AN INTRODUCTION TO COCO

Dr. Jasper van Baten, AmsterCHEM, Las Rozas, Spain

Summary

COCO is a CAPE-OPEN based steady state flowsheet simulation environment. COCO consists out of 4 CAPE-OPEN based software components: a flowsheeting environment (COFE), a thermodynamic system (TEA), a set of unit operations (COUSCOUS) and a reaction package manager (CORN). COCO is created with CAPE-OPEN interoperability testing and development in mind, but features a fully functional flowsheet simulation environment. TEA comes with an extensive thermodynamic model library, available in CAPE-OPEN thermodynamic standard versions 1.0 and 1.1. The thermodynamic property calculations and compound database are based on over 10 year experience of the distillation column simulation package ChemSep (http://www.chemsep.com/).

Whereas other simulation environments offer access to simulation components via CAPE-OPEN interfaces, COCO is modeled around CAPE-OPEN interfaces. The flowsheeting environment does not have integrated unit operation models or thermodynamic calculations: all such calculations are done only via CAPE-OPEN interfaces. This setup allows for using each of the COCO components in combination with any other equivalent CAPE-OPEN compliant components.

COCO can be downloaded for free at http://www.cocosimulator.org/. Within the CAPE-OPEN community, COCO is extensively used for interoperability testing. As a result of its free availability and extensive usage, COCO frequently receives feedback on CAPE-OPEN interfacing and interoperability issues. For the COCO development team this provides a means to remain up-to-date with the latest CAPE-OPEN developments; the COCO developers actively take part in CAPE-OPEN Laboratories Network activities and especially in its various Special Interest Groups (SIGs).

Introduction

A typical simulation environment supporting CAPE-OPEN[1,2] Process Modeling Clients, or PMCs, is sketched in Figure 1:

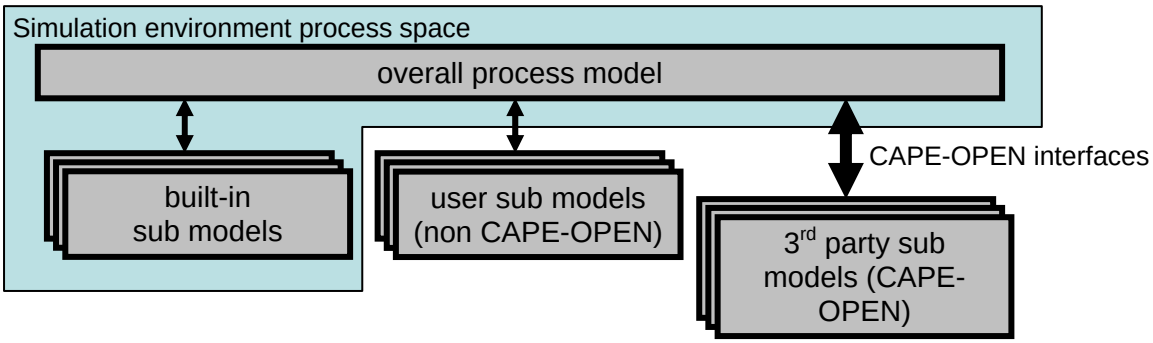


Figure 1: typical setup for process engineering modeling tools supporting CAPE-OPEN models.

COCO is a steady state simulation environment, for CAPE-OPEN interoperability testing and development as well as for simulation purposes. The setup of COCO is much like the typical setup in Figure 1, except for that COCO's flowsheeting environment COFE does not require any built-in sub models or thermodynamics or proprietary interfaces; COCO is entirely modeled around CAPE-OPEN. Therefore, you can run COFE with COCO's thermodynamics library TEA, or with any third-party CAPE-OPEN compliant thermodynamic components; you can run COFE with COCO's unit operation models COUSCOUS, or with any other third-party CAPE-OPEN compliant unit operation models. Similarly, you can use COCO's thermodynamics TEA or COCO's unit operation models COUSCOUS in COFE, but also in any other third-party CAPE-OPEN compliant simulation environment.

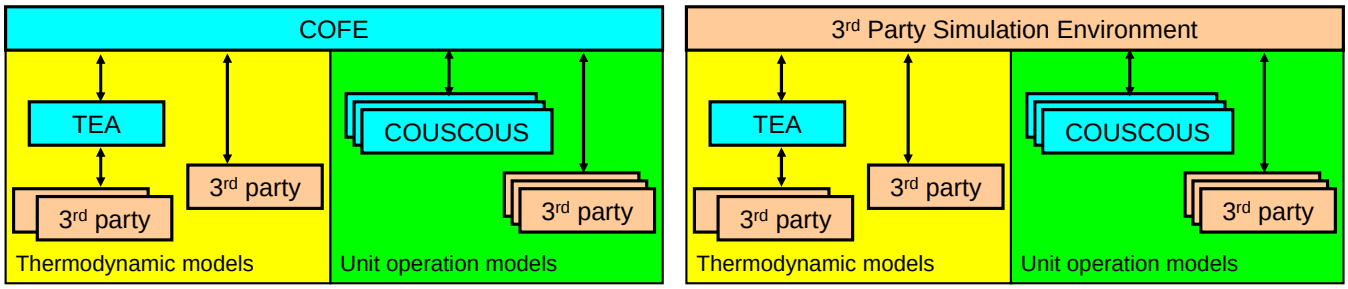


Figure 2: Schematic representation of simulation environments with thermodynamic models and unit operation models. All of COCO's components are exchangeable. Support for external models as indicated for third-party simulation environments differs from product to product.

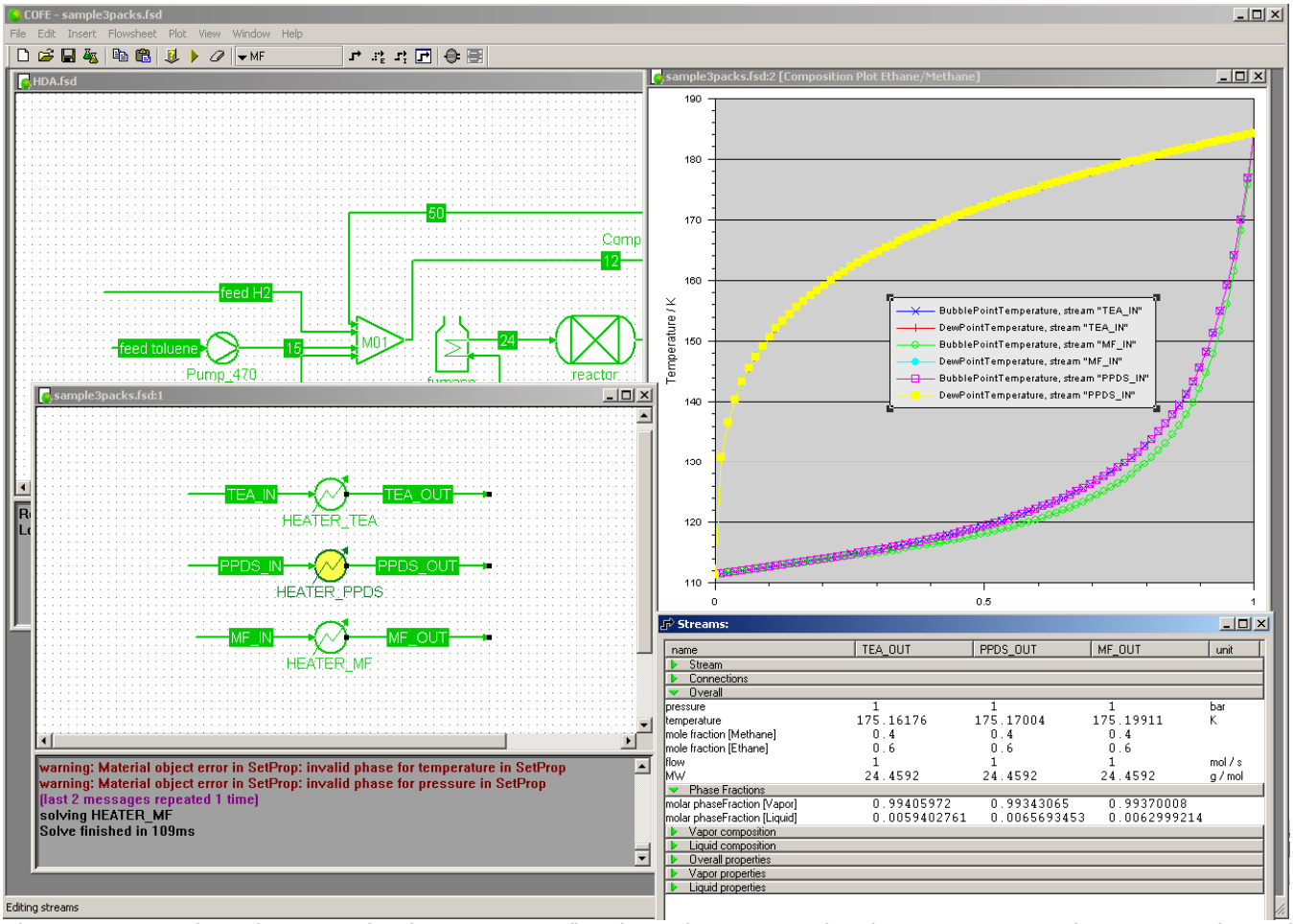
At this moment, all COCO's CAPE-OPEN interfaces are COM interfaces, and therefore run on Microsoft Windows® platforms[3]. COCO received the CO-LaN CAPE-OPEN 2006 Award.

COFE: CAPE-OPEN Flowsheeting Environment

COFE is a steady state flowsheeting environment. It has an intuitive graphical front-end for flowsheet building. Steady state flowsheets are solved by partitioning, followed by cutting and tearing for partitions containing recycles. Recycles are detected by structurally traversing the partition's streams, considering groups of unit operations as a single entity. After removing self-recycles from the equation, recycle tearing aims for an optimal tearing set by selecting tear streams on criteria like cutting recycles as few times as possible, cutting as few variables as possible, and having as few cut streams as possible. Recycles are solved using a hybrid approach, switching between Wegstein substitution and full Newton iterations.

COFE supports CAPE-OPEN thermodynamic property packages (versions 1.0 and 1.1), CAPE-OPEN unit operations and CAPE-OPEN reaction packages. Configuration data of each CAPE-OPEN PMC is easily accessed, either through CAPE-OPEN parameter interfaces or using the model's native editing methods.

COFE features property graphing, a built-in property calculator, multiple material types allowing for sub-sets of compounds and easy switching of thermodynamic models, and standard Windows features like graphical printing and print preview, OLE support, copy / paste, as well as an extensive on-line help. An Automation interface allows accessing COFE flowsheets in a programmatic manner; a direct application hereof is the ability to incorporate flowsheets in a Microsoft Excel workbook, and perform thermodynamic calculations as well as access stream and unit operation data.



name	TEA_OUT	PPDS_OUT	MF_OUT	unit
Stream				
Connections				
Overall				
pressure	1	1	1	bar
temperature	175.16176	175.17004	175.19911	K
mole fraction [Methane]	0.4	0.4	0.4	
mole fraction [Ethane]	0.6	0.6	0.6	
flow	1	1	1	mol / s
MW	24.4592	24.4592	24.4592	g / mol
Phase Fractions				
molar phaseFraction [Vapor]	0.99405972	0.99343065	0.99370008	
molar phaseFraction [Liquid]	0.0059402761	0.0065693453	0.0062999214	
Vapor composition				
Liquid composition				
Overall properties				
Vapor properties				
Liquid properties				

Figure 3: screenshot of COCO showing two open flowsheet documents. The document on top shows comparison of thermodynamic calculations of three different vendors. The stream view on the bottom right lists the results of the stream exiting the heaters (with equal configuration and equally defined inlet streams). The plot on the top right shows the phase envelopes for the three thermo systems at inlet stream conditions.

COFE is built not only for simulation purposes, but also with CAPE-OPEN testing and development in mind. Therefore, COFE does extensive error checking and logging. Errors and warnings are collected separately for each unit operation at the last iteration of their solution. CAPE-OPEN interface errors clearly show in red text in the log window that sits at the bottom of every flowsheet document. Messages sent to COFE by external models show in blue in the log window. Information messages show in black. Critical CAPE-OPEN errors are shown in a message box.

Figure 3 shows a screen shot of COFE. Figure 4 shows an example of COFE's Automation; running COFE in Microsoft Excel.

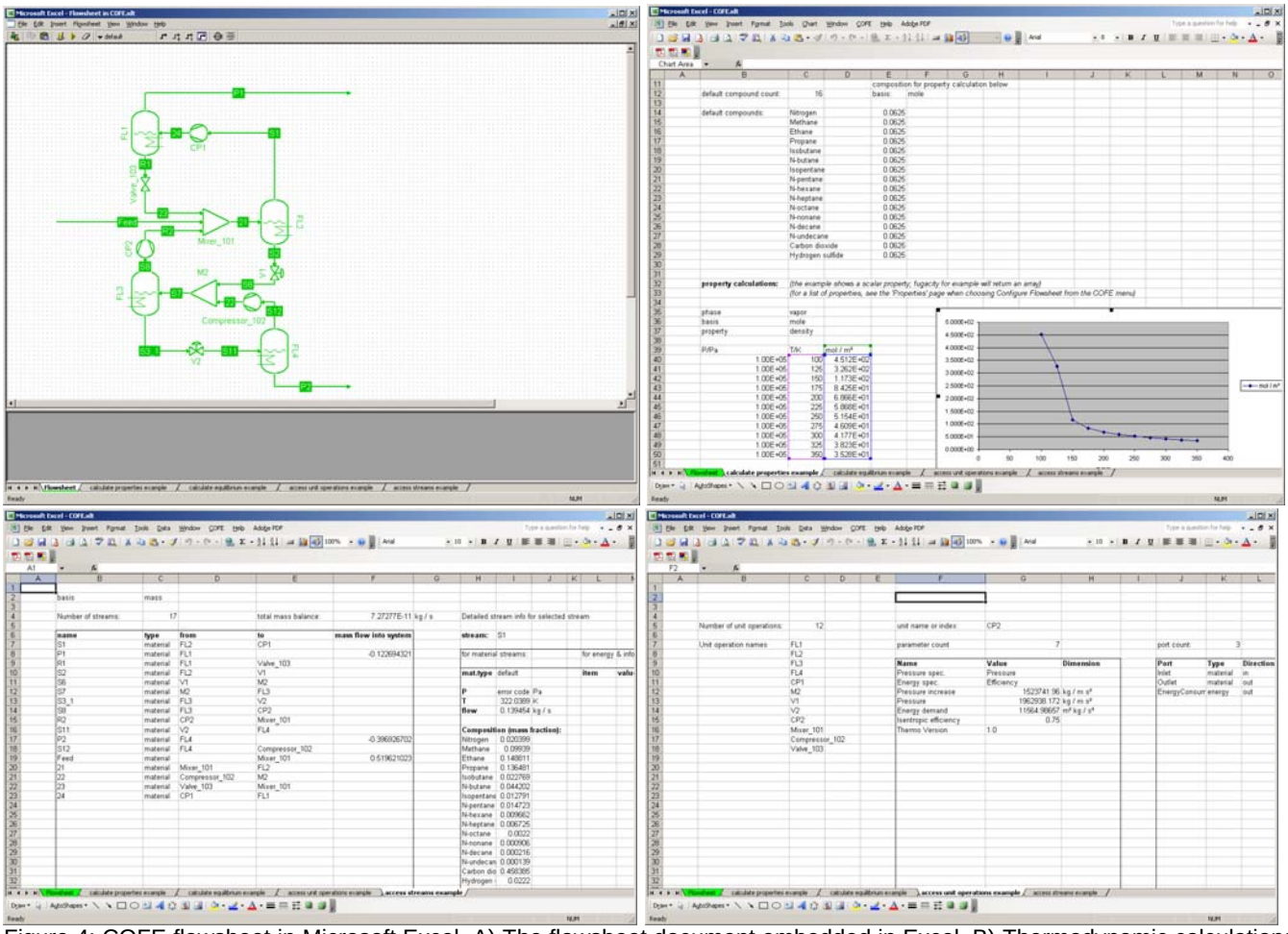


Figure 4: COFE flowsheet in Microsoft Excel. A) The flowsheet document embedded in Excel. B) Thermodynamic calculations utilizing the flowsheet's thermodynamic setup C) accessing stream data from the flowsheet D) accessing unit operation data from the flowsheet.

TEA: Thermodynamics for Engineering Applications

TEA is COCO's thermodynamic calculation engine. It implements a CAPE-OPEN version 1.0 Thermo System as well as a CAPE-OPEN version 1.1 Property Package Manager. With an extensive library of property calculation routines, TEA exports more than 25 different properties with their pressure-, temperature- and composition derivatives. Each property calculation method can be selected individually, allowing the user to pick from more than 100 property calculation routines. TEA comes with a pure compound database that can be extended with user data or by using commercially available compound databases (DIPPR). TEA includes binary interaction coefficients for various models, which the user can override. Also all compound properties and coefficients to correlations can be overridden by the user. Most of the calculation routines that are built into TEA are based on the implementation of ChemSep (http://www.chemsep.com/), a distillation column simulation program. In doing so TEA shared in more than 10 years of experience of the ChemSep development team. Pseudo properties are implemented for infeasible solution regions of cubic equations of state[4], and TEA comes with a built-in vapor-liquid equilibrium calculator using inside-out flash calculations[5,6], with as backup a full Newton solution to flash calculations.

TEA supports plugging in external property Calculation Routines (CAPE-OPEN version 1.0) as well as external Property Calculation Routines and Equilibrium Calculation Routines

(CAPE-OPEN version 1.1). This allows overriding property calculations that are done by TEA by any other third-party calculation server, as well as overriding the equilibrium model. As a result, you can use TEA for your thermodynamic calculations, but you can also use TEA as a means to combine multiple third-party property packages or calculation routines to define a custom set of thermodynamic property calculations.

COUSCOUS: CAPE-OPEN Unit operations (Simple)

COUSCOUS is a library of unit operations. COUSCOUS aims to allow for the most common process engineering calculations. Most of the COUSCOUS models are simple and straight-forward, including unit operations such as compressors, pumps, turbines, expanders, simple reactor models, flash unit operations, heaters, coolers, heat-exchangers, mixers and splitters. COUSCOUS includes a no-operation unit operation, which is intended for testing CAPE-OPEN operation only. More-over, it contains a unit operation specifically to test property package implementations. This unit operation will systematically calculate all properties and compare obtained property derivatives with derivatives that are calculated by perturbation. Unit operations like this aid in CAPE-OPEN development and are not intended to contribute to process simulations. All COUSCOUS' unit operations can deal with CAPE-OPEN thermodynamic versions 1.0 and 1.1.

COUSCOUS does not include a distillation column. COCO however ships with a LITE version of ChemSep; this allows for calculation equilibrium distillation columns with a limited number of compounds and stages. A full version of ChemSep, featuring reactive distillation and non-equilibrium calculations, can be purchased separately.

CORN: CAPE-OPEN Reaction Numerics

CORN is COCO's reaction packages; it features kinetic and equilibrium reactions. For reaction kinetics, equilibrium constants and heats of reactions, formulas can be entered depend on pressure, temperature, concentration, mole fraction or activity. CORN deals with CAPE-OPEN thermodynamic versions 1.0 and 1.1.

Currently, there is not a wide support for reaction packages. The main application for CORN at the moment therefore is to run COUSCOUS reactors in COCO. CORN can aid in development of CAPE-OPEN simulation environments that aim to implement support for reaction packages.

COCO: CAPE-OPEN to CAPE-OPEN environment

COCO is the collection of COFE, TEA, COUSCOUS and CORN. In addition to that, it contains utilities like CORK (CAPE-OPEN Resource Kit), a utility to inspect and manipulate CAPE-OPEN object registration. The COCO distribution also includes third-party contributions. Currently, it includes the LITE version of the ChemSep distillation column simulation program (http://www.chemsep.com/) and COSMO*Logic*'s activity calculation routine COSMO*Therm* (http://www.cosmologic.de). Developers and software vendors are encouraged to include freely available, functional, CAPE-OPEN compliant software components in the COCO distribution.

Interoperability

COCO comes with a number of test-problems (available from the web site), such as the Hydro De-Alkylation plant[7], and the Cavett test-problem for flowsheet convergence[8]. Each of

these test problems can be used to insert any other thermodynamic model or unit operation for interoperability testing.

COCO and its components have been submitted to extensive cross-testing against third-party products. Often these tests are successful; sometimes the tests expose items that are amendable for improvement. As a testing platform, COCO is popular within the CAPE-OPEN community. As a result, COCO often gets feedback on things that do or do not function properly in inter-model communication. Sometimes this leads to discussions that involve multiple software vendors and the CAPE-OPEN special interest groups (SIGs) on how the standard or its documentation can be improved upon. COCO has recently launched a CAPE-OPEN interoperability testing program. For more details, please see http://www.cocosimulator.org/.

Shown in Figure 3 is a test example in which three different thermodynamic systems; COFE allows for loading multiple thermodynamics sets at the same time. You can create multiple types of material definitions, and assign a thermodynamic property package to each material definition. Cross-testing can be done by setting up the problem twice (as in Figure 3) or by re-assigning the thermodynamic set to the material type and rerunning the problem. An example of TEA thermodynamics running in AspenPlus 2004.1 is shown in Figure 5; in this example TEA imports activity coefficients from COSMO*Therm*.

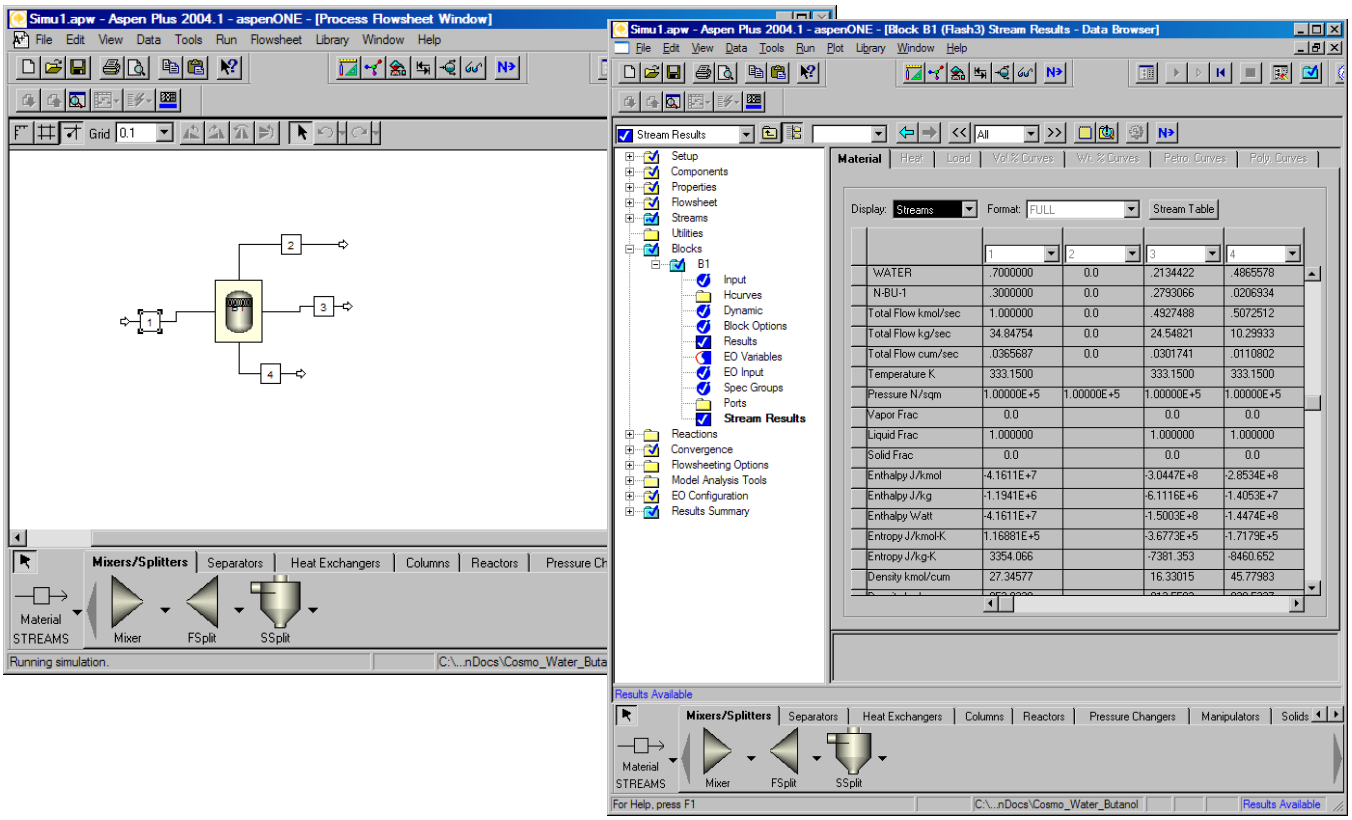


Figure 5: AspenTech's AspenPlus 2004.1 three phase flash using TEA thermodynamics combined with COSMO*Logic*'s activity calculation routine COSMO*Therm*, as presented by Frank Eckert at the annual CAPE-OPEN conference in Cannes (France), March 2006.

In allowing each of the software components to be used and tested in any desired environment, COCO makes it possible for developers without access to proprietary simulation environments to reliably develop new process models and thermodynamic models. Because of the activities of the COCO developers in the CAPE-OPEN special interest groups and frequent

discussions with software developers, COCO contributes to enhancements and additions to the CAPE-OPEN standard specifications and its documentation. By means of its recent testing program, COCO contributes to the steadily improving quality of existing CAPE-OPEN implementations currently available, and promotes new implementations to be released.

Availability

COCO is available for download free of charge from http://www.cocosimulator.org/.

Conclusions

COCO is a collection of CAPE-OPEN software components for steady state process simulation and CAPE-OPEN interoperability testing. It is the award-winning simulation environment that is entirely based on CAPE-OPEN, allowing developers and industry to fully test and exploit the power and versatility of CAPE-OPEN technology.

COCO is available free of charge. It contains all requirements for basic steady state flowsheet simulations, and is therefore suitable for academic use and educational courses on thermodynamics, reactions, separations and process design and synthesis.

CAPE-OPEN builds bridges between commercial industrial software and academia for development of dedicated process software in reactor engineering and separation technologies. COCO contributes because of its availability and because is it open to contributions from third parties.

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