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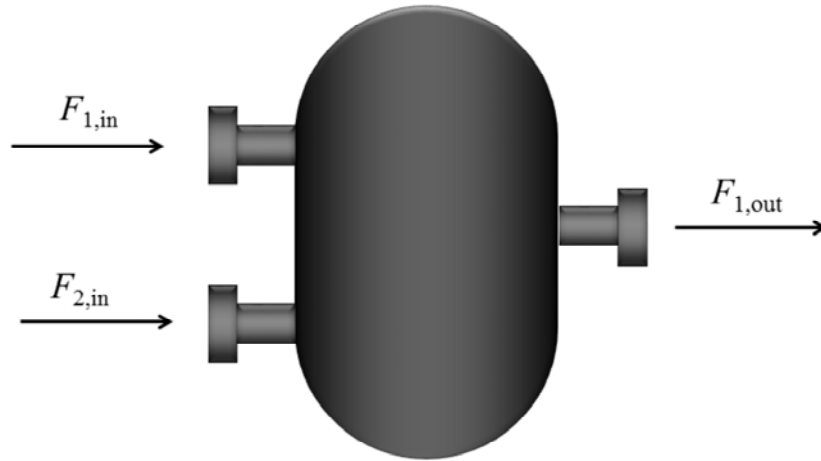
**COCO**  
**THE POWER OF COMPONENT  
BASED FLOWSHEETING**

**Jasper van Baten & Richard Baur**

Hi. My name is Jasper van Baten. Together with Richard Baur I was introduced to CAPE-OPEN in 2004, ten years ago. Nowadays, CAPE-OPEN is a well defined and mature standard set, but back then CAPE-OPEN was in its early days and implementations were just emerging. We built a CAPE-OPEN test platform, which soon grew into a modest process simulator. With the generous help of the authors of the separation software Chemsep, thermodynamics were added and COCO became interesting as a process simulation platform, which was first presented on the CO-LaN annual meeting in Cannes, in 2006. COCO was quickly accepted in the CAPE-OPEN community, as it provided a means for CAPE-OPEN developers to test against one single implementation that everybody could use. COCO was after all, and still is, and will always be, free-of-charge. COCO started leading two lives: as CAPE-OPEN testing platform it was always up to speed with the latest interface developments in thermodynamics, reactions, unit operations etc, but it also gained interest in the rest of the world as steady state flowsheet simulator. It is today both: the defacto CAPE-OPEN interop testing platform, and a simulation platform that is used all around the world. But I am getting carried away. Let us start at the start: flowsheeting.

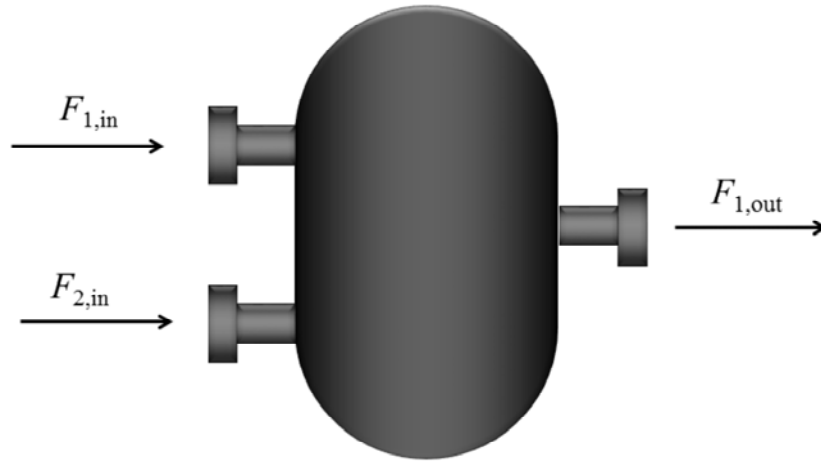


This is chemical factory. As you can see this is a rather complex combination of equipment and pipes. The complexity arises from the many interconnected pieces. Mass and energy is conserved, as you probably know. If we put crude oil in this factory, we want to get diesel and gasoline out. We also get waste products. The total amount of what goes in and what comes out is equal. We prefer however much of the valuable diesel and gasoline to come out, rather than lots of waste products.



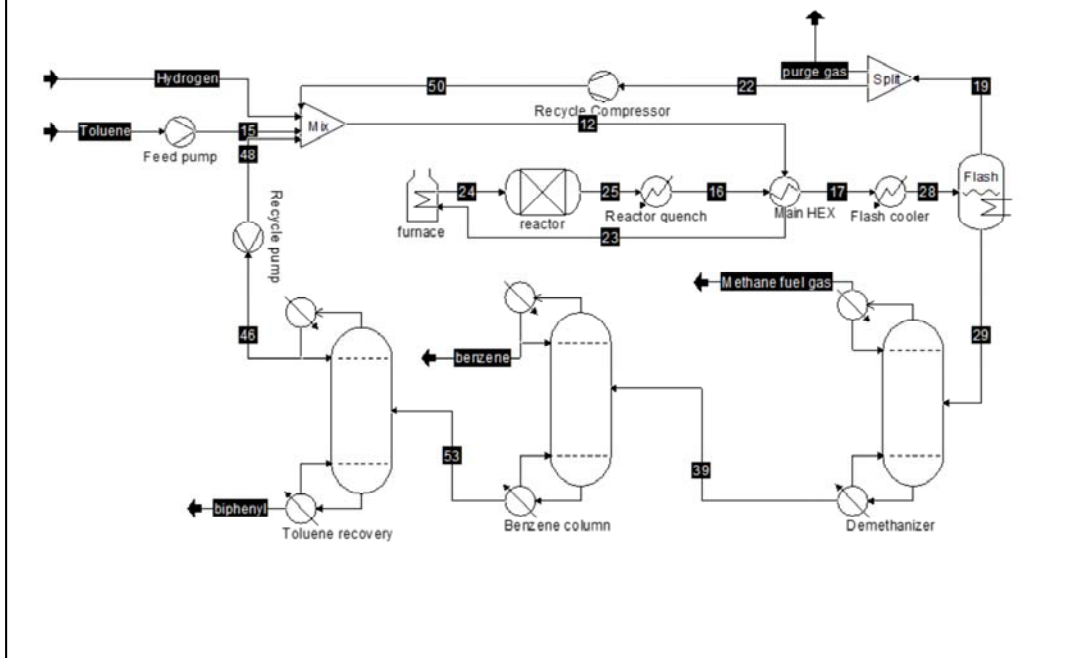
$$\text{accumulation} = \text{in} - \text{out}$$

We can break the factory down into smaller pieces. Such a piece is called a unit operation. Also around a unit operation, mass and energy are conserved. The accumulation of mass and energy in the equipment equals what goes in minus what comes out.



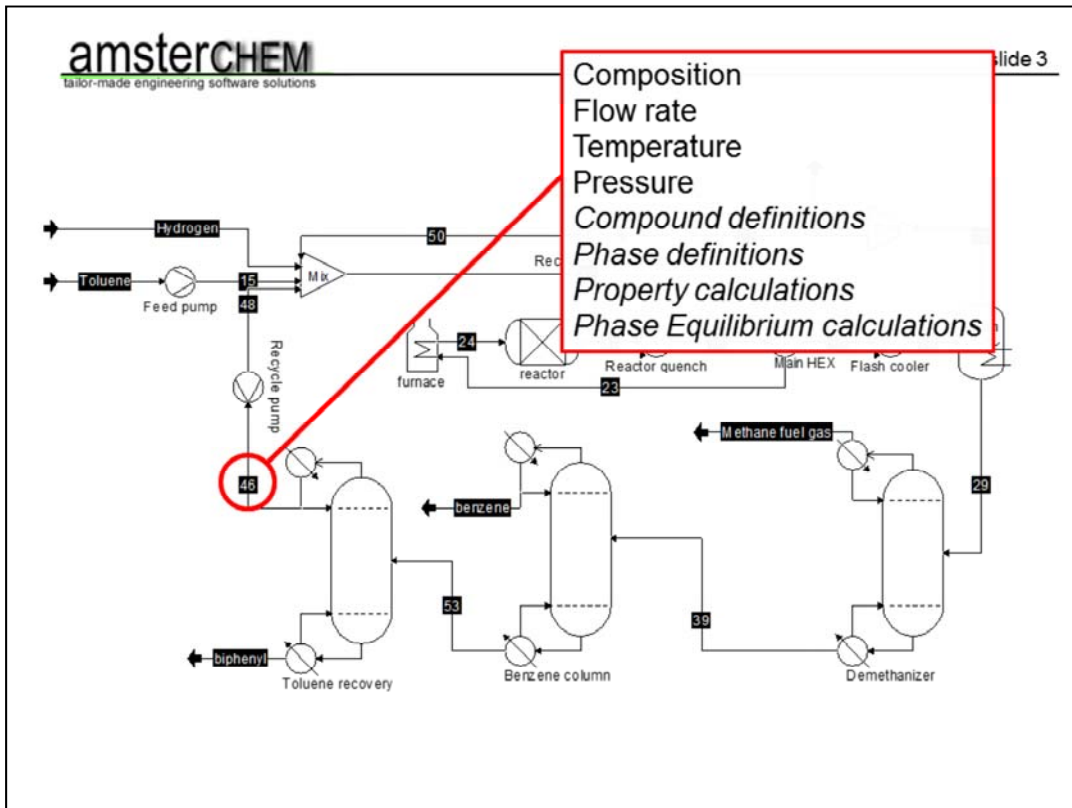
$$0 = \text{accumulation} = \text{in} - \text{out}$$

If the factory operates stably, eventually steady state is reached. The accumulation becomes zero, and the complexity is now simplified to what comes in equals what goes out.

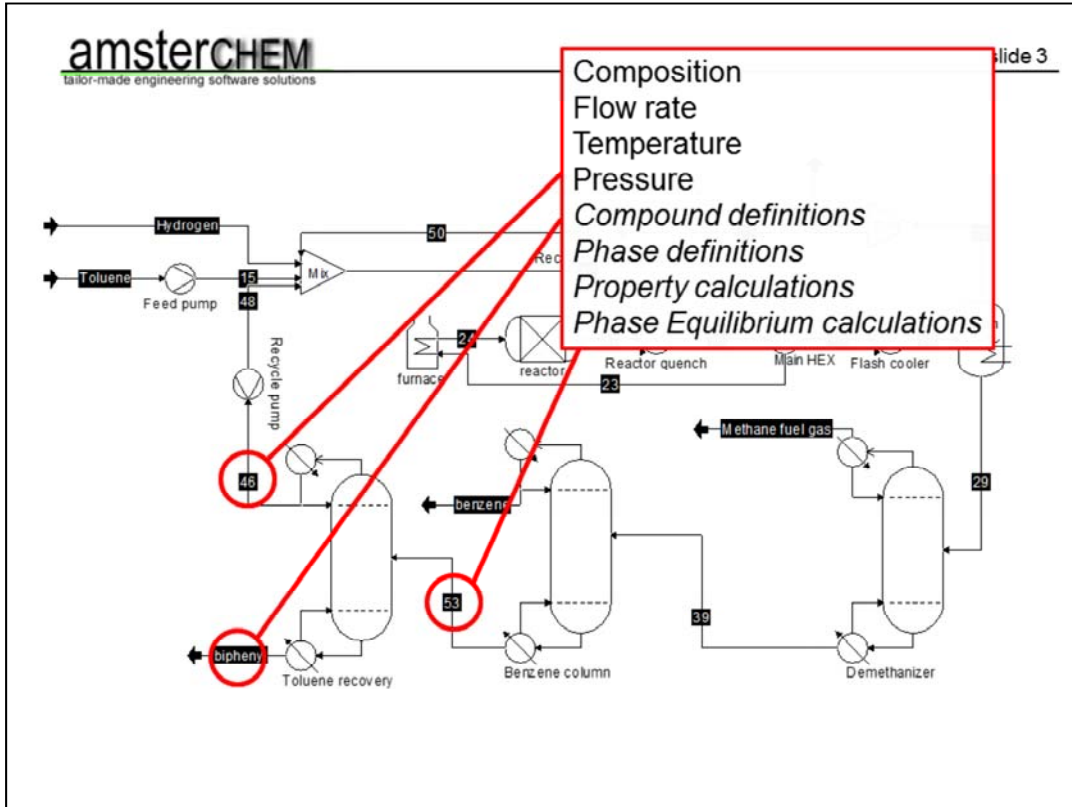


For a single unit operation, the mass and energy balances may be easy to solve. However, in a real process we typically deal with recycles. This is where flowsheet modelling comes in. A flowsheet model gives us a mathematical description of the factory. We can use the mathematical model to design and optimize the process, to do if-then studies and to come to a better overall understanding of the factory.

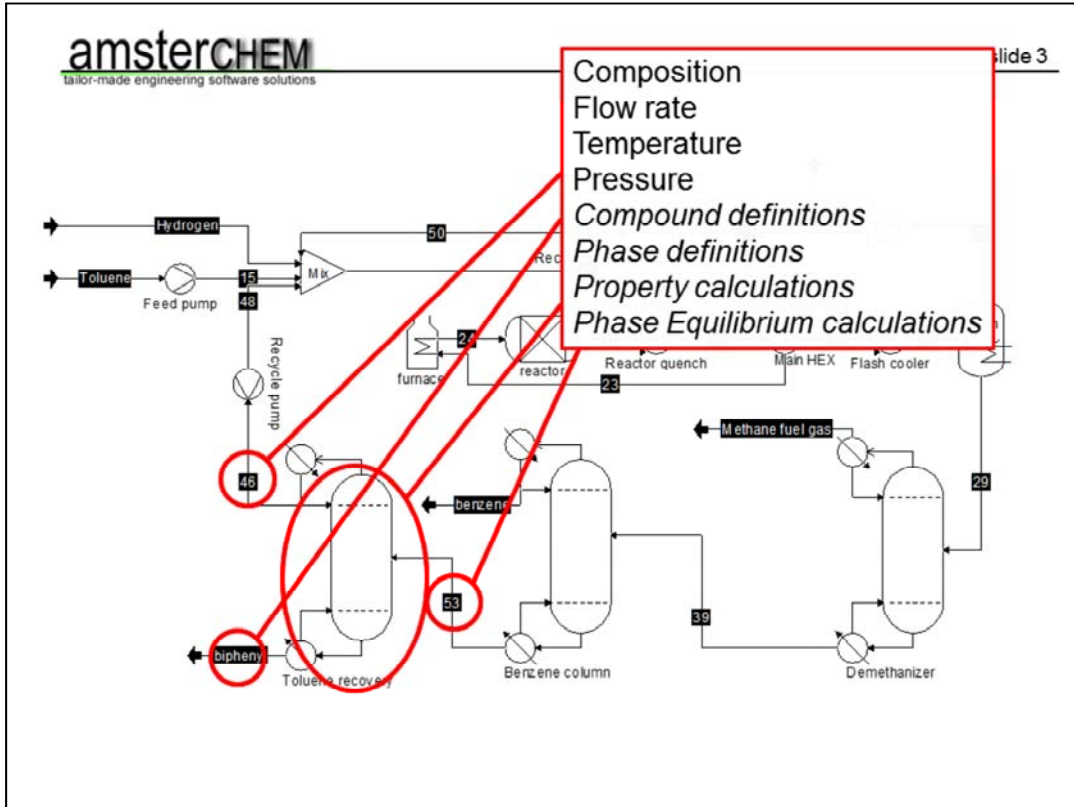
Given the feeds, we want to establish the solution for each of these unit operations. Doing so, we do not only solve the mass and energy balances around each unit operation, but we solve the mass and energy balances of the entire flowsheet.



Clearly, any material stream is represented not only by a flow rate, but also by a composition, and additional conditions like temperature and pressure. In addition to the conditions, there is an underlying definition of the thermodynamics. This includes chemical compound and phase definitions, but also a selection of models that allows for the prediction of physical and thermodynamic properties and phase equilibria.

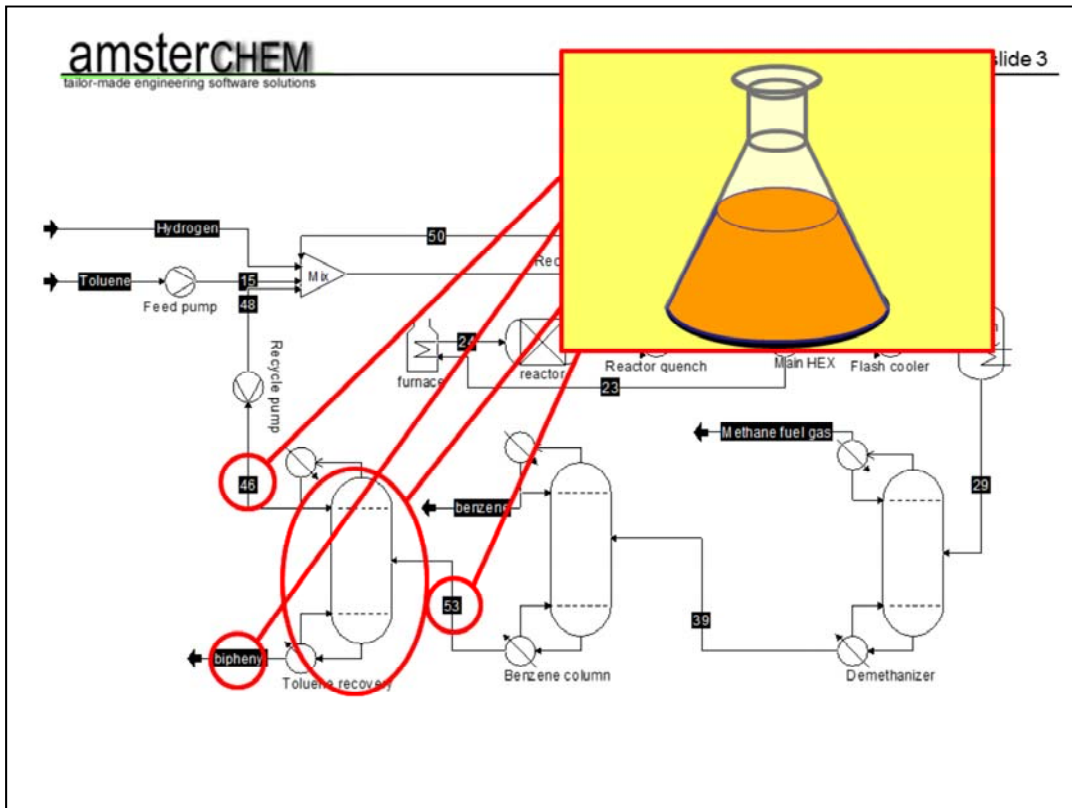


It stands to reason that if we are interested in closing energy balances, that the definition of thermodynamics must be consistent on the streams that go into and come out of a given model. Otherwise we are comparing apples and pears in the enthalpy balance.

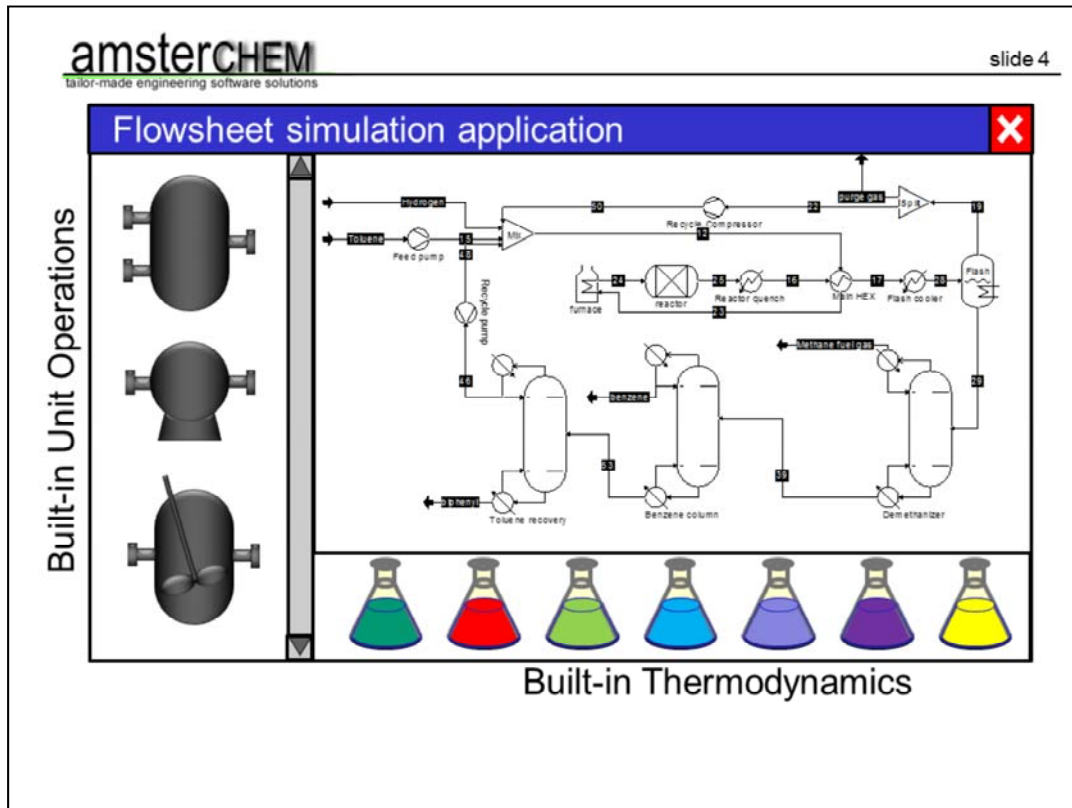


And remember that it is the unit operation that actually performs the local balance. So it too must have access to the thermodynamic property calculations



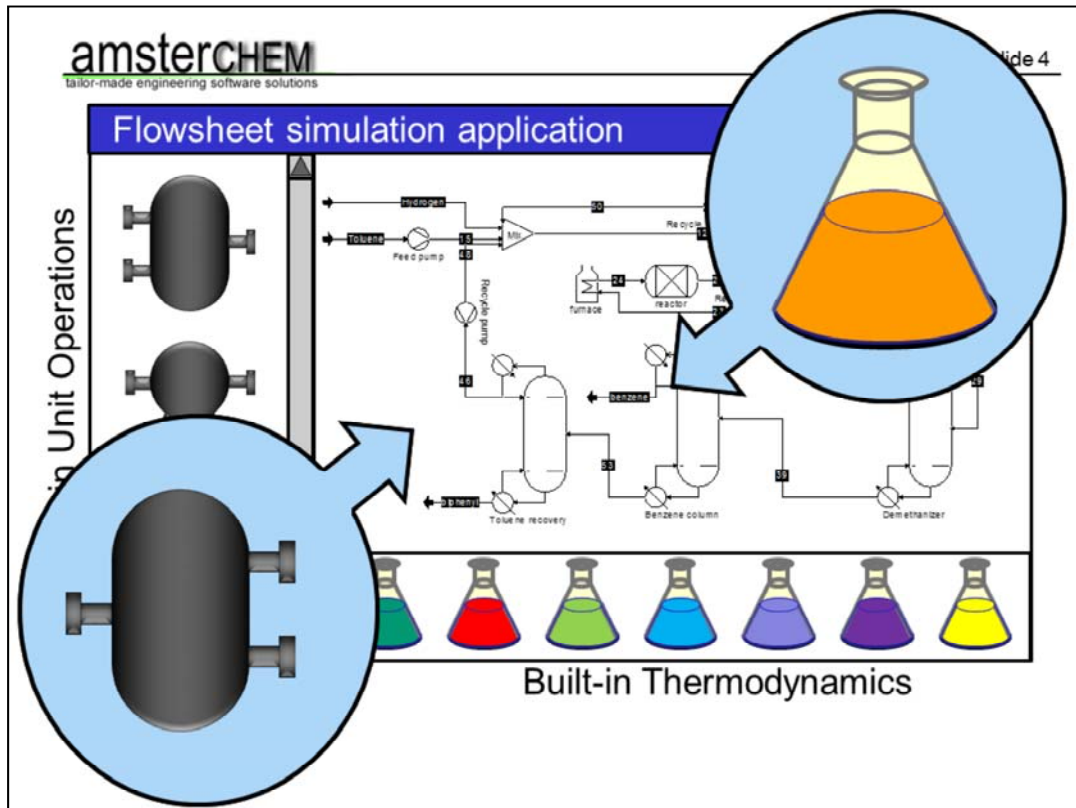


Clearly we need thermodynamic definitions at the level of a flowsheet simulation, that are accessible to all streams and to the unit operation. This is the only manner in which thermodynamic consistency can be obtained.

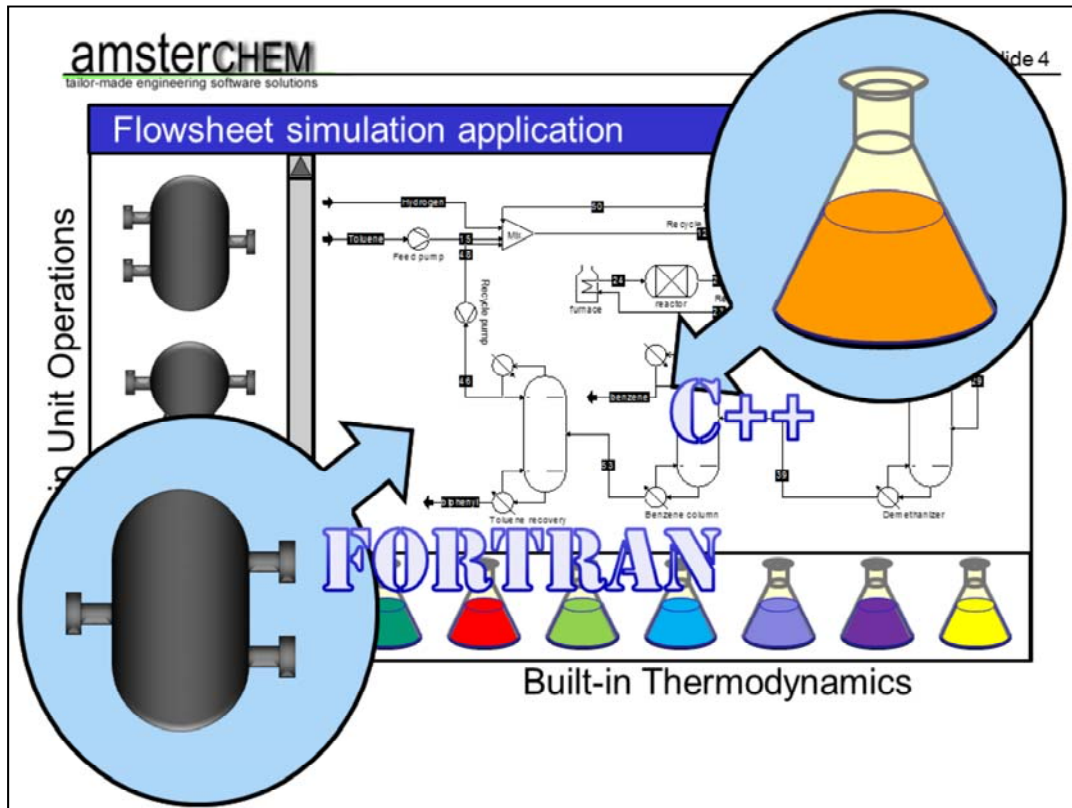


So this is what flowsheet simulation applications typically offer. The ability to solve flowsheets, given a number of built-in unit operation models and thermodynamic models. Typically this is not sufficient though. Clearly it is impossible to cover all possible reactor models, separator models or unit operations by a fixed set of built-in models. You may also find that you are in need of specialty thermodynamics to model a particular system, which is not covered by your simulation application. Or you know that there is another company that simply does the thermodynamic better than your simulation software vendor, and you want to use their thermodynamics instead. Or you are in a company in which multiple simulation applications are used, and it is imperative that the results are consistent over all applications.

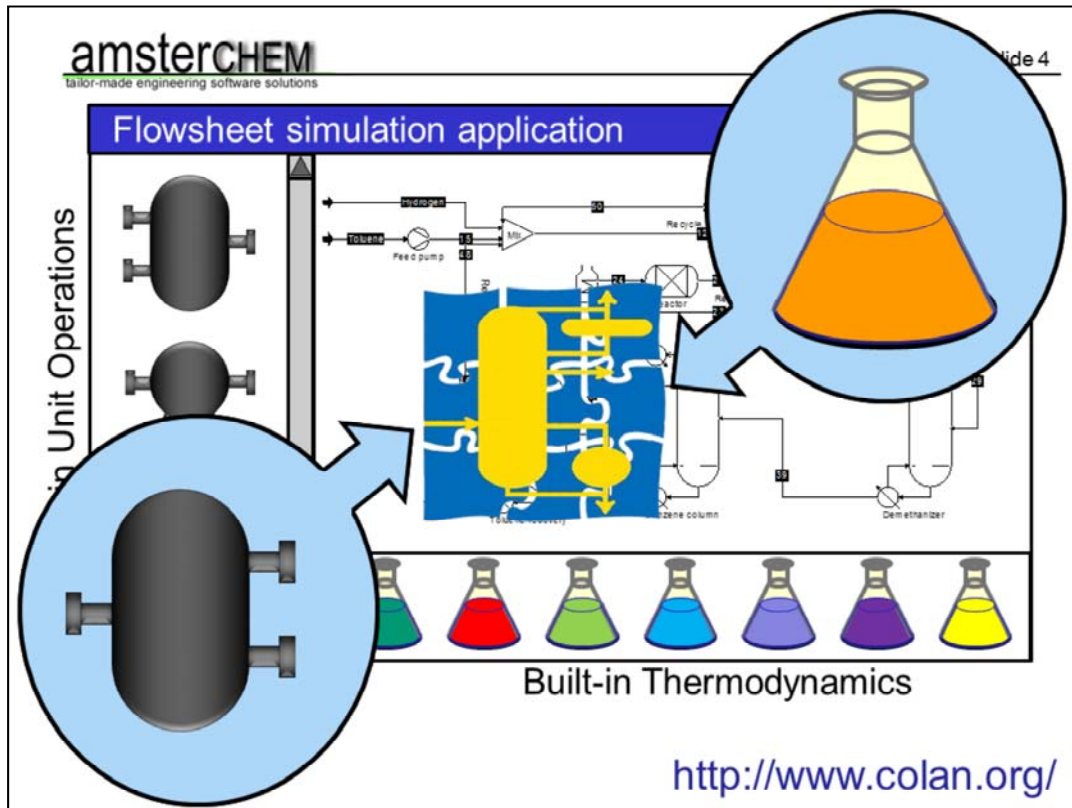
Let us consider our factory of the first slide again. We put crude oil in, we get diesel out. If you want to be able to sell the diesel, the sulphur content must be below 8 ppm. Clearly you are not going to simulate this with any standard reactor model. You will need a tailor made desulphurization model.



So, we need to be able to introduce custom or third part unit operation models and thermodynamic models into our simulation. As the need for this is rather obvious, all simulation environments support this.

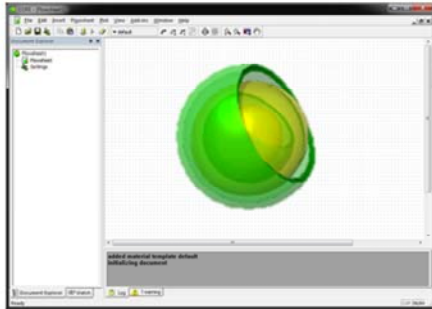


The classic approach is that you have to write some code, either in Fortran, or C, or C++. You tell the simulation application that this code exists and where it is, and you can use your models via this code. This is of course not very flexible, as such code is specific to the simulation application. If you want your custom model to work in multiple simulation applications, you will have to write such code for each simulation application that you are targeting. This makes it nearly impossible to use *any* custom or commercially available 3<sup>rd</sup> party model in *any* simulation environment. It would be better to have universal interface between simulation software components.



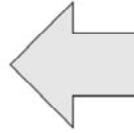
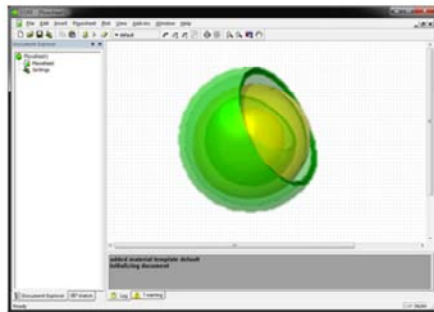
Fortunately such a universal interface exists. It is called CAPE-OPEN. It is an industrial, freely available, open software standard that allows exchange of chemical engineering software components, particularly unit operation models and thermodynamic models, between simulation applications. It is maintained by the CAPE-OPEN organization CO-LaN, and available from their web site.

## COFE

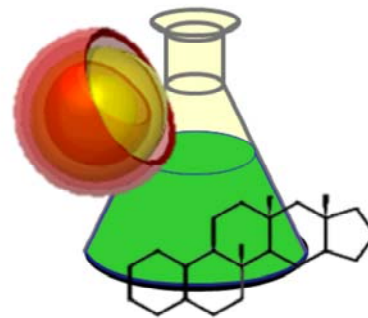


COCO is a bit different from other simulation environments. It is assuming from the start that you want to mix and match. We have as the basis, COFE, the CAPE-OPEN Flowsheet Environment. COFE does not feature any built-in unit operation models or thermodynamics. It does not make any assumptions on the type of unit operations, number of compounds, maximum number or types of phases or anything else, as this is defined by external software components.

COFE

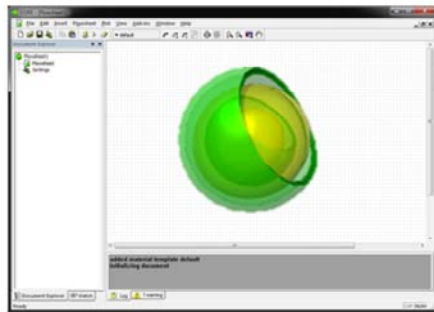


TEA

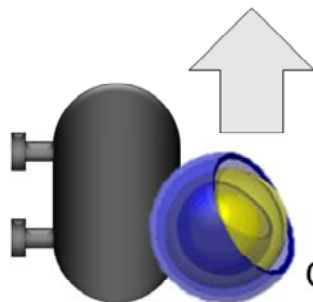
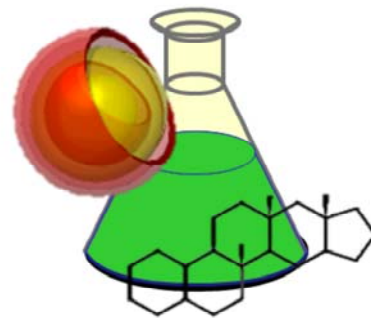


The thermodynamics that come with COCO are provided by TEA, Thermodynamics for Engineering Applications. TEA includes more than 100 property calculation methods. The default data bank contains over 400 compounds, and can easily be extended.

COFE



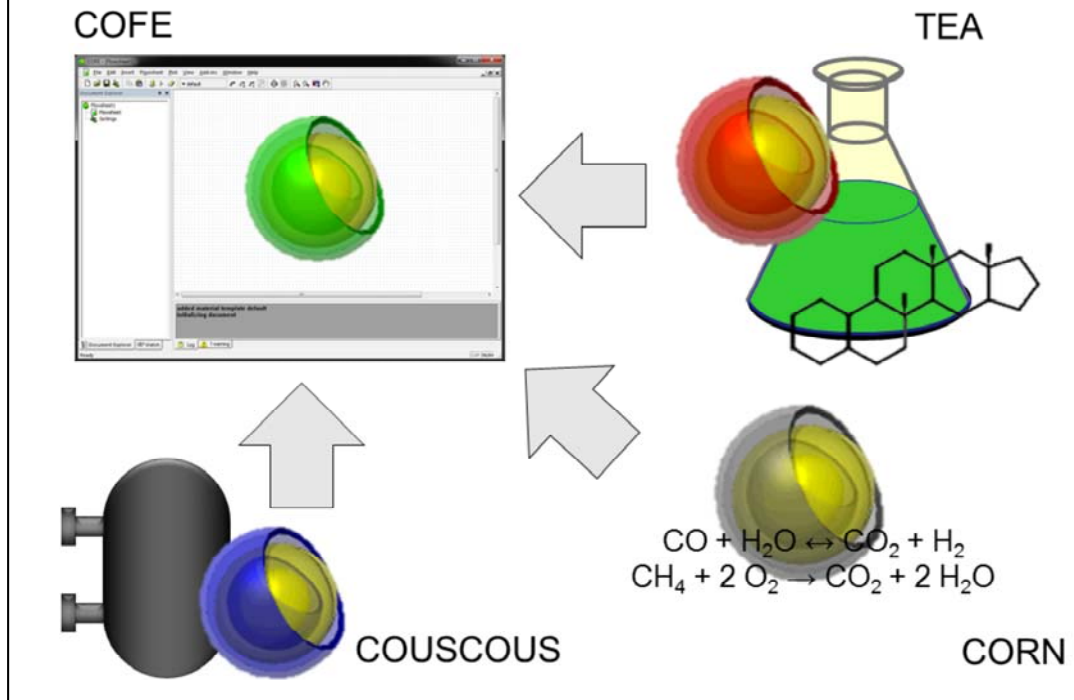
TEA



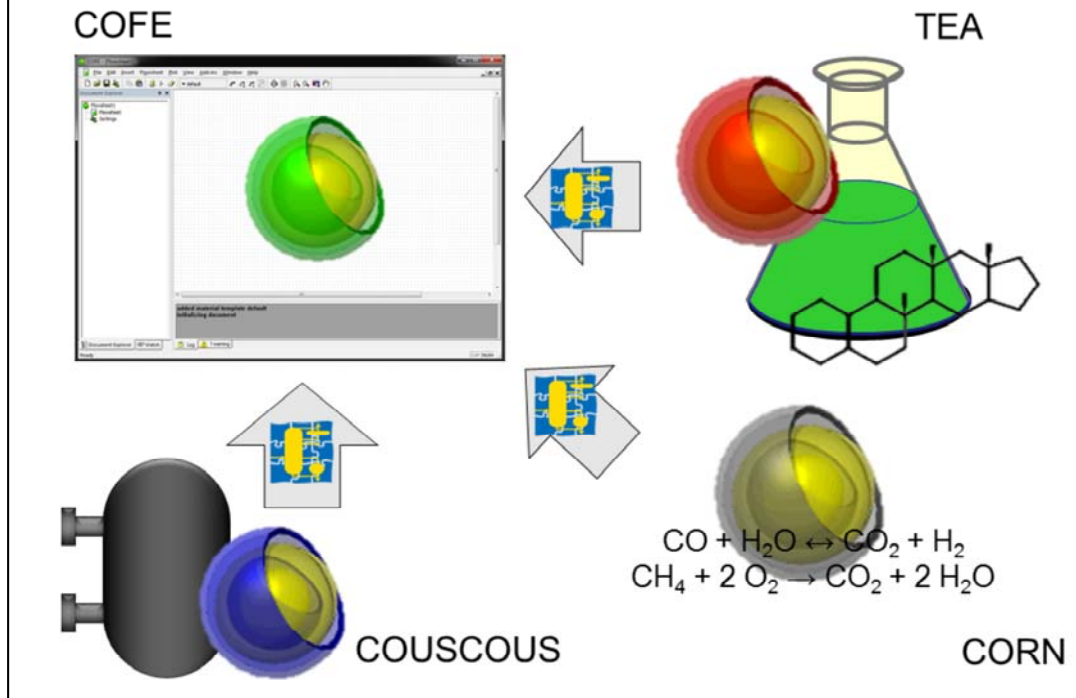
COUSCOUS

The unit operations are served by COUSCOUS.



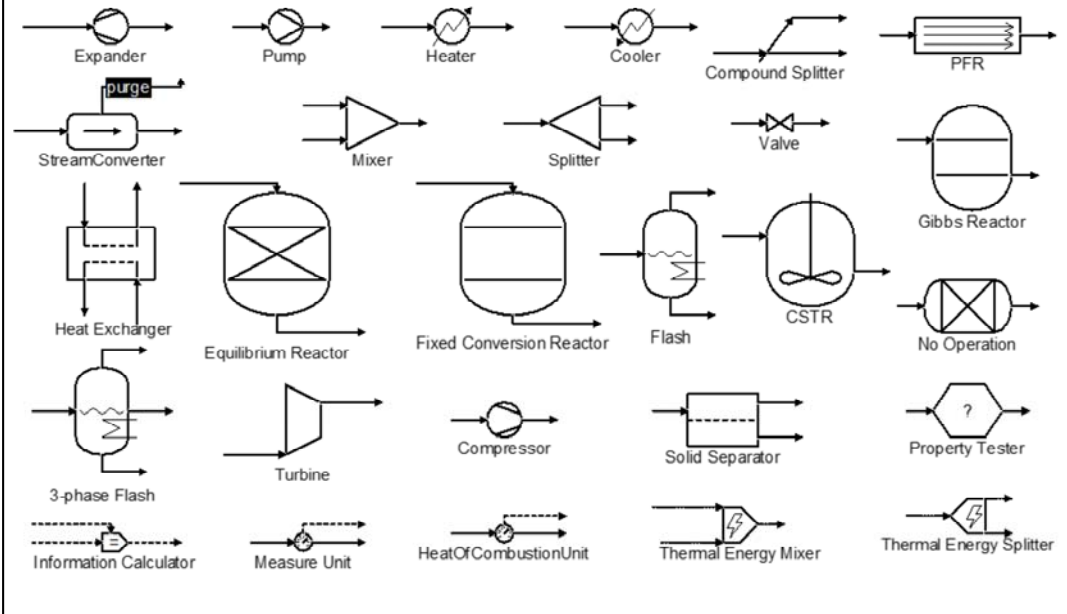


And the reaction package is called CORN; CAPE-OPEN reaction numerics.



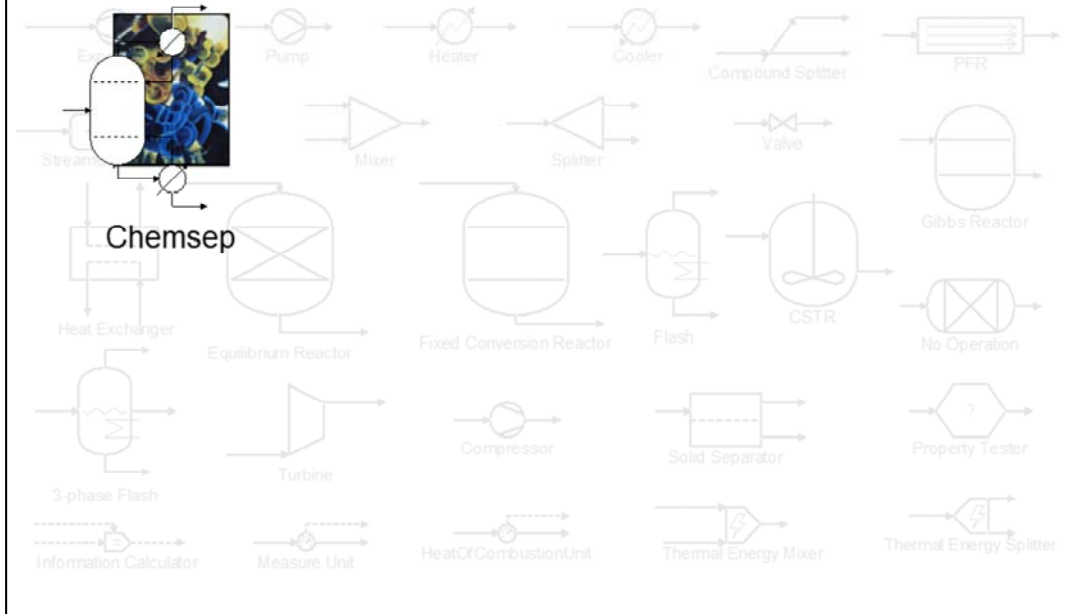
All these components talk to each other using the open and freely available CAPE-OPEN standard. This implies we can mix and match.

## Unit operations: COUSCOUS



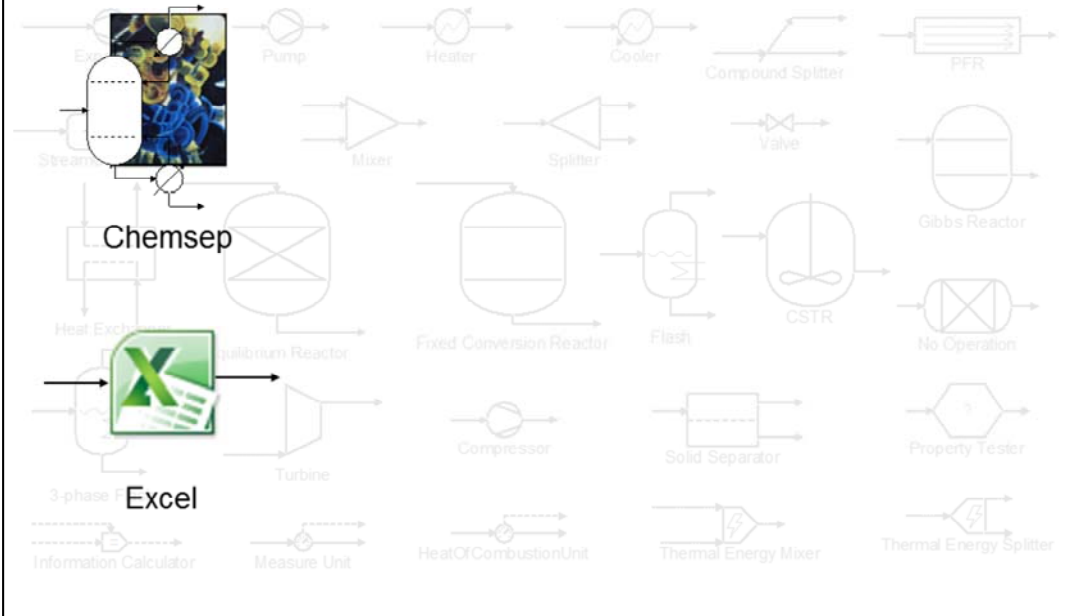
These are for example the unit operations that come with COUSCOUS. Arguably quite a few, but surely not complete. Via CAPE-OPEN we have access to

Unit operations:



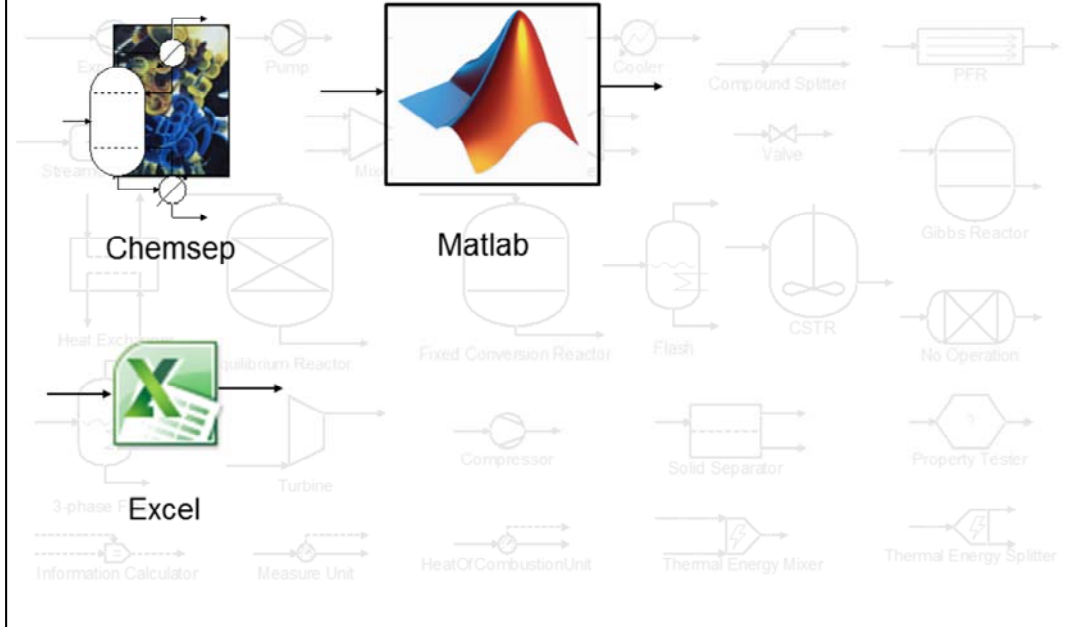
the Chemsep unit operation for distillation and extraction columns. The authors of Chemsep contributed immensely to the development of COCO, and the thermodynamics are still largely based on their code and data. The ChemSep unit operation is the main separation device in COCO.

Unit operations:



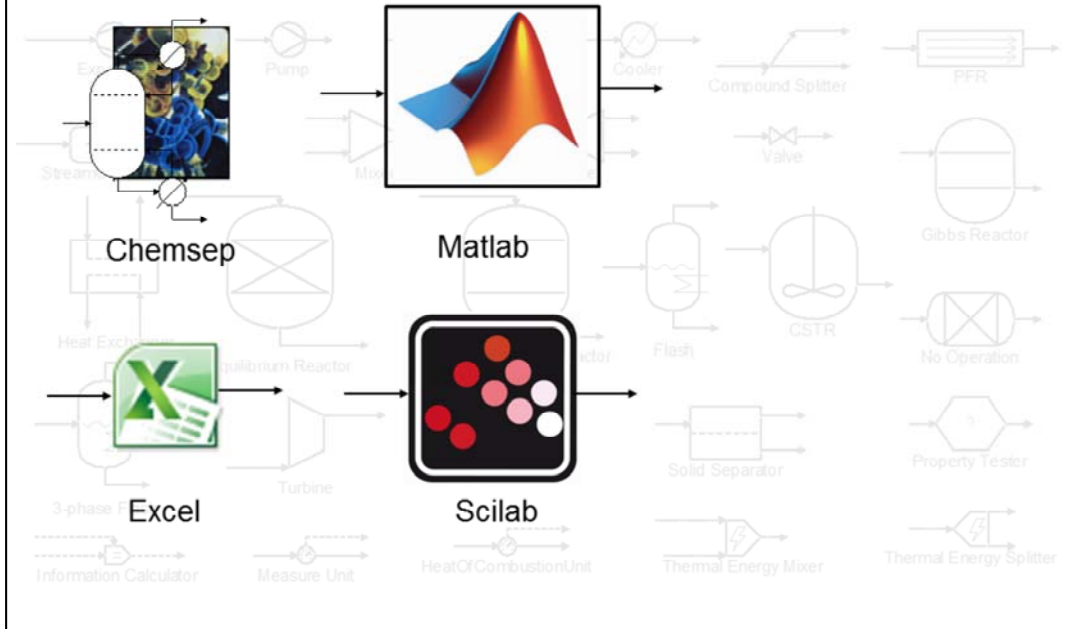
Then there is the Excel based unit operation, in which you can type your unit operation equations in Excel, which also ships with COCO. Here your unit operation equations can be formulated as excel inputs, and solved using the excel solver.

Unit operations:



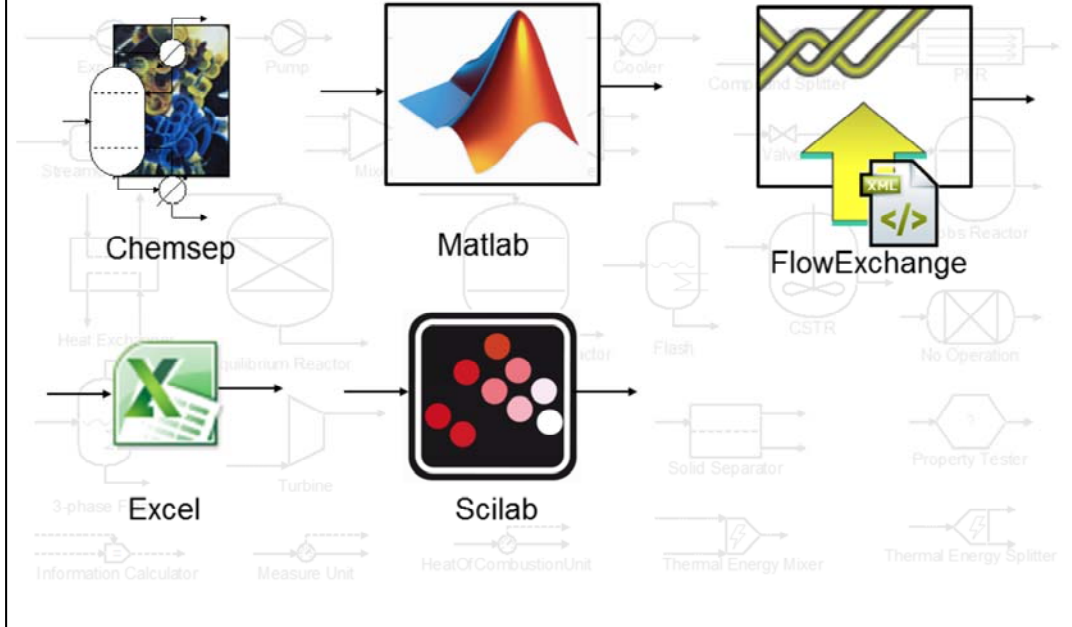
There is the Matlab based unit operation, in which you can use Matlab calculations for your unit operations, and use the suite of solvers that comes with Matlab.

Unit operations:



There is the Scilab unit operation, which is similar to Matlab, but Scilab is free-of-charge,

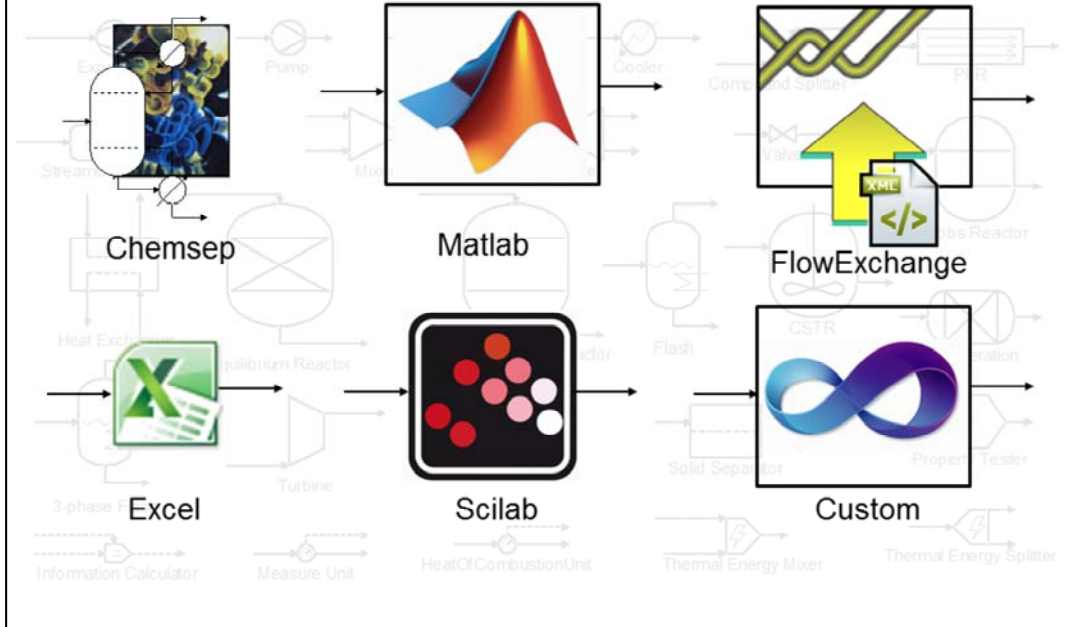
Unit operations:



the open source FlowExchange unit operation, that can be used to import and export stream data from and to XML, and therefore can also be used to exchange stream data between different simulations, even in different simulation programs,

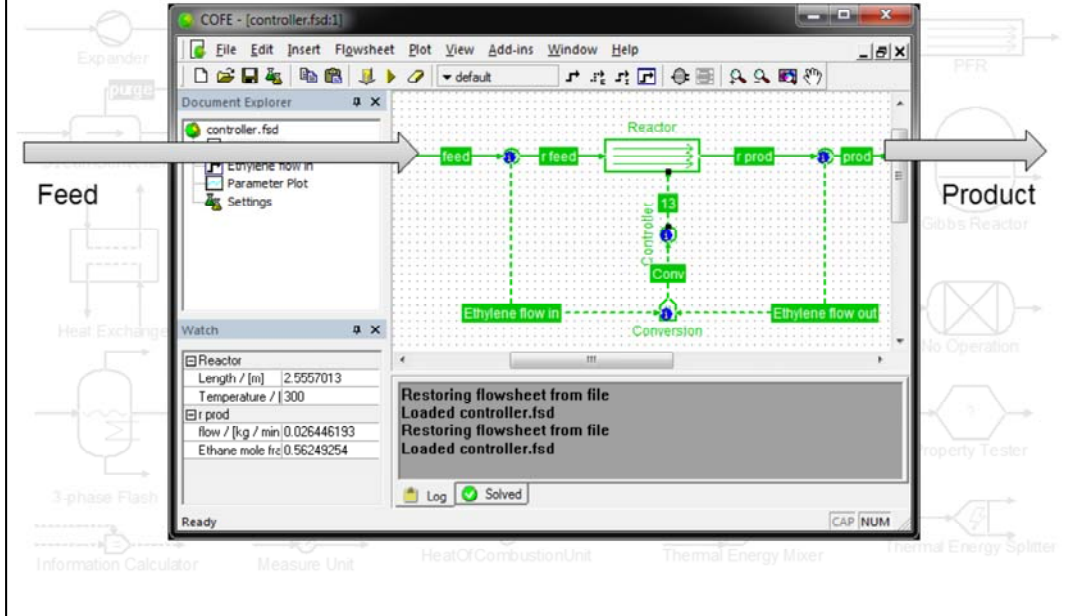


Unit operations:



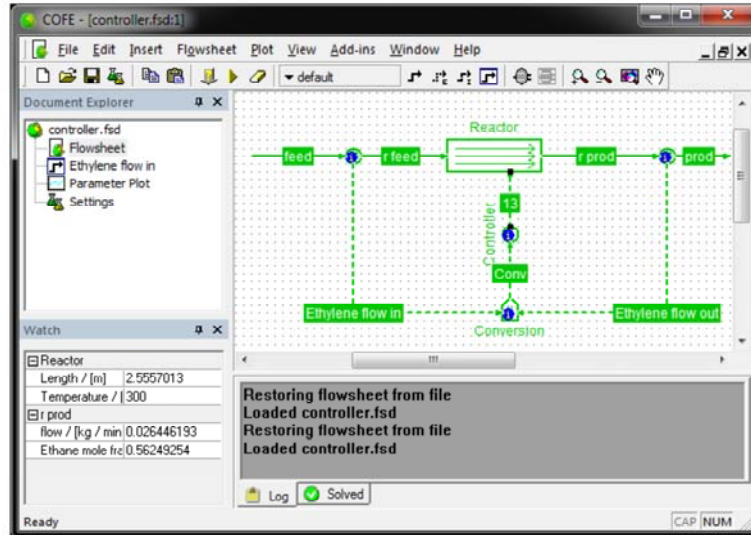
or any custom unit operation that you code yourself that implements the CAPE-OPEN interfaces for unit operations.

Unit operations:



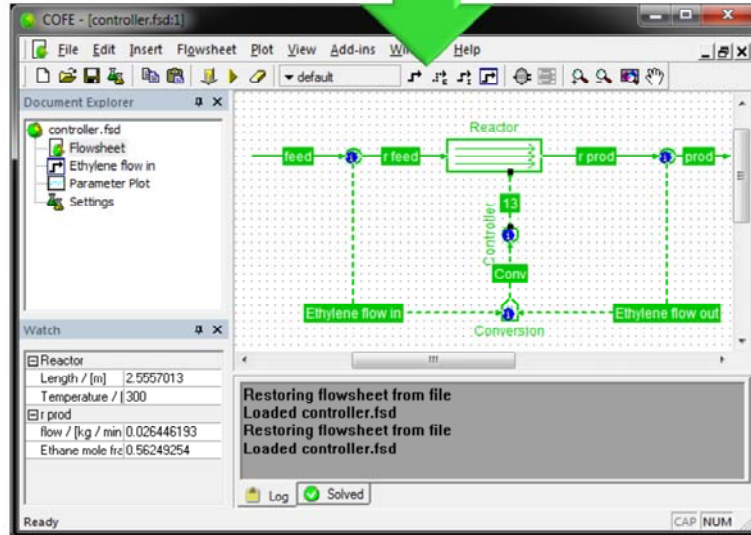
You can even use an entire COFE simulation as a unit operation inside another simulation. And of course there is a variety of third party unit operations available. This argument of course also holds for the thermodynamics; you do not have to use TEA; you can use third party thermodynamics or your own.

Features:



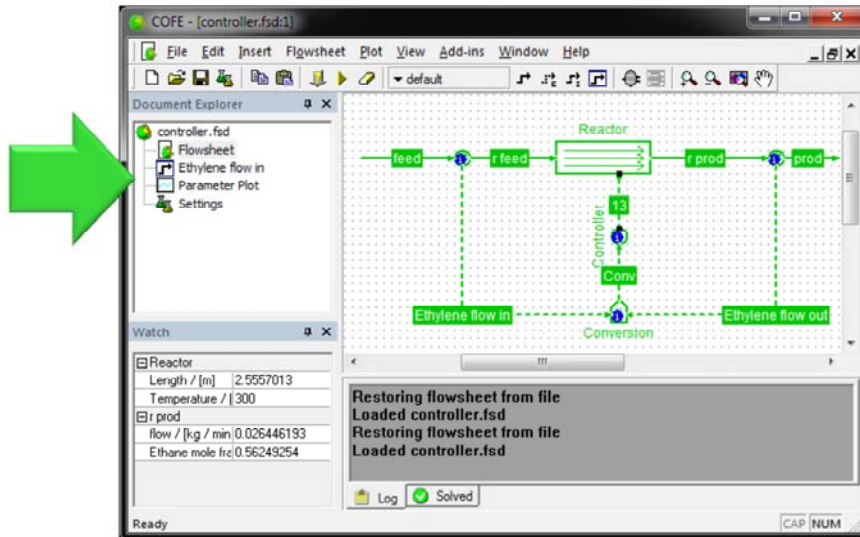
Also the large amount of features and user friendliness of the COFE flowsheeting environment deserves some attention. In the main window, we see

Features:



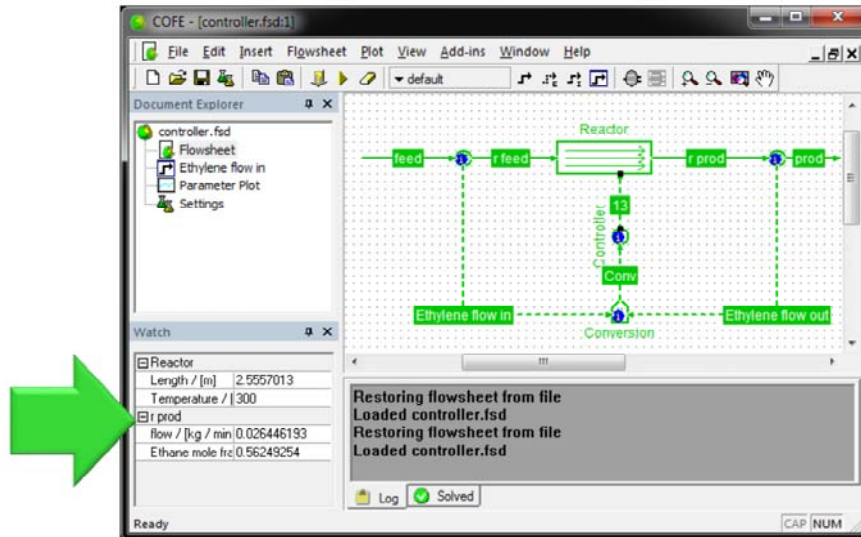
intuitive toolbar buttons for inserting objects like streams and unit operations,

Features:



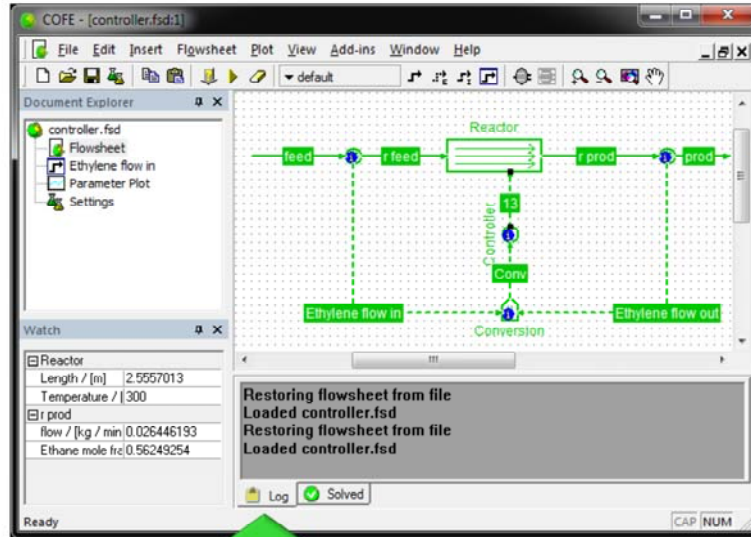
an easy to access navigation pane of the open document and its views

## Features:



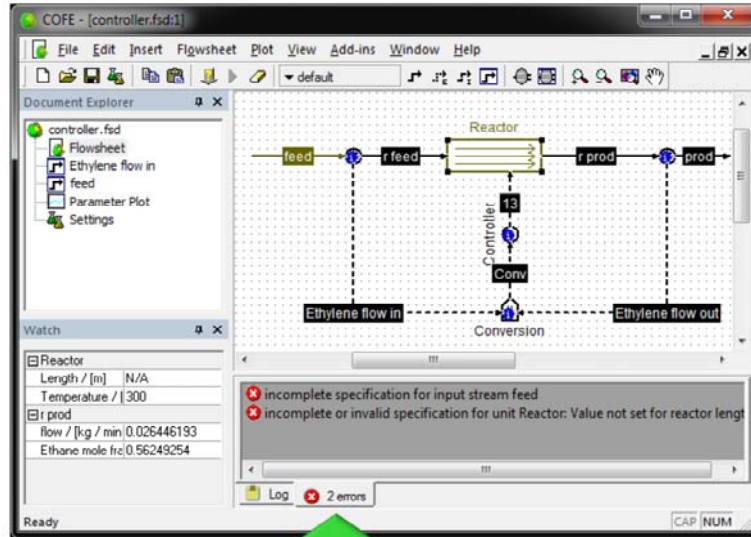
a watch window to access all variables of interest in the flowsheet immediately

Features:



a log window that will keep track of what has happened

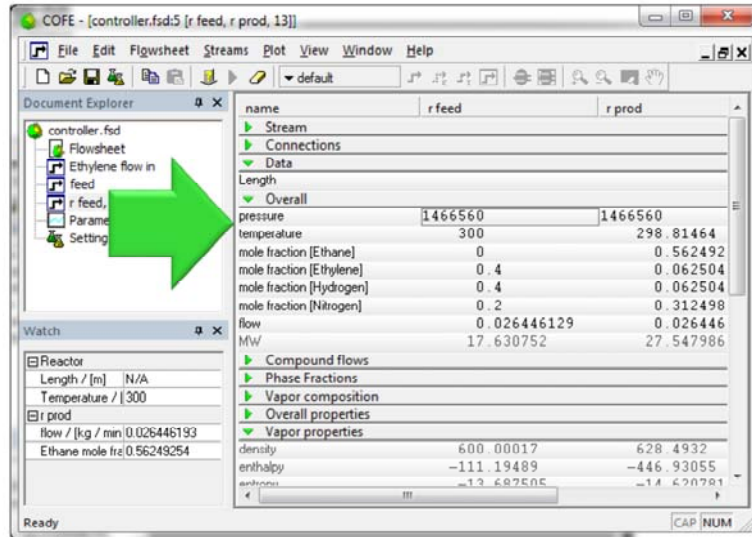
### Features:



and a list of issues that need to be addressed before you can run your simulation.

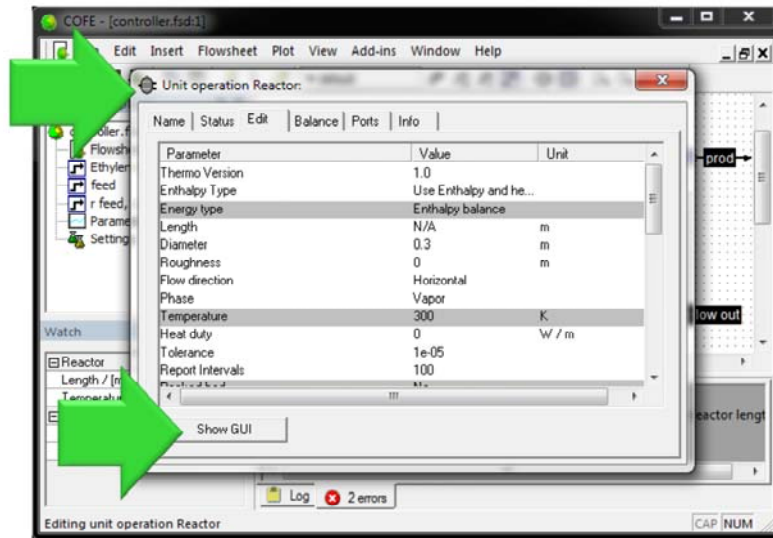


Features:



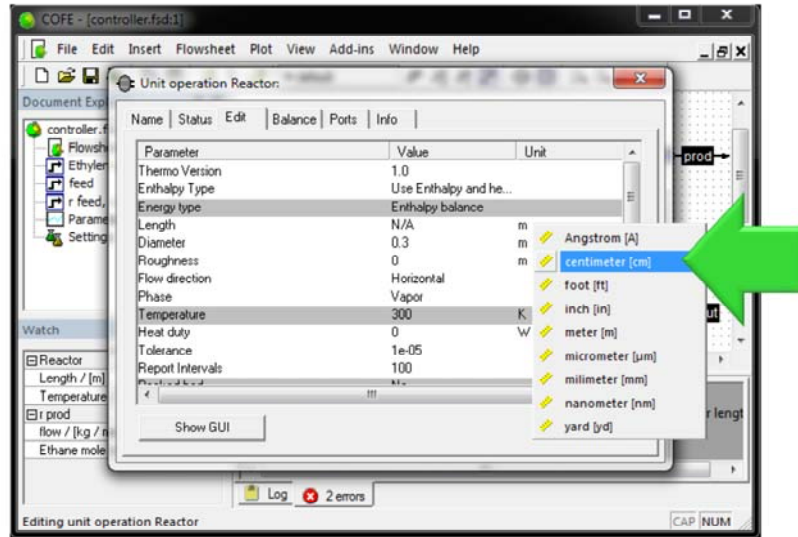
Double clicking a stream will open a stream view. You can also open this for multiple streams at the same time. This view serves both to enter stream specifications and to inspect stream results.

Features:



Double clicking a unit operation will of course open the unit operation data entry window. At first you will see what COFE sees, but as the unit operations are not part of COFE itself, they all have their own input window as well.

Features:

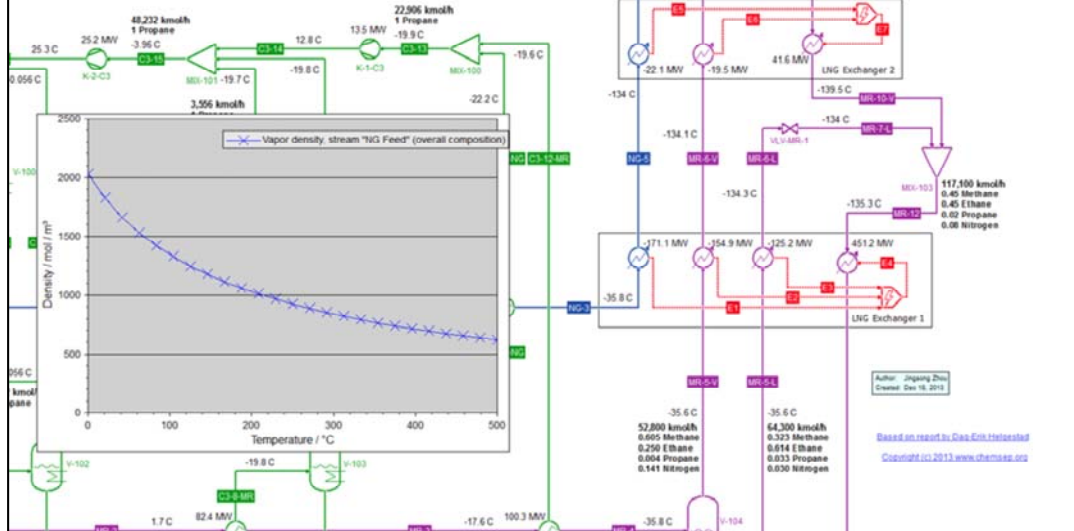


The flexible built-in unit conversion system lets you work in your preferred units of measure just by click on a unit of measure.

**Features:**

**C3MR LNG Refrigeration Process**


Stream	SI Feed	SI-5	SI-6	Unit
Pressure	400	330	280	kPa
Temperature	20	-124	-128.8	°C
Flow rate	10000	10000	10000	kmol/h
Mole Frae Methane	0.887	0.887	0.887	
Mole Frae Ethane	0.093	0.093	0.093	
Mole Frae Propane	0.014	0.014	0.014	
Mole Frae Isobutane	0.001	0.001	0.001	
Mole Frae Nitrogen	0.002	0.002	0.002	



Inside the flowsheet graph you can use custom colouring of unit operations, stream reports, unit operation reports and others kinds of tables, graphs with dynamically updating data, text and drawing items to clear things up, hyper links, and any OLE objects imported from file or pasted from another application.

## cape open to cape open simulation environment





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### COCO

Welcome to COCO.

COCO is a [CAPE-OPEN](#) compatible simulation environment. It consists of the following 4 parts:

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

The following additional utilities are available:

-  **Water:** IAPWS-97 based steam and water property package
-  **CORK:** the CAPE-OPEN Registry Kit
-  **QATS:** out-of-process thermo server and CAPE-OPEN logging tool; includes unit operation logger tool COULIS
-  **COFE\_xlt:** a Microsoft Excel™ spread-sheet template designed to include a COFE document in an Excel workbook
-  **JULIE:** an editor for unit operation icons
-  **TERNary:** TERNary Plugin. Creation of phase diagrams, property plots and residue curves of ternary systems
-  **ConfigureTEA:** a utility application to configure and maintain TEA property packages
-  **ConfigureCORN:** a utility application to configure and maintain CORN reaction packages
-  **CUUP:** COCO Update utility for online software updates

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- Adding series to a plot

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- Utility applications
- 64-bit versus 32-bit software
- Disclaimer

Hopefully this brief overview of what you can do with COCO wets your appetite. You can check out more of COCO's features, including the documentation of all used unit operation and thermodynamic models in the online help that comes with the program. You can also access this directly on the web site.

**COCO**

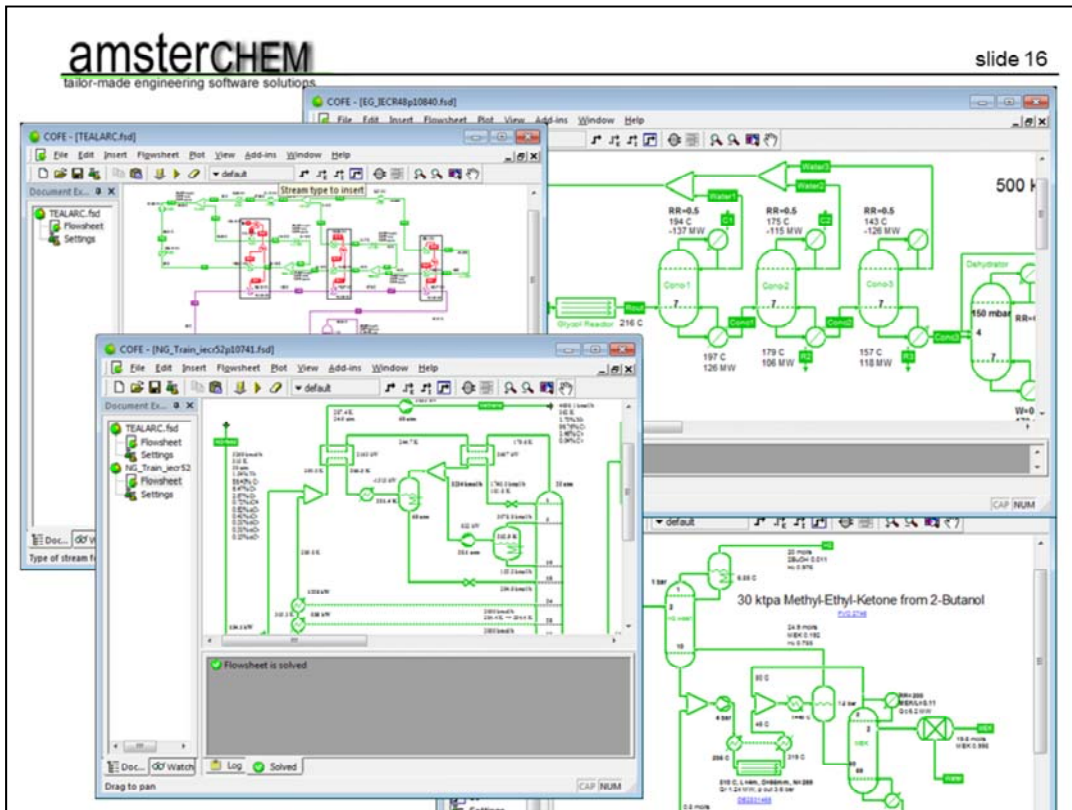
Moderator: jasper

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<b>Plotting Issues</b> by nrgeng » 23 March 2014, 14:23	1	54	by jasper 23 March 2014, 15:28
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<b>Information Calculator Unit: Warning "Mole flow"</b> by nrgeng » 09 February 2014, 17:24	1	70	by jasper 10 February 2014, 18:31
<b>Information Calculator Unit Configuration</b>	12	308	by jasper

This is not your only resource to get help. The CAPE-OPEN forum hosts a section dedicated to COCO where many users posts their problems and get answers.



The COCO web site itself has a support section and it hosts many examples, and allows you to subscribe to a mailing list to stay up-to-date with new releases.

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

Thank you for your time. I hope you have enjoyed this presentation. If you have any further questions or doubts, feel free to contact us. We invite you to download and use the software, it is free of charge. Please participate with your own CAPE-OPEN based models, create your own flowsheets and we are looking forward to seeing you at the CAPE-OPEN forum.