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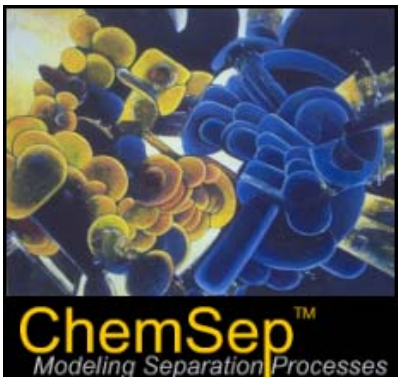
ChemSep
Modeling Separation Processes

Flowsheeting with

COCO and



Ross Taylor, Clarkson University

Jasper van Baten, AmsterCHEM

Rev5 – Apr 14 2010

Flowsheeting with COCO and ChemSep

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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

This presentation will provide an overview how to use the combination of ChemSep and COCO for simulation of steady state chemical processes.

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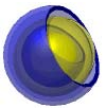
Introduction to COCO:

Simulation environment (COFE)

Thermodynamic property package (TEA)

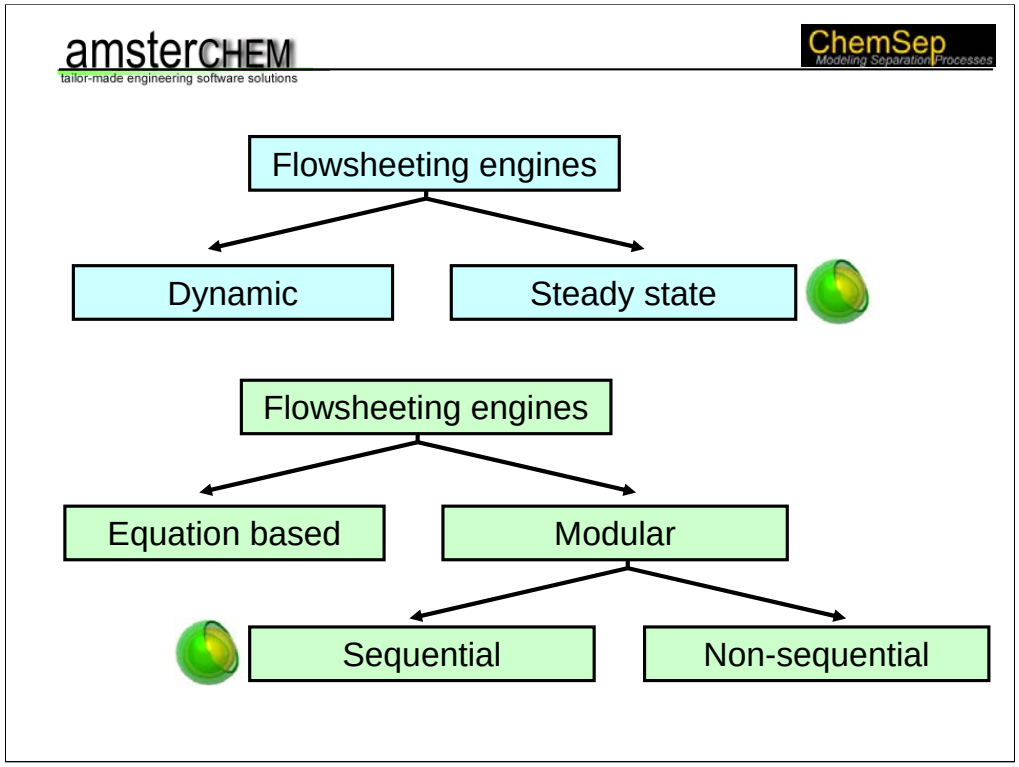


Collection of unit operations (COUSCOUS)

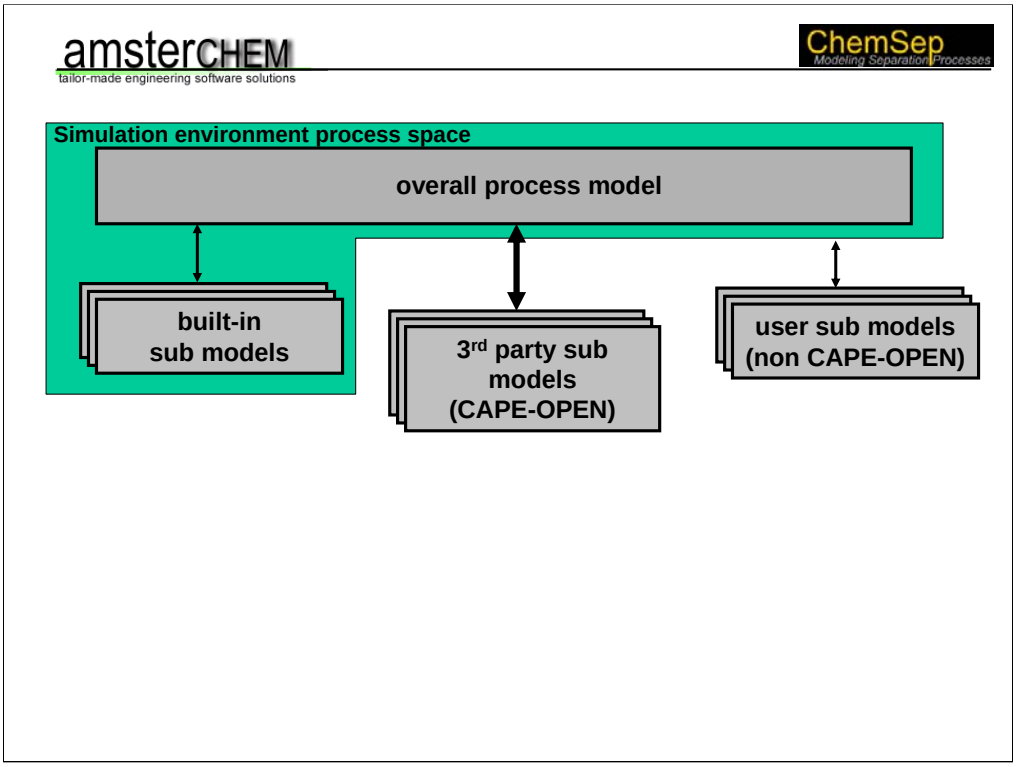
Reaction package (CORN)

… and utilities

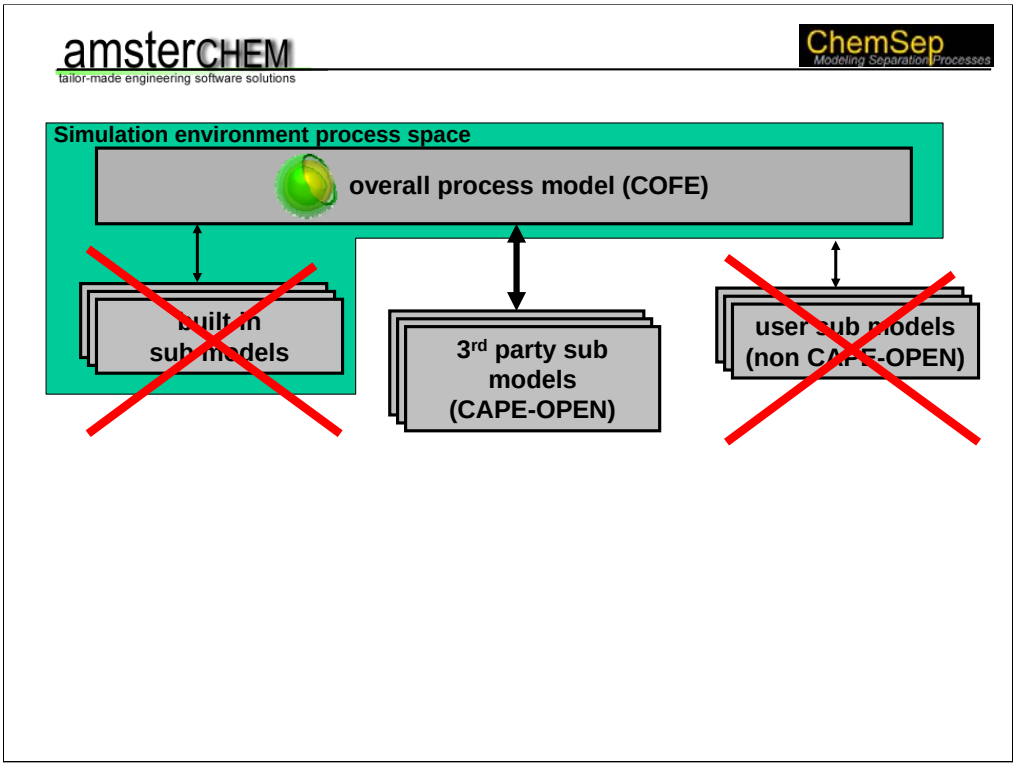
COCO is a collection of software components for setting up steady state chemical engineering flowsheet simulations. It consists out of 4 main components. The CAPE-OPEN flowsheeting engine is called COFE. The thermodynamic system is called TEA (Thermodynamics for Engineering Applications). The collection of unit operations that comes with COCO is called COUSCOUS. And then there is the CAPE-OPEN Reaction Numerics package: CORN. These are the 4 main components that will allow you to set up flowsheet calculations. The COCO distribution also includes the LITE version of ChemSep, and quite a few utilities. ChemSep will be discussed in detail later. The utilities are outside the scope of this presentation, but all are documented in the COCO online help.



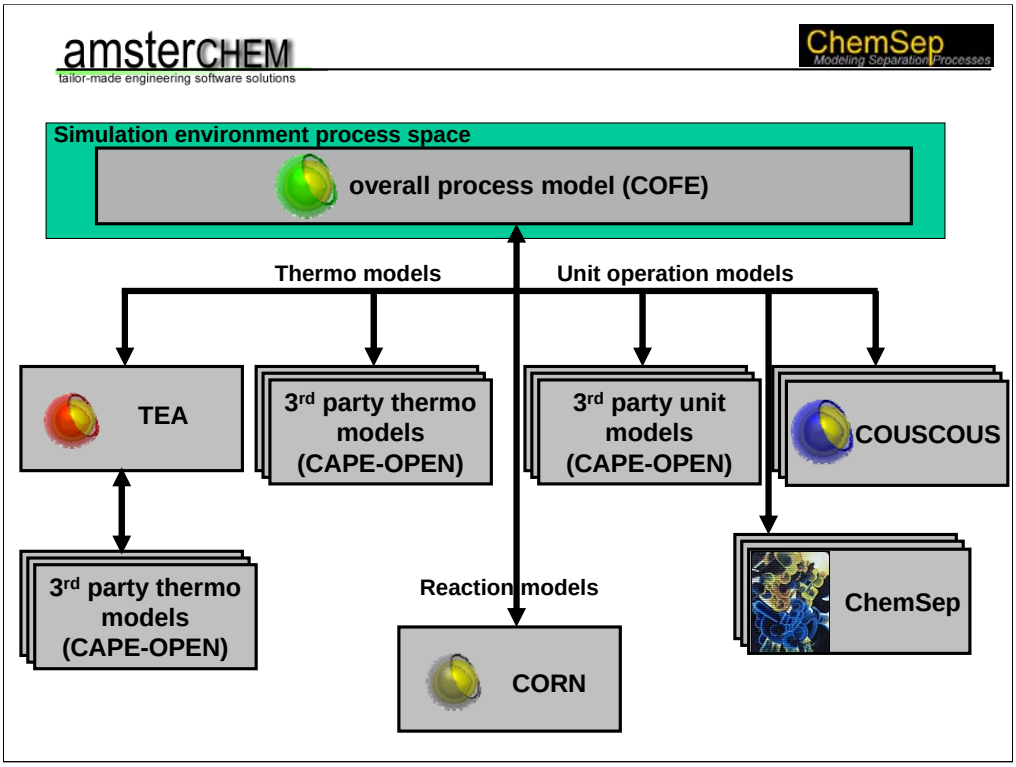
There are many steady state flowsheet engines available. Generally they can be divided into several categories. There are steady state flowsheeting engines versus dynamic flowsheeting engines. With dynamic flowsheeting engines the solution is time dependent. Here, we will focus on steady state simulations. Then there is the class of modular flowsheeting engines, versus equation based flowsheeting engines. For equation based flowsheets, the whole flowsheet (or independent sections thereof) translates to a set of equations that are solved simultaneously. In the modular approach, each sub-model in the process, e.g. a unit operation, is considered a black box, and recycles are solved by an iterative procedure. The modular flowsheeting engines can be divided in two more categories: sequential ones and non-sequential ones. COCO's flowsheeting engine COFE is a steady state sequential modular flowsheet system.



Often a flowsheeting environment is built up hierarchically as shown here. The overall process model – the flowsheet – runs in the application space, shown here in green. The flowsheet will require thermodynamic sub-models and unit operation sub-models. Typically, most of those are provided by the application, and these also run in the application space, as shown on the left. Most flowsheeting engines will allow the user to add user-defined sub-models, for example unit operations. Usually there is a proprietary way to allow the user to enter these models. More often than not this is accomplished by compiling Fortran modules that are specific to the flowsheet at hand. These models are shown on the right. Then there is a third category of sub-models: those that are CAPE-OPEN compliant. The interfacing of a CAPE-OPEN compliant sub-model does not use the flowsheet engine's proprietary interface, and therefore typically can be run in a variety of flowsheet simulation packages. This class of models is shown in the center.



COFE does not use built-in thermodynamic or unit operation models. Nor does it provide a proprietary way to enter user-defined models. COFE works only with CAPE-OPEN models.

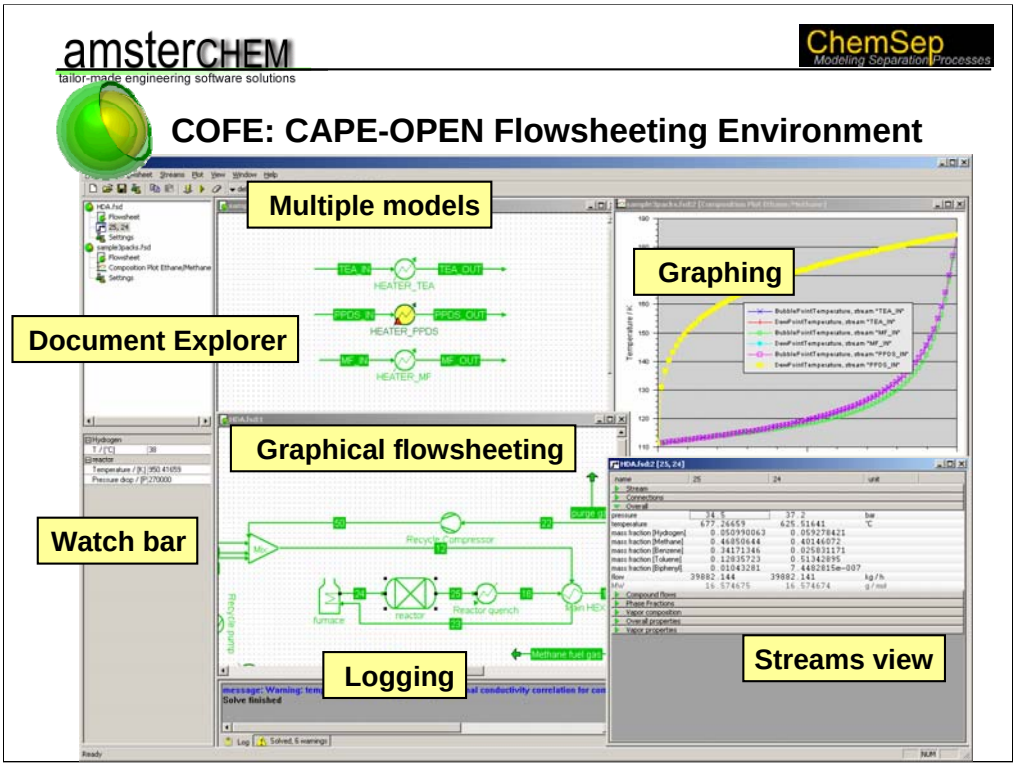


If we look at the most commonly used CAPE-OPEN sub-models, we can find thermodynamic models, unit operation models, and a class of models that allows for specifying reactions, e.g. stoichiometry, reaction rates, heats of reaction and so on.

COCO comes with the TEA thermodynamics package. You can choose to use this, or you can choose to use third party thermo models. You can even plug in third party thermo models in TEA to calculate the phase equilibria or specific properties.

For unit operations, the choices are the unit selections that come with COCO: COUSCOUS. ChemSep can be used to model many separation columns. There are also third party unit CAPE-OPEN compliant unit operation models around that can be used. An example here is the advanced heat transfer units of the specialists at HTRI.

Reaction models are only required when using COUSCOUS reactors. Currently there are not many such packages. The reaction package manager of COCO is called CORN. It will be briefly discussed.



Here we see a COFE screenshot. COFE can load multiple flowsheets, within a graphical user interface. Within one flowsheet, we can load multiple models. The example here shows a heater that is solved with thermodynamics of TEA and two other vendors. COFE comes with graphing facilities. Here we see the phase envelopes calculated using the three thermo models. If we edit one or multiple streams we get a stream view in which we can enter data in various ways and units-of-measurement of choice. The stream view does not only allow you to enter data, it will also immediately calculate the phase equilibrium on entering data.

The document explorer on the top left provides easy navigation through the open documents and document views.

The watch window allows quickly setting and inspecting variables of special interest.

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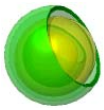

COFE: CAPE-OPEN Flowsheeting Environment

- 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

The techniques used in COFE are proven technology. Recycles are broken, and solved using either a Wegstein or Newton method, or a combination thereof. Reduced Newton methods like Broyden also are available. You can load multiple thermodynamic models, and assign them to different material types. You can also make material types using a sub-set of the chemical compounds present in a thermodynamic package. Other than material streams, we can work with energy streams – mostly heat streams – and information streams. Energy streams allow us to set up heat integration, and information streams allow us – for example – to use controllers (well – the steady state equivalent thereof).

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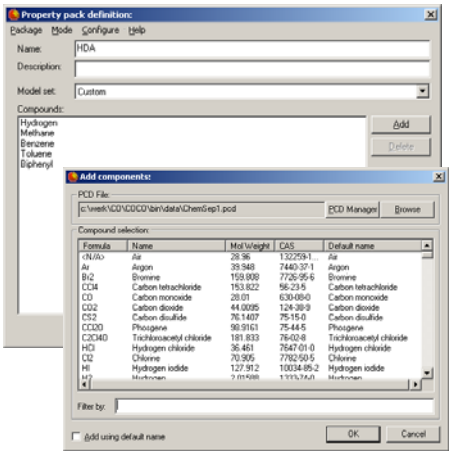
TEA: Thermodynamics for Engineering Applications

- **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 is the thermodynamics system that comes with COCO. It uses compound information that is compatible with that of ChemSep, and by default COCO ships with the compound data base that is ChemSep's. You can however extend this. You can for example use the DIPPR database, or you can use ChemSep's PCD manager to define your own compounds or download information from the NIST web site.

TEA contains more than a 100 property calculation methods, describing over 25 different properties. These property calculation methods are based on those of ChemSep, the COCO programmers had access to the ChemSep source code during the implementation, and the major part of the property calculation routines are very similar, if not the same. There are some differences in the calculations of chemical equilibria. TEA still uses the old ChemSep full Newton approach for equilibrium calculations as backup method, but ChemSep internally chose to use one algorithm to improve on equilibrium calculation performance and stability, whereas TEA took a different approach.

We can also use third party thermo to enhance TEA, by using them for external property calculations, phase equilibrium calculations or both.

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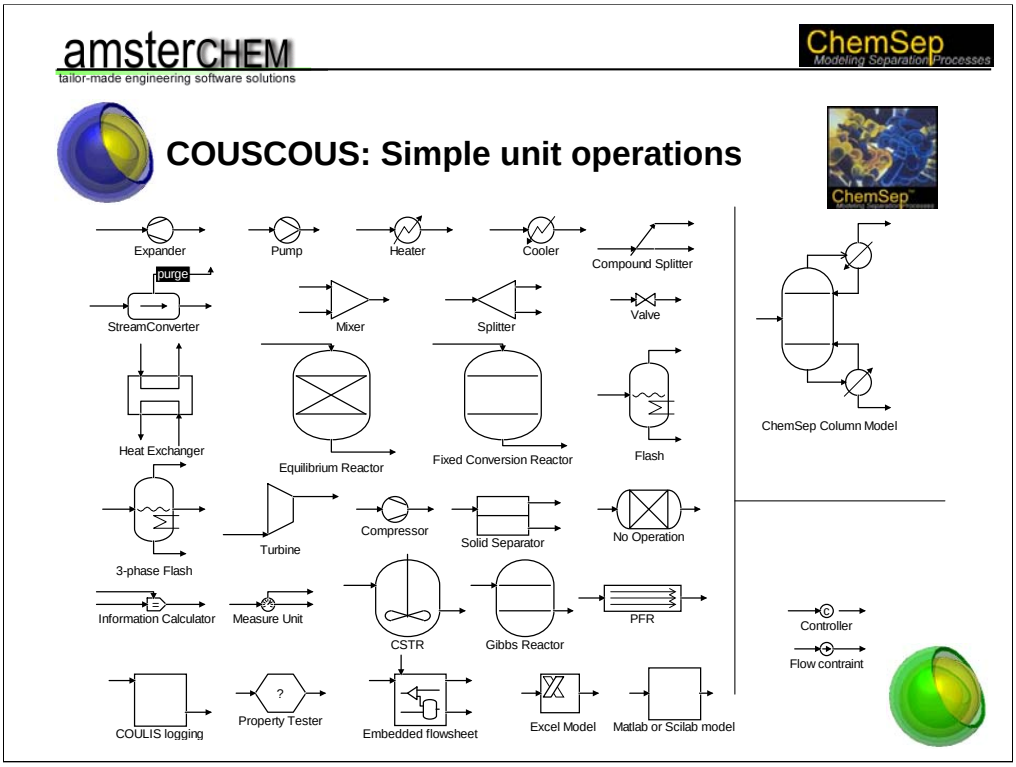
TEA: Thermodynamics for Engineering Applications

VLE equilibrium calculations

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

TEA supports a wide variety of flash calculations, for which it uses a Boston & Britt type inside-out approach. As a back-up it can use ChemSep's full Newton approach. The solutions are post-checked, for example by back-calculating enthalpy at the solution of a PH flash, and checking that against the specified enthalpy. COFE also carries out some back-checking of phase equilibrium calculations. The mass balance for each equilibrium calculation is checked by COFE.



COUSCOUS is the set of unit operations that comes with COCO. It comes with a range of the most common unit operation types, including pumps, compressors, expanders, heating and cooling devices, reactors, mixers and splitters. What COUSCOUS does not include is separation columns. For that, ChemSep is available. COFE does not come with built-in unit operations, with one exception. The controller unit operation and flow constraint unit operation are special cases, because it does not fit in the CAPE-OPEN framework of a sequential modular unit operation. This is because of the way it affects the flowsheet equations being solved.

You can also add third party unit operations and user unit operations to the mix, as long as they are CAPE-OPEN compliant. Examples shown are Excel, Matlab or Scilab models, but specialized CAPE-OPEN Unit Operation models are available from other vendors.

Notice how the unit operations come with graphical representations (which have nothing to do with CAPE OPEN). You can associate a default unit operation icon with each type of unit operation, or change the icon associated with a specific unit operation at will.

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- 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

COCO is available free-of-charge, from the cocosimulator.org web site. COCO has been written mostly by Jasper van Baten, from AmsterCHEM. He has also written the CAPE-OPEN interface of ChemSep..

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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

Now let us take a closer look at CAPE-OPEN, and why it is a good development for the chemical engineering simulation world.

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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

If we look up CAPE, you get different answers, depending on the source. Two of them are listed here. Computer Applications in Production and Engineering, or more commonly (and as specified in the CAPE-OPEN leaflet): Computer-Aided Process Engineering. OPEN we do not have to look up. In this context it means it is an interface specification that is freely available to everybody concerned, and everybody can contribute if they like. This is not the same as Open Source. Open Source deals with source code of software, and CAPE-OPEN is a set of interface definitions. It specifies how two pieces of software must talk to each other. CAPE-OPEN itself is not a piece of software.

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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)

From the CO-LaN leaflet, we can get this description about the nature of CAPE-OPEN: “The CAPE-OPEN standard is the de facto standard for interfacing process modeling software components for use in the design and operation of chemical processes. It is based on universally recognized software technologies, such as COM and CORBA. The CO standard is open, multi-platform, uniform and available free of charge.”. In practice, this means COM and not CORBA (since COM is limited to Microsoft Windows platforms).

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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)

The same CO-LaN leaflet continues with the following: “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 modeling software tools”. The text mentioned various software components, including numerical solvers, but in practice the implementations are limited to thermodynamic and physical property packages and unit operation implementations.

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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

Conclusion: we are talking about a set of interface definitions if we are talking about CAPE-OPEN. These interface definitions allow thermodynamic packages and unit operation models to be used in different simulation environments. The current status is that all major simulation environments come with CAPE-OPEN socket implementations. Unfortunately, not all of them are mature. The interface definitions are available in CORBA as well as COM. COM and CORBA are Common Object Models (this leaves the acronym of COM; CORBA stands for Common Object Request Broker Architecture). CORBA is used in the linux and java world, but is not as standardized as COM in Windows. So practical implementations at this point are restricted to Windows platforms, or WINE under Linux, Wine being a WINdows Emulation.

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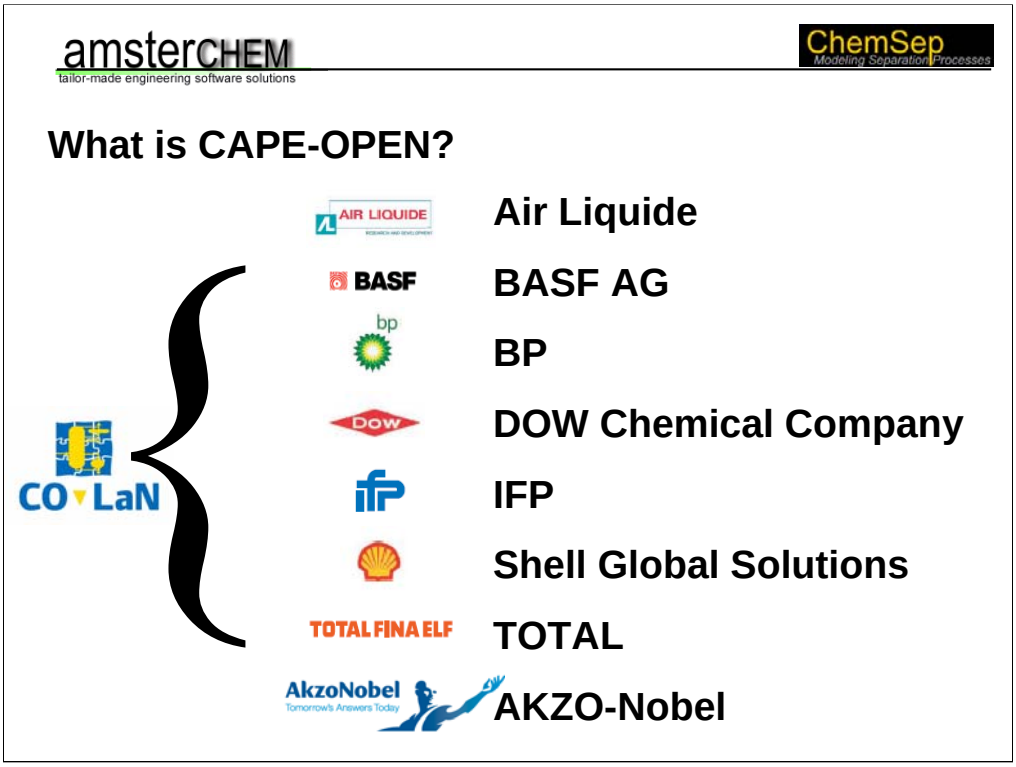
What is CAPE-OPEN?

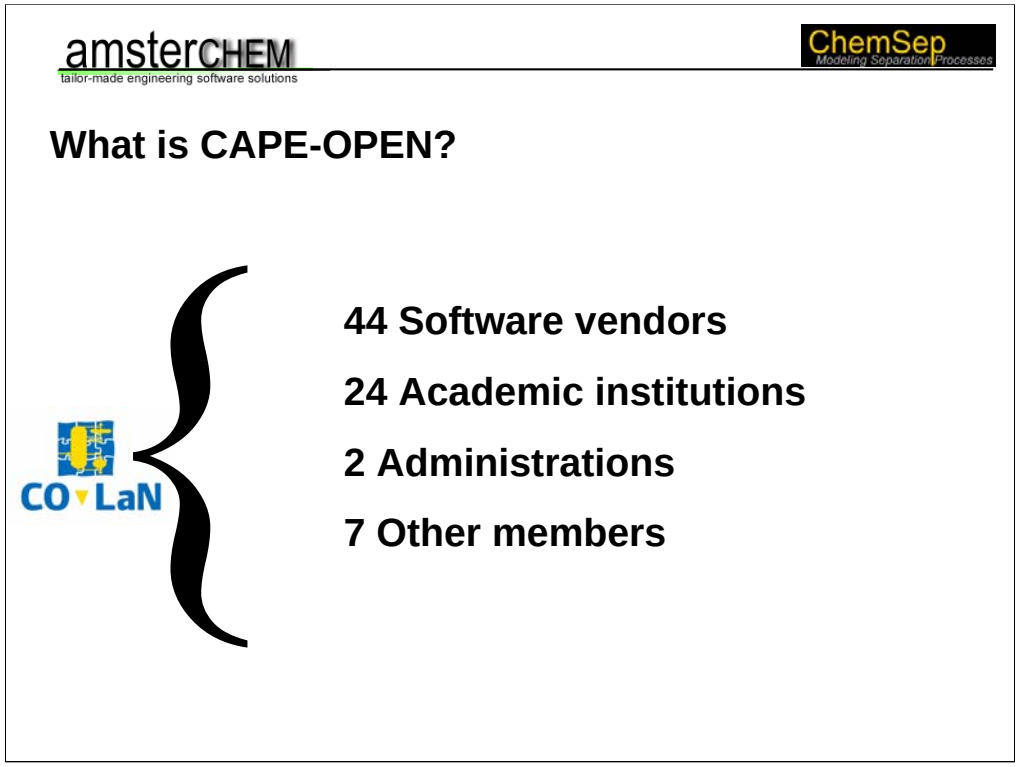
CAPE-OPEN Laboratories Network

http://www.colan.org/

The CAPE-OPEN interface standard definitions are maintained and published by CO-LaN: the CAPE-OPEN Laboratories Network. All the standard definitions can be downloaded from the www.colan.org web site.



CO-LaN has 8 paying members. Each full member pays EUR 10,000 per year. This supports the organization and technical management, the CO-LaN web site and the yearly Euro and US conferences (the latter being a topical at the AIChE annual fall meetings). If you are a paying CO-LaN member, you get to be on the board and you are involved in the decision making process of setting the strategy. On top of that, due to the nature of the interfaces, you have access to a lot of information on how to go about modeling chemical processes.



You do not have to pay to be a CO-LaN member. There are currently 44 software vendors (including the major simulation engine vendors), 24 universities, 2 adminstrations and 7 otherwise qualified members to CO-LaN. Together with the paying full members, the associate members have access to the CO-LaN member part of the web site. Both paying and associate members can take part in the Special Interest Groups, the so-called SIGs. This is where the standards are developed.

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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

CAPE-OPEN is becoming more mature and more widely accepted. This is for some good reasons. If you are a model developer, like ChemSep, you can write a CAPE-OPEN front-end to your model that allows you to run in multiple simulation environments. The opposite of course also holds: you do not trust the thermo of your current flowsheet setup? Simply replace it with thermo of another vendor. This way you can easily and affordably reproduce and validate your results.

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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

Before we can set up a simulation, we need to define the thermodynamic system we are going to use. We will be doing this in TEA. TEA is not the only option though.

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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

TEA comes with COCO. It is free of charge. The license is flexible and does allow for commercial use (validate at cocosimulator.org). TEA's property calculation routines are based on those of ChemSep. ChemSep has a long history of validation of thermo calculations. In inheriting most of its property calculation routines from ChemSep, TEA also shares in the validated results. As TEA is free of charge, it does not come with a guarantee. However, if you find problems with any of TEA's calculations, you can tell the developers. The feedback time to get things fixed is generally considerably shorter than with most other packages. Last but not least, TEA is highly configurable. We will get to that later.

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Reasons not to use TEA

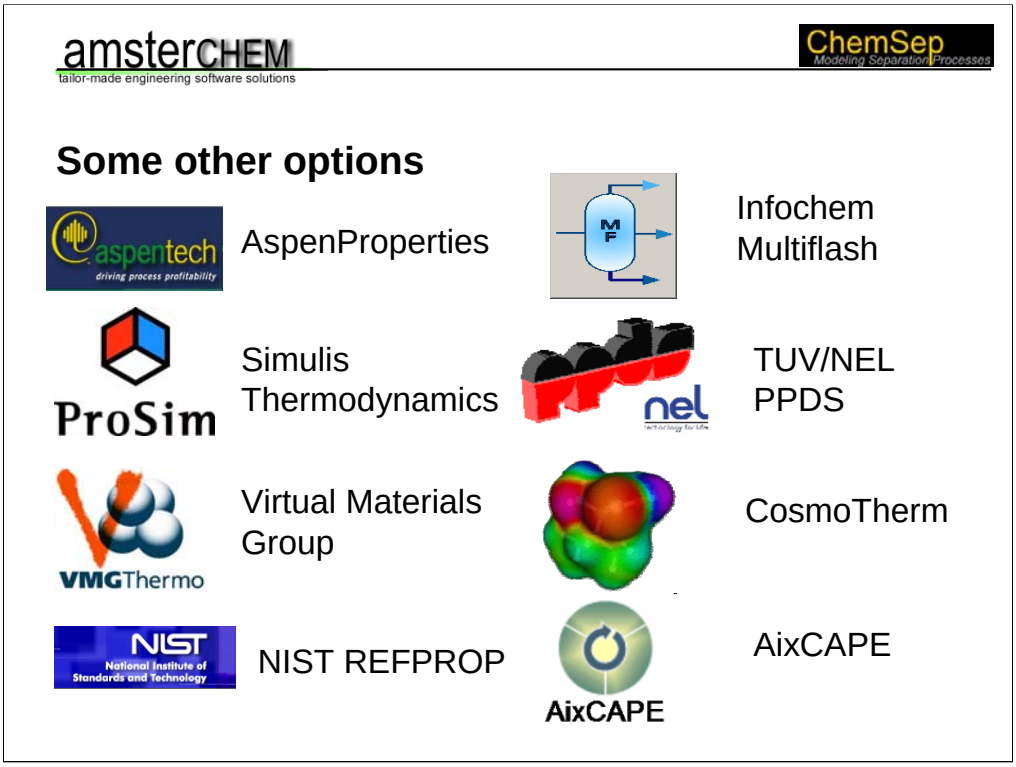
- TEA's equilibrium routines current restricted to V-L systems
- All CAPE-OPEN thermo is supported under COFE
- Validate your results
- Availability

As mentioned, TEA is not the only option. Any thermo package that is CAPE-OPEN compliant can be used in COFE to supply thermodynamics properties. One good reason to switch to another thermo system is the equilibrium calculation routines. If you are happy with vapor-liquid equilibria only, TEA is a good choice. Currently, it will not allow you to go beyond that, for example TEA will not calculate equilibria including solid or multiple liquid phases. This may change in the future though.

Another good reason to use different thermodynamic is because you have another package that you trust. If that package is CAPE-OPEN compliant it can be used in COFE. A good reason to do this is if you own licenses to thermodynamic calculation packages, or if you have in-house packages for special purpose calculations.

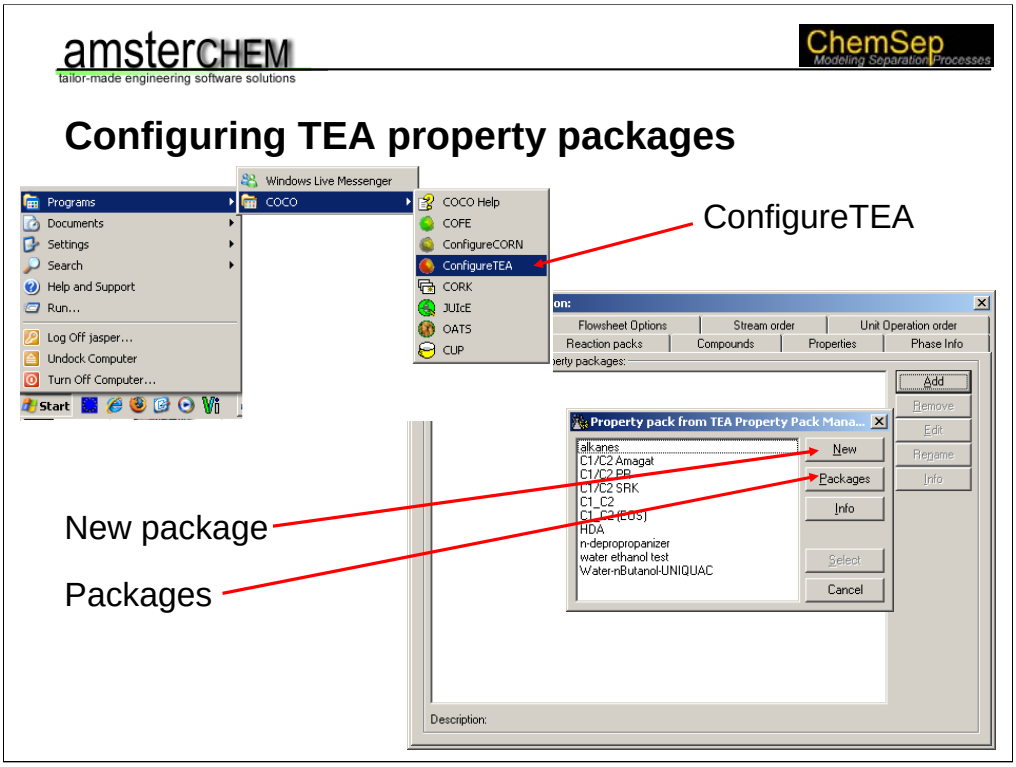
You may also want to switch thermodynamic packages to check the answers TEA is giving.

A last reason to use a thermodynamics package is simply because you can. Let's take a look at the alternatives.



This list of alternatives is not exclusive, but possible alternatives are – in no particular order – AspenProperties, or COM Thermo from AspenTech, Simulis Thermodynamic from ProSim, the thermodynamics engine of the Virtual Materials Group, Infochem's Multiflash, PPDS by TUV/NEL, AixCAPE thermo, and REFPROP by NIST. Various companies use in-house CAPE-OPEN compliant thermo.

Also packages that will give you access to specific properties can be used, in combination with TEA. An example is CosmoTherm by CosmoLogic, allowing a-priori activity coefficient calculations based on surface charge distribution considerations which in turn come from quantum chemistry calculations.



Back to TEA. Before we can use a property package, we need to configure it. A property package is a set of chemical compound definitions, property definitions, corresponding property calculation routines, and equilibrium calculation routines. All of this is pre-configured into a Property package, which you can subsequently load into your simulation. We can use two – equivalent – mechanisms to configure a TEA property package. We can use the utility ConfigureTEA from the COCO start-menu, or, we can go in COFE to the flowsheet configuration, select TEA for the system we want to use. At the point COFE shows us the available packages in TEA, it also shows a button labeled Packages. Both of these choices put us in the TEA configuration window.

Or we can directly create a new package from scratch using the New button

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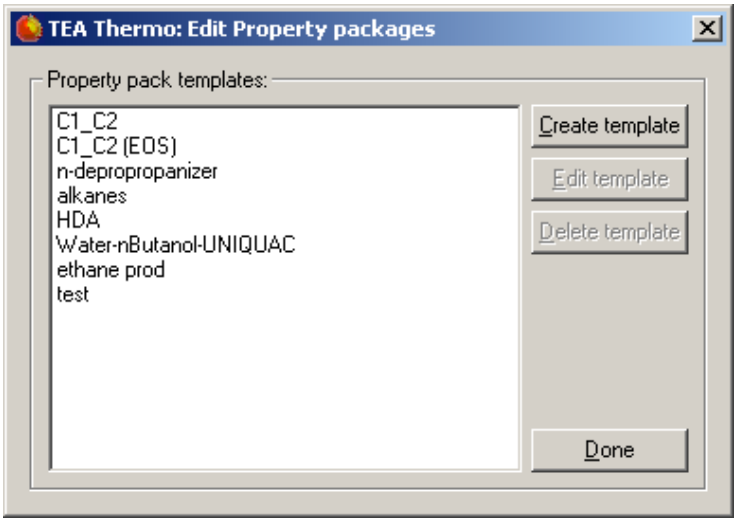
Configuring TEA property packages



This is what the TEA packages configuration window looks like. We see the packages that already exist. Notice the term templates. Actual TEA property package instances are stored within a COFE document. So inside a document you can change the compounds or property calculations of the TEA package used. The pre-configured property package templates are therefore called: templates.

In this window, we can change the definition of existing templates, but we are rather interested in creating our own. For that, we hit the Create template button.

If we are not interested in re-using the package, we do not need to create a template. Instead, we can directly use a new one-off package in our document by using the New button as shown in the previous slide.

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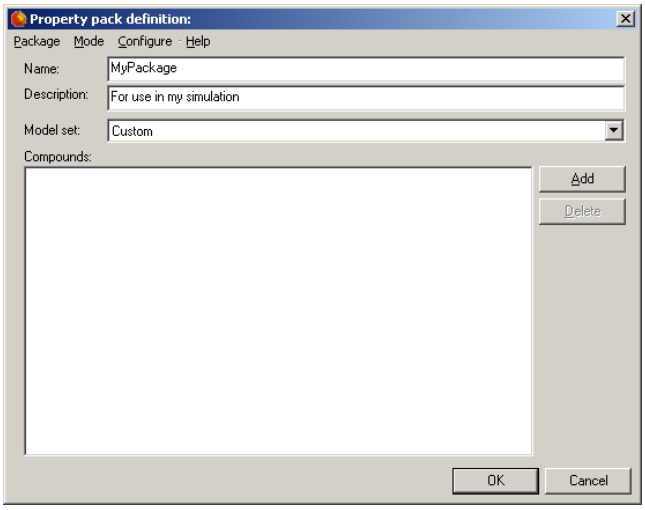
Configuring TEA property packages



The TEA package configuration dialog pops up. We first give our property package a name and a description.

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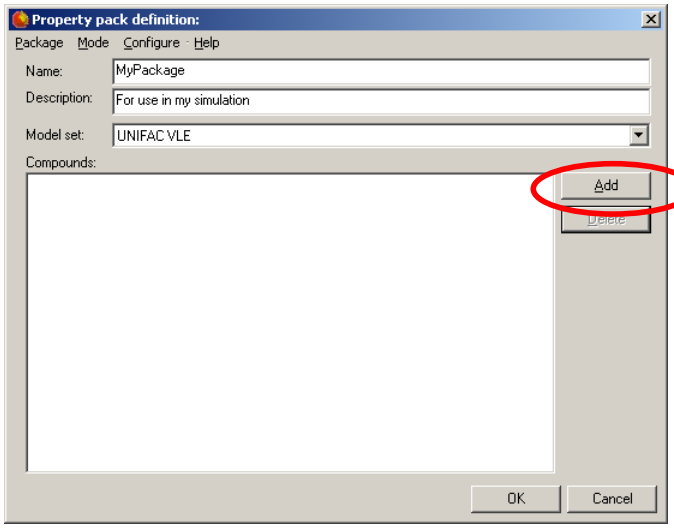
Configuring TEA property packages



We then proceed to add compounds to our package. We can add a compound by hitting the Add button.

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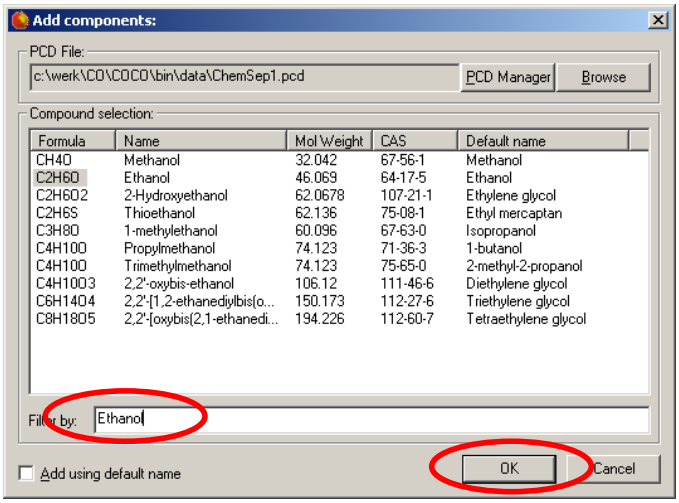
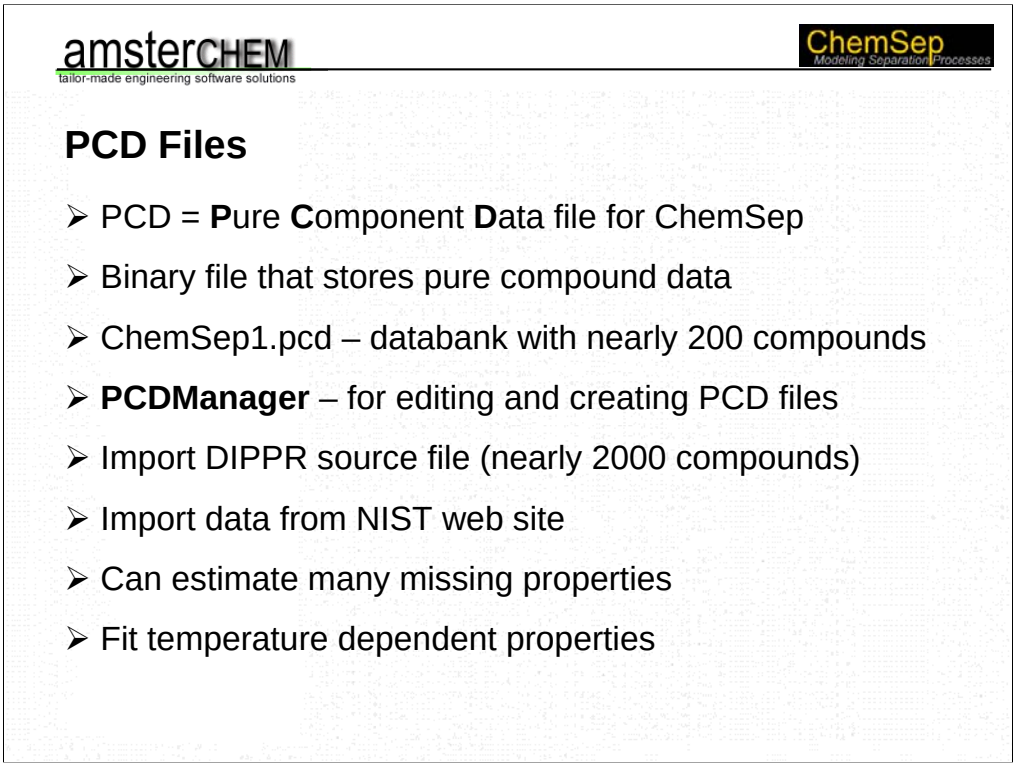
Configuring TEA property packages

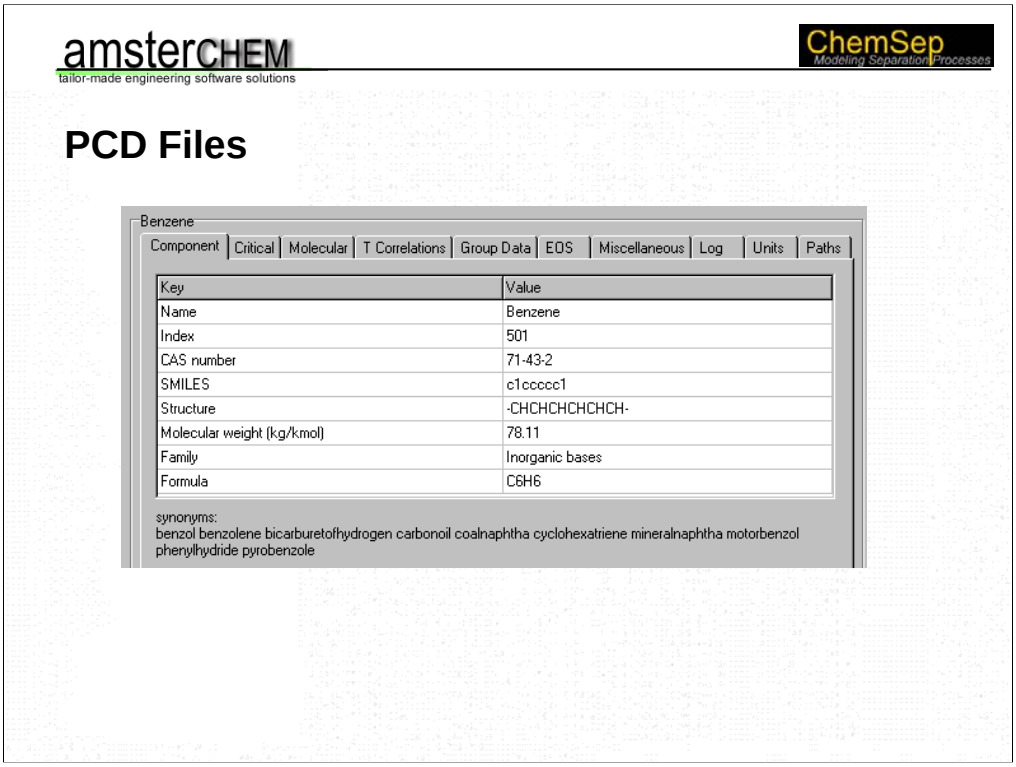


If we press Add, we get the a dialog from which we can load one or multiple compounds. We can search for our compounds by putting in a formula, a CAS number or part of the compound name. Here we have entered “Ethanol” which gives several partial matches and one exact match, which is automatically highlighted. Click OK to add.

Compounds are loaded from PCD files (PCD stands for Pure Compound Database). By default, the ChemSep PCD file is selected.



PCD files are Pure Component Data files. They contain chemical compounds, and for each chemical compound, properties like formula, name, critical pressure, as well as coefficients to correlations for property calculations. The PCD file format is binary, but ChemSep (LITE) comes with a package to edit and compile PCD files; the PCD manager. From here, you can manage you compounds, import NIST data, DIPPR data, estimate properties, fit coefficients to measurements, and more.



The *Component* panel displays the most basic information about the compound, its name, index number (usually this is the index number assigned by DIPPR), its CAS number, SMILES string, structural formula, molecular weight, family (from the DIPPR list) and formula. The formula is constructed from the structural formula and cannot be entered from the keyboard. With that sole exception all of the other entries can be altered simply to clicking in a cell to the right and typing a new entry. To accept a new entry press *Enter* or click in another cell.

At the foot of this tab page is a list of synonyms for the compound on display. These synonyms are from the file chemsep.syn that is located in the pcd subdirectory. This is a plain text file that can be edited using a text editor (such as Notepad, but not Word).

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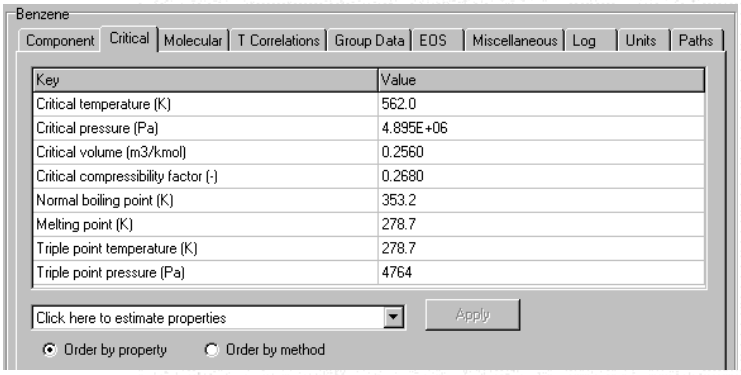
PCD Files



This panel displays some of the most important properties, namely the critical constants, normal boiling point, melting point, and the triple point temperature and pressure. The critical constants are needed in any application of an equation of state to estimate thermodynamic properties.

Note the white line near the foot of this panel that says *Click here to estimate properties*. As this line suggests, you can click here to obtain estimates of the various properties that are listed on this panel (the same opportunity to estimate properties is available on several other panels). This ability to estimate missing properties is one of the most valuable aspects of PCDmanager.

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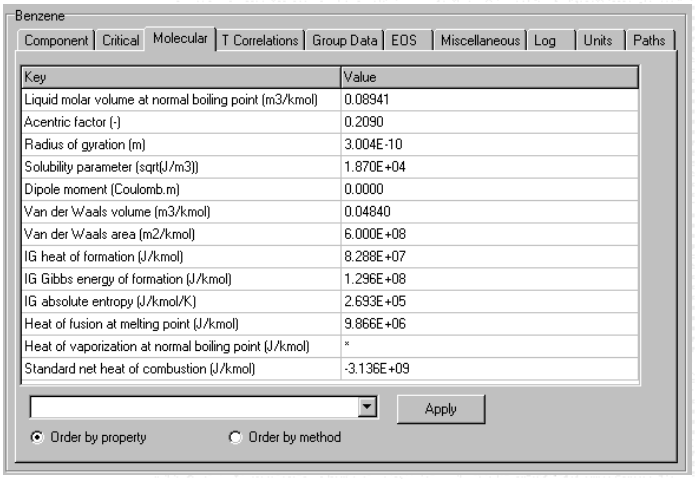
PCD Files



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

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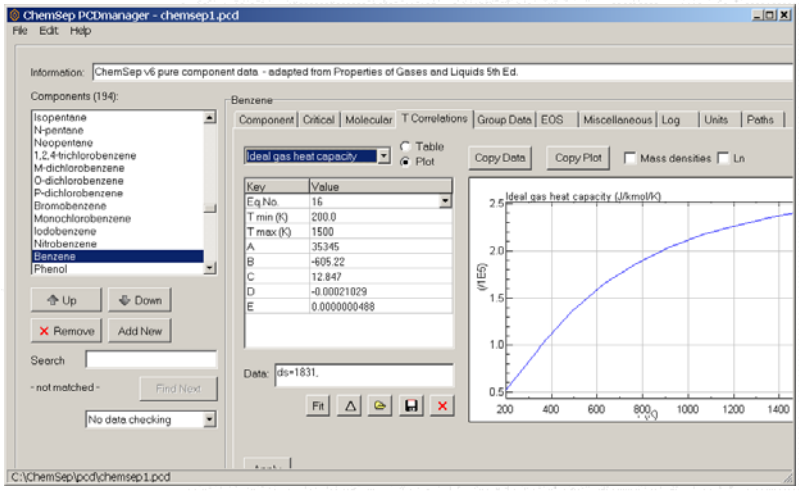
PCD Files



PCD files also contain constants for temperature dependent properties like density and viscosity.

Later versions of PCDManager will also be able to fit pure component property data to a wide range of correlation equations.

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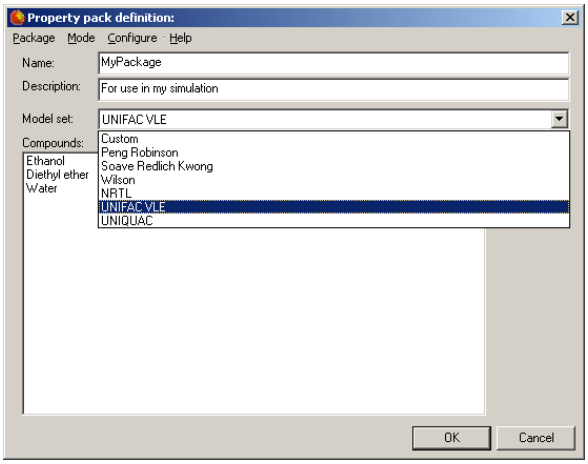
Configuring TEA property packages



Back to TEA. When we are done adding compounds (Ethanol, Diethyl ether and Water) to our property package, we can proceed with configuring the properties and models. For this particular example we will select the UNIFAC VLE model set. This will automatically configure default properties and calculation methods. We can inspect and change these if we like, by using the advanced configuration mode of TEA, which we can access via the various sub-menus of the Configure menu.

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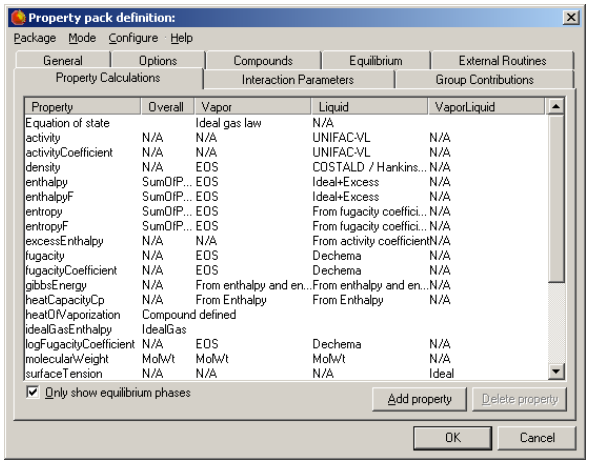
Configuring TEA property packages



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.

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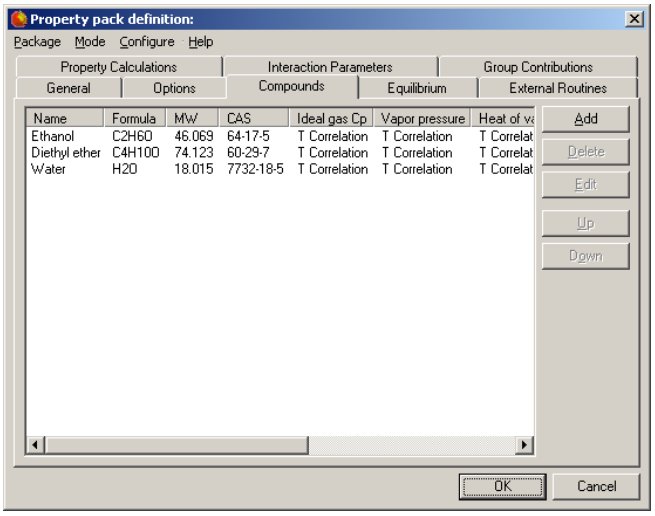
Configuring TEA property packages



Notice that 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.

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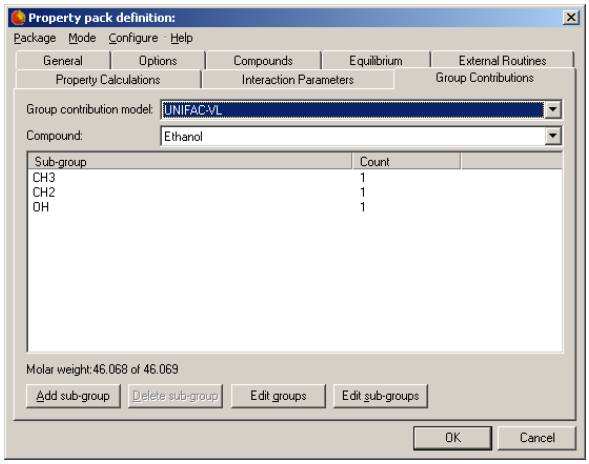
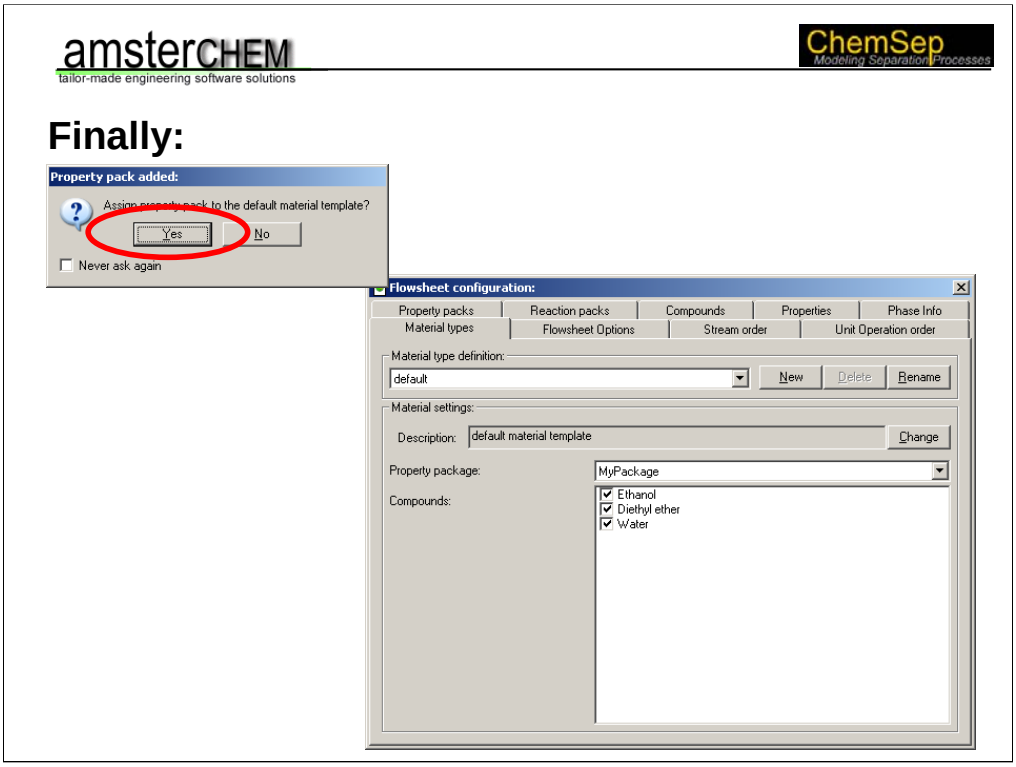
Configuring TEA property packages



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.



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.

On the Material Types tab we then see that the default material is associated with MyPackage and defined by compounds Ethanol, Diethyl ether and Water.

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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

We have prepared our thermo package, now we need to go to the next step. Setting up the flowsheet. For this, we start COFE.

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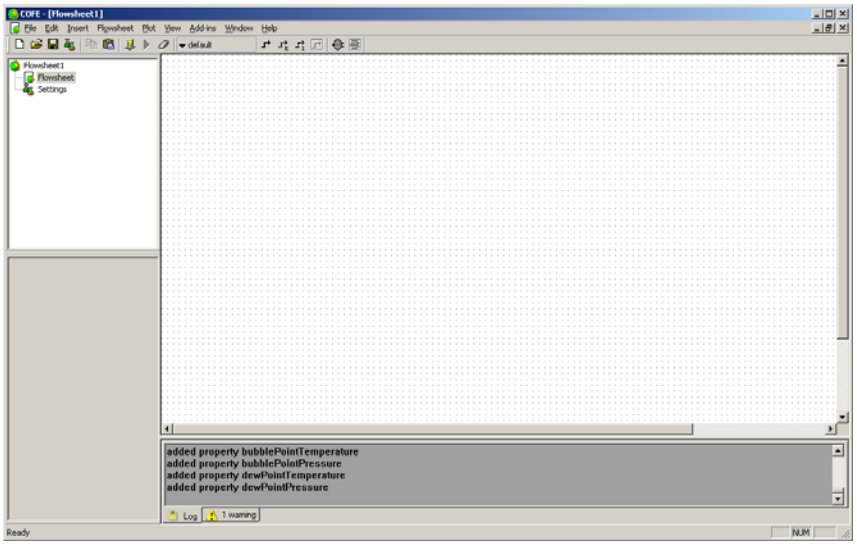
Empty COFE document



Time to make a flowsheet. After inserting the property package, we have an empty flowsheet in front of us. We see a couple of things.

A toolbar with the most common functions. An empty grid in which we can make our flowsheet. And in the bottom we see the log for the flowsheet document. If something goes wrong, it will appear in the log. It may be useful to keep an eye on the log from time to time. In addition to the log, there is an errors and warnings pane that will show the currently active errors and warnings. Currently it has one warning: “Flowsheet is empty”.

On the top left, we see the document explorer. This allows us to easily navigate through the open documents and document views. The watch window in the bottom left we can use later on to add variables of interest.

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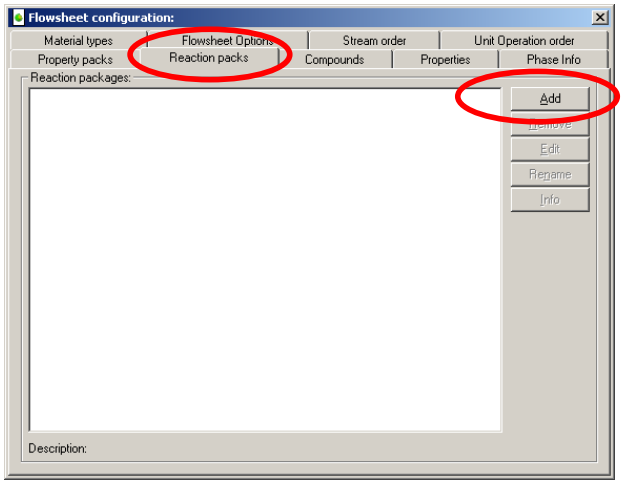
Setting up reactions



We are going to use reactions in our example. Much like using thermodynamic property packages for our thermodynamics, we need to use a reaction package for setting up our reactions. A reaction package is just another CAPE-OPEN component. We go to the flowsheet configuration page (hit the toolbar button, hit Ctrl+K or select Configure from the Flowsheet menu; or hit Settings in the Document Explorer). On the reactions page, we see no reaction packages have been aded.

Hit the Add button to add one.

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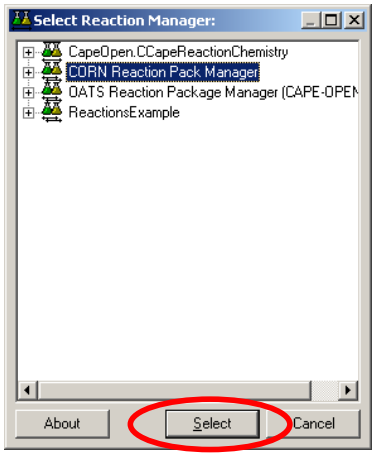
CORN: CAPE-OPEN Reaction Numerics



We have seen that TEA Is the thermodynamic property package manager that comes with COCO. CORN is the Reaction Manager that comes with COCO. Let's use it. Select it and hit OK.

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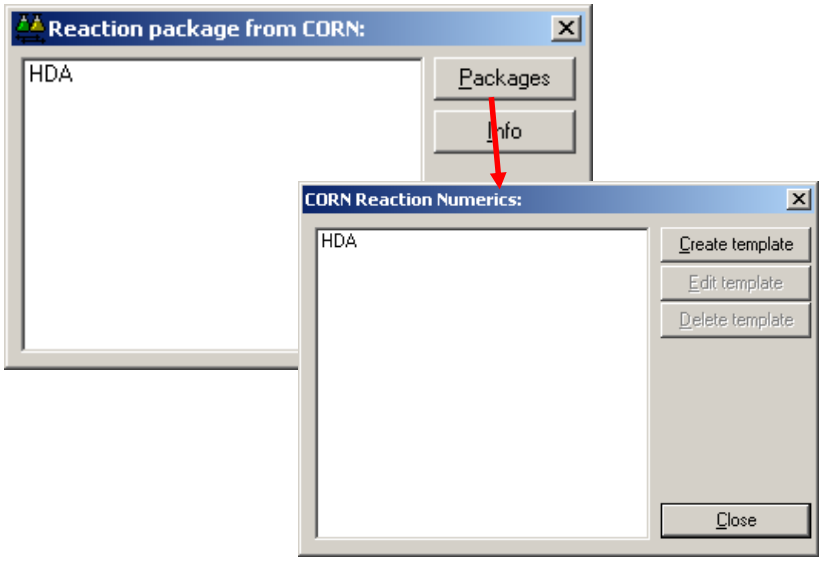
Setting up CORN



We will see the CORN reaction package manager show up with a list of all reaction packages that are defined. We want reactions from Ethanol to Dimethyl Ether, which is not there yet. Hit the Packages button to configure a new package. This will show up the CORN Configuration window. You can also access this by choosing ConfigureCORN from the start menu.

For the purpose of our flowsheet we need a new reaction package template. Reaction packages in COFE are saved with the flowsheet document. A reaction package template is used to create a reaction package from. Once the reaction package is in the document, you can modify it and the changes will be saved with the flowsheet. These changes will not affect the template.

We will however start with a template. Hit Create Template please.

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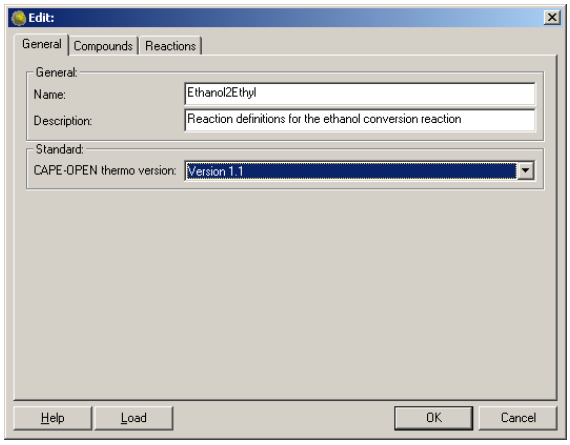
Editing a reaction package (1/4):



First, create a name and description for the reaction package template.

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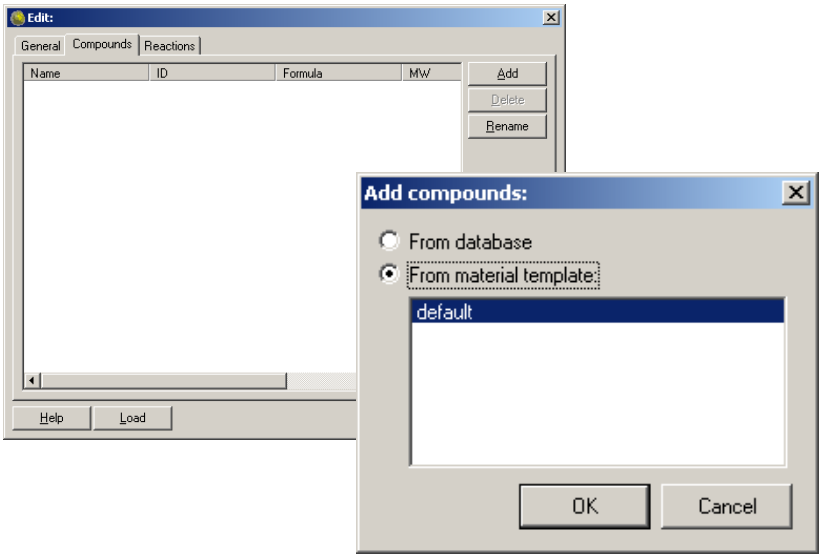
Editing a reaction package (2/4):



Then we add the compounds. Hit Add on the Compounds page. As we are currently running inside a simulation, we may as well take advantage of it and use the compounds that are defined in the simulation. So choose a material template as the source for compounds and hit OK.

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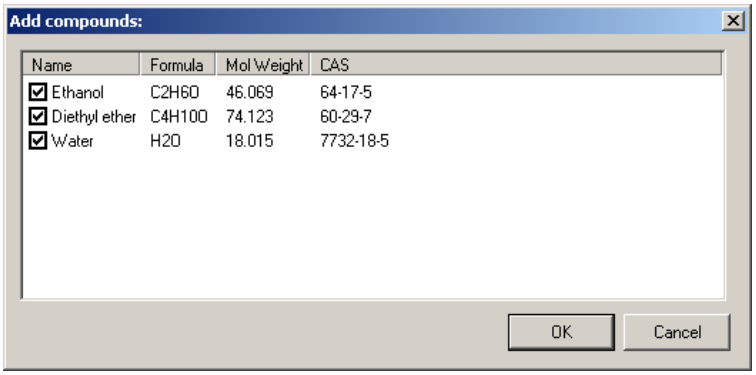
Editing a reaction package (3/4):



All the compounds in our simulation will take part in the reaction. Select all of them and hit OK.

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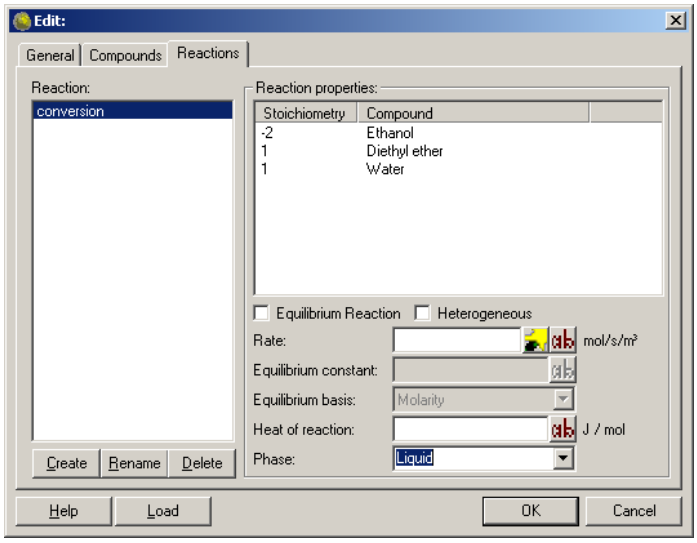
Editing a reaction package (4/4):



All that remains is to define the reaction. On the reaction page, click Create. We choose ‘conversion’ for the name of our only reaction. The default stoichiometry is 0 for all compounds. We change this in the proper amounts: 2 ethanol will react to 1 Diethyl ether and 1 water molecule. So -2 for ethanol, and 1 for the others. We select the reaction phase to be the liquid phase. We will be performing our reaction in a very simple reactor in which we specify conversion, so currently we do not have to fill in a reaction rate, equilibrium constant or heat of reaction. Hit OK to accept the new property package definition.

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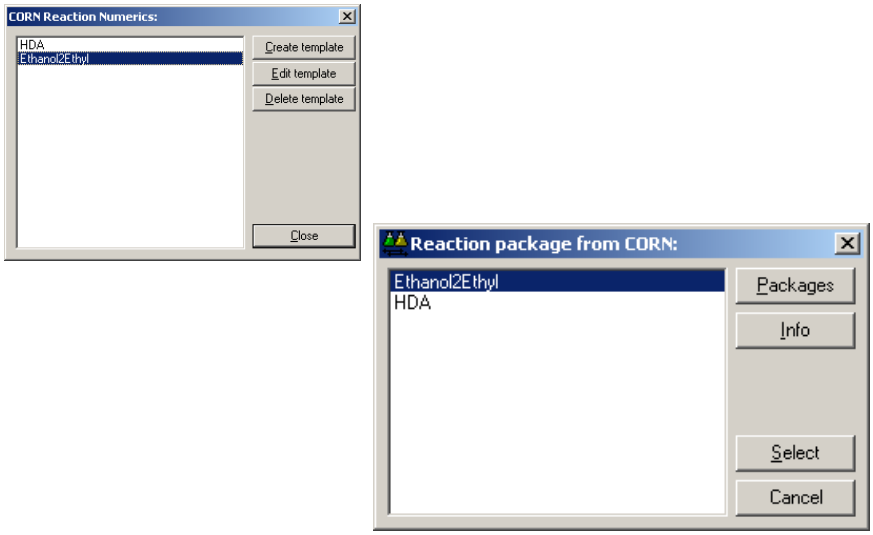
Add it to the simulation



We are now back in the list of reaction packages that are defined. Our new package shows up. Hit close as we are done configuring packages. That puts us back in the window to select a package. Select our new package and hit Select.

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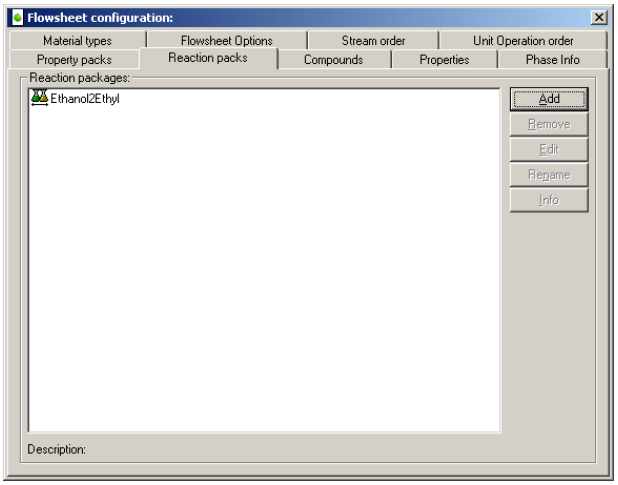
We have a reaction package:



As we return to COFE, we see that the new package has been added. Our flowsheet configuration is now complete, and we can close this window.

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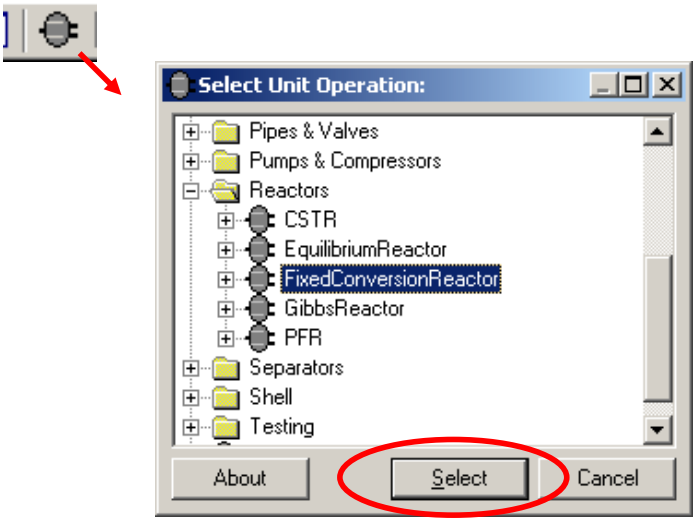
Inserting our reactor:



We are now going to insert our reactor. Start by going to the Insert menu and select the Unit Operation item to bring up this list. Or hit the Insert Unit Operation button on the toolbar. This list shows the main categories of unit operation. Click on a + sign to see an expanded view of the options under each category. From the reactors category, there are several reactors to choose from. We will use a very simple reactor model, one in which we specify the conversion of a given compound. In our case that will be ethanol. we select the FixedConversionReactor. Hit Select to confirm.

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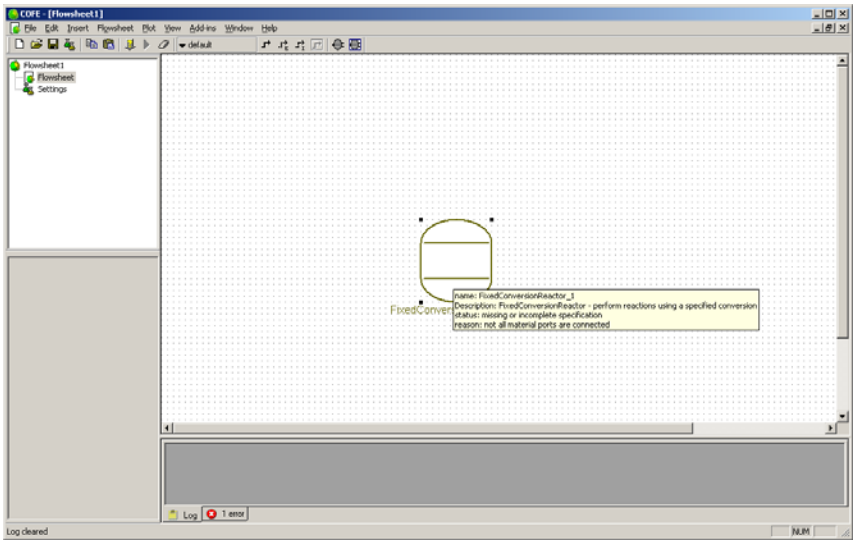
Inserting our reactor:



We can use the mouse to place the unit operation somewhere in the flowsheet.

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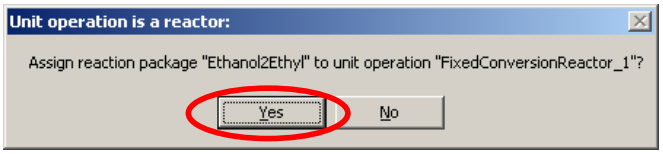
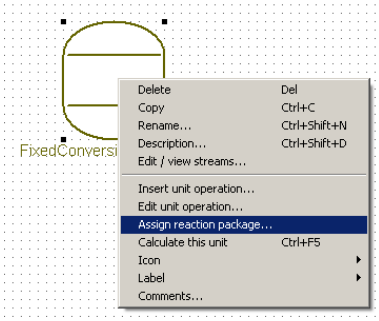
Inserting our reactor:





As the unit operation we have just inserted is a reactor, it will need to know about reactions. We have previously added a reaction package, and as this is the only reaction package in our simulation, COFE will ask us if we want to use that reaction package for our reactor. We do, so we choose Yes. We can at any point assign a different reaction package to our unit operation. We do this by clicking on the unit operation with the right mouse button, and select Assign Reaction Package.

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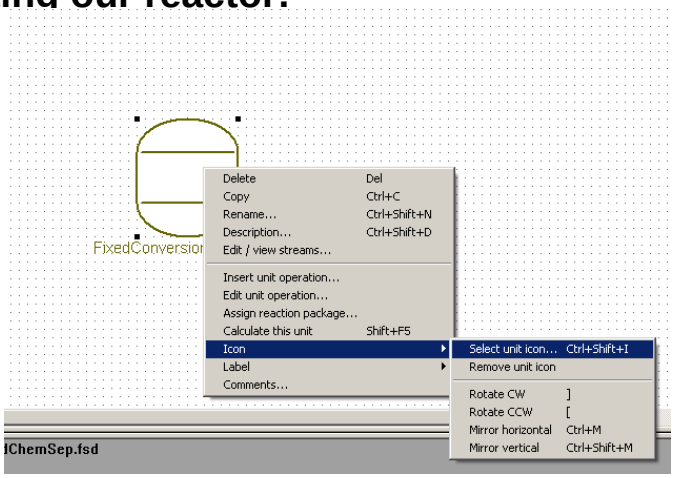
Inserting our reactor:



We can also change the appearance of the reactor. Right click on the reactor to pop up the unit operation menu. From the Icon sub menu, we can pick Select Unit Icon.

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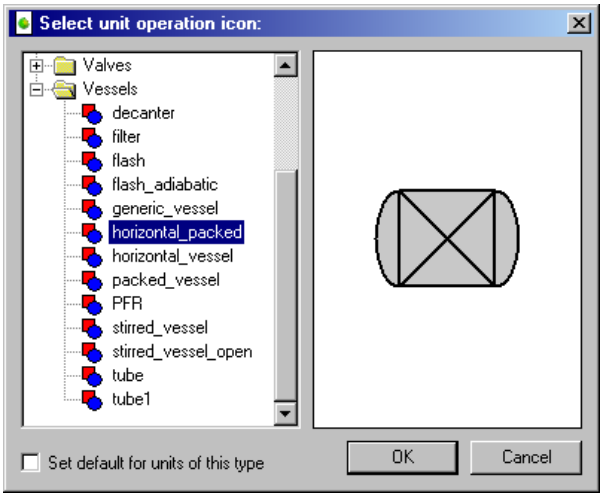
Inserting our reactor:



We want a horizontal layout in out flowsheet, so we select vessels, and assign the horizontal_packed icon to the reactor. Click OK.

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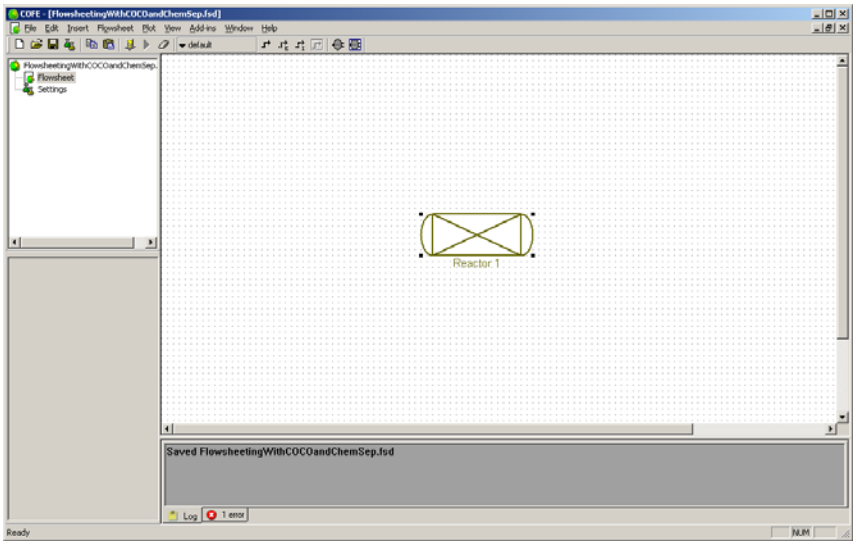
Inserting our reactor:



We can rename the reactor (pick rename from the right mouse button menu) to Reactor 1. We can use the mouse to stretch the reactor a bit, and we will end up with a view that looks like this.

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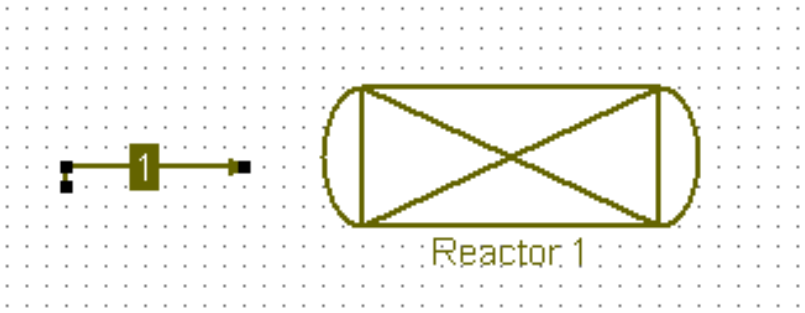
Inserting the reactor feed:



The next step is to add a feed to and product stream from the reactor.

To add a stream go to Insert and select Stream (or hold Ctrl-I or click on the stream icon on the icon bar below the main menu line). The cursor will change in a cross. Locate the cross where you want the stream to start and click on the mouse button. Then locate the mouse somewhere else (the temporary end of the stream) and click again; a numbered line should appear on the flowsheet.

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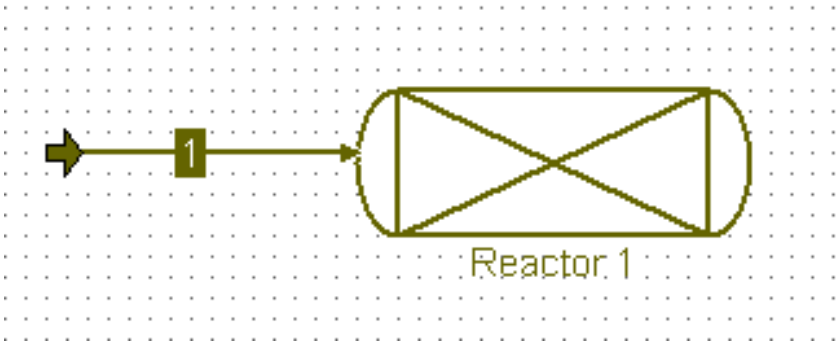
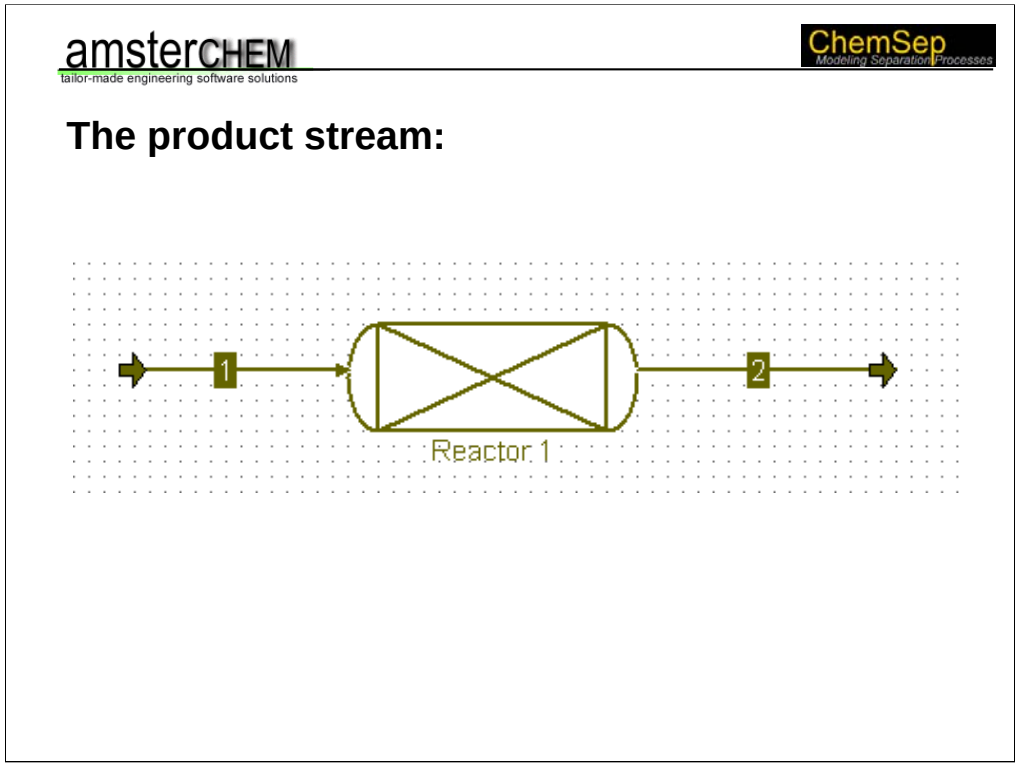
Connecting the feed:



To connect this stream to the reactor simply use the mouse to grab hold of the arrow end and drag it towards the reactor; when the arrow touches the reactor it will turn red. Release the mouse button and the stream will be attached to the reactor as shown below. If we select Feed and Product Indicators from the View menu, the feeds and products are clearly indicated by a larger arrow head.



Add another stream in the same way as before; drag the end of the stream arrow to the right hand side of the reactor to connect it. This will be recognized as the product stream.

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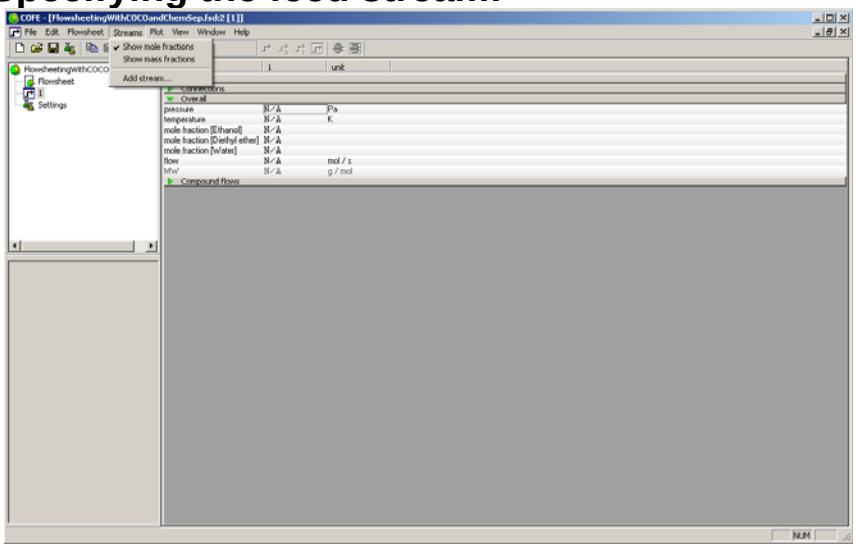
Specifying the feed stream:



To enter the details about the feed stream, double click on stream 1. A stream view will show up. We have all the details about the feed available to us in the process description. Click on any field that shows N/A and type in the appropriate values. The units can also be changed by clicking on them. Notice that by default mole fractions will be shown. Use the Streams menu if you prefer mass fractions. This choice applies to both compositions and phase fractions.

The new view will show up in the document explorer on the left, indicated by title “1” as this view is only showing stream 1. We can either close the stream view, or leave it open. If we click on the Flowsheet view in the document explorer, we will switch to that view.

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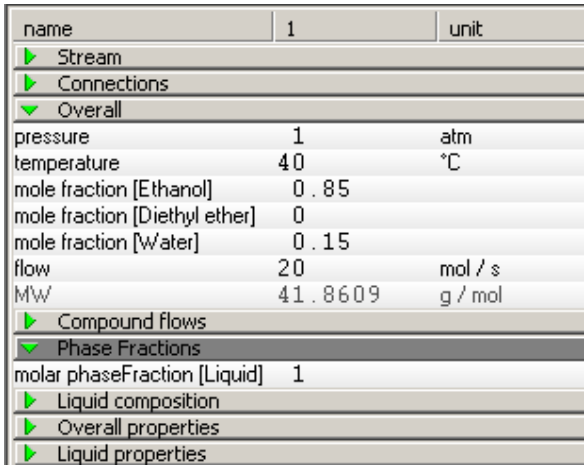
Specifying the feed stream:



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		

We change the units of measure to atm for pressure, centigrades for temperature. We enter 1 atm for pressure, 40 C for the temperature. We enter a mole fraction of 0.85 for ethanol. Right click on the water composition and choose Remaining. This will also fill in the missing number for diethyl ether. We specify a 20 mol/s flow and end up with the specification as shown here.

The stream specification at this point is complete. This will signal COFE to flash the stream. If we unfold the phase fractions section, we see that the stream is all liquid. We also notice some numbers are displayed in gray and some in black. The black ones we can modify, the gray ones are results of the equilibrium calculation. See that the liquid phase fraction is black. If we would click on it, we can perform a vapor phase fraction flash, either keeping the temperature or the pressure as specified.

The feed stream specification is now complete and we can turn our attention to the reactor itself.

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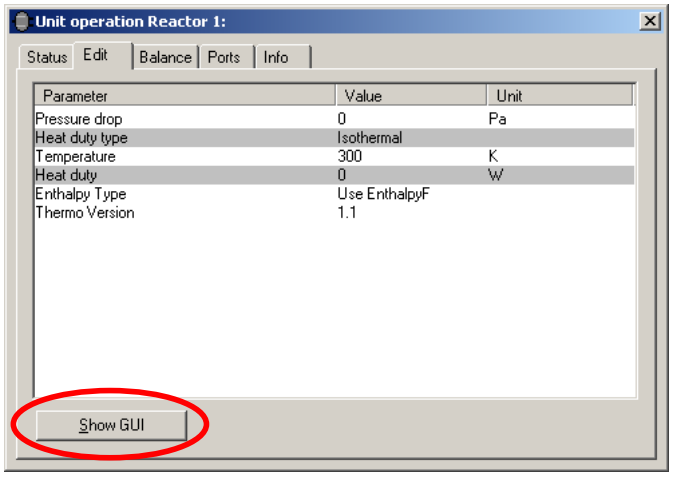
ChemSep
Modeling Separation Processes

Reactor specifications:



Switch back to the flowsheet view, and double click on the reactor to bring up the reactor properties. COFE will automatically bring up its own dialog for unit operations. This dialog has some advantages; we can add numbers in a unit-of-measure of choice. It will also always tell us which ports are exposed by the unit operation and what they are connected to. It will show us the reports exposed by the unit operation. And it will show us mass and energy balances. Normally, a unit operation also comes with its own interface. This is accessed by clicking on the Show GUI button in the bottom.

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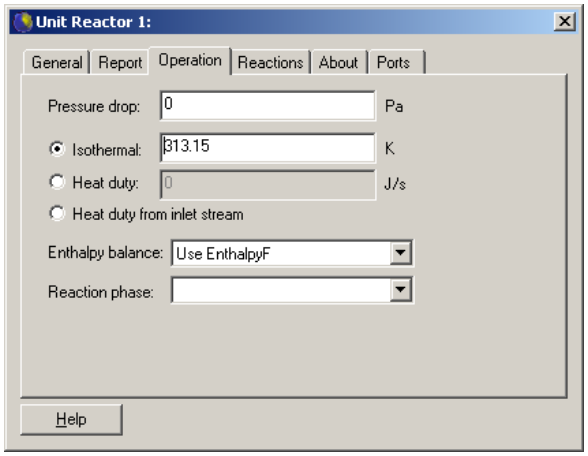
ChemSep
Modeling Separation Processes

Reactor specifications:



Here we specify the details of the reactor. This is a very simple conversion reactor so there is not a great deal to say about it here. For present purposes we will assume that the reactor is isothermal and operates at 40 C. Thus we need to change the default temperature shown in the above screen to 313.15 K.

We have several options to specify how the heat balance should be calculated. In this case – as we have configured it before – we can use the flavour of enthalpy that includes heat of formation, and we do not have to worry about specifying heat of formation explicitly.

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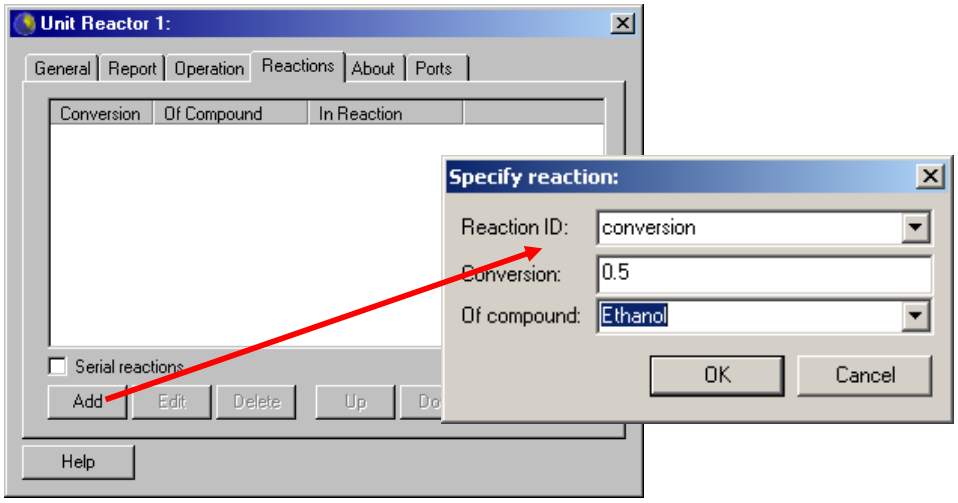
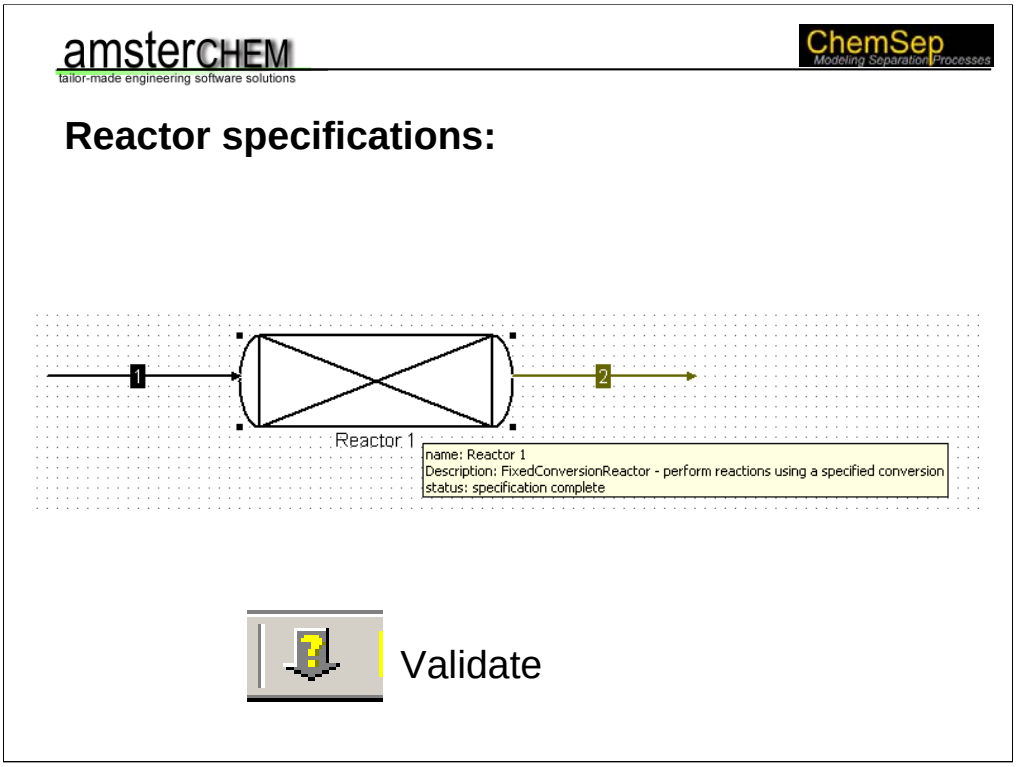
ChemSep
Modeling Separation Processes

Reactor specifications:



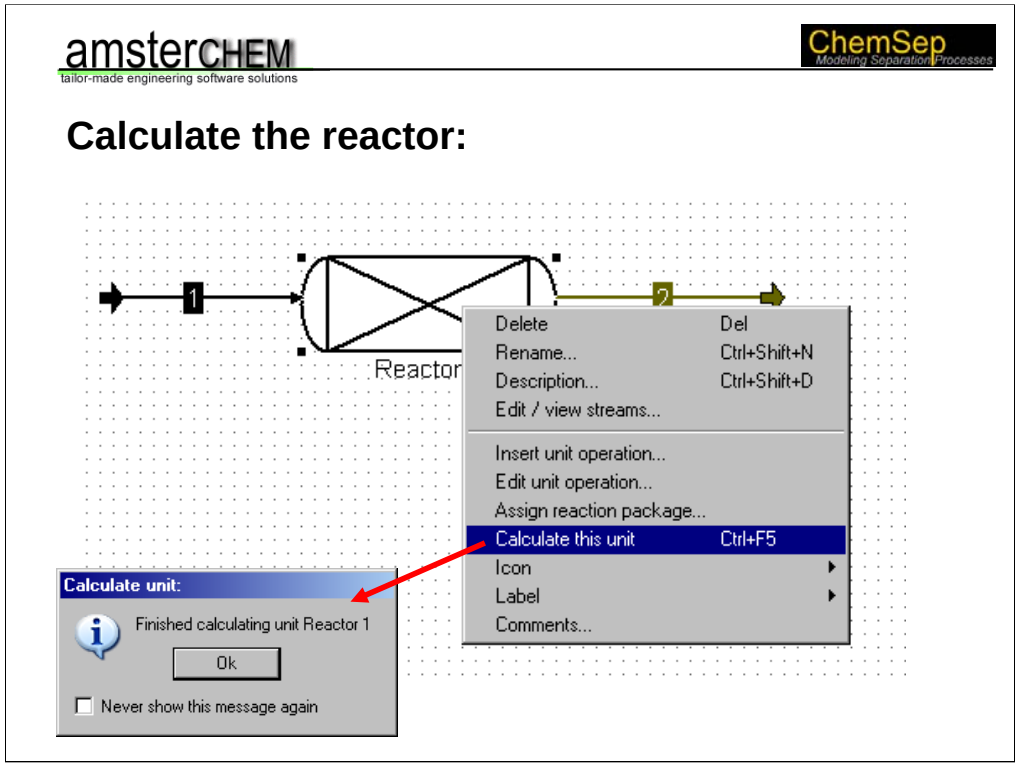
If we go to the Reactions page, we see that no reaction is specified. We had noticed before a reaction package has already been assigned to the reactor, so click Add to add a reaction. We choose the only reaction available, which is called ‘conversion’. We specify a conversion of 0.5 for compound Ethanol. Hit OK to accept the reaction specification. If we would have multiple reactions, we would need to be concerned about whether the conversion specification is of serial or parallel type. For now we do not worry about it. For the details, hit Help in the reactor window. This will pop up the help for the Fixed Conversion Reactor, which explains what that choice is all about.

As we are done specifying reactor inputs, close the dialog by clicking on the X in the corner of the window.



The reactor has now changed color from brown to black. If we hold our mouse over the reactor, a message pops up. From there, we can derive that the change in color signifies that the specification of the reactor is now complete. That is: enough details have been specified to calculate the reactor.

If the reactor specification would not be complete, this balloon help would show us what we still need to specify. For the whole flowsheet, we can always use the Validate button to get all messages about specification issues.



We can hit solve at this point, but we can also calculate individual unit operations by right-clicking on the unit operation and selecting Calculate this unit. Calculation of individual units may help trouble shooting flowsheet solutions. When COFE is done calculating the unit, it will tell us so.

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ChemSep
Modeling Separation Processes

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			

To inspect the calculation results for the reactor, we can bring up the stream dialog for each individual stream by double clicking the stream. We can also bring up the stream dialog for multiple streams. For all streams connected to the reactor, select the reactor and hit the stream dialog button on the toolbar. We verify that indeed half of our ethanol has been converted.

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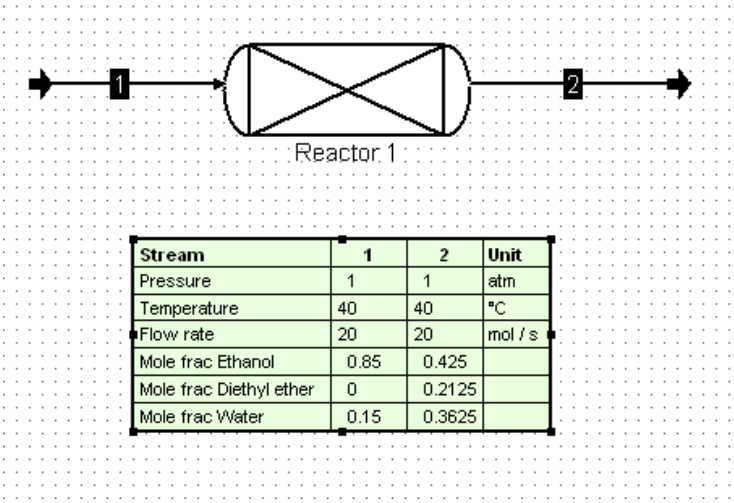
ChemSep
Modeling Separation Processes

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	

Alternatively, we can select Stream report from the insert menu and place a stream report directly on the flowsheet. This reporter asks us to specify the streams to report (there are only two here and both are important, but in more complicated processes we might not want to see the details of all of the streams).

We can see from these results that the product stream still contains a great deal of ethanol and some water; these compounds need to be removed in order to recover the diethyl ether. Thus, the next step is to add a separator. In this case we will use ChemSep to model a distillation column.

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ChemSep
Modeling Separation Processes

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

This brings us to setting up ChemSep. This requires you to have either the Full version or Lite version of ChemSep to be installed at your system. The LITE version has some limitations; it will only run equilibrium models, and it has a limitation on the number of trays and compounds. It is however free-of-charge and is installed with COCO.

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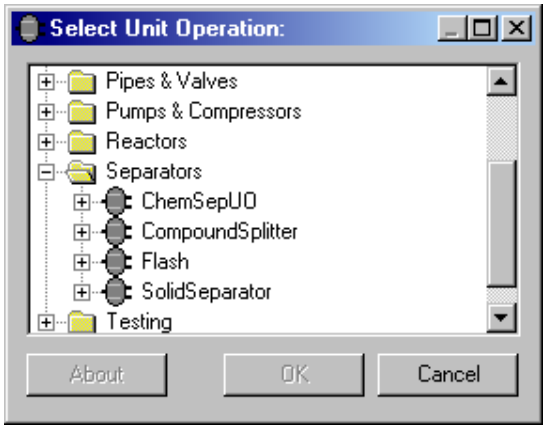
ChemSep
Modeling Separation Processes

Inserting a ChemSep column:



Return to the flowsheet menu and select Insert Unit operation. From the separators category, we pick ChemSepUO. Place the unit operation on the right of the reactor.

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ChemSep
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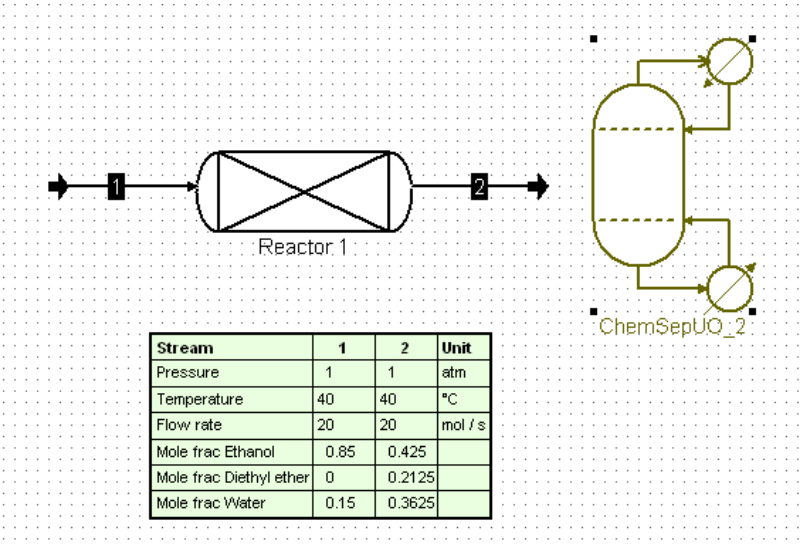
Inserting a ChemSep column:



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	

This is what it will initially look like, but as we configure the column, its appearance will change.

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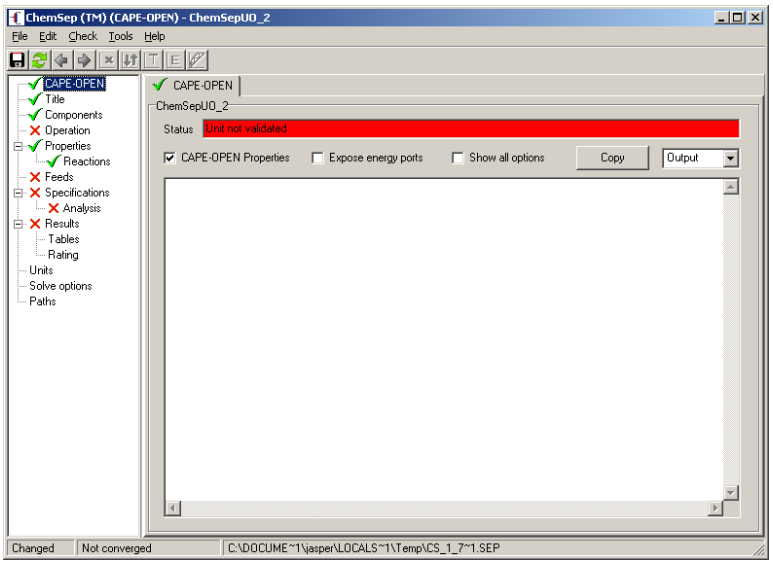
ChemSep
Modeling Separation Processes

Inserting a ChemSep column:



If we now try connecting stream 2 to the column by dragging the arrow of stream 2 to the ChemSep UO symbol, we will see that this proves not to be possible. The reason is that COFE does not yet know anything about this column. To configure the column, double click the column. This will bring up the COFE unit operation dialog. Select Show GUI to bring up the ChemSep Program. At this point – as the ChemSep column has not yet been configured – you will be asked whether you want to load a sep file describing a ChemSep column, or whether to start a new column. We select that we want to start a new column. The ChemSep interface starts.

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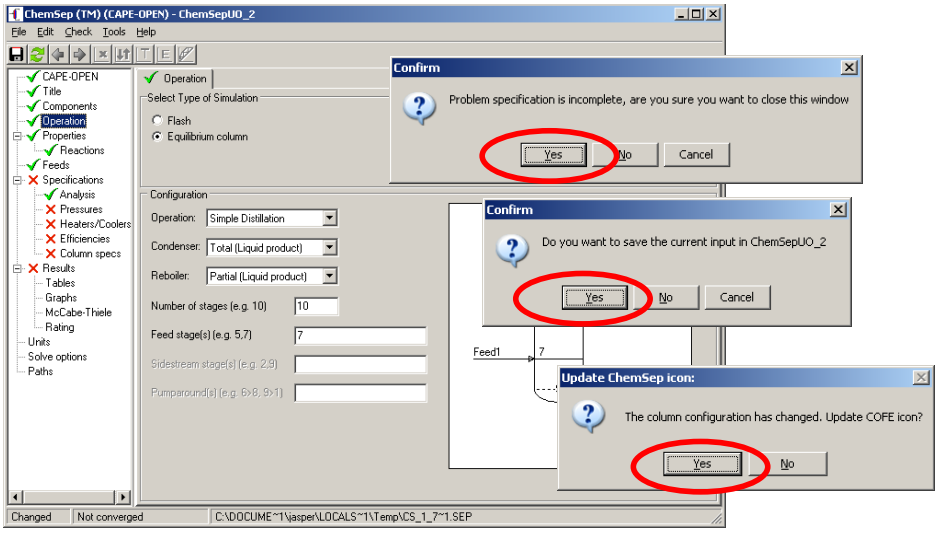
ChemSep
Modeling Separation Processes

Configuring the ChemSep column:



We only need to specify the column configuration at this stage. Click on the Operation tab and provide some details about the column. Select Equilibrium column, Simple distillation, Total Condenser, Partial Reboiler, 10 stages, feed stage 7. The specification of the column is not yet complete, but we will return to that later. For now, close the ChemSep interface, and save the file when prompted. The new column knows what it should look like, and we accept Chemsep's offer to adjust the icon inside COFE.

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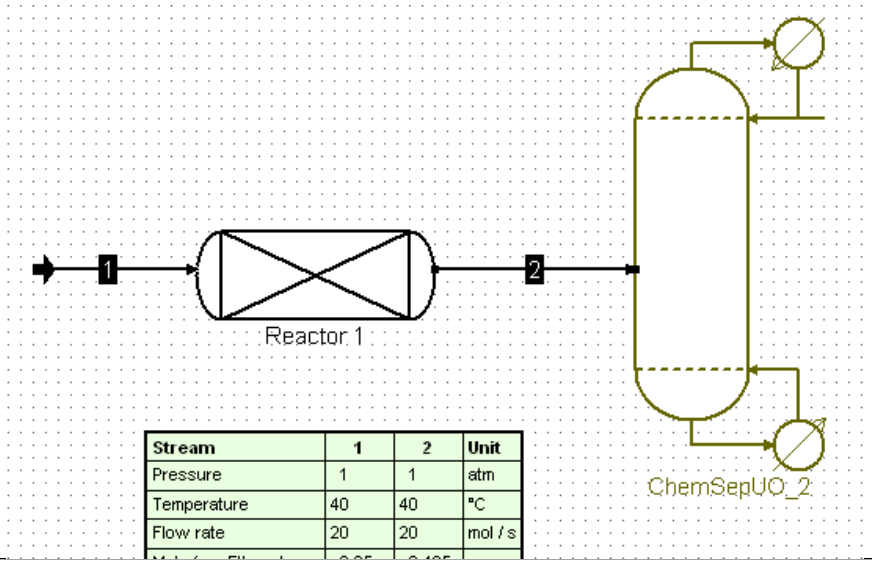
ChemSep
Modeling Separation Processes

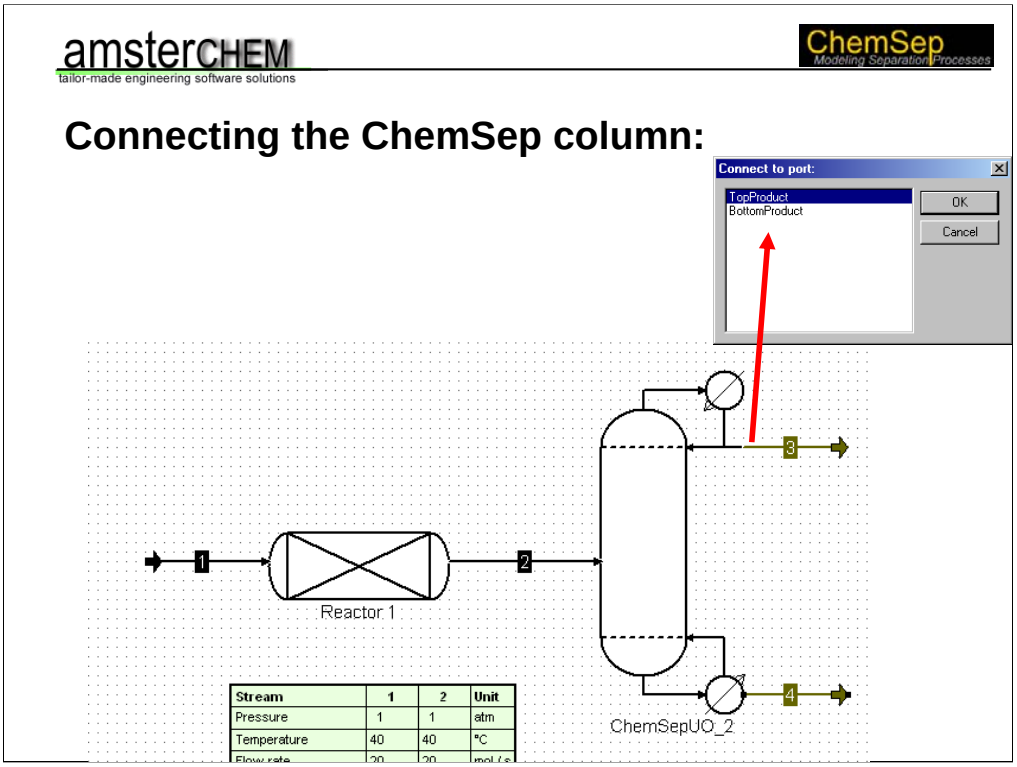
Connecting the ChemSep column:



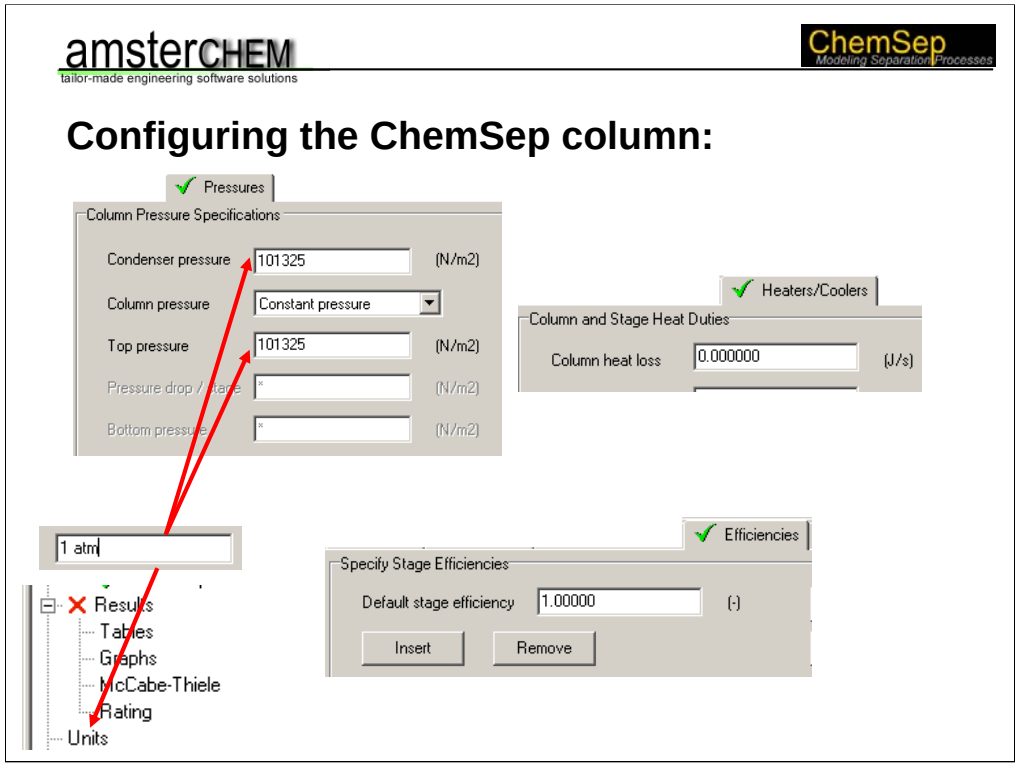
Stream	1	2	Unit
Pressure	1	1	atm
Temperature	40	40	°C
Flow rate	20	20	mol / s

We can use the mouse to resize the new icon to our likings.

Now, the column has a feed port, as well as top and bottom product ports. We can now connect stream 2 to be the feed of the separation column.



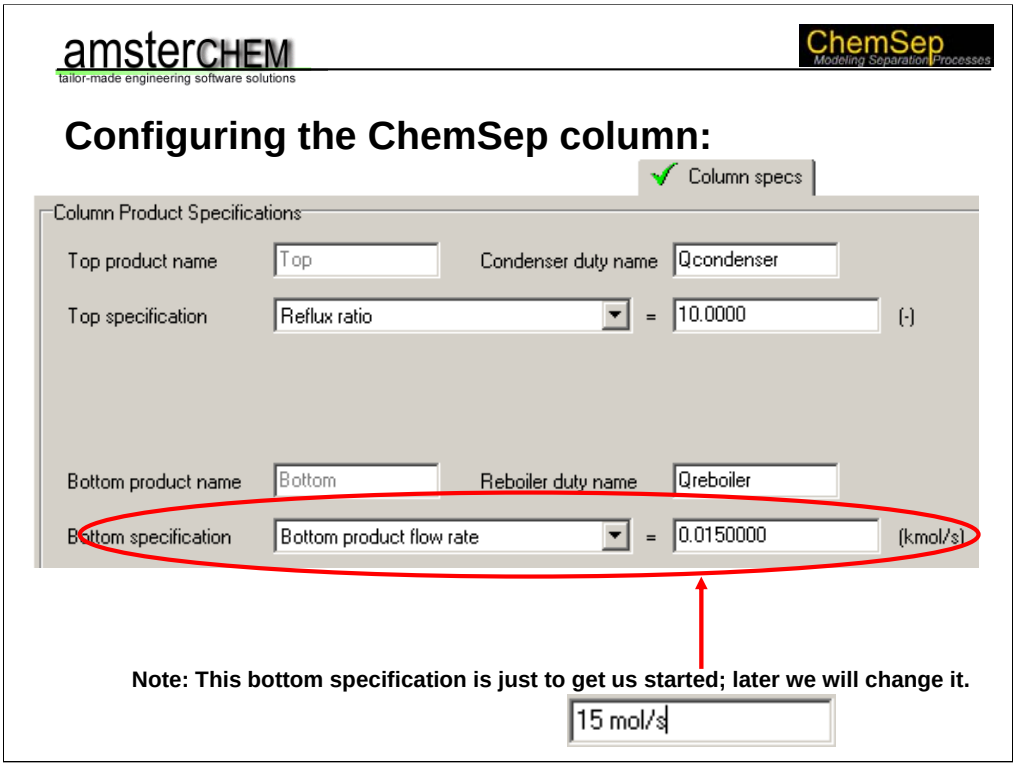
The column, of course, has two products so we need to add two more streams. Following the procedure described earlier for adding streams we add two more to the flowsheet. When connecting the first of the two product streams, we need to select which of the product streams this is. For the second product stream, there is only one product left. No ambiguities, so we will not be prompted again by COFE to select a product.



Complete the column specifications. Note that the feed to the column will come from reactor product stream and we do not need to (and, in fact, are not able to) specify anything it in ChemSep. Also, the thermodynamic models have already been selected in COFE and ChemSep will call up the TEA property package to compute the properties when needed (unless we selected the option to use the property models that are inside ChemSep).

We start the ChemSep GUI again. We will in a 1 atm constant column pressure. If the default pressure units are not set to atm, we can either change the units configuration (by clicking on the corresponding node in the tree), or we can just enter the value with the unit of measure, .e.g. 1 atm, and Chemsep will convert the value to the selected units.

In addition to that, we specify no heat loss, and a stage efficiency of 1.



We will set the top reflux ratio to 10, and to get started, we will specify that 75 % of the flow goes over the bottom. Remember that we had specified 20 mol/s for the reactor feed flow rate and that the reactor product flow was also 20 mol/s. We enter 15 mol/s for the feed flow rate.

Save the configuration, exit the ChemSep GUI, close the Edit Unit Operation dialog.

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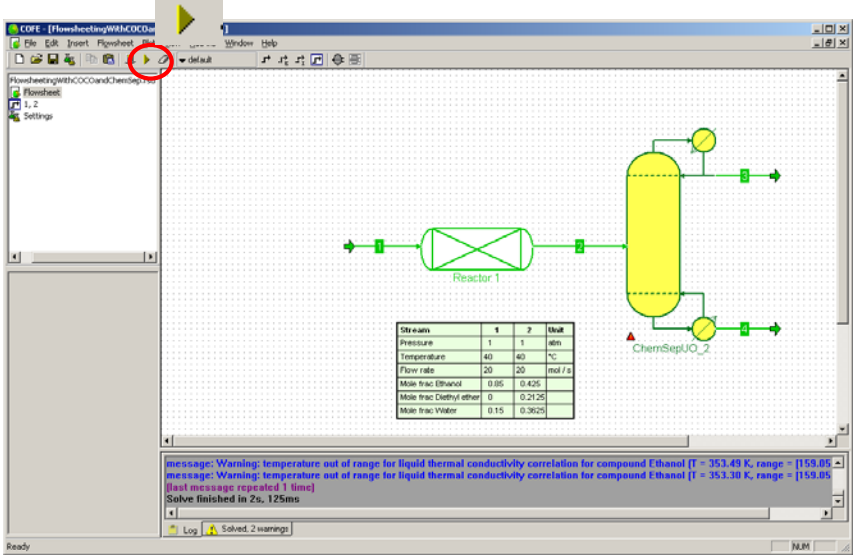
ChemSep
Modeling Separation Processes

We can now run the column:



Hit Solve to solve what we have so far. Notice that after solving, the column turns yellow. This indicates that some warnings have been encountered when solving the column. This is also shown by the exclamation mark at the column and the text in the log in the bottom of the window.

We can double click the stream report, and add the two new streams. Our product is now in stream 3. Stream 4 contains the remaining water and ethanol. We are only using ethanol. We had water in our feed. We are producing water. Ergo, we want to get rid of the water. For that we will use another column.

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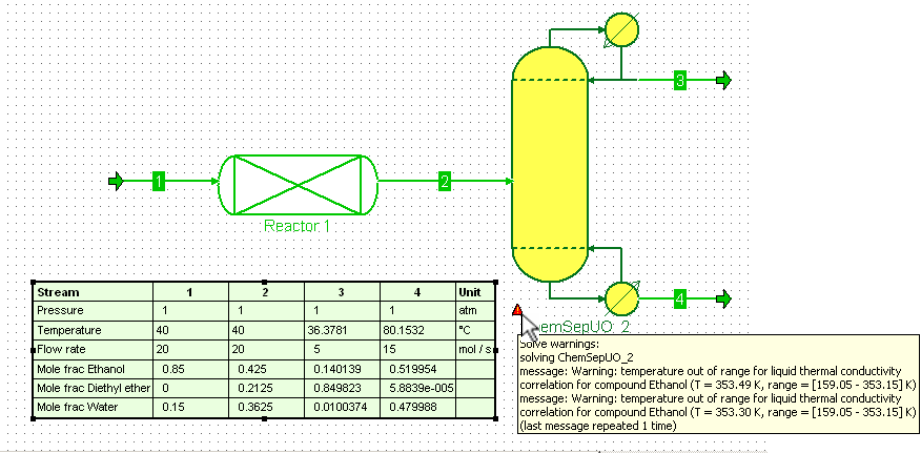
ChemSep
Modeling Separation Processes

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	

When holding the mouse over the column's warning indicator, we can read the warnings. During evaluation of the column, thermal conductivities of ethanol were used 353 and a bit Kelvin, a fraction of a degree higher than the range in which the thermal conductivity correlation is available. For a difference this small, we can safely ignore it. For temperatures that are out of range by a bigger distance, we would be wise to check that the used properties make sense, for example by making a graph of – in this case – ethanol thermal conductivity versus temperature.

We can double click the stream report, and add the two new streams. Our product is now in stream 3. Stream 4 contains the remaining water and ethanol. We are only using ethanol. We had water in our feed. We are producing water. Ergo, we want to get rid of the water. For that we will use another column.

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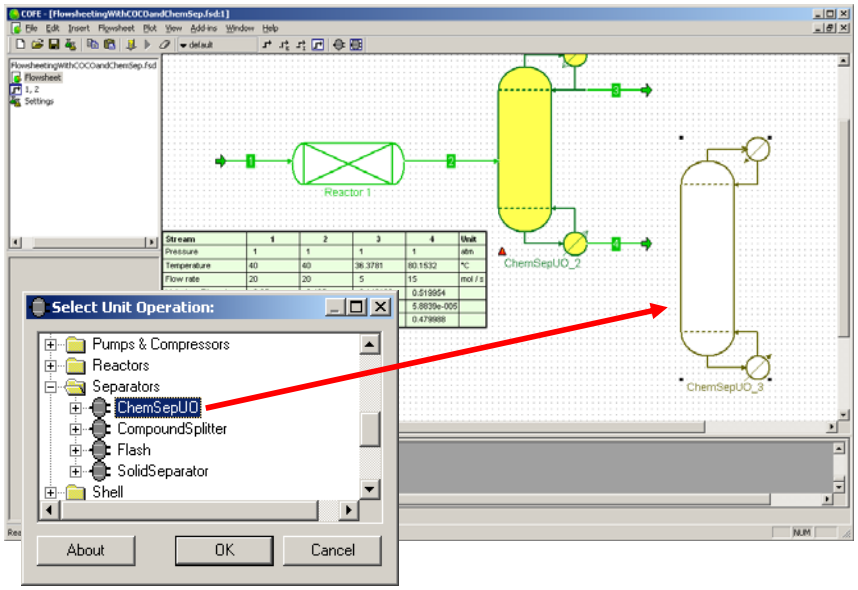
ChemSep
Modeling Separation Processes

Inserting the second column:



Hit the Insert Unit Operation button on the toolbar, and from the Separators section, pick another ChemSepUO column. Using the mouse, we maneuver it to be in the right location, and we stretch it a bit to have a nicer aspect ratio. Double click the new column. On the Edit tab, hit Show GUI. Select that we will use a new column configuration. For setting up the column, hit ChemSep Interface.

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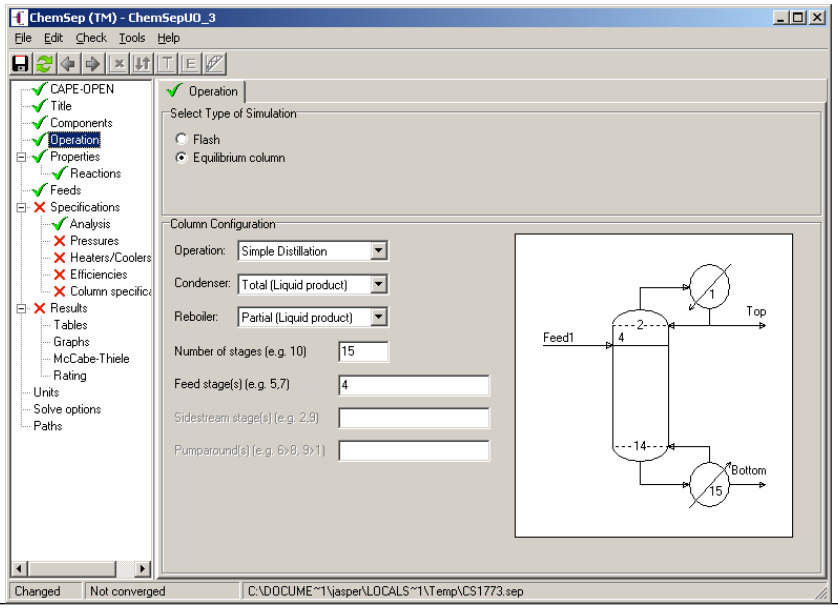
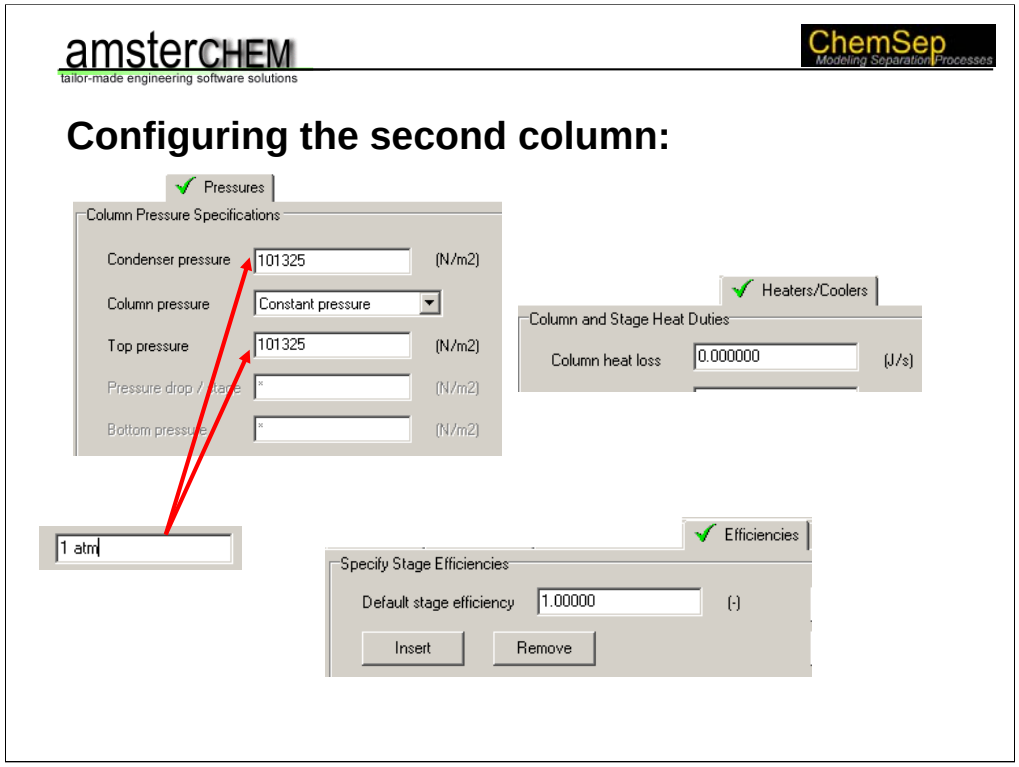
ChemSep
Modeling Separation Processes

Configuring the second column:



We will choose again an equilibrium column. We pick a total condensor and a partial reboiler. This time we will use 15 stages, with the feed on stage 4. This time around will we complete the column specification before we return to the simulator. The left column shows us the part of the specification that is incomplete. Let's start with specifying the column pressure, by clicking on it in the tree view.



We will use the same simple column specification as earlier: constant pressure operation at 1 atm. No heat loss, and a default efficiency of unity.

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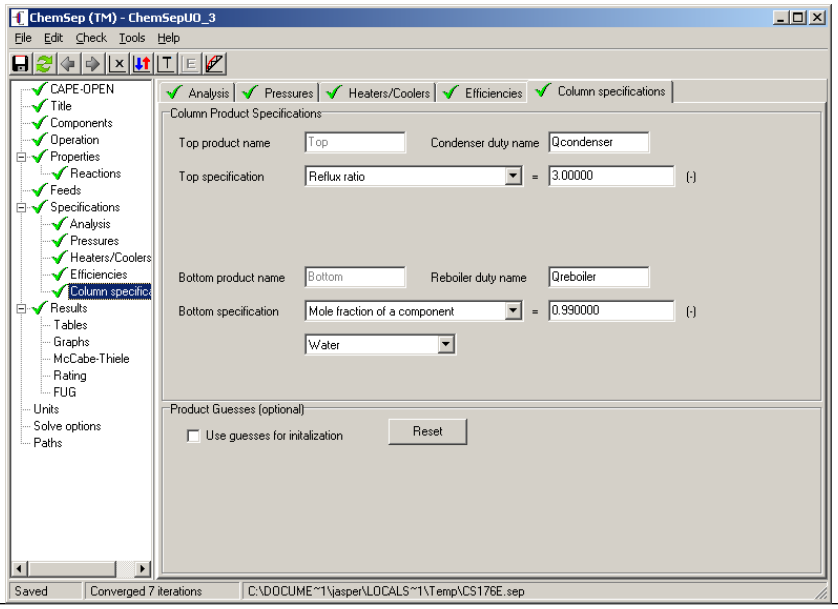
ChemSep
Modeling Separation Processes

Configuring the second column:



We choose a reflux ratio of 3 for the top specification. For the bottom specification we do not want to waste to much ethanol. So we specify the water mole fraction to be 99%. Notice that at this point the ChemSep column is already aware of the compounds that are present in the simulation, even though we did not connect the streams yet. This is because ChemSep can access the underlying thermo system in COFE and query the components from there. It will use the default material template for that. This functionality is not implemented by most other simulation environments, so if you need to make a a compounds based specification for ChemSep in other simulators, it is useful to first connect at least one stream.

In the left column we see that all specifications are at this point complete. We do not have results for this column yet, because we did not run the column yet. We are happy with this specification for now, so we will save the configuration, exit the ChemSep program, and close the Edit Unit Operation dialog.

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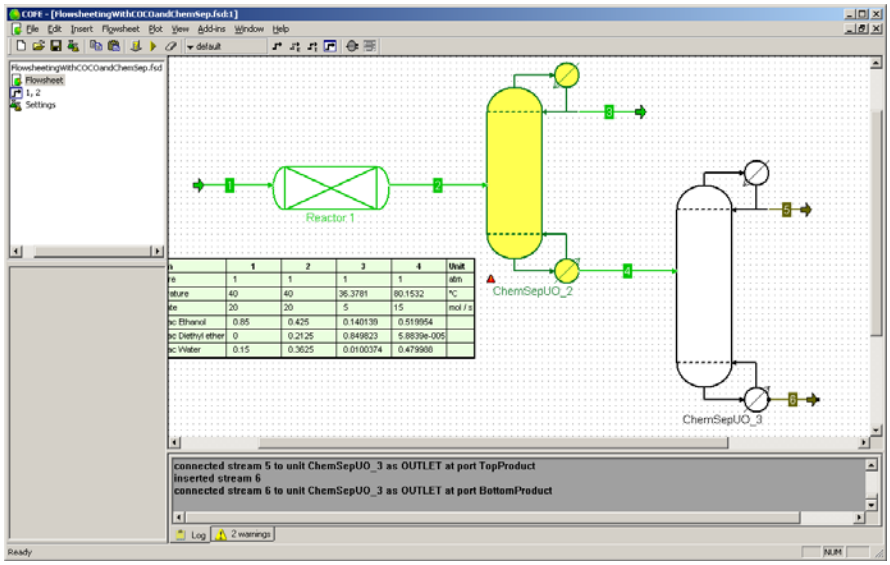
ChemSep
Modeling Separation Processes

Connecting the streams:



Now that the column is fully specified, we can drag the end of stream 4 to the feed location of the new column, and connect it. We can also insert stream 5 as the vapor product, and stream 6 as the liquid product. The black color of the last column tells us its specification is complete, but it has not been solved yet. The brown color of the product streams indicates no values are there yet at all, but solving the column will take care of that.

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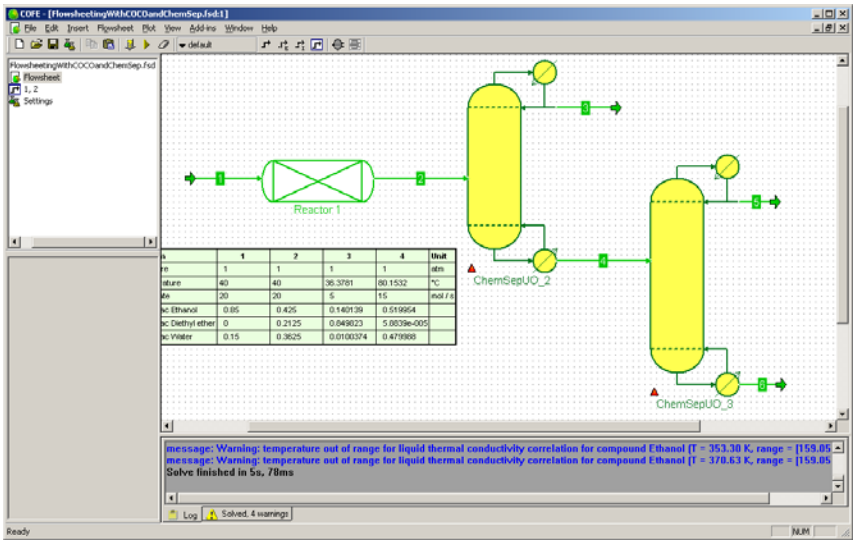
ChemSep
Modeling Separation Processes

Solving the second column:



Solving the second column also shows that temperatures are out of range for correlations for Ethanol. On inspection (see the text in the log or hover the mouse over the exclamation mark near the column) we see that in this case the transport properties thermal conductivity and viscosity have been evaluated out of range. For the second column, values are somewhat further out of range than the first column.

The transport properties are being calculated for the equilibrium column only for the purpose of tray profiles. They are not actually being used in calculations; this would be different if we would simulate the column using a non-equilibrium model.

In this particular case, we can safely ignore the warnings about the transport properties of Ethanol being evaluated out of valid correlation range.

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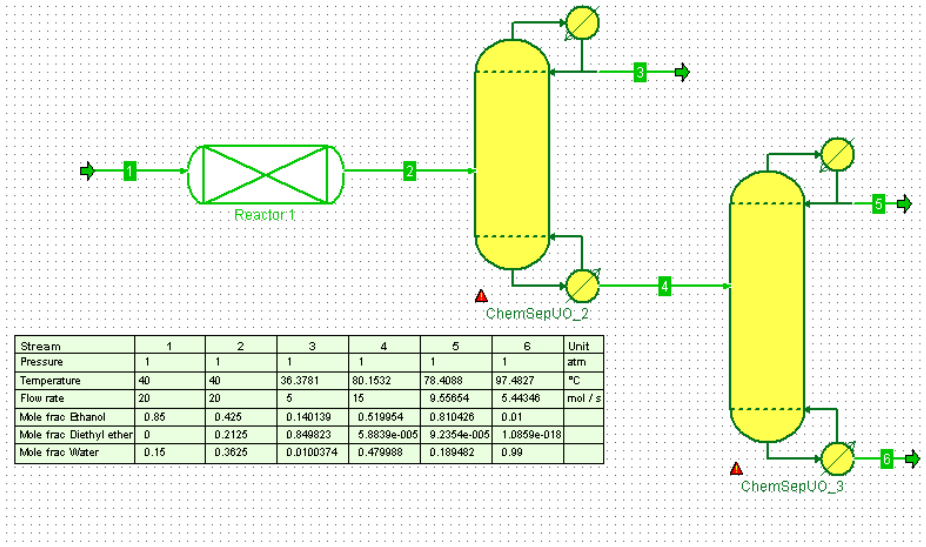
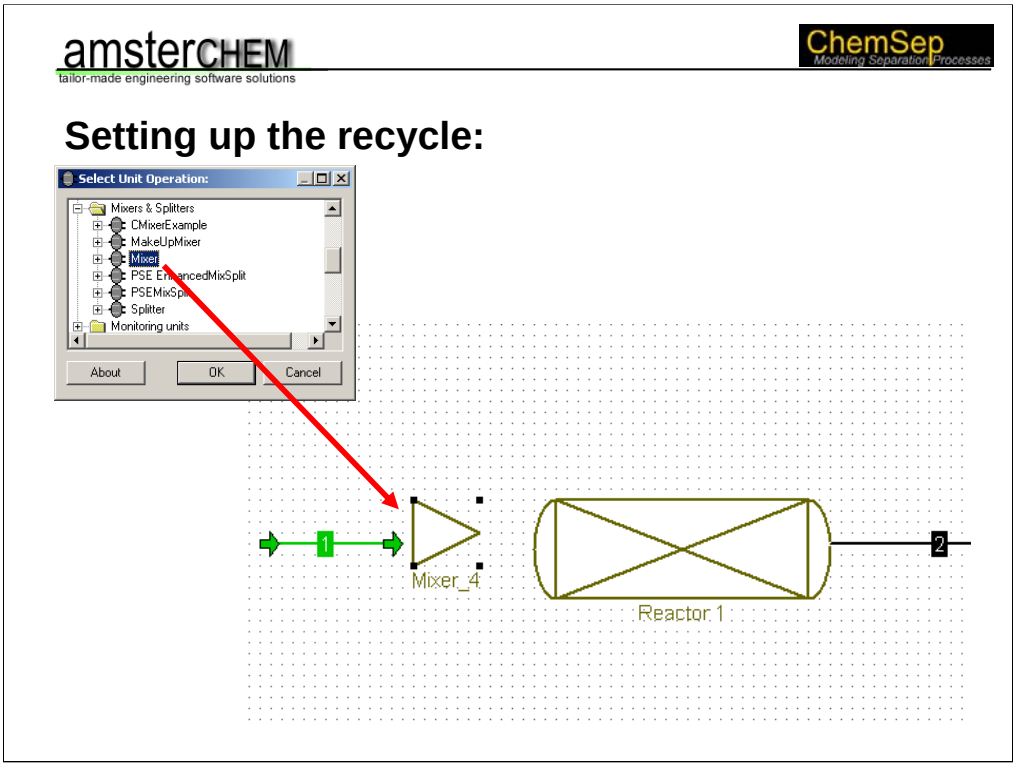
ChemSep
Modeling Separation Processes

Let's see what we get:

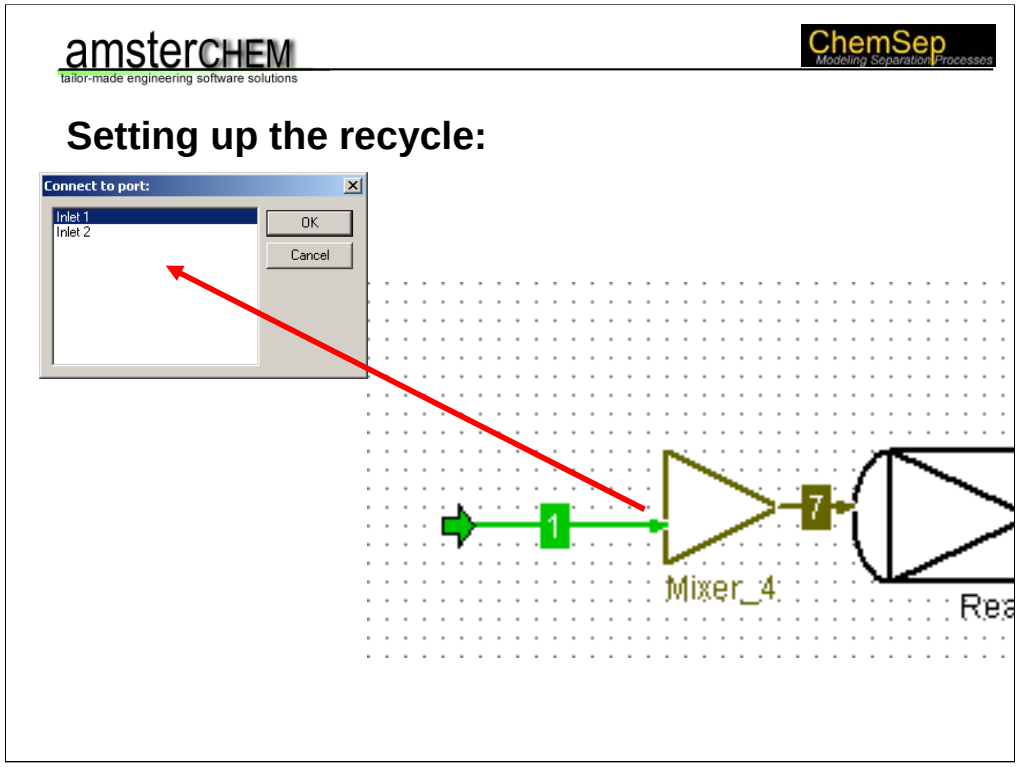


Stream	1	2	3	4	5	6	Unit
Pressure	1	1	1	1	1	1	atm
Temperature	40	40	36.3781	80.1532	78.4088	97.4827	°C
Flow rate	20	20	5	15	9.55654	5.44346	mol / s
Mole frac Ethanol	0.85	0.425	0.140139	0.519954	0.810426	0.01	
Mole frac Diethyl ether	0	0.2125	0.849823	5.8839e-005	9.2354e-005	1.0859e-018	
Mole frac Water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

We can add the new streams to the stream table so that we can inspect them. We see that the liquid product of the last column is exactly what we specified: 99% water. The remaining 1% is nearly all ethanol. We can live with that. The distillate is more than 78% ethanol that we can recycle.



We can pick up the end of the feed stream and move it away from the reactor. This will disconnect the stream from the reactor, and we see that the reactor responds to that by changing color. The color indicates the specification of this unit is not complete. If we hold our mouse over it we can see that it is because the feed is not connected. We will connect the feed in a bit. But fist we insert a mixer. Click the insert unit operation dialog, and from the Mixers & Splitters section, we pick a mixer. We place it in front of the reactor. By default, the mixer has two inlets and one outlet. We can change the number of inlets if we like, but there is no need to for this example. By default it will have a zero pressure drop and will operate adiabatically, which is also fine.



As we drag the end of feed stream 1 on top of the mixer, COFE sees the mixer has two inlets. So we need to pick one to connect to. The inlets of the mixer are of course equivalent and it does not matter which one we pick. We can insert another stream between the outlet of the mixer and the feed of the reactor. At this point, the black color of the reactor tells us the reactor specification is complete again. The mixer specification is not. It lacks the second feed.

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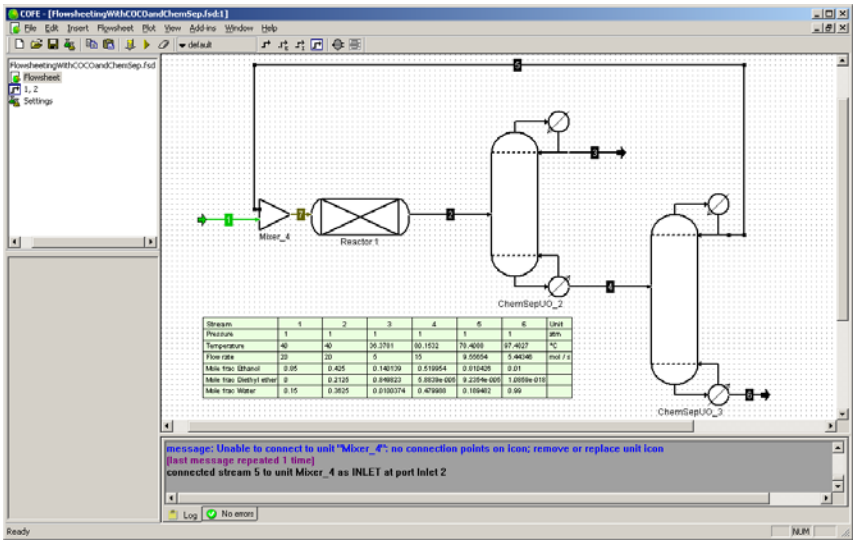
Closing the recycle:



We can now close the recycle: drag the end of stream 5 to the start of the mixer and drop it on top of a feed location. The mixer specification is now complete. However, before we can solve the flowsheet we need to change the specifications on Column 1.

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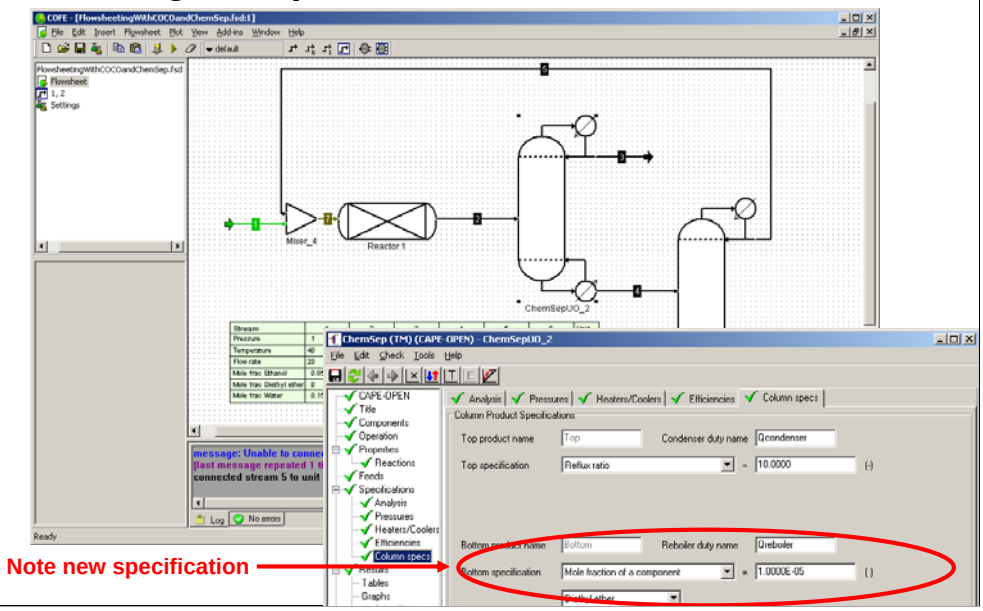
Redoing the specifications for Column 1:



Now that we have a recycle in place (leading to an increased flow through the reactor and to column 1) the bottom flow rate from column 1 specified earlier no longer is appropriate. Since we wish to take the Diethyl Ether (DE) as the top product from column 1 we change the specifications to make sure that very little DE leaves in the bottom product.

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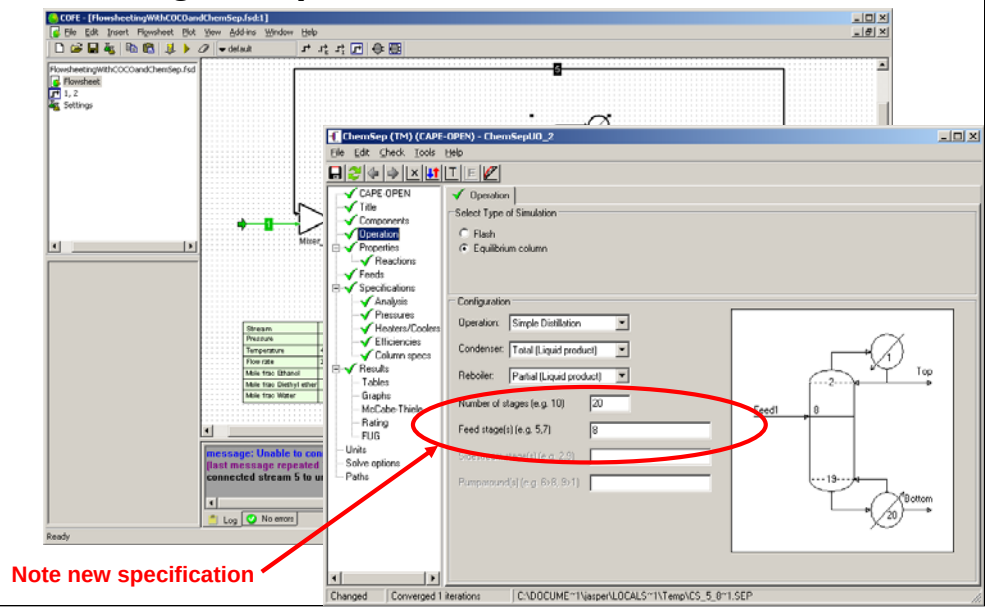
Redoing the specifications for Column 1:



We also add some stages to make sure our new specification can be met. We increase the number of stages to 20, with the feed on stage 8. Once this new specification has been set we are ready to solve the flowsheet.

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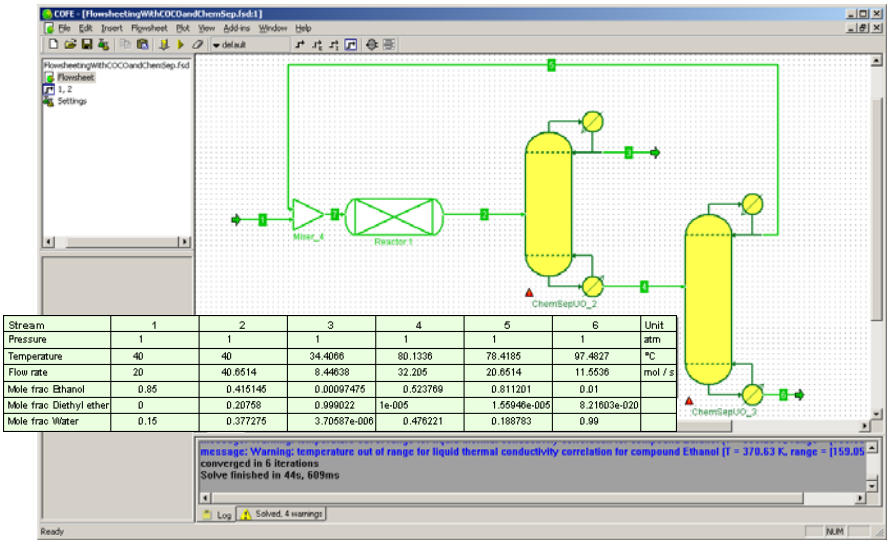
The solution:



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	

If we hit solve, the simulation converges in this case in 6 iterations. Inspecting the log, we will find some warnings about temperatures being outside of the proper range for correlations. The warnings of the last The solution shows that still 99% of the liquid stream 6 leaving the second column is water. This is what we specified. The product stream 3 is 99.9% pure diethyl ether. So we have converted nearly all our ethanol in the feed, and separated the water that was in the feed in the process as well. With some minor revisions to the column specifications we can obtain even higher purity products should we wish to do so.

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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**

Now that we have seen how to configure Property Packages, how to set up a flowsheet and how to set up ChemSep inside a flowsheet, we have covered all the basics. We will shortly touch on some more advanced features

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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

Material streams in COFE show as solid lines. In our example we have only used material stream so far. These streams were all of the same default material type. You can however set up multiple material templates in COFE. Each material template is associated with a specific Property Package: this way you can use multiple Property Packages in your simulation. An example application would be to use two Property Packages of different vendors using the same configuration, to validate your results. Or you could setup two different parts of your process where a different selection of property calculation routines would be more suitable to describe the process. Or the Property Packages could have a different set of compounds altogether.

Another way to make material types with different compounds is by selecting a sub-set of compounds that is available from the associated Property Package. If you know that in a part of your process, hydrogen does not play a role, you can set up one material type with and one without hydrogen, and use them where appropriate.

By default, COFE will not let you hook up different material types to one unit operation. But you can override this behaviour. If you do, it is up to the unit operation to check whether what you are doing makes sense. A unit operation with hydrogen and methane at the inlet, and only hydrogen sulfide at the outlet does not make sense. But a heat exchanger with one type of material at the cold in and outlet, and another at the hot in and outlet does make sense.

You will need to convert in some cases one type of material into the other. COUSCOUS has a special unit operation for that, the stream converter. In the example above, you may want to convert the stream type that cannot contain hydrogen, to one that can. Subsequently you can mix the resulting stream with one that does contain hydrogen.

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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

Energy streams in COFE show as dotted lines. Energy streams are mostly used for heat integration. To use energy streams, you will need unit operations that expose energy ports. You can only connect energy streams to energy ports. Many of the COUSCOUS units have energy ports that you can connect or leave disconnected. ChemSep also exposes energy ports. Energy streams have a direction, like any other stream in a sequential modular flowsheeter. Depending on the sign of the energy, you can transport energy production or energy consumption. One unit operation will need to define how much heat is transported, and the unit operation at the other end of the energy stream can use that heat. For example, you can use the heat produced by the condensor of a ChemSep column to heat up another stream using a Heater unit operation with an energy stream inlet.

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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

Information streams in COFE show as dashed lines. Information streams contain information. Typically, one number. This number comes with a unit of measure. There are several ways set the data on an information stream. You can set it by hand, or you can use the COUSCOUS MeasureUnit to – for example – measure temperature of a stream. You can also take multiple information streams and produce another information stream from that. This is done with the InformationCalculator unit. For example, you can measure two temperatures, and subtract them to calculate a temperature difference.

An important use of information streams is for the controller unit operation that is built in to COFE. This unit takes an information stream as measurement, and exposes one as manipulated variable. For that it requires a set point.

So what does one control? It could be any parameter of another unit operation for example. COFE allows exposing parameters as information streams. This could be input information or output information, depending on the parameter. Example: you can measure a flow somewhere in your process, and transfer that information via an information stream to the measured variable of a controller. The manipulated variable of the controller could be a split factor of a Splitter unit operation somewhere else in your flowsheet.

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Graphs

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

You can insert graphs into your flowsheet. These graphs could show property calculations as a function of temperature, pressure or binary composition. This way you could graph phase envelopes in a number of ways. You can also plot parameters of unit operations. Most interesting are of course array parameters. This way, for ChemSep, you can plot concentrations of temperature profiles along the column height, as ChemSep exposes this information via array parameters.

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Reports and graphical elements

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

As we have seen in the example, COFE allows for inserting stream reports into the flowsheet. These reports can be configured to show any stream and a variety of properties. There are also various unit operation reports to choose from: you can insert reports that show unit operation parameters, or reports that show textual reports as produced by the unit operation.

Basic shapes like boxes, circles and arrows as well as formatted text boxes allow you to clarify things in your flowsheet. You can also embed documents made by other applications, through Object Linking and Embedding. To further clarify things, you can associate a comment with each stream or unit operation. Once you have added a comment, the stream or unit operation will show a little information icon. Hold your mouse over it to see the comments.

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Parametric studies

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

If you want to study the effect of inputs to the flowsheet on outputs, you can use a parametric study. Inputs are independent variables, such as feed conditions, or parameters to unit opertions. Changes in multiple inputs can be studies at the same time. First, solve the flowsheet. Then, pick Parametric Study from the flowsheet menu. Define which inputs you are interested in. For each input value, specify the minimum and maximum value, and the amount of steps to modify the value between its minimum and maximum. Then, define all of the outputs you are interested in. After solving the parametric study, the results can be exported as a text file, copied directly to the clipboard, or used in plots.

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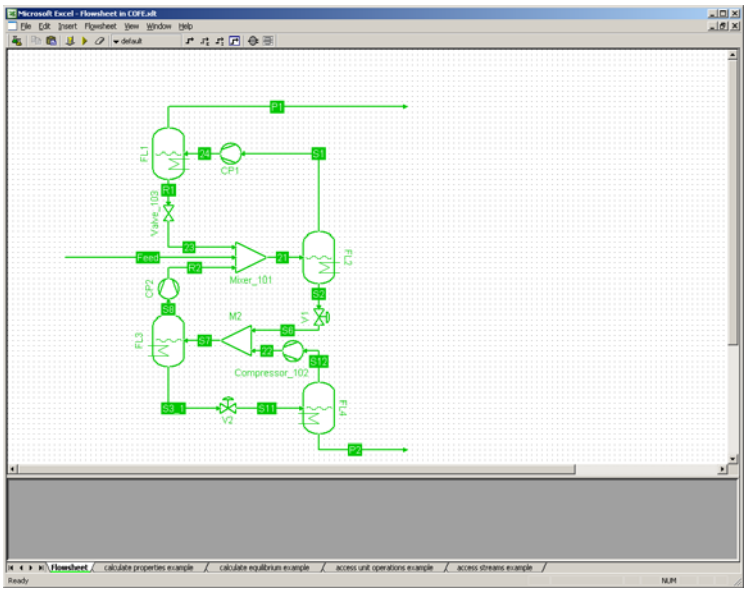
Embedding flowsheets in Excel



What you see on this slide is Microsoft Excel. It is a COFE flowsheet embedded in Excel. COFE comes with an Excel template that you can use for creating a new flowsheet in Excel, or load an existing one.

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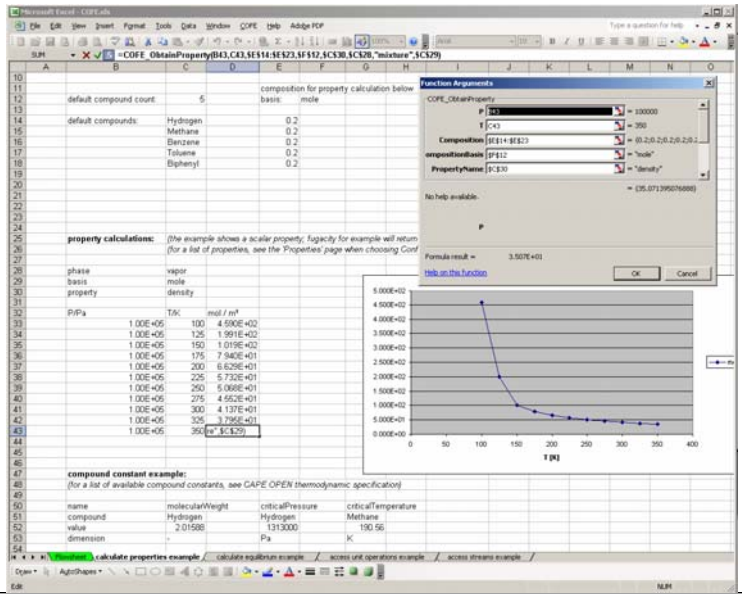
Embedding flowsheets in Excel



Once you have embedded a flowsheet in Excel, you can access all stream and unit operation data. You can also perform thermodynamic property calculations, using whatever material types you have configured in the flowsheet. The Excel template comes with examples on how to go about that. The Excel function wizard will help you fill in the function arguments for property calculations.

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This brings us to the end of this presentation. We hope it was useful and it will allow you to use COCO and ChemSep in a more productive manner.