Flowsheeting for Free with COCO

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Why COCO or "Do we really need another flowsheeting progam, even if it is free?"

In previous articles in CACHE News we have described ChemSep™**,** a software system for modeling distillation, absorption, and extraction operations. ChemSep was designed to be easy to use by students with little or no experience of engineering software, while having sufficient flexibility and power to appeal to expert users and engineers in industry.

ChemSep was not a flowsheet simulation program but a standalone one-column-at-a-time simulator so intuitive to use that students could pick it up in 5 minutes or less. Therefore, it was more difficult to model complicated processes involving multiple units and recycle streams than one would like. To deal with this limitation ChemSep came with a rather rudimentary flowsheeting system described in The ChemSep Book (Kooijman and Taylor, Books on Demand, 2000). However, this was not an easy-to-use program (it did not have a user-friendly interface).

The main requirement for an industrial ChemSep user is that ChemSep use the thermodynamic models available in the main flowsheet simulator with the associated databases with pure compound data and interaction parameters. The importance here being that this data & models have been validated. The protocols developed under the CAPE OPEN (CO) movement have made it possible for ChemSep to function as a user model in any CO compliant process simulation environment (this includes all major and some of the less well known packages available today). In addition, any CO compliant thermodynamics package could be used with ChemSep. In CACHE News for Spring 2006 we showed ChemSep as the column model in an Aspen Plus flowsheet for the well-known HDA process.

During the development of a CO compliant version of ChemSep we had need for a CO flowsheet simulation program (because we had no immediate access to Aspen Plus or other similar package). The authors of the CO interface for ChemSep were fascinated by the concept of CO based flowsheeting. An environment was required for ChemSep to perform flowsheet based simulations. And there was a need for in-house code to facilitate CO based development, testing and debugging. Hence, a CO based simulation program was created. The package is known as **COCO** (CAPE OPEN to CAPE OPEN) and is the subject of this article.

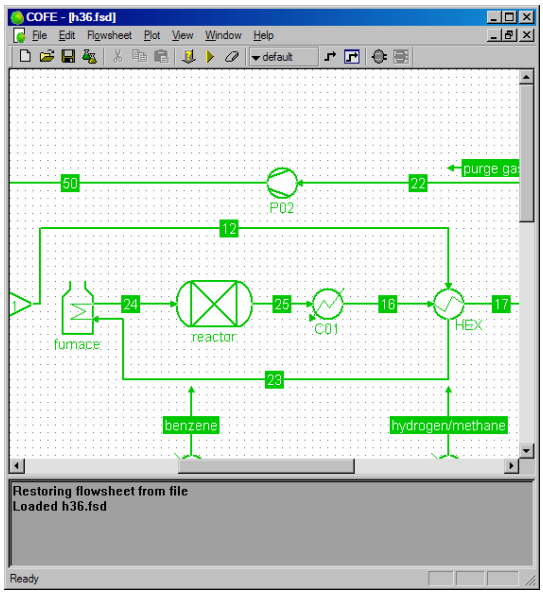
The COCO Kitchen

There are four parts to COCO:

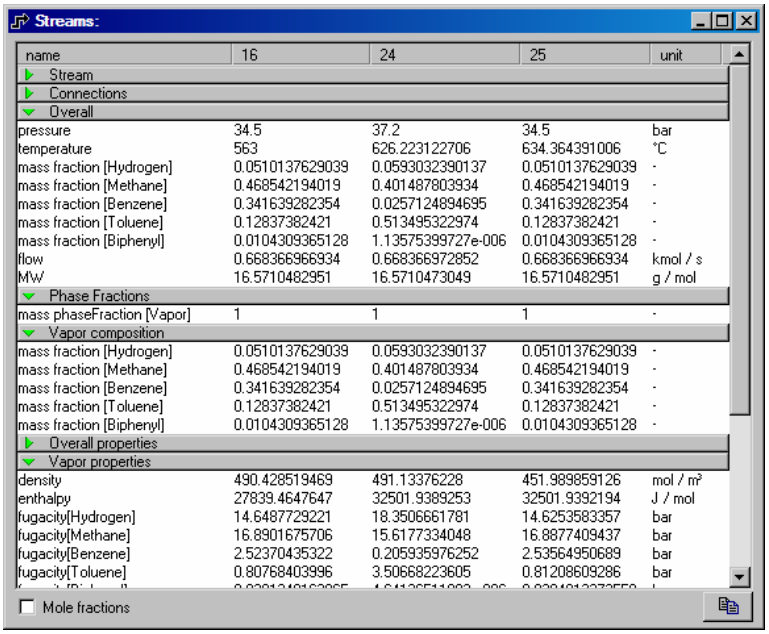
- A simulation environment (COFE, CAPE OPEN Flowsheeting Environment)
- A thermodynamic property package (TEA, Thermodynamics for Engineering Applications)
- A collection of unit operations (COUSCOUS, CAPE OPEN Unit operationS)
- A reaction package (CORN, CAPE OPEN Reaction Numerics)

The Flowsheeting Environment (COFE) features:

- Graphical flowsheet editing:

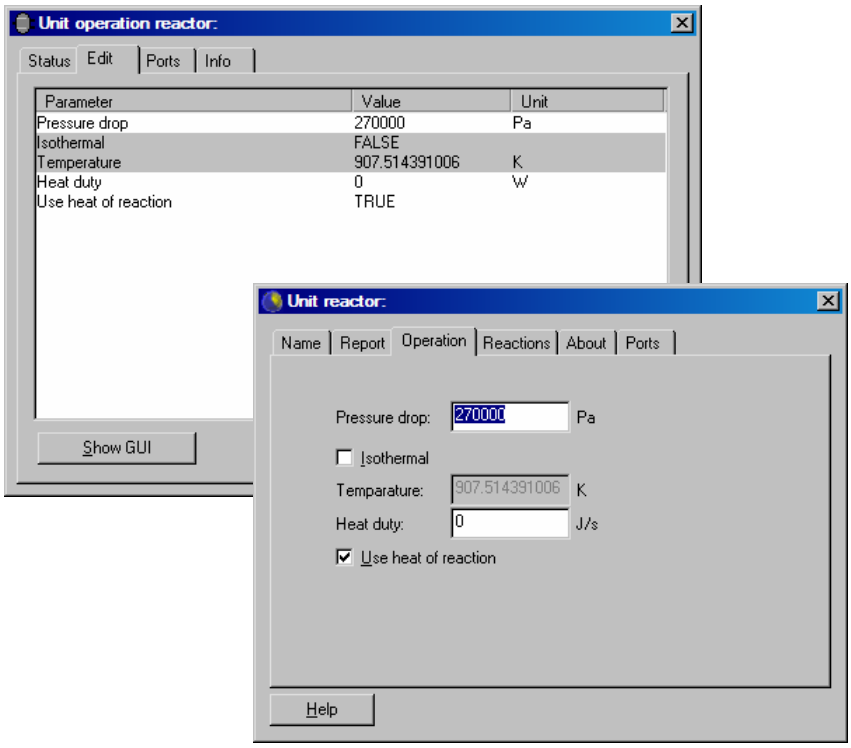


- Compact display of stream information:

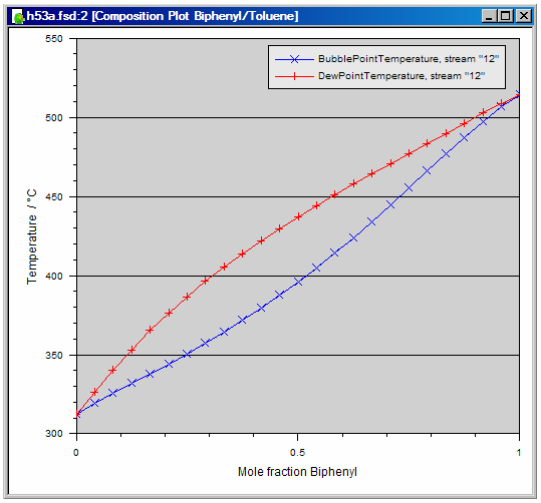


name	16	24	25	unit
Stream				
Connections				
Overall				
pressure	34.5	37.2	34.5	bar
temperature	563	626.223122706	634.364391006	°C
mass fraction [Hydrogen]	0.0510137629039	0.0593032390137	0.0510137629039	-
mass fraction [Methane]	0.468542194019	0.401487803934	0.468542194019	-
mass fraction [Benzene]	0.341639282354	0.0257124894695	0.341639282354	-
mass fraction [Toluene]	0.12837382421	0.513495322974	0.12837382421	-
mass fraction [Biphenyl]	0.0104309365128	1.13575399727e-006	0.0104309365128	-
flow	0.668366966934	0.668366972852	0.668366966934	kmol / s
MW	16.5710482951	16.5710473049	16.5710482951	g / mol
Phase Fractions				
mass phaseFraction [Vapor]	1	1	1	-
Vapor composition				
mass fraction [Hydrogen]	0.0510137629039	0.0593032390137	0.0510137629039	-
mass fraction [Methane]	0.468542194019	0.401487803934	0.468542194019	-
mass fraction [Benzene]	0.341639282354	0.0257124894695	0.341639282354	-
mass fraction [Toluene]	0.12837382421	0.513495322974	0.12837382421	-
mass fraction [Biphenyl]	0.0104309365128	1.13575399727e-006	0.0104309365128	-
Overall properties				
Vapor properties				
density	490.428519469	491.13376228	451.989859126	mol / m³
enthalpy	27839.4647647	32501.9389253	32501.9392194	J / mol
fugacity[Hydrogen]	14.6487729221	18.3506661781	14.6253583357	bar
fugacity[Methane]	16.8901675706	15.6177334048	16.8877409437	bar
fugacity[Benzene]	2.52370435322	0.205935976252	2.53564950689	bar
fugacity[Toluene]	0.80768403996	3.50668223605	0.81208609286	bar

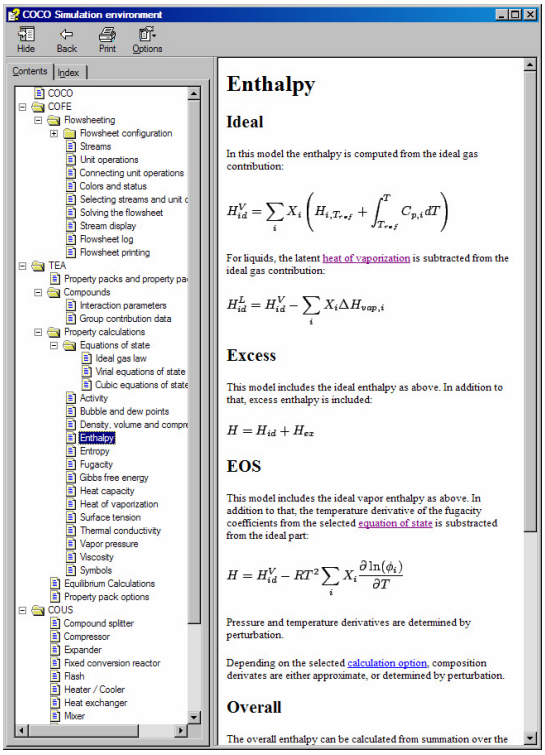
- Access to CO objects such as a reactor unit operation model:



Plotting and printing of physical properties:



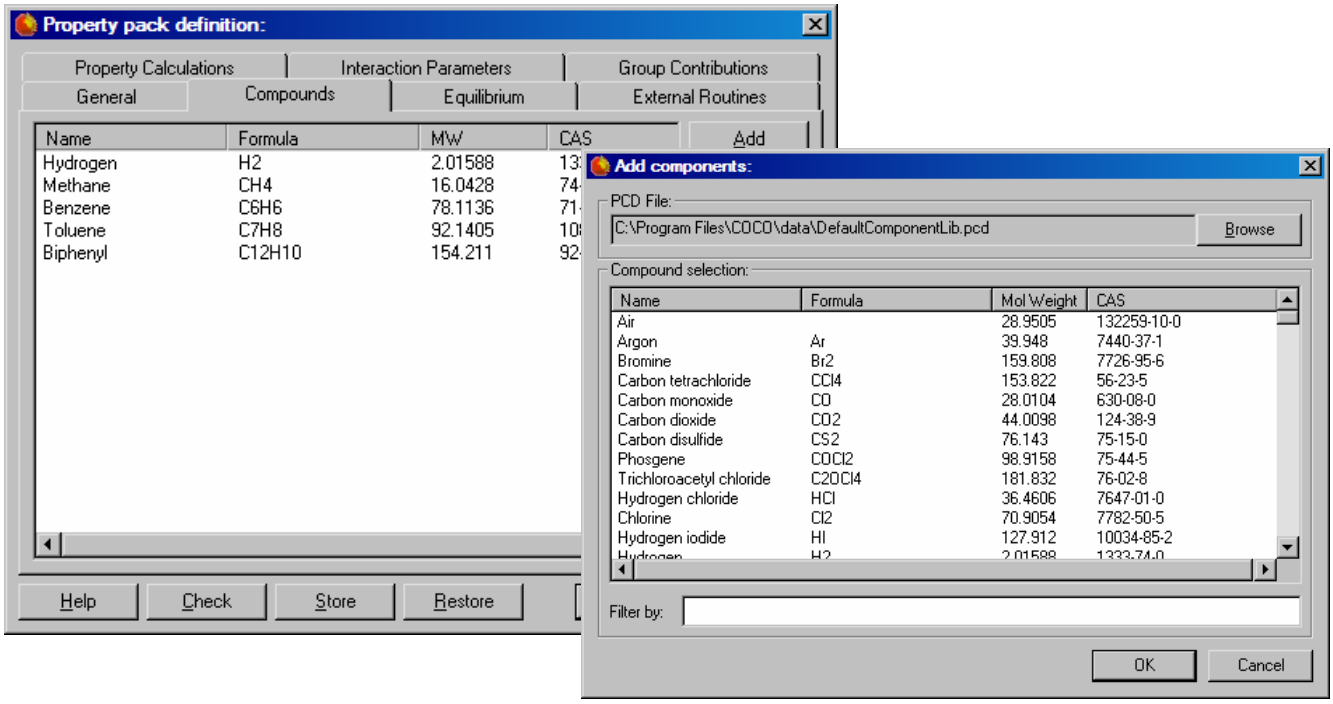
- And a help system:



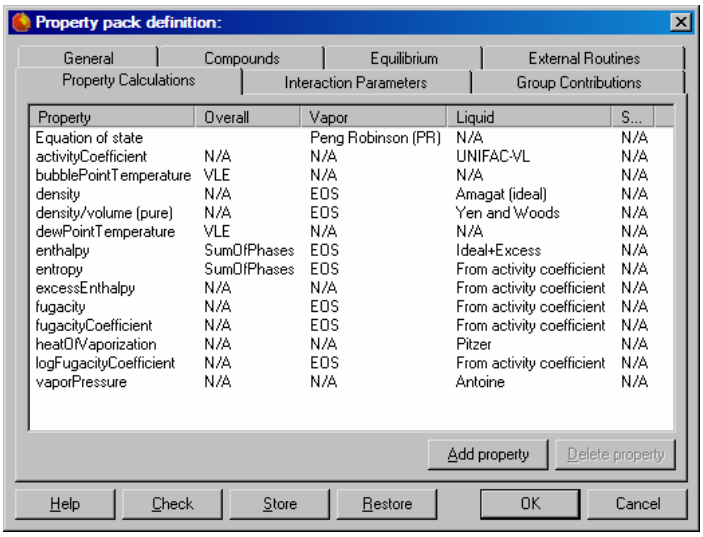
- Steady state process flowsheets are solved using a tearing method (much like the methods used in most commercial simulation programs).

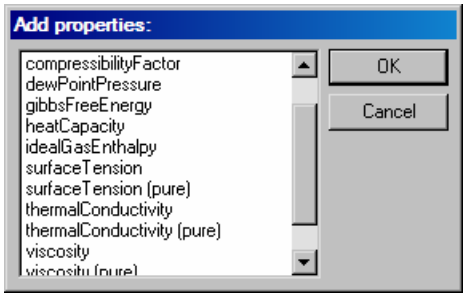
The property package (TEA):

- Includes an extendible pure compound data library:



- Over 100 methods available for the estimation of more than 25 different properties:

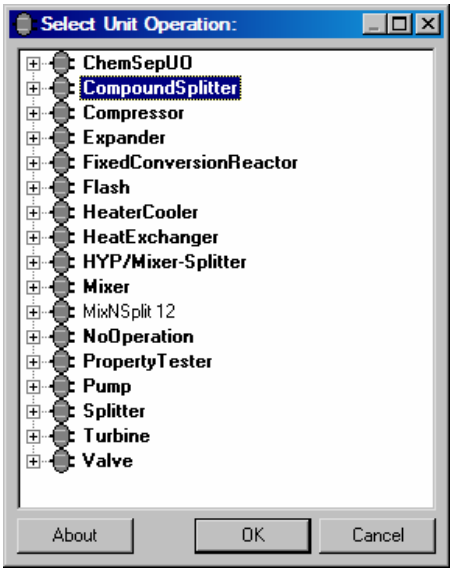


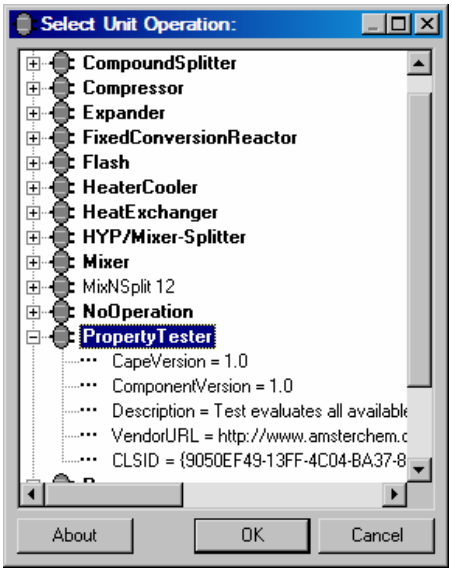


- Property derivatives
- Support for external (CAPE OPEN compliant) physical property packages.

TEA is a reimplementation in C++ of the property package in ChemSep, combined with the pure component databank from ChemSep. TEA can be (and has been) used in any other CO compliant process modeling system.

The Unit Operations package (COUSCOUS) contains general-purpose unit operations such as a mixer, splitter, heat exchanger, a flash, and a property tester:

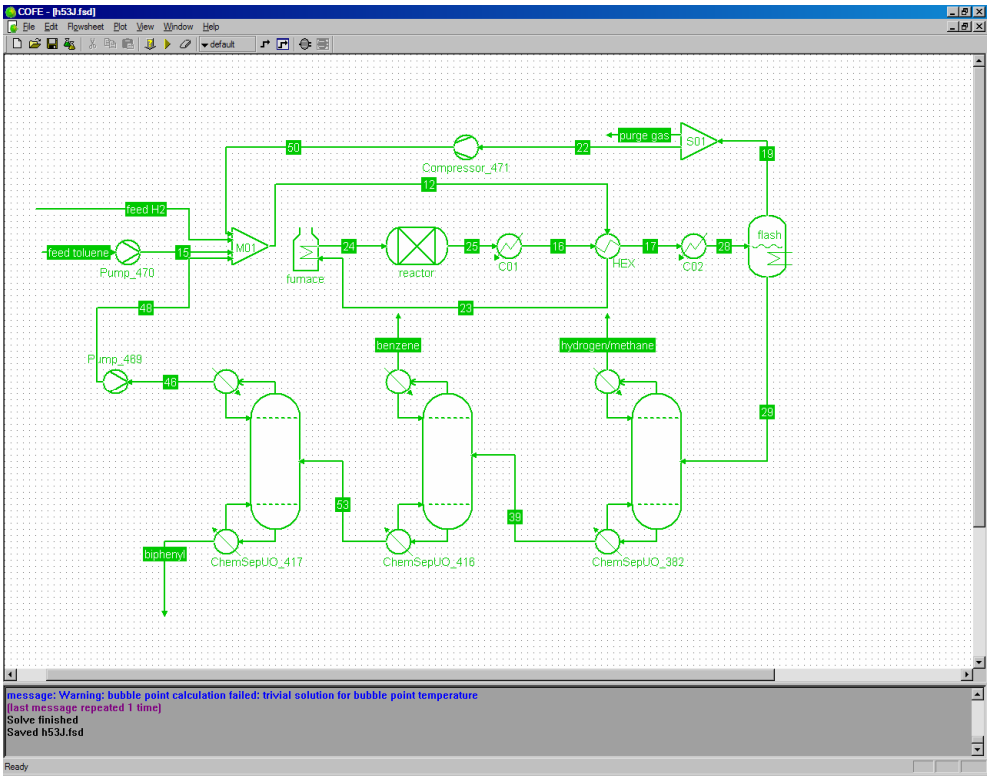




Due to the nature of CO interfacing, COUSCOUS unit operations can be mixed transparently with 3rd party unit operations. COUSCOUS currently provides only a limited number of unit operations (there is currently only one reactor for which conversions have to be specified) but since the interfaces are open, end users can add their own unit operation models.

COCO does *not* include a model for distillation, absorption, and extraction columns. Those units can be simulated using ChemSep.

The illustration below shows COCO being used to model the HDA process. This flowsheet has 3 columns, all modeled using ChemSep.



In summary, The COCO Kitchen serves:

- CAPE-OPEN based flowsheeting environment
- Good interoperability; include units from different sources
- Many flavors of thermodynamic and physical properties
- Support for external (CAPE OPEN compatible) thermodynamic routines (property calculations and equilibrium calculations)
- The ultimate tester for CAPE-OPEN compatibility

Still on the stove are:

- Excel interface to COFE
- Petroleum fractions
- Additional unit operations
- Import/export of numeric interfaces

Acknowledgement

The authors would like to acknowledge the contribution of Richard Baur to the development of COCO.

Availability

COCO is freely available from http://www.cocosimulator.org/

ChemSep-Lite is included in the COCO installation program, and also is freely available from http://www.chemsep.com/. The full version of ChemSep is available for educational use from the CACHE corporation (http://www.cache.org/). For ChemSep licenses for non-educational use please write to taylor@clarkson.edu.

For more information on CAPE OPEN visit http://www.colan.org/.