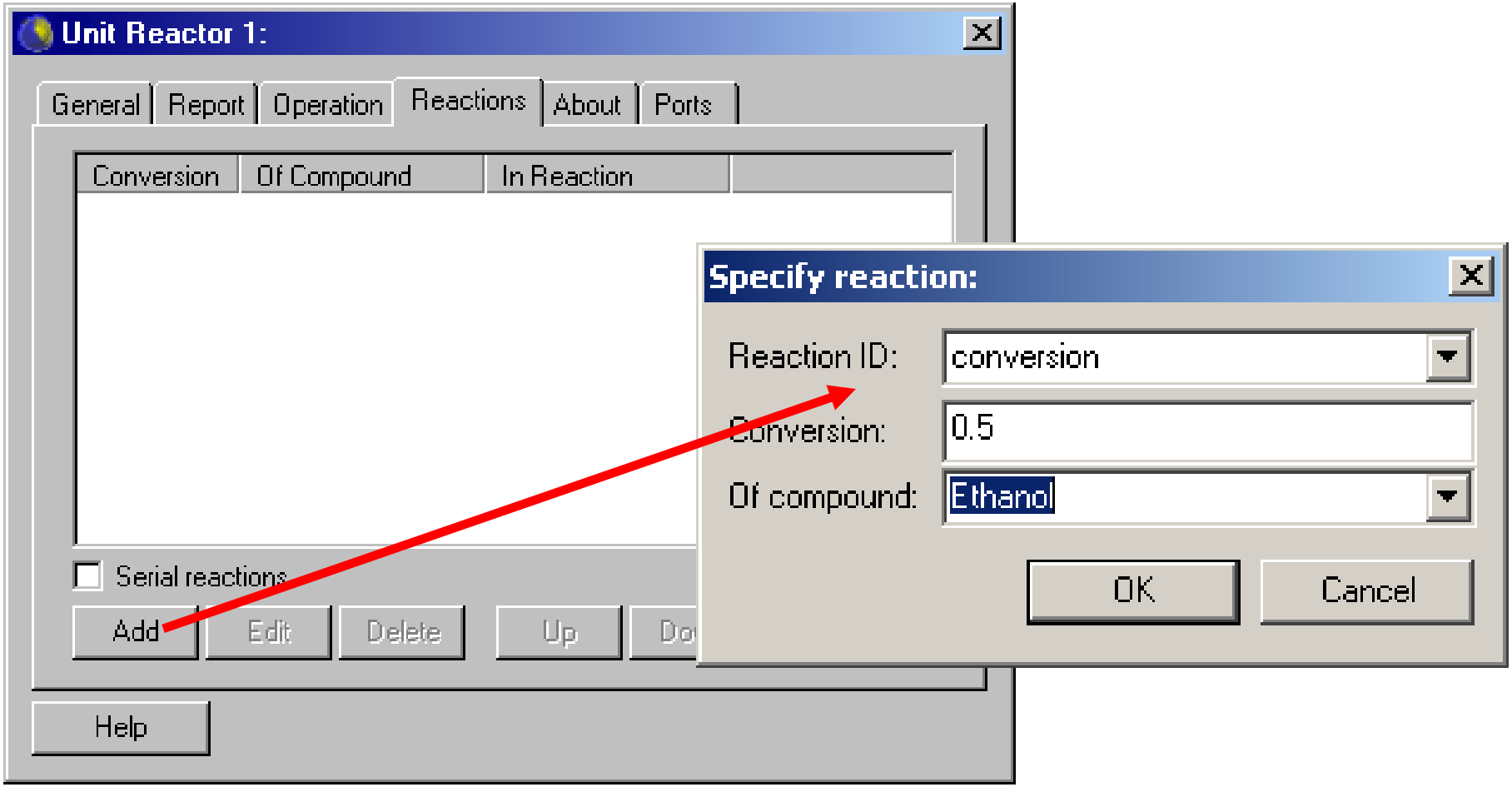
Reactor specifications:



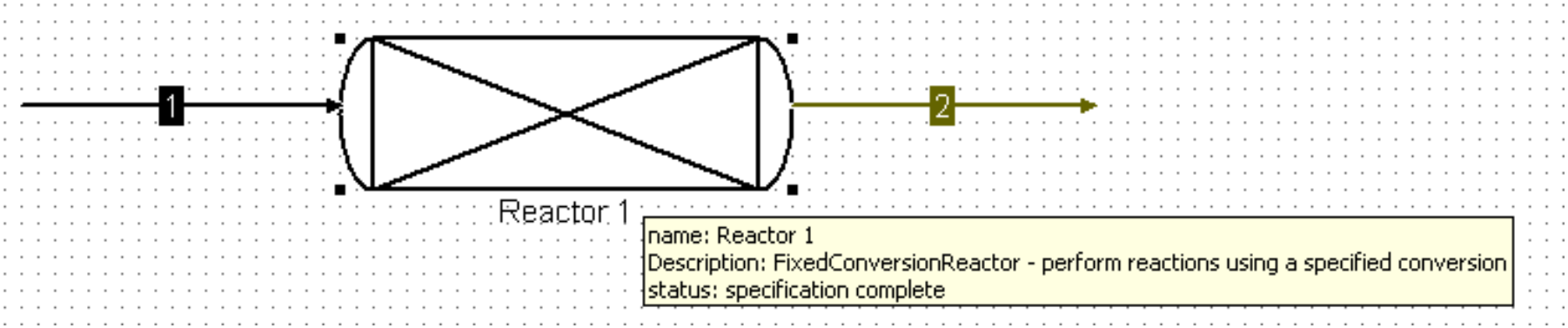
Reactor specifications:

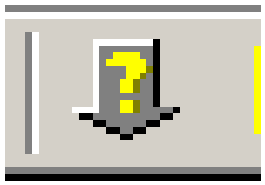


Reactor specifications:



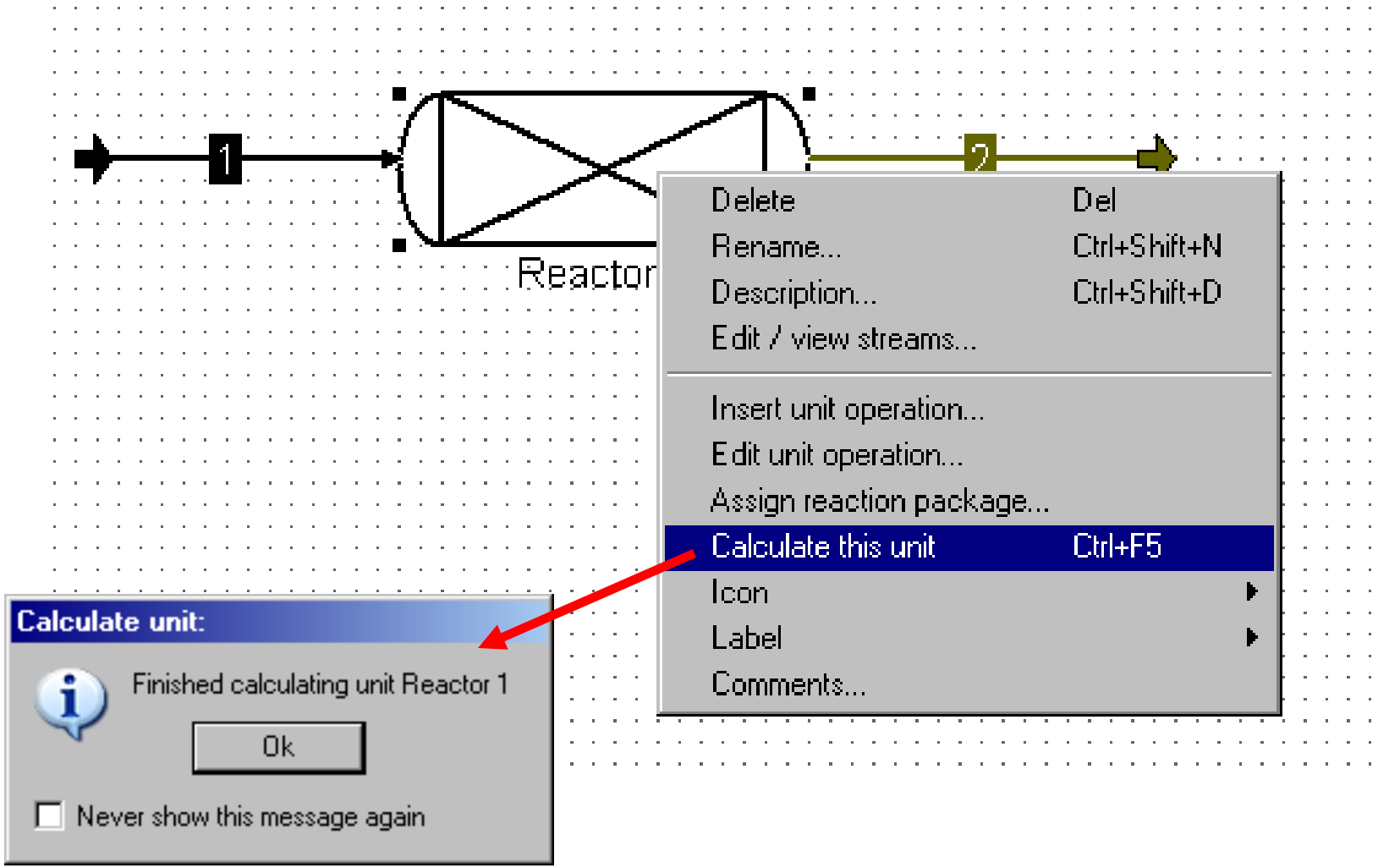
Reactor specifications:



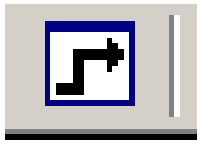


Validate

Calculate the reactor:

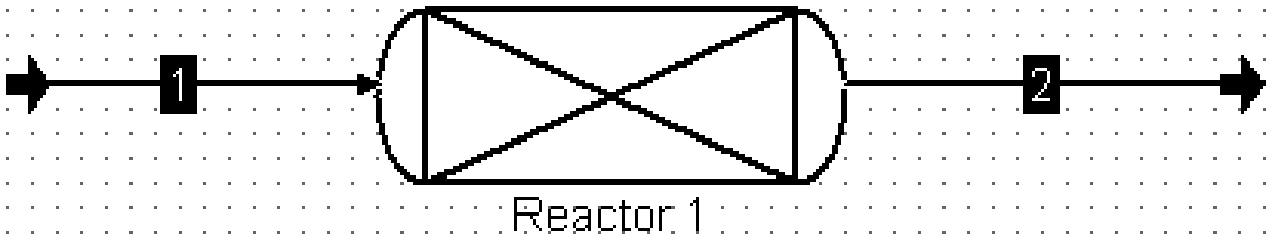


Reactor results:



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:

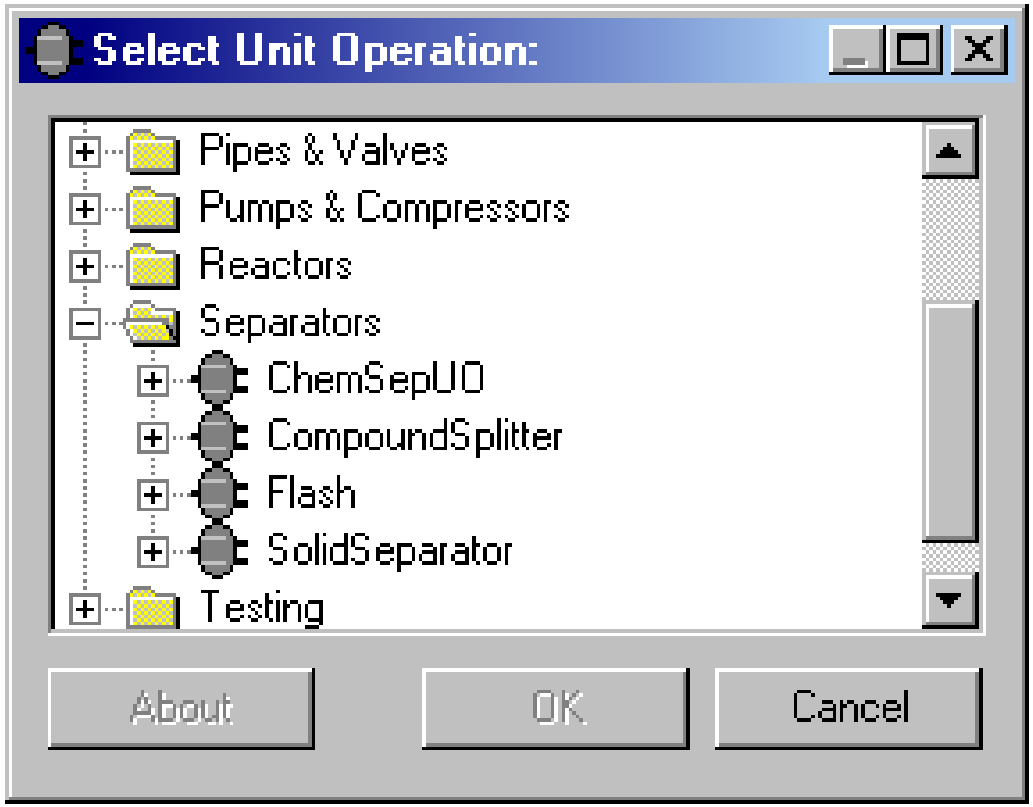


Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

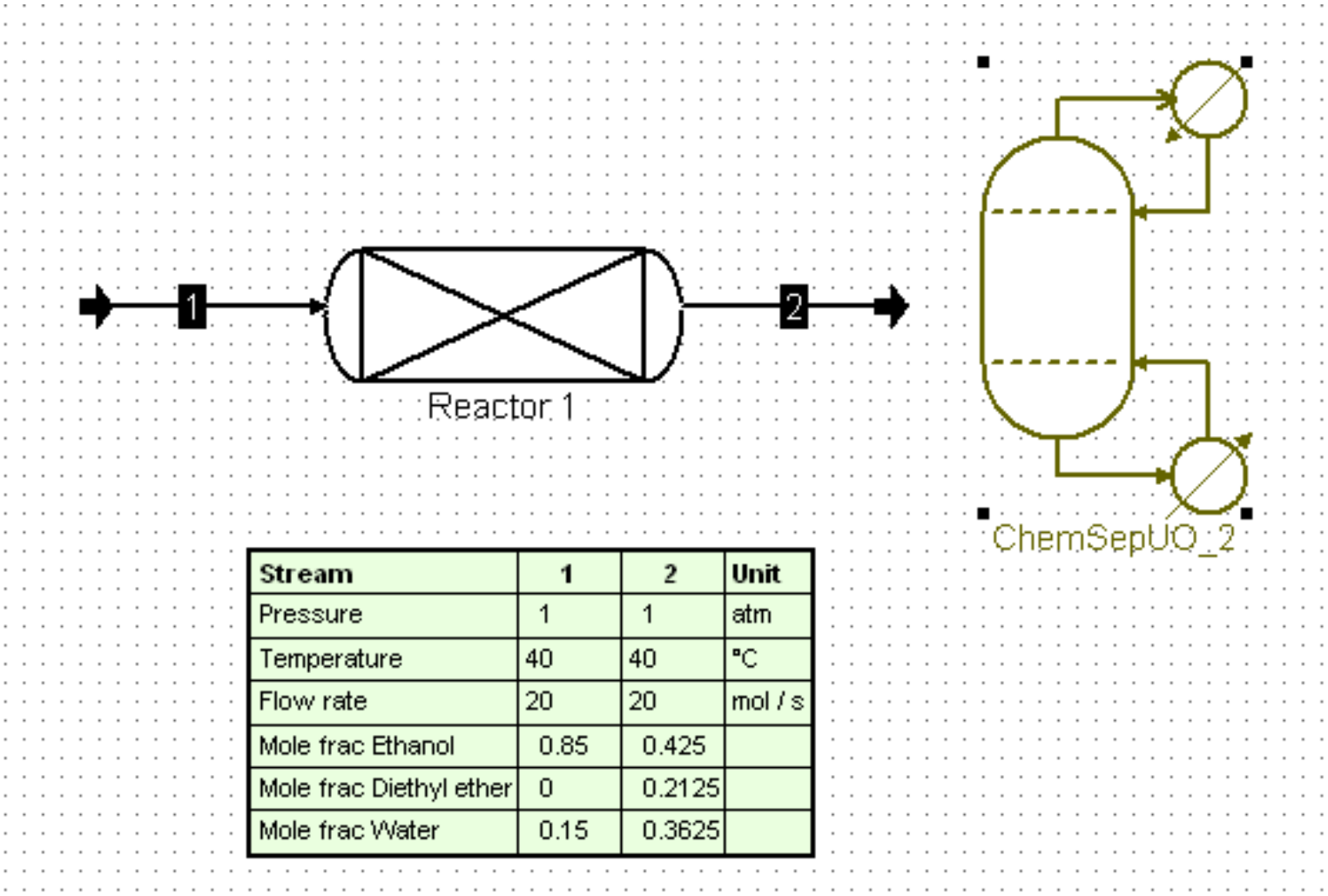
Presentation outline

- 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:

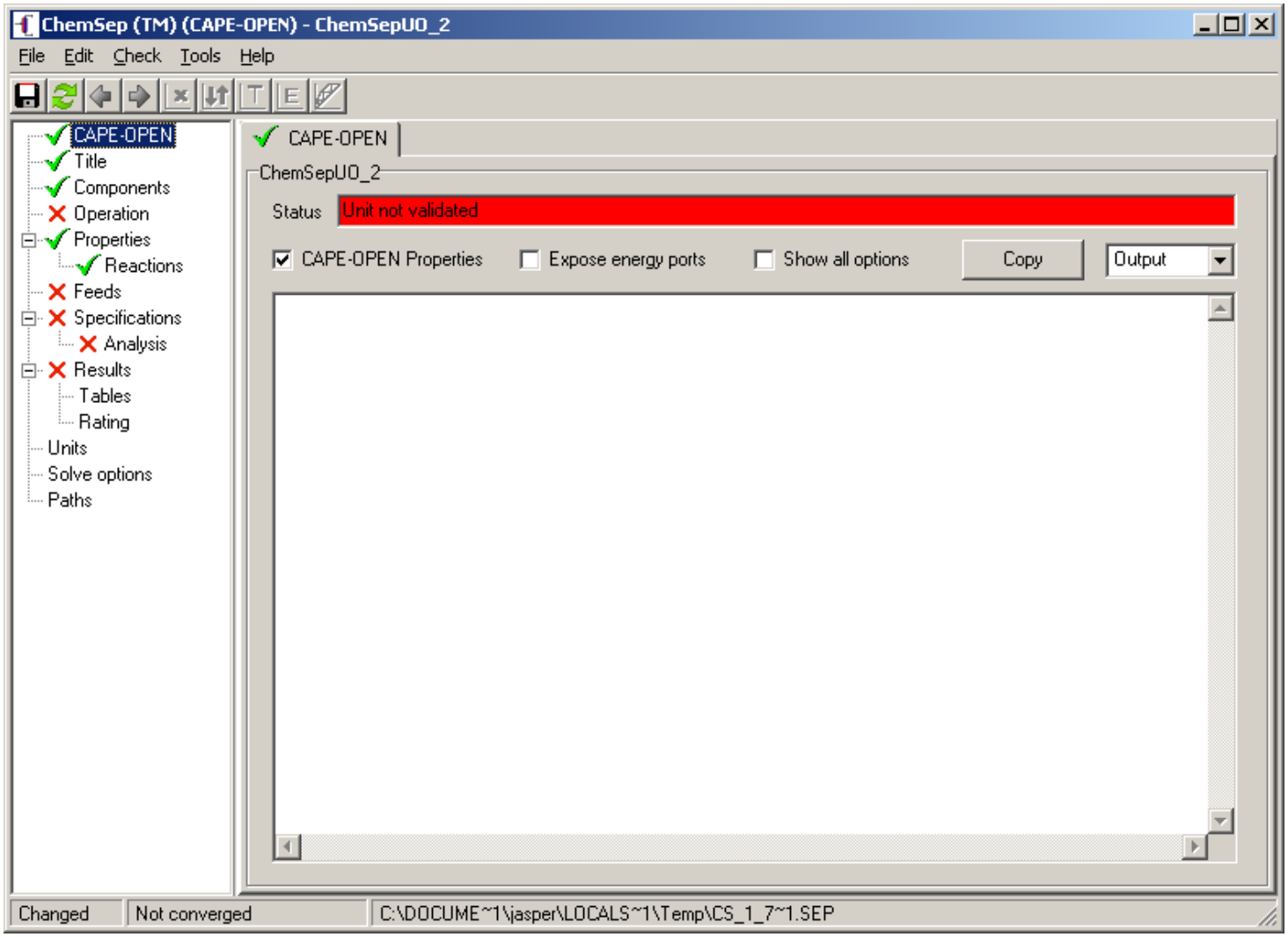


Inserting a ChemSep column:

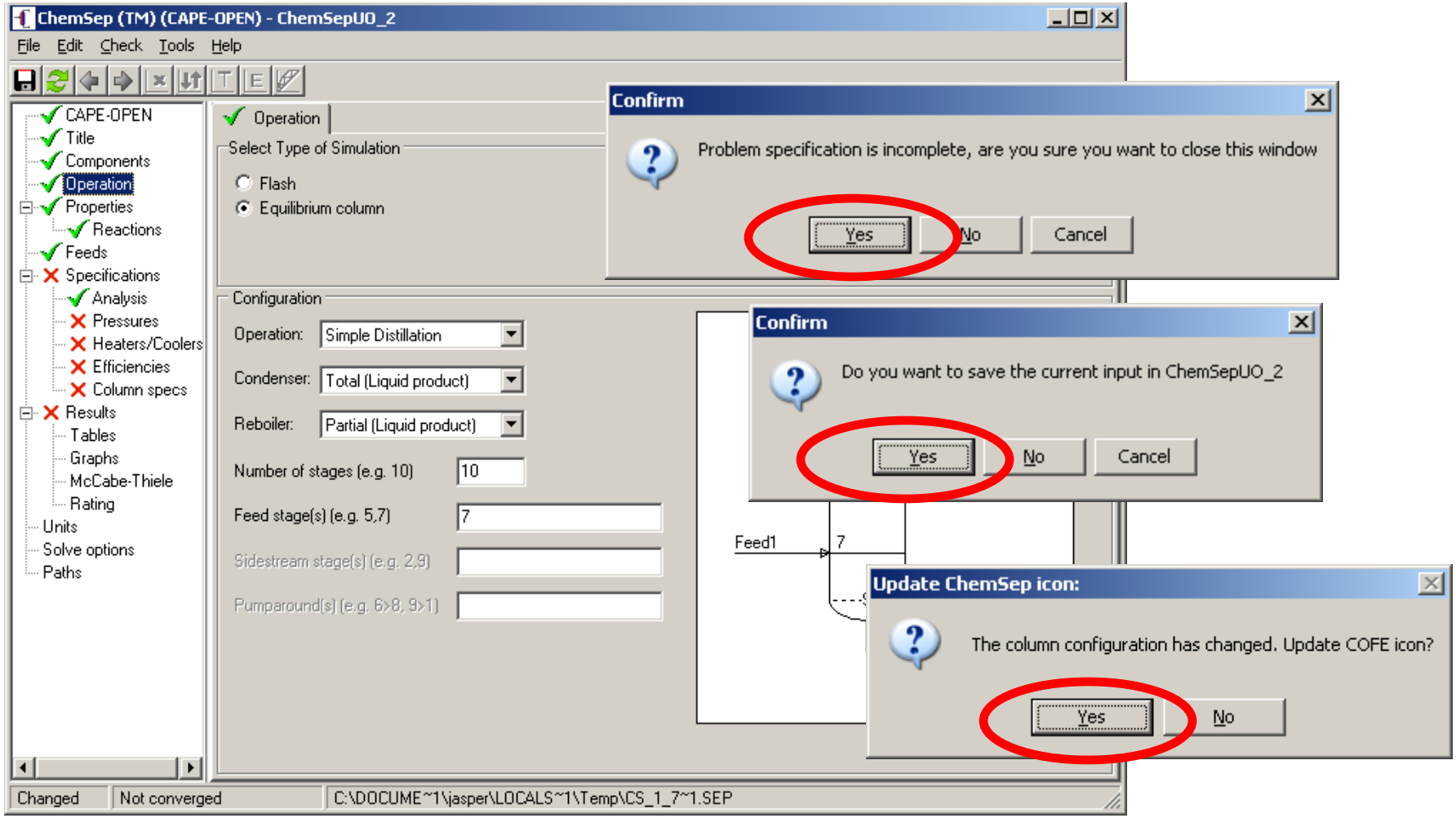


Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s
Mole frac Ethanol	0.85	0.425	
Mole frac Diethyl ether	0	0.2125	
Mole frac Water	0.15	0.3625	

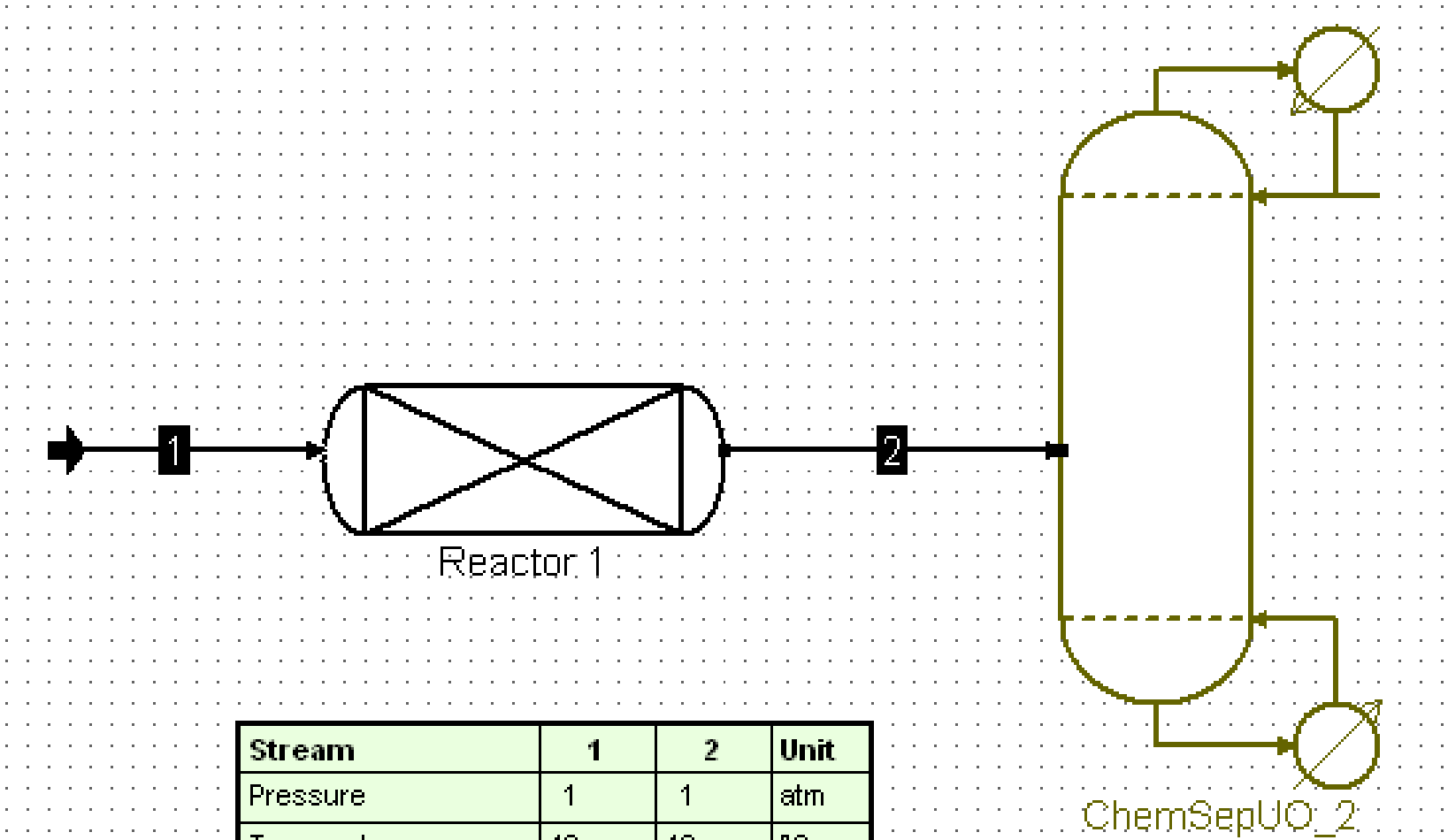
Inserting a ChemSep column:



Configuring the ChemSep column:

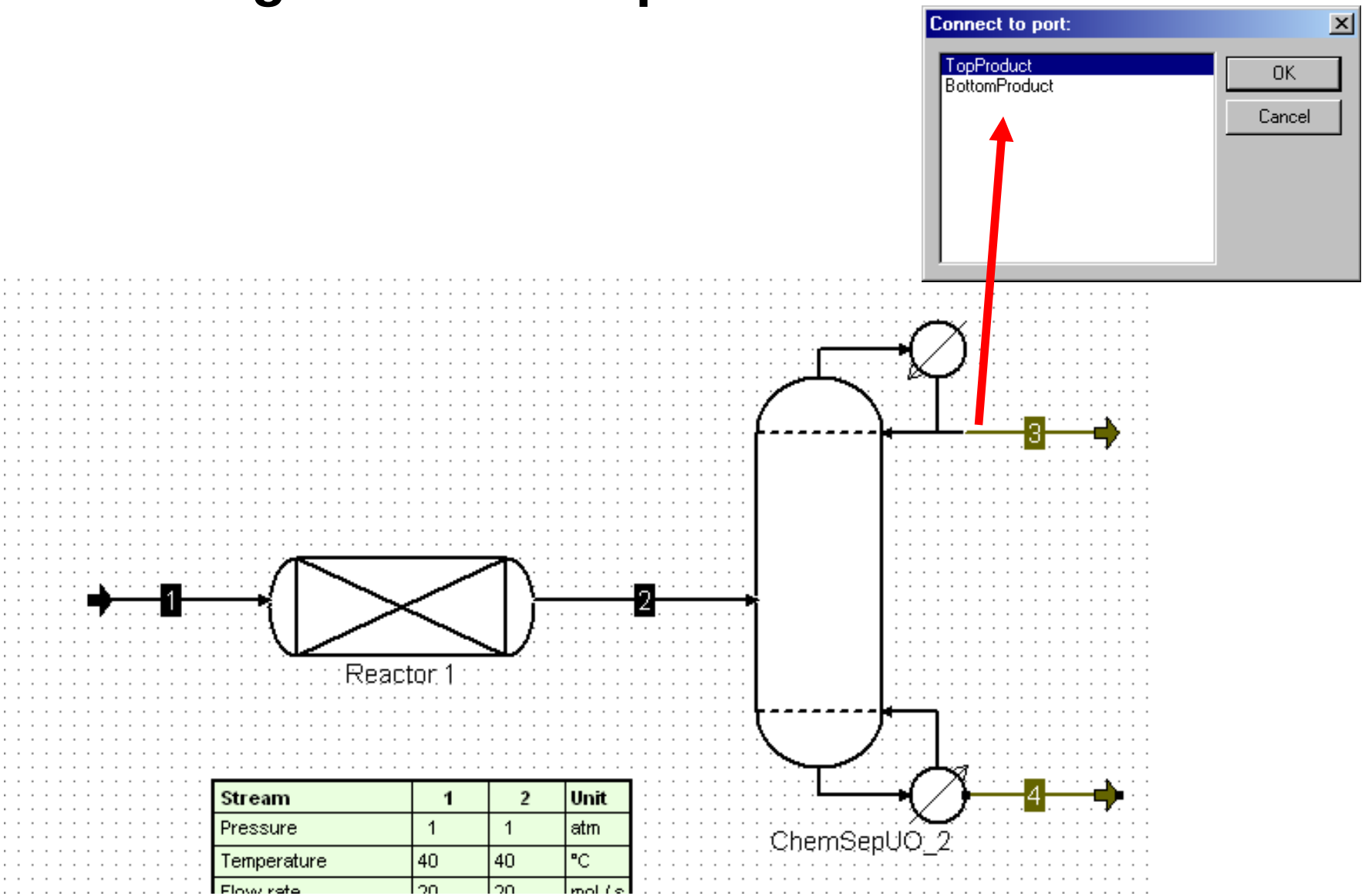


Connecting the ChemSep column:

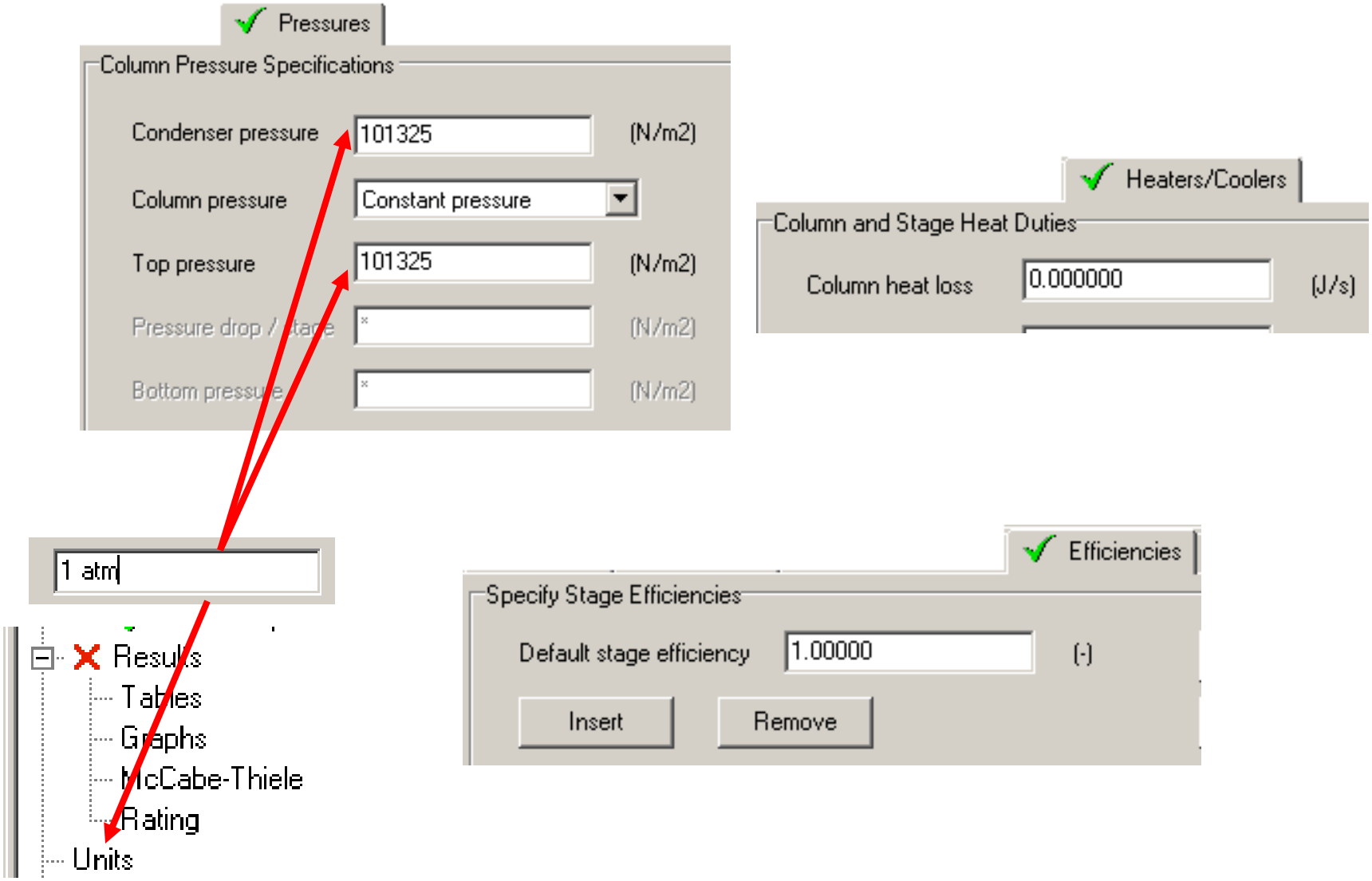


Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s

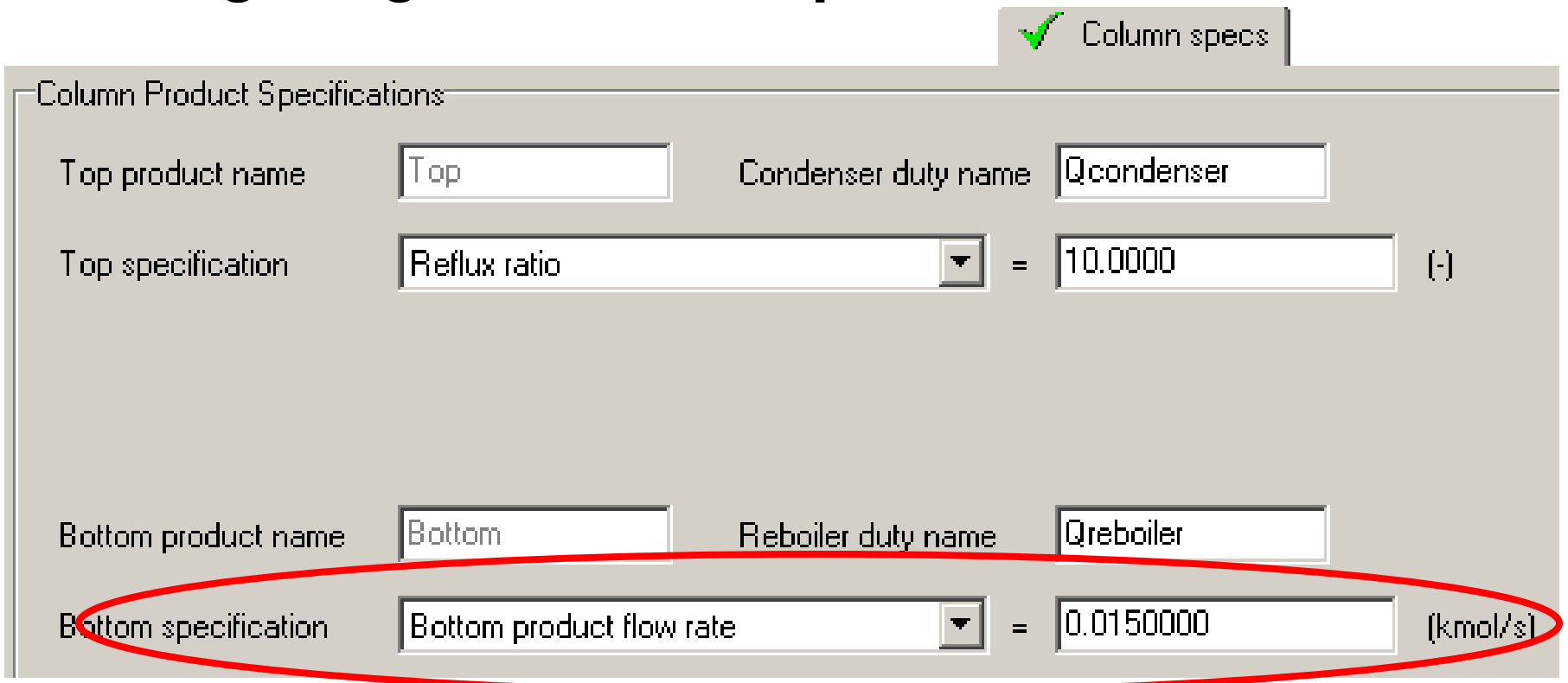
Connecting the ChemSep column:



Configuring the ChemSep column:



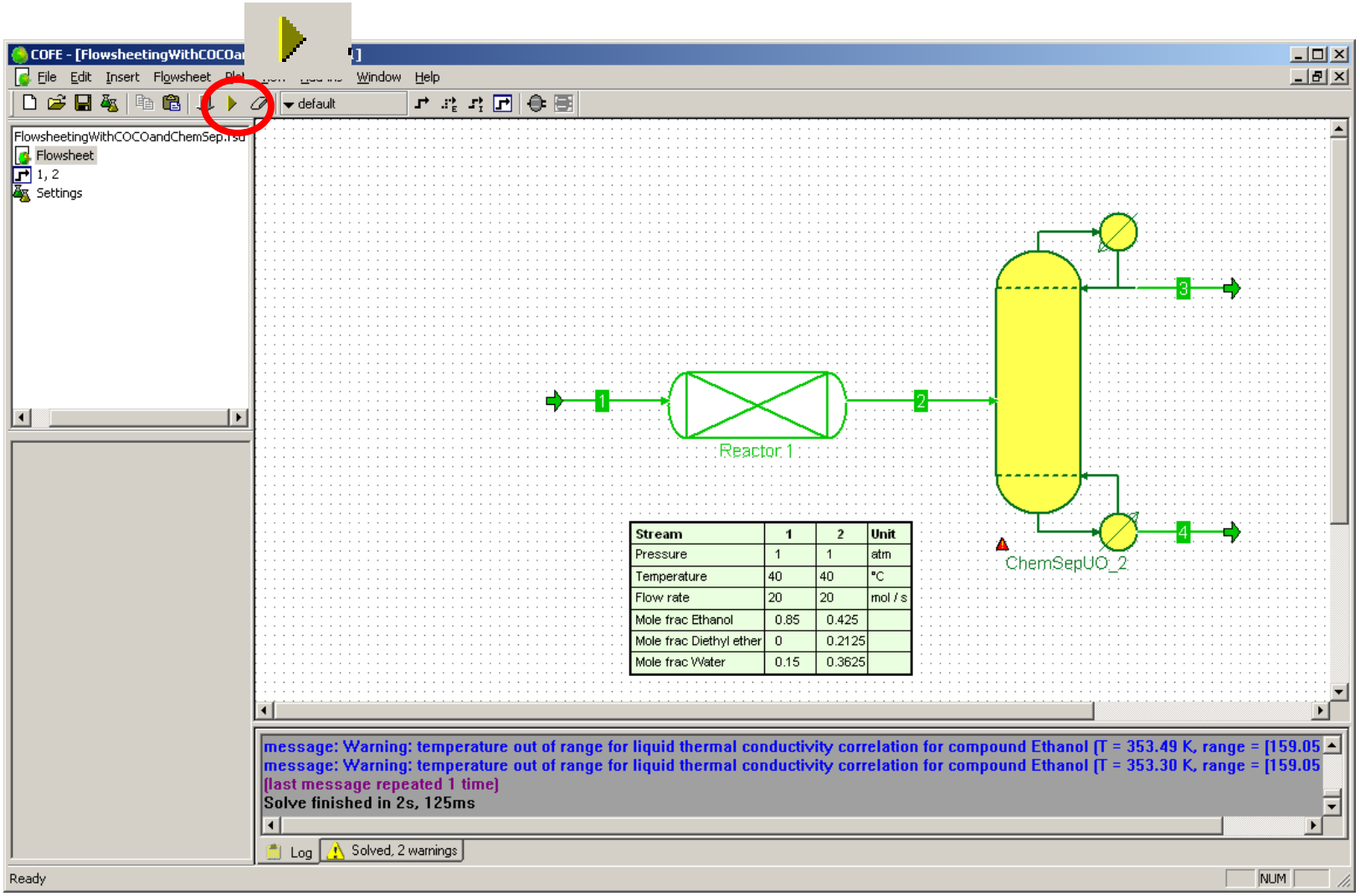
Configuring the ChemSep column:



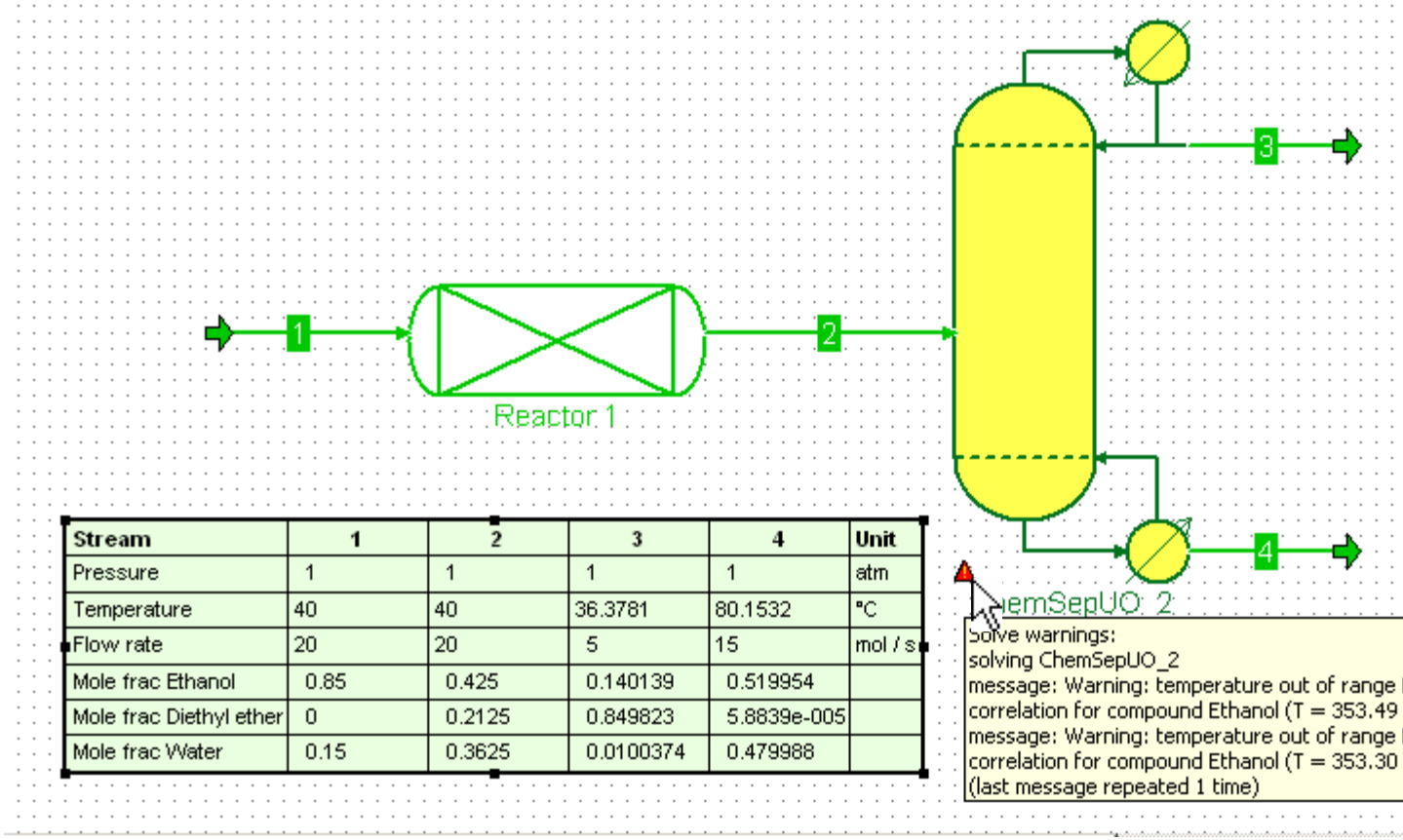
Note: This bottom specification is just to get us started; later we will change it.

15 mol/s

We can now run the column:

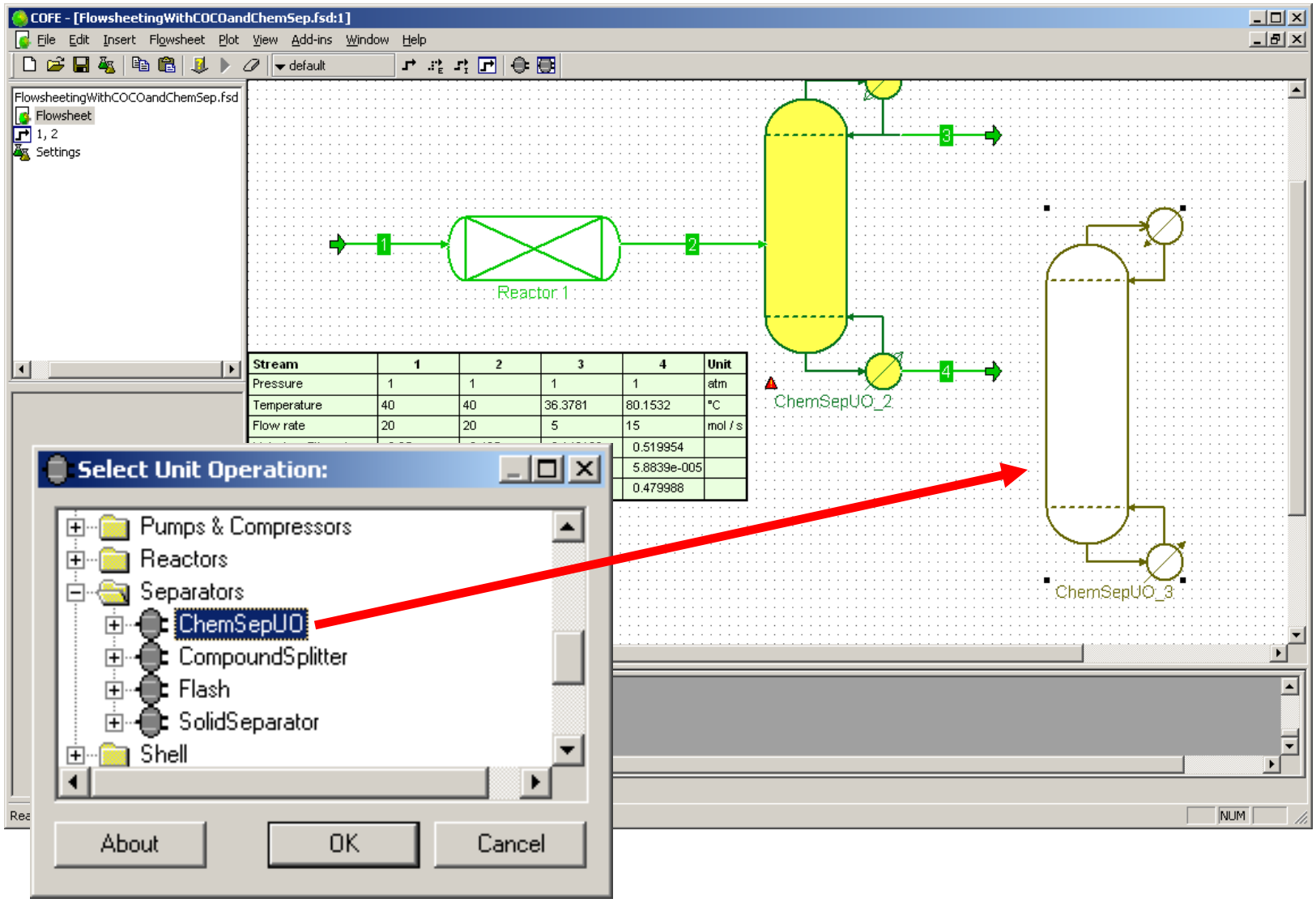


Checking the column results:

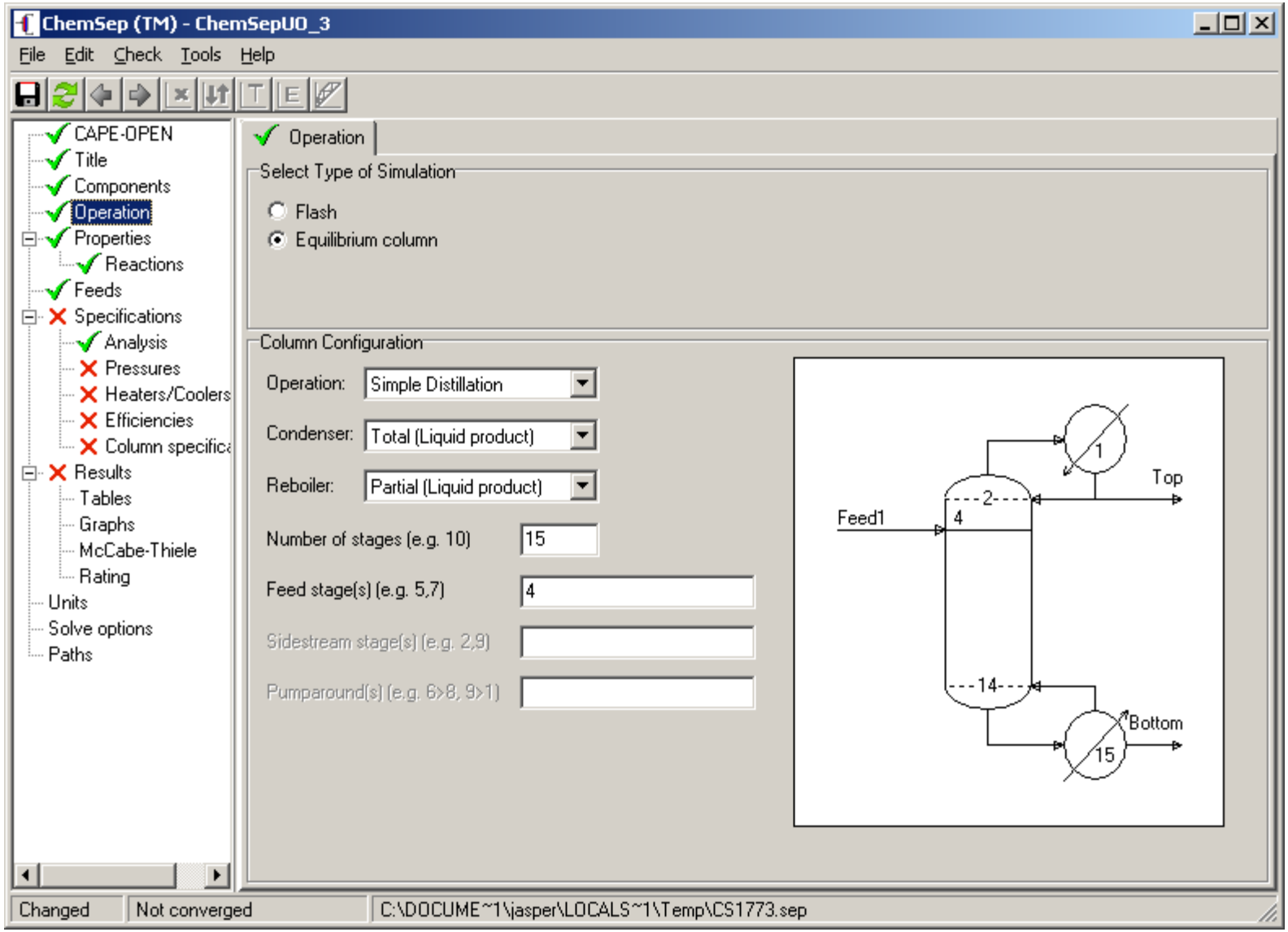


Stream	1	2	3	4	Unit
Pressure	1	1	1	1	atm
Temperature	40	40	36.3781	80.1532	°C
Flow rate	20	20	5	15	mol / s
Mole frac Ethanol	0.85	0.425	0.140139	0.519954	
Mole frac Diethyl ether	0	0.2125	0.849823	5.8839e-005	
Mole frac Water	0.15	0.3625	0.0100374	0.479988	

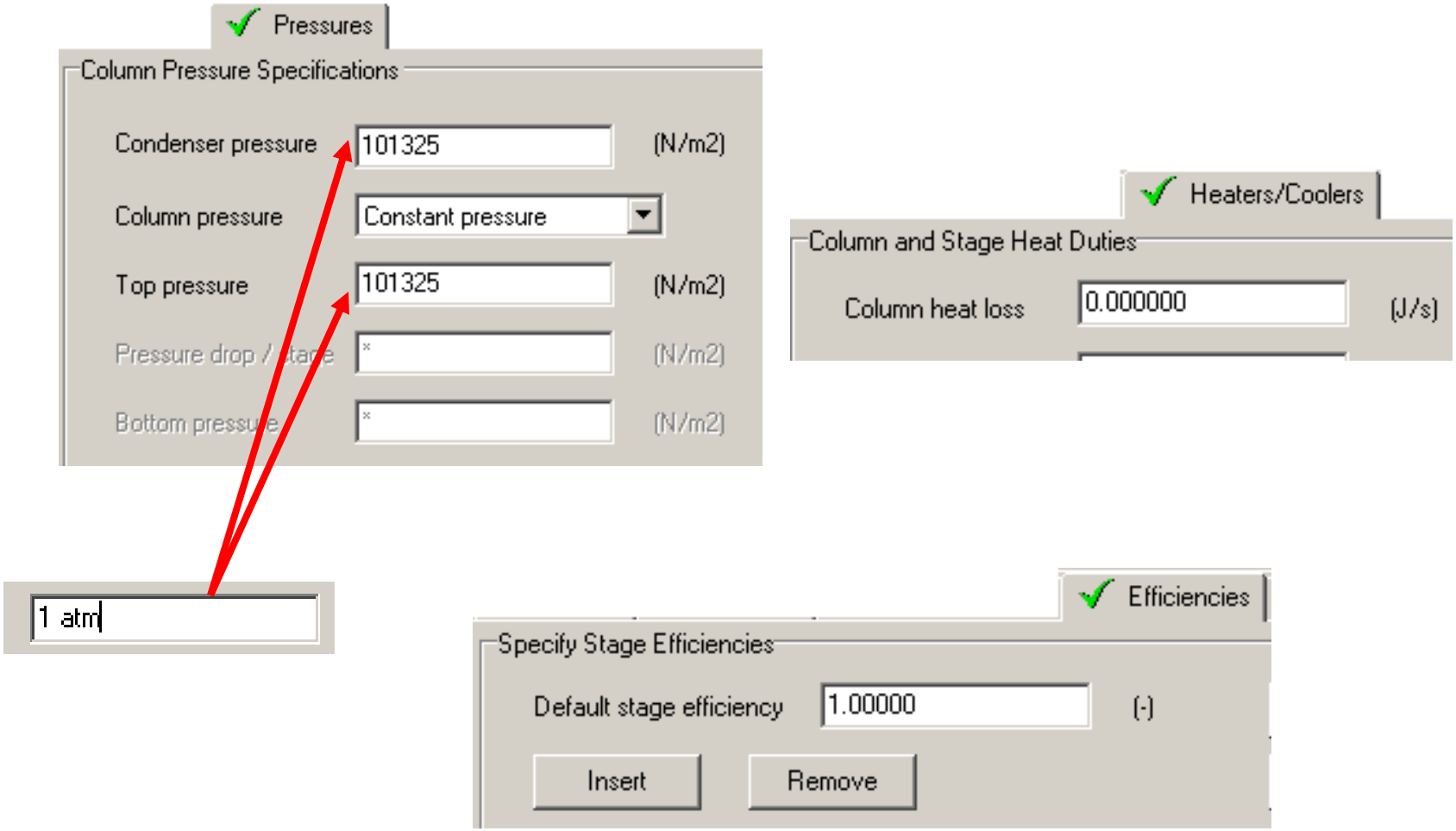
Inserting the second column:



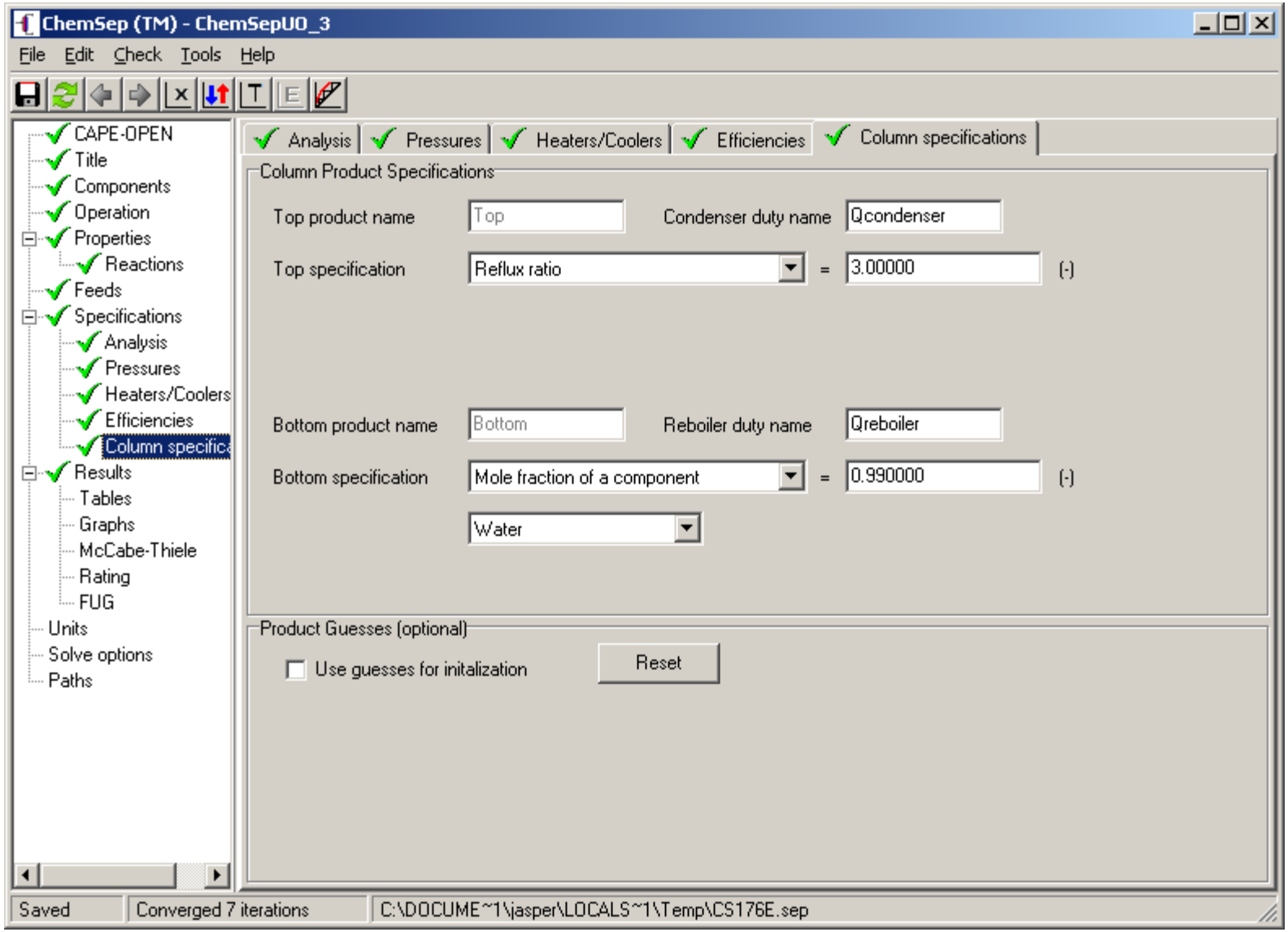
Configuring the second column:



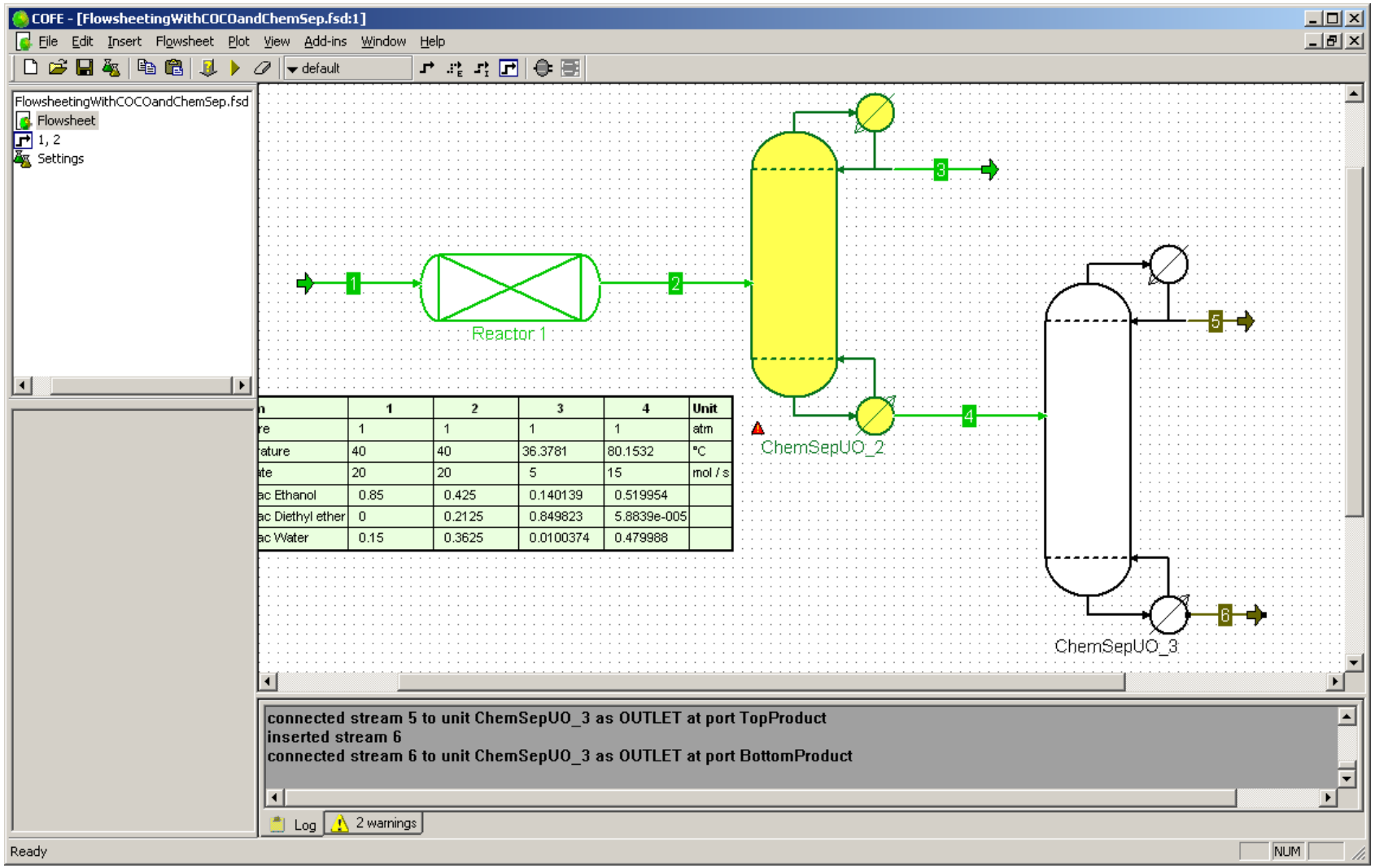
Configuring the second column:



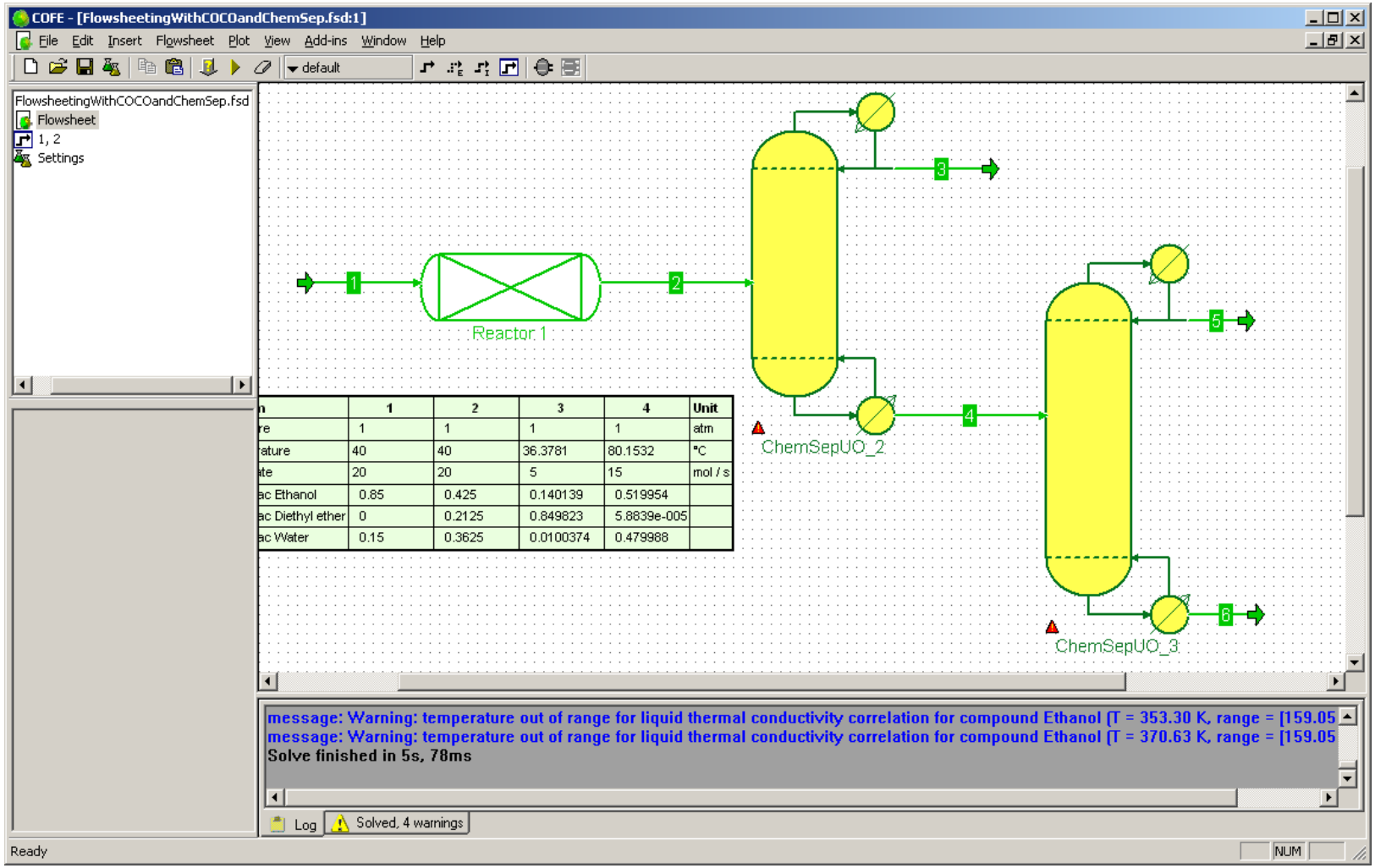
Configuring the second column:



Connecting the streams:

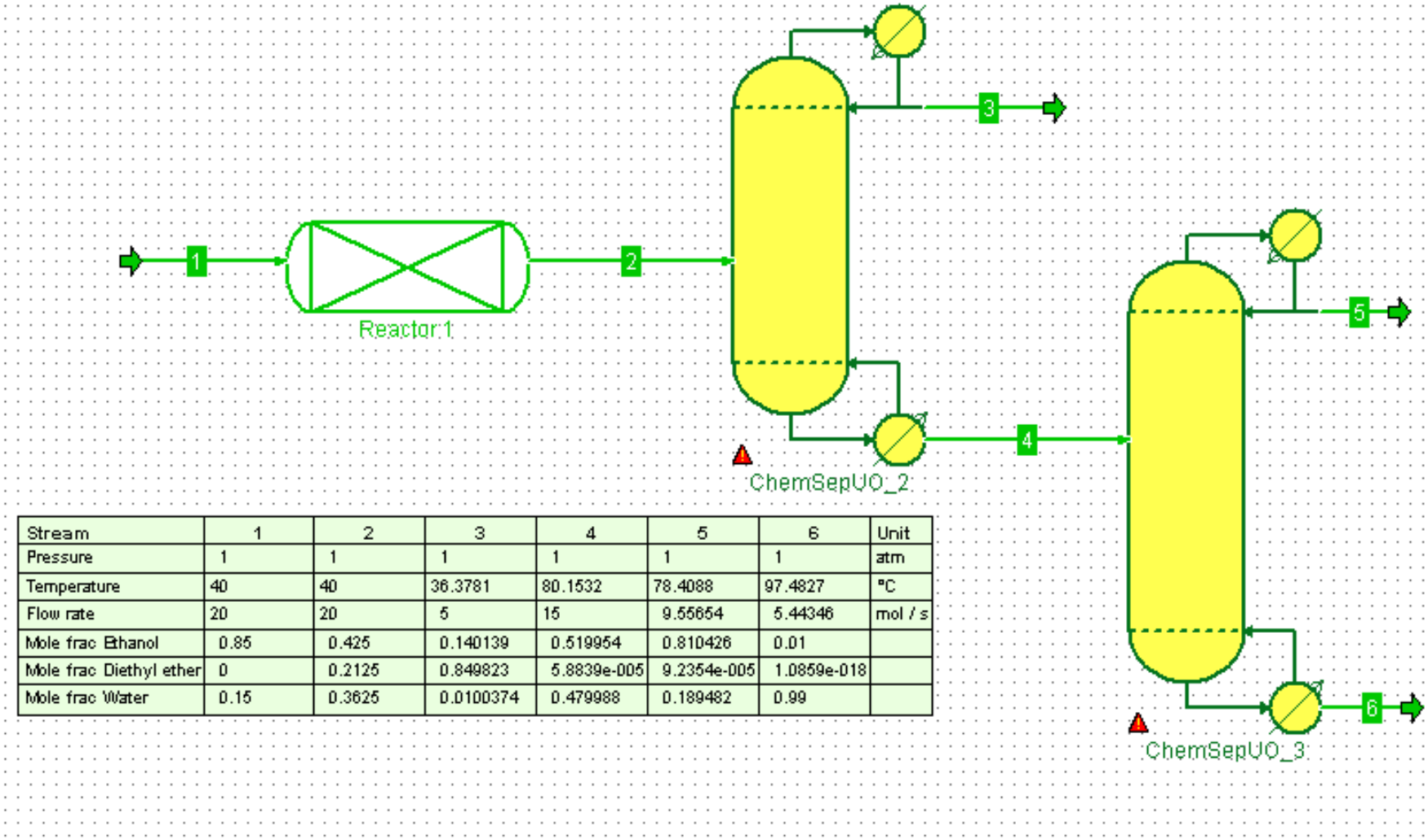


Solving the second column:



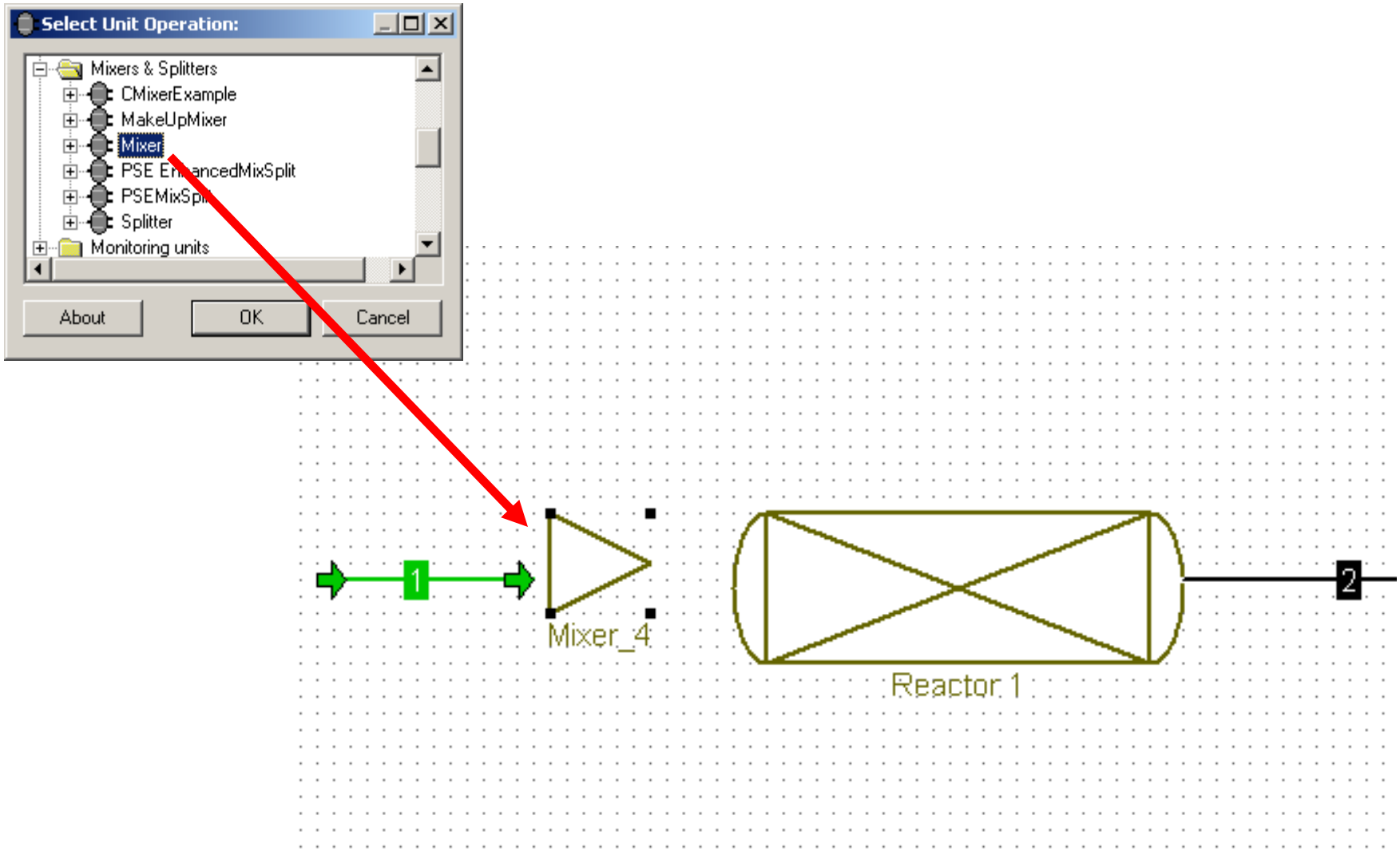
	1	2	3	4	Unit
re	1	1	1	1	atm
ature	40	40	36.3781	80.1532	°C
te	20	20	5	15	mol / s
ac Ethanol	0.85	0.425	0.140139	0.519954	
ac Diethyl ether	0	0.2125	0.849823	5.8839e-005	
ac Water	0.15	0.3625	0.0100374	0.479988	

Let's see what we get:

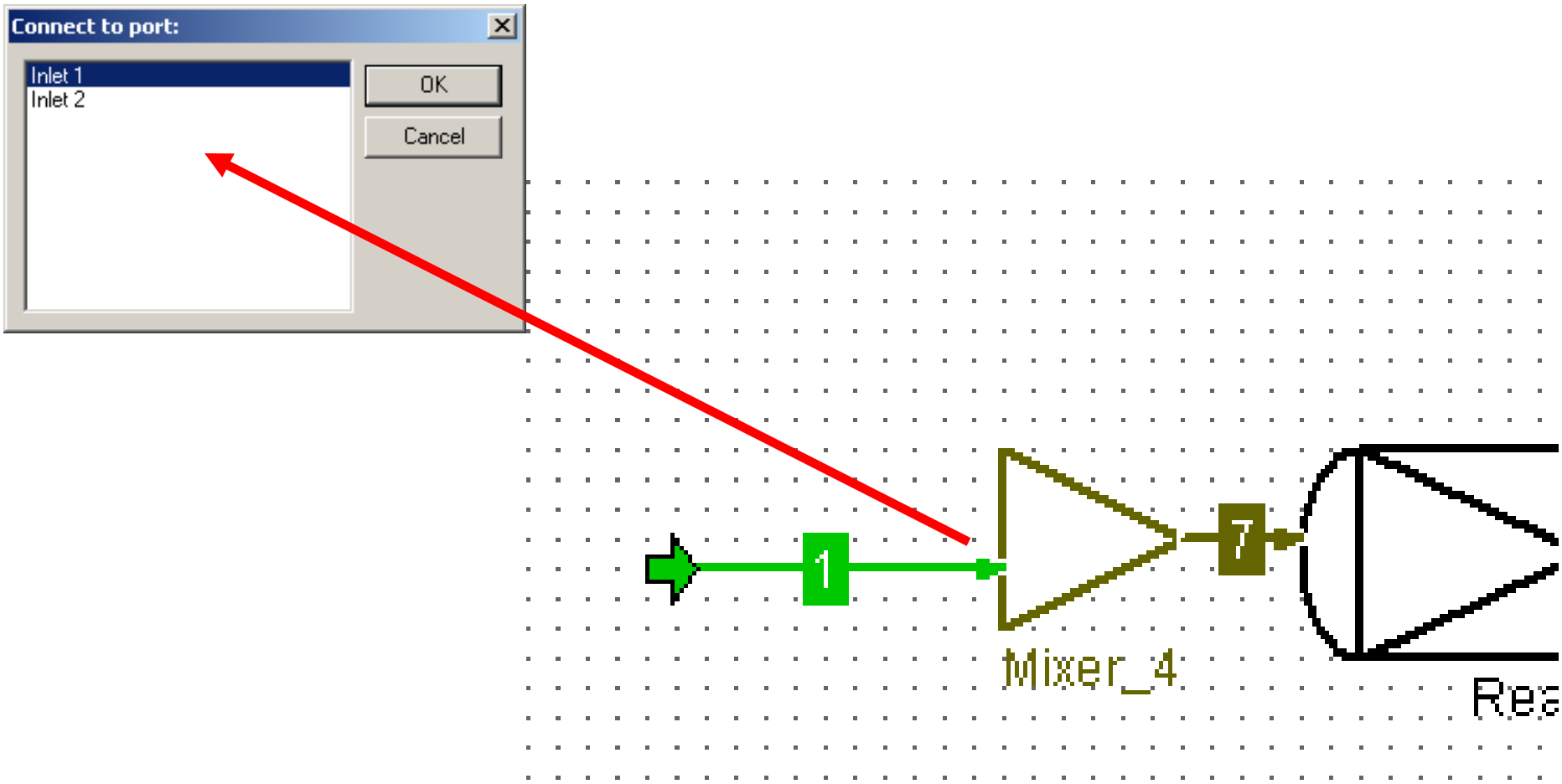


Stream	1	2	3	4	5	6	Unit
Pressure	1	1	1	1	1	1	atm
Temperature	40	40	36.3781	80.1532	78.4088	97.4827	°C
Flow rate	20	20	5	15	9.55654	5.44346	mol / s
Mole frac Ethanol	0.85	0.425	0.140139	0.519954	0.810426	0.01	
Mole frac Diethyl ether	0	0.2125	0.849823	5.8839e-005	9.2354e-005	1.0859e-018	
Mole frac Water	0.15	0.3625	0.0100374	0.479988	0.189482	0.99	

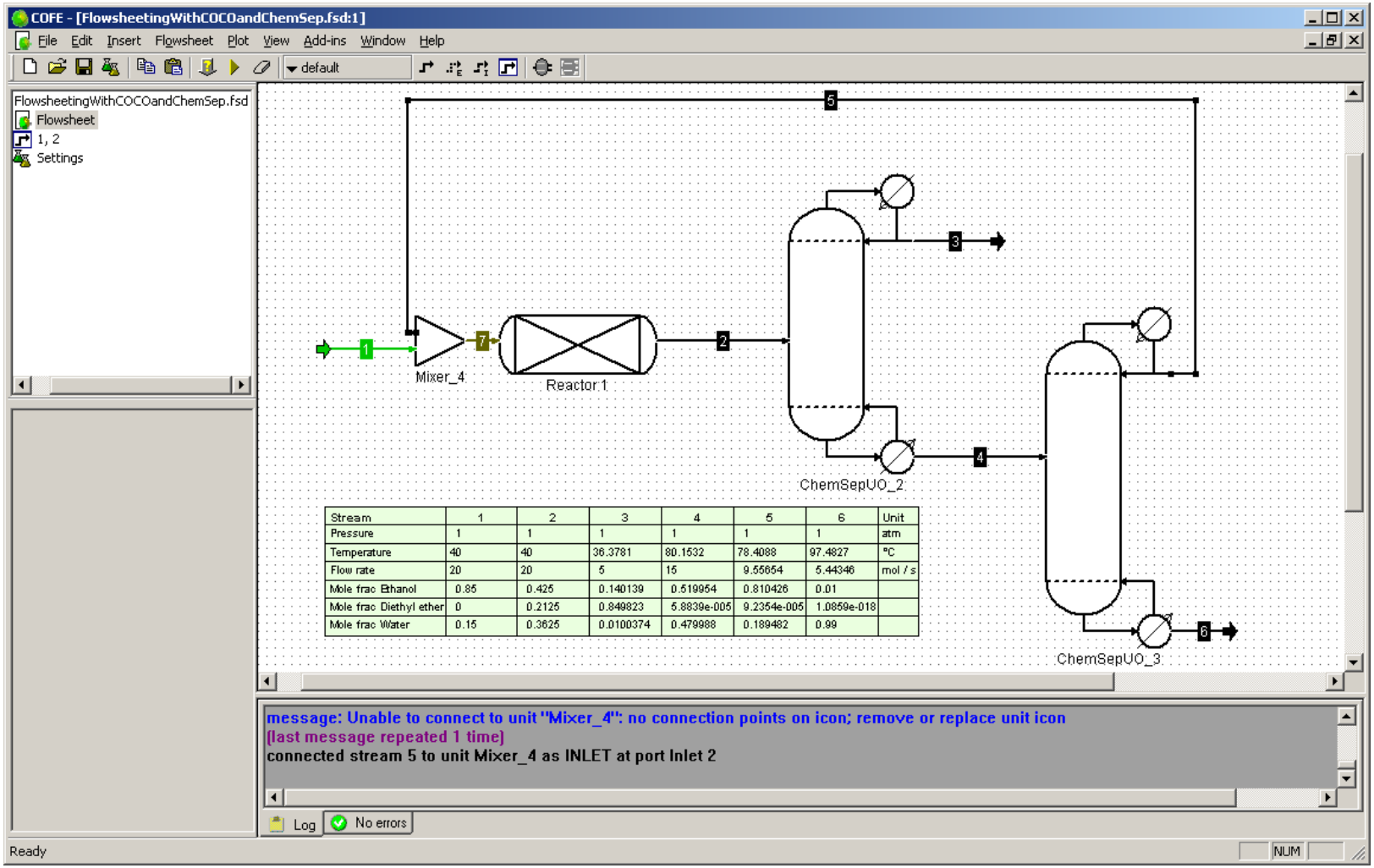
Setting up the recycle:



Setting up the recycle:

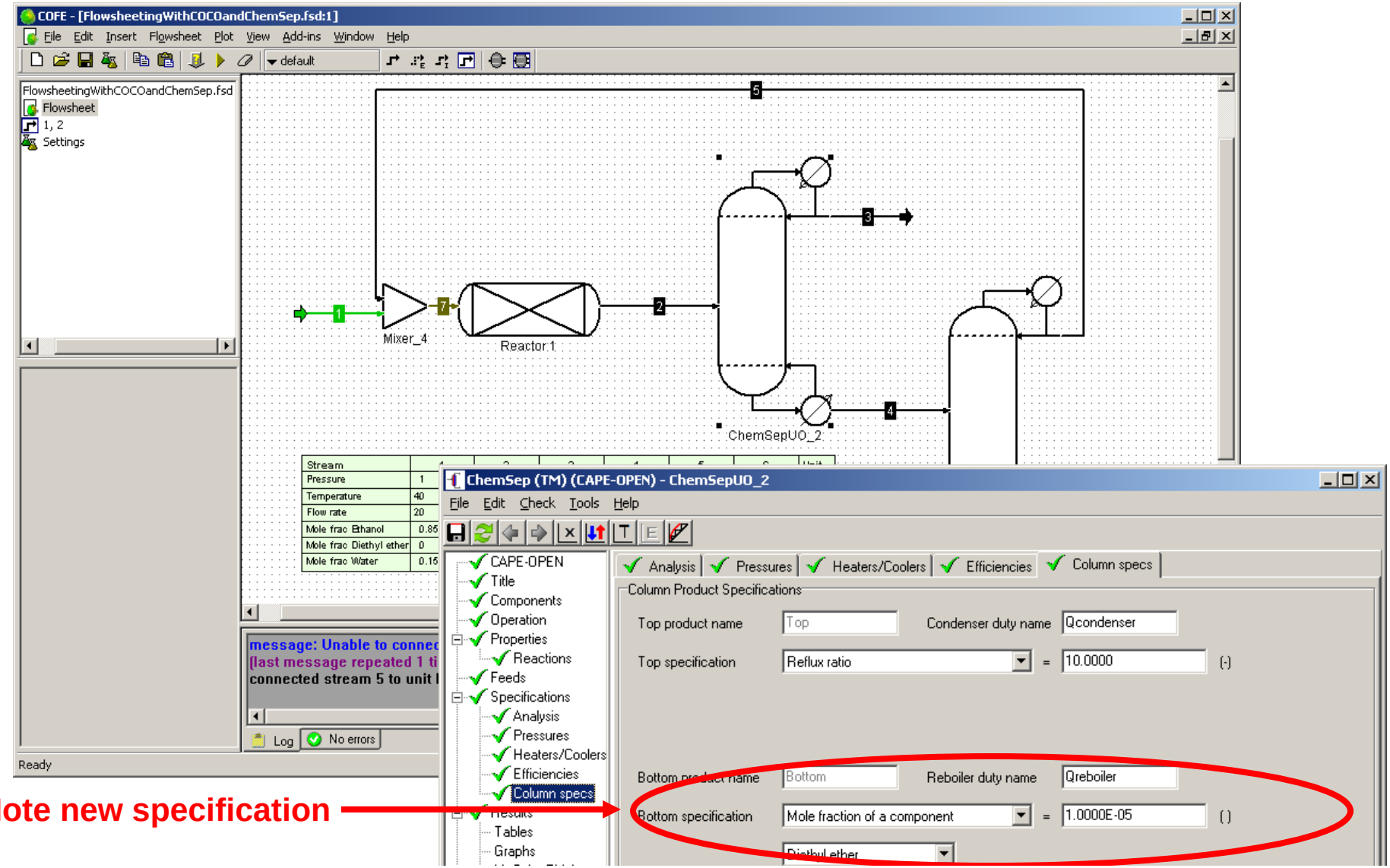


Closing the recycle:



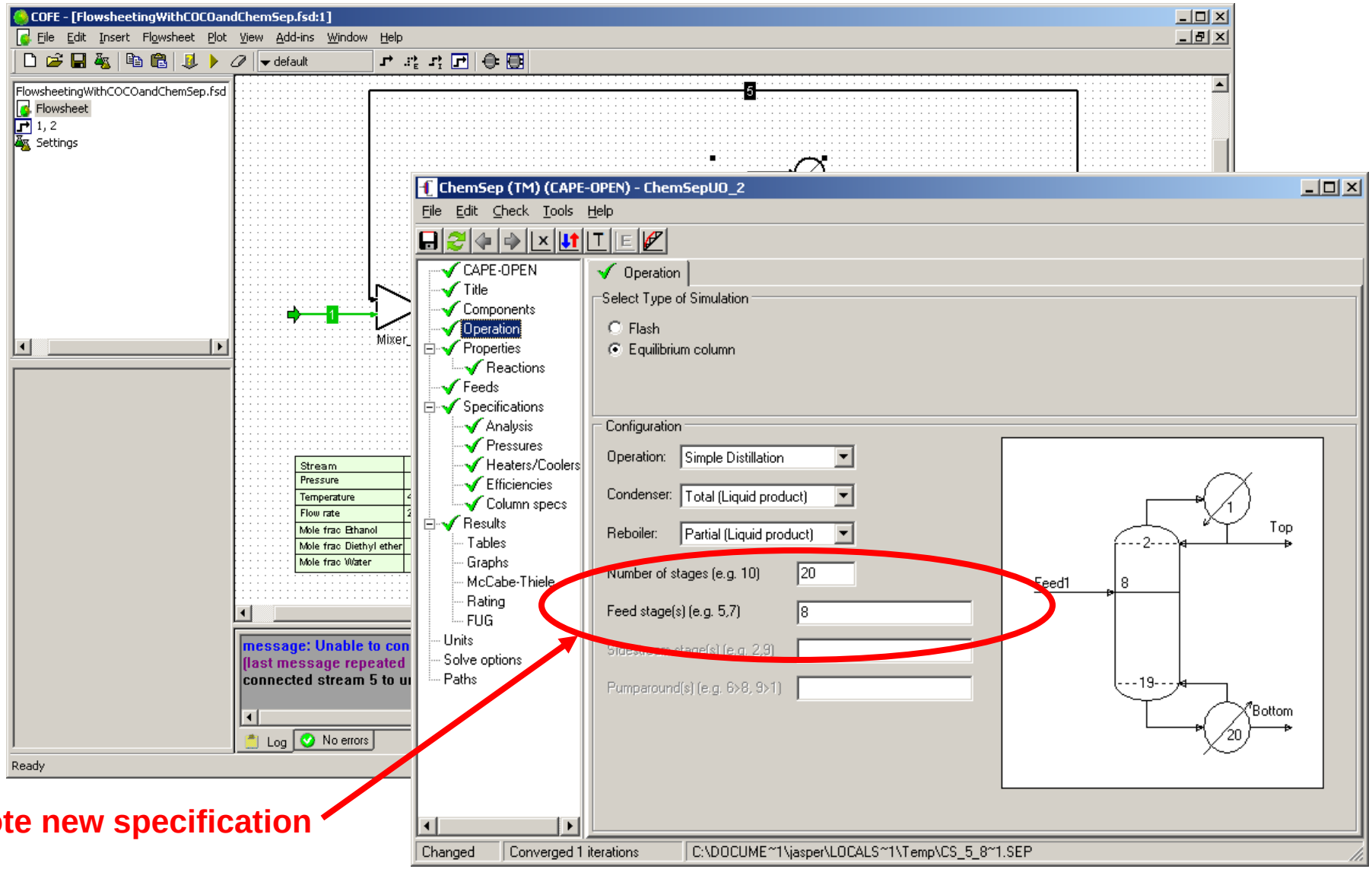
Stream	1	2	3	4	5	6	Unit
Pressure	1	1	1	1	1	1	atm
Temperature	40	40	36.3781	80.1532	78.4088	97.4827	°C
Flow rate	20	20	5	15	9.55654	5.44346	mol / s
Mole frac Ethanol	0.85	0.425	0.140139	0.519954	0.810426	0.01	
Mole frac Diethyl ether	0	0.2125	0.849823	5.8839e-005	9.2354e-005	1.0859e-018	
Mole frac Water	0.15	0.3625	0.0100374	0.479988	0.189482	0.99	

Redoing the specifications for Column 1:



Note new specification

Redoing the specifications for Column 1:



Note new specification

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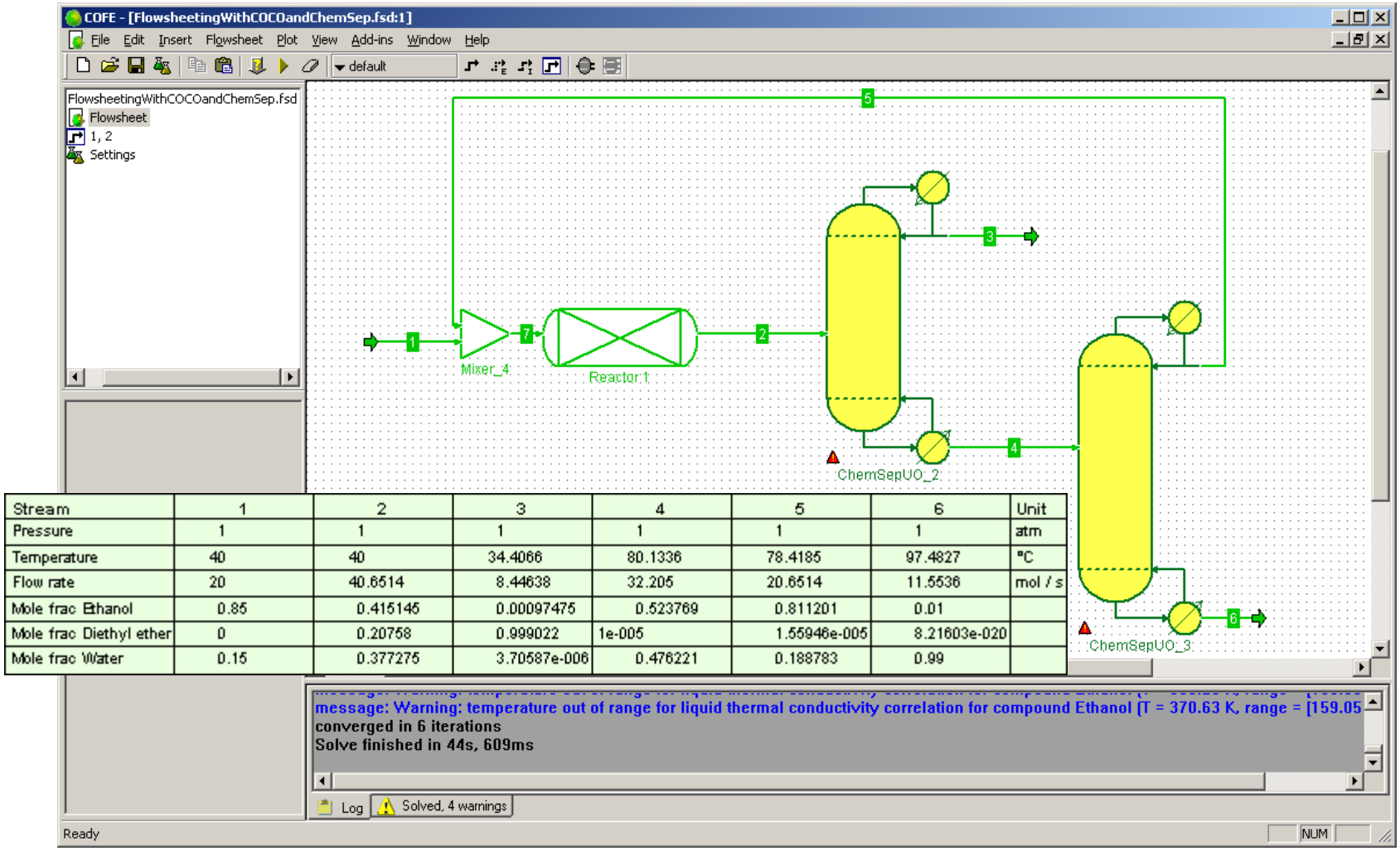
Modeling Separation Processes

The solution:



Stream	1	2	3	4	5	6	Unit
Pressure	1	1	1	1	1	1	atm
Temperature	40	40	34.4066	80.1336	78.4185	97.4827	°C
Flow rate	20	40.6514	8.44638	32.205	20.6514	11.5536	mol / s
Mole frac Ethanol	0.85	0.415145	0.00097475	0.523769	0.811201	0.01	
Mole frac Diethyl ether	0	0.20758	0.999022	1e-005	1.55946e-005	8.21603e-020	
Mole frac Water	0.15	0.377275	3.70587e-006	0.476221	0.188783	0.99	

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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
- …

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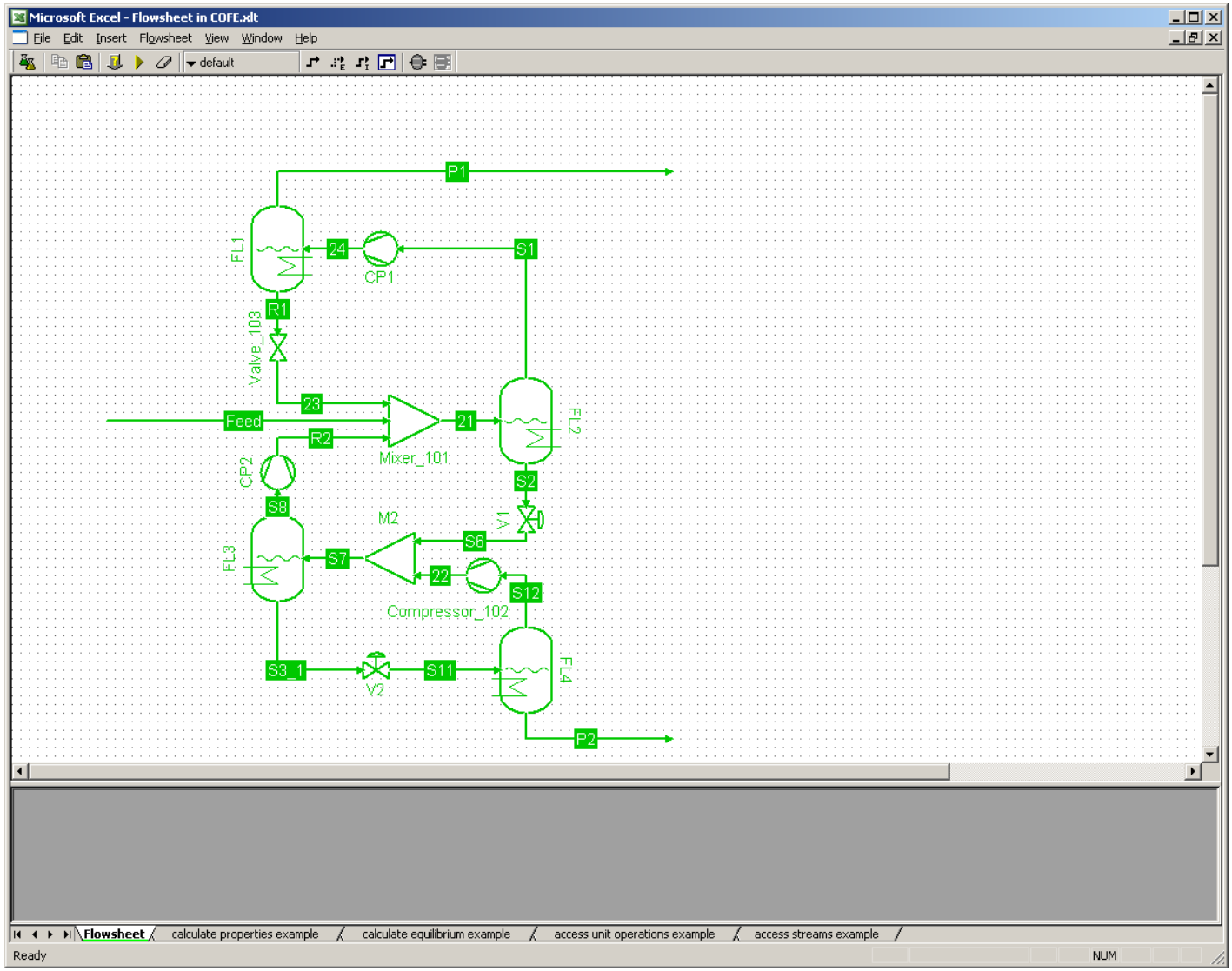
ChemSep
Modeling Separation Processes

Embedding flowsheets in Excel



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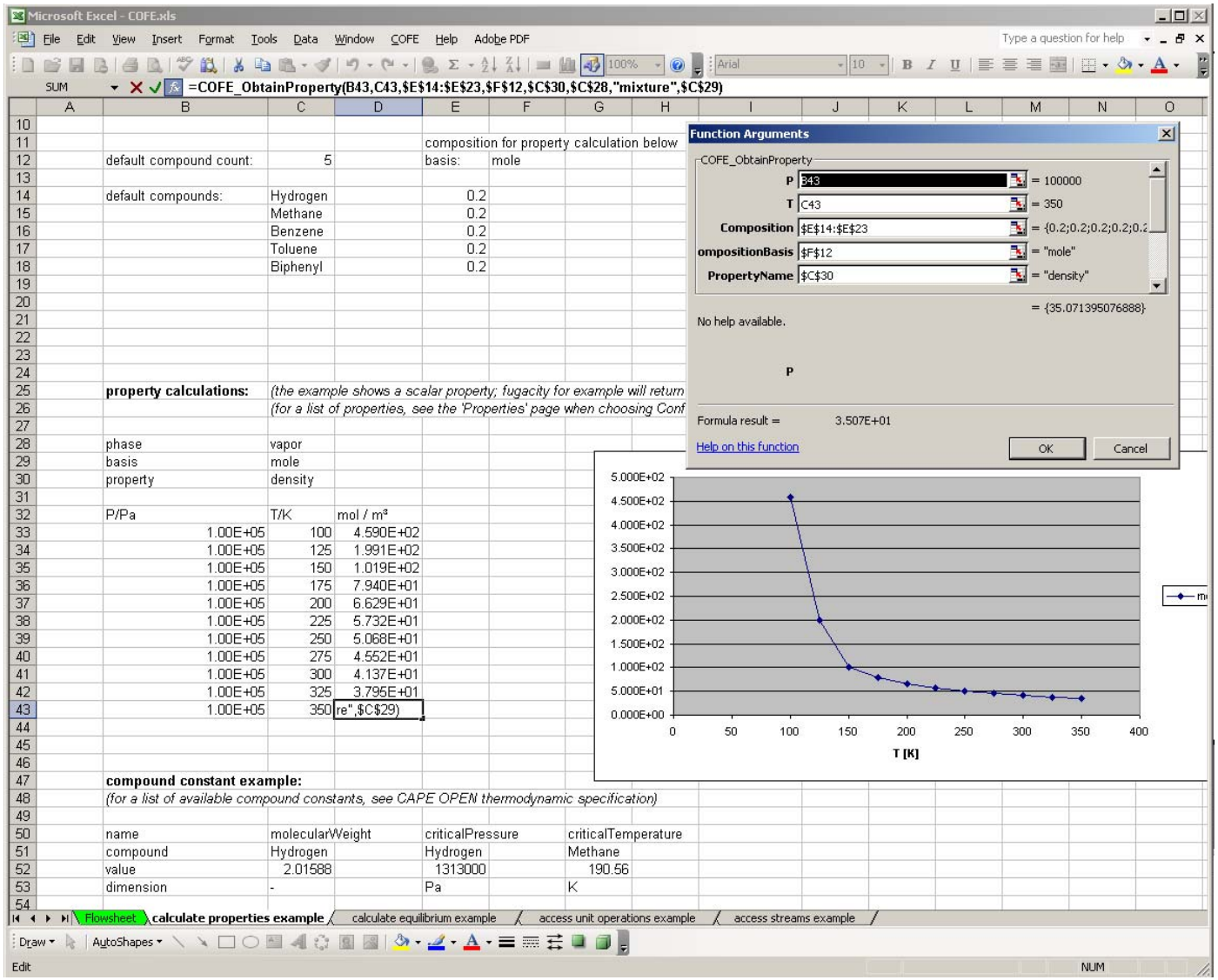
ChemSep
Modeling Separation Processes

Embedding flowsheets in Excel



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