

A look into the CAPE-OPEN kitchen of



COCO

Jasper van Baten, AmsterCHEM

CAPE-OPEN to CAPE-OPEN (COCO):



Simulation environment (COFE)



Thermodynamic property package (TEA)



Collection of unit operations (COUS)



Reaction package (CORN)



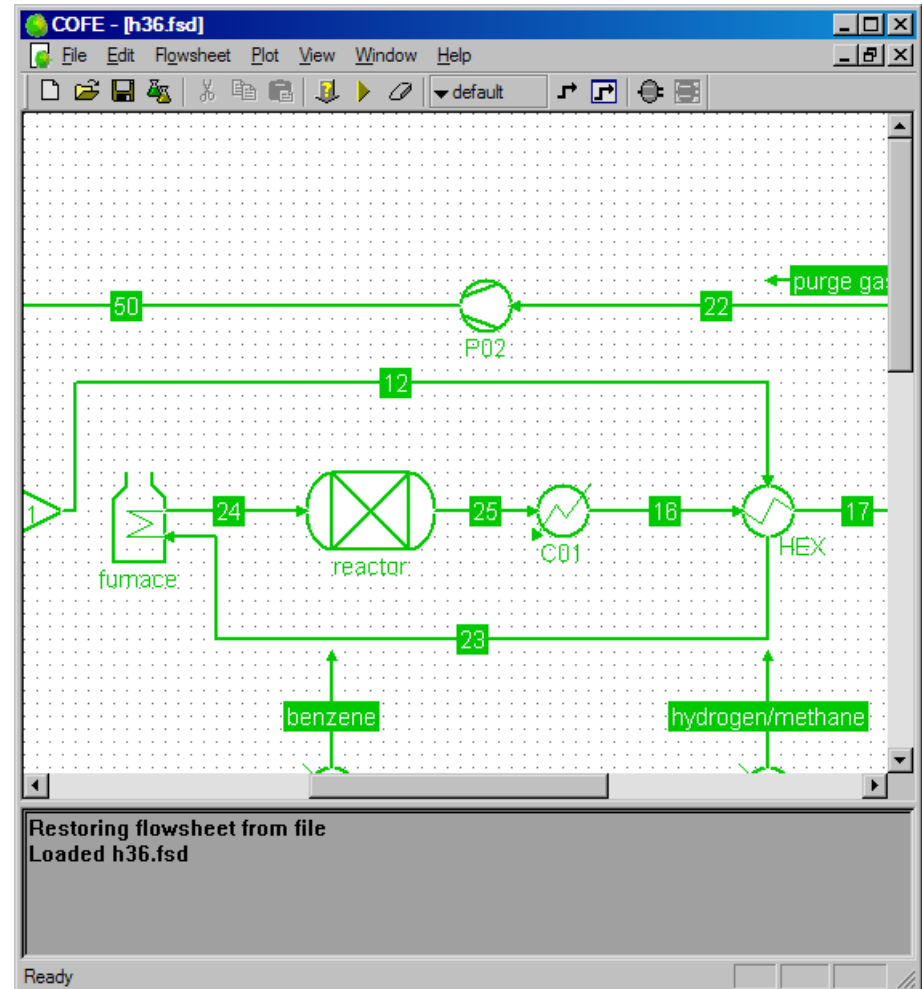
COFE: CAPE-OPEN Flowsheeting Environment

GUI:

- Graphical flowsheet editing
- Compact display of streams
- Quick access to CO objects
- Property graphing & printing
- Extensive help

Flowsheeting:

- Steady state
- Solution by tearing algorithm
- Multiple material templates





COFE: CAPE-OPEN Flowsheeting Engine

GUI:

- Graphical flowsheet editing
- **Compact display of streams**
- Quick access to CO objects
- Property graphing & printing
- Extensive help

Flowsheeting:

- Steady state
- Solution by tearing algorithm
- Multiple material templates

The screenshot shows the COFE software interface with a 'Streams' window open. The window displays a table of process data for three streams (16, 24, 25). The table is organized into several sections: Overall, Phase Fractions, Vapor composition, and Vapor properties. The 'Overall' section includes pressure, temperature, mass fractions of Hydrogen, Methane, Benzene, Toluene, and Biphenyl, flow, and MW. The 'Phase Fractions' section shows mass phase fraction [Vapor] for each stream. The 'Vapor composition' section shows mass fractions of Hydrogen, Methane, Benzene, Toluene, and Biphenyl. The 'Vapor properties' section shows density, enthalpy, and fugacity for Hydrogen, Methane, Benzene, and Toluene. The 'Mole fractions' checkbox is unchecked.

	16	24	25	unit
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	-
Vapor properties				
density	490.428519469	491.13376228	451.989859126	mol / m ³
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	0.205335976252	2.53564950689	bar
fugacity[Toluene]	0.80768403996	3.50668223605	0.81208609286	bar



COFE: CAPE-OPEN Flowsheeting Engine

GUI:

- Graphical flowsheet editing
- Compact display of streams
- **Quick access to CO objects**
- Property graphing & printing
- Extensive help

Flowsheeting:

- Steady state
- Solution by tearing algorithm
- Multiple material templates

The screenshot displays the COFE software interface. The main window is titled 'COFE - [h36.fsd]' and contains a 'Unit operation reactor' window. This window shows a table of parameters for the reactor:

Parameter	Value	Unit
Pressure drop	270000	Pa
Isothermal	FALSE	
Temperature	907.514391006	K
Heat duty	0	W
Use heat of reaction	TRUE	

Below the table is a 'Show GUI' button. To the right of the table, a green arrow points to a 'purge gas' label. In the foreground, a 'Unit reactor' configuration dialog is open, showing the same parameters as the table, with input fields for 'Pressure drop' (270000 Pa), 'Temperature' (907.514391006 K), and 'Heat duty' (0 J/s). The 'Use heat of reaction' checkbox is checked. A 'Help' button is at the bottom of the dialog. At the bottom of the main window, a status bar reads 'Ready' and a message says 'Restoring flowsheet from... Loaded h36.fsd'.



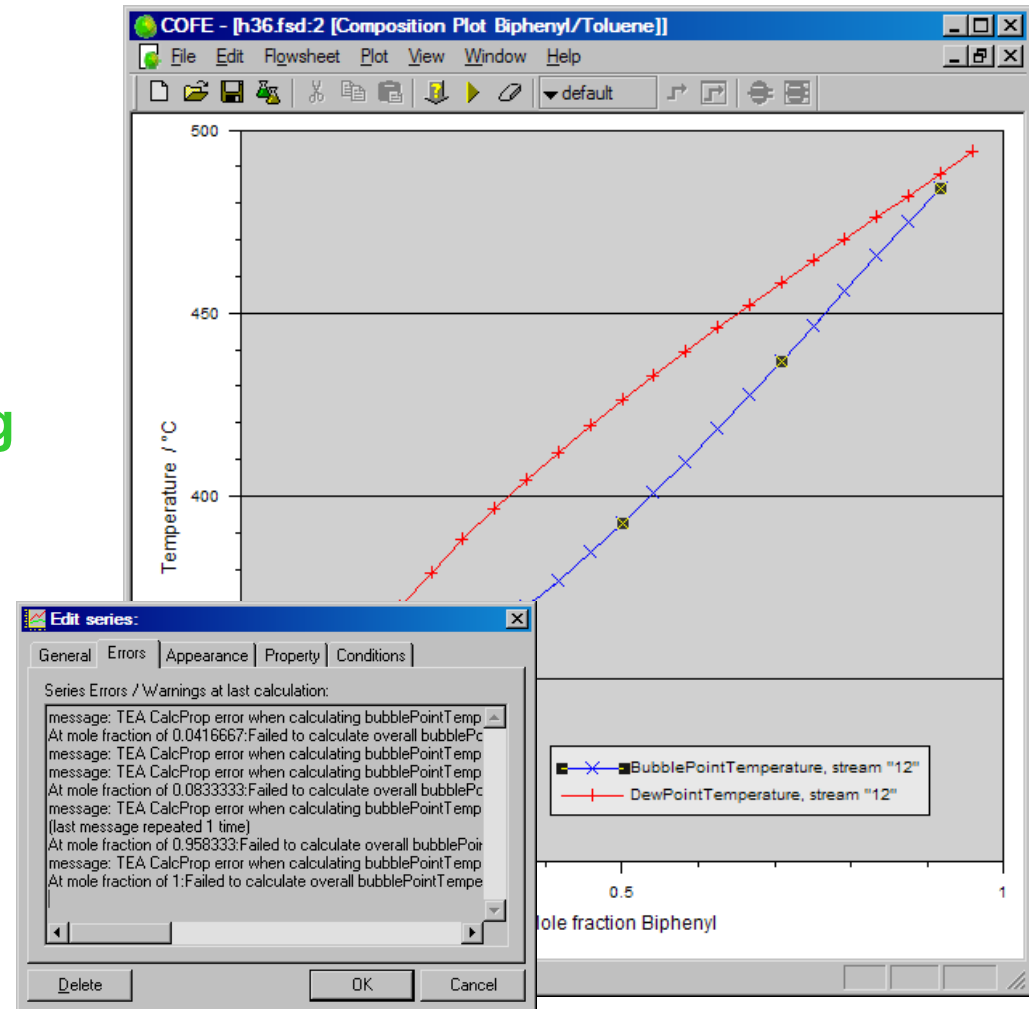
COFE: CAPE-OPEN Flowsheeting Engine

GUI:

- Graphical flowsheet editing
- Compact display of streams
- Quick access to CO objects
- **Property graphing & printing**
- Extensive help

Flowsheeting:

- Steady state
- Solution by tearing algorithm
- Multiple material templates





COFE: CAPE-OPEN Flow Editor

GUI:

- Graphical flowsheet editing
- Compact display of streams
- Quick access to CO objects
- Property graphing & printing
- **Extensive help**

Flowsheeting:

- Steady state
- Solution by tearing algorithm
- Multiple material templates

Enthalpy

Ideal

In this model the enthalpy is computed from the ideal gas contribution:

$$H_{id}^V = \sum_i X_i \left(H_{i,T_{ref}} + \int_{T_{ref}}^T C_{p,i} dT \right)$$

For liquids, the latent [heat of vaporization](#) is subtracted from the ideal gas contribution:

$$H_{id}^L = H_{id}^V - \sum_i X_i \Delta H_{vap,i}$$

Excess

This model includes the ideal enthalpy as above. In addition to that, excess enthalpy is included:

$$H = H_{id} + H_{ex}$$

EOS

This model includes the ideal vapor enthalpy as above. In addition to that, the temperature derivative of the fugacity coefficients from the selected [equation of state](#) is subtracted from the ideal part:

$$H = H_{id}^V - RT^2 \sum_i X_i \frac{\partial \ln(\phi_i)}{\partial T}$$

Pressure and temperature derivatives are determined by perturbation.

Depending on the selected [calculation option](#), composition derivatives are either approximate, or determined by perturbation.

Overall

The overall enthalpy can be calculated from summation over the



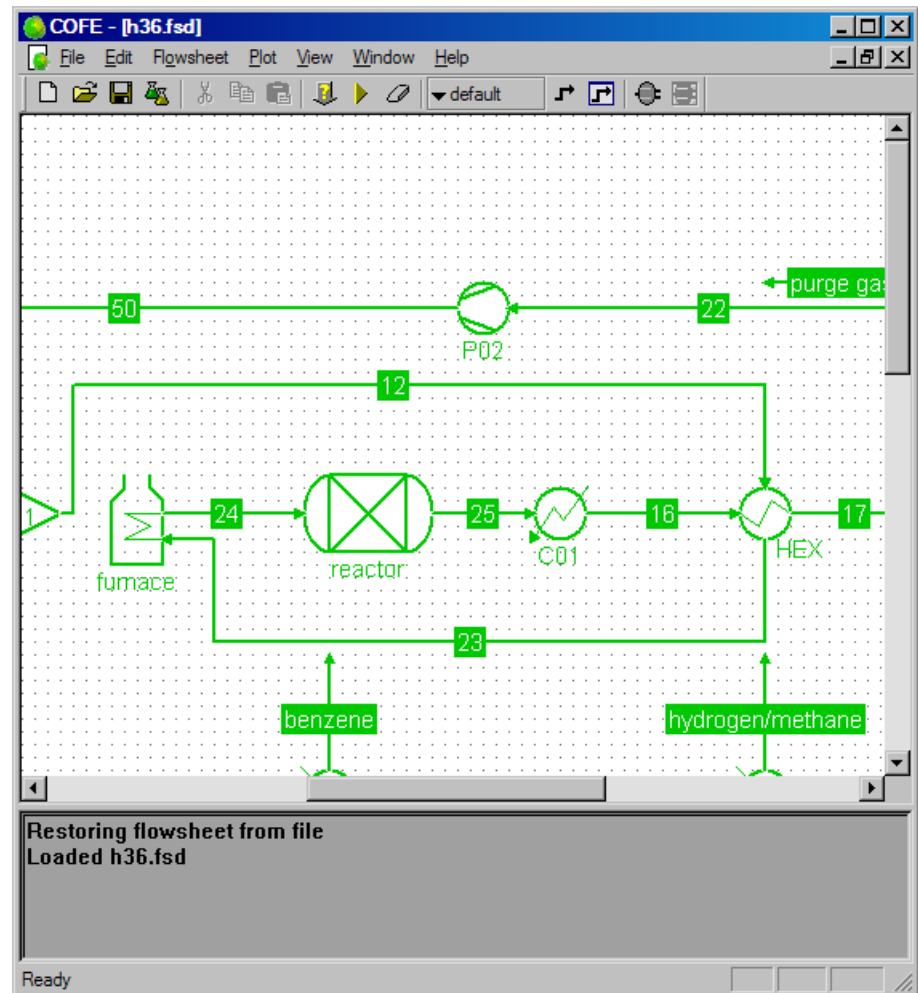
COFE: CAPE-OPEN Flowsheeting Engine

GUI:

- Graphical flowsheet editing
- Compact display of streams
- Quick access to CO objects
- Property graphing & printing
- Extensive help

Flowsheeting:

- **Steady state**
- **Solution by tearing algorithm**
- **Multiple material templates**





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 (ICapeThermoCalculationRoutines)

The screenshot shows two overlapping windows from the TEA software. The top window is titled 'Property pack definition:' and contains a table of compounds with columns for Name, Formula, MW, and CAS. The bottom window is titled 'Add components:' and shows a 'PCD File' path and a 'Compound selection' table with columns for Name, Formula, Mol Weight, and CAS.

Name	Formula	MW	CAS
Hydrogen	H2	2.01588	1333-74-0
Methane	CH4	16.0428	74-82-8
Benzene	C6H6	78.1136	71-43-2
Toluene	C7H8	92.1405	108-88-3
Biphenyl	C12H10	154.211	92-52-4

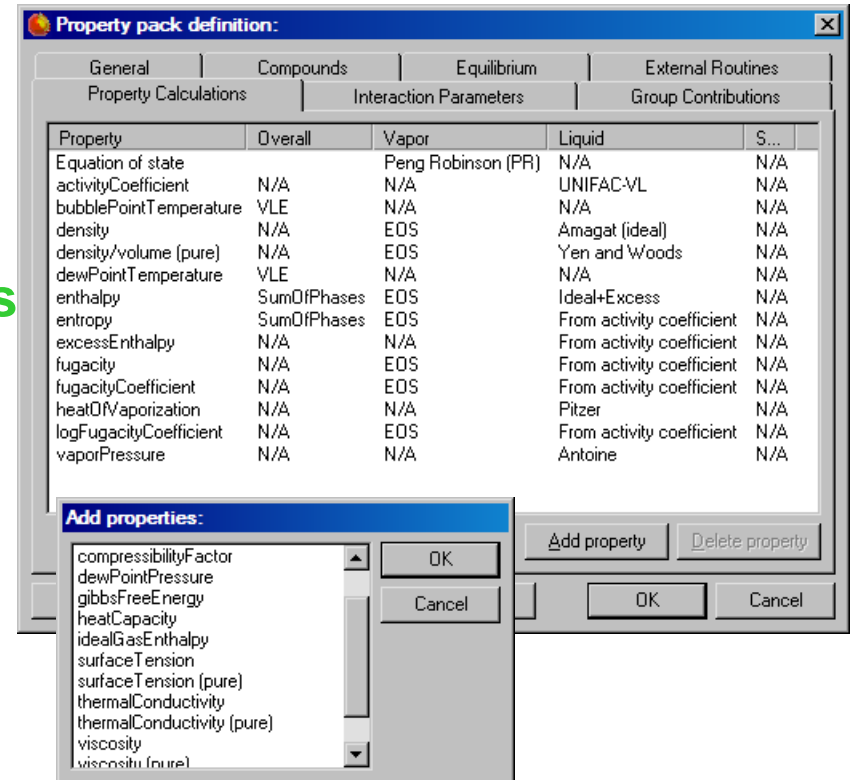
Name	Formula	Mol Weight	CAS
Air		28.9505	132259-10-0
Argon	Ar	39.948	7440-37-1
Bromine	Br2	159.808	7726-95-6
Carbon tetrachloride	CCl4	153.822	56-23-5
Carbon monoxide	CO	28.0104	630-08-0
Carbon dioxide	CO2	44.0098	124-38-9
Carbon disulfide	CS2	76.143	75-15-0
Phosgene	COCl2	98.9158	75-44-5
Trichloroacetyl chloride	C2OCl4	181.832	76-02-8
Hydrogen chloride	HCl	36.4606	7647-01-0
Chlorine	Cl2	70.9054	7782-50-5
Hydrogen iodide	HI	127.912	10034-85-2
Hydrogen	H2	2.01588	1333-74-0

Thermodynamic models and compounds from ChemSep



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 (ICapeThermoCalculationRoutines)



Thermodynamic models and compounds from ChemSep



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 (ICapeThermoCalculationRoutines)

Flowsheet configuration:

Property packs | Reaction packs | Compounds | Properties | Material types | Solve Options |

Chemical / physical properties:

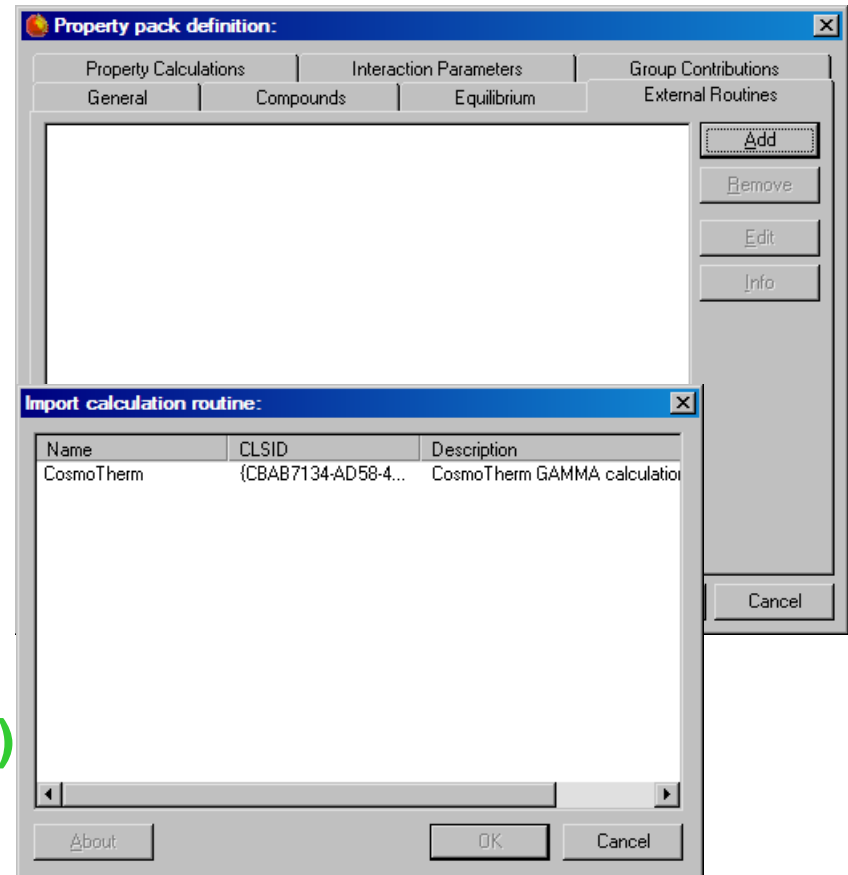
Name	Sho...	Sho...	Sho...	S...	Unit
bubblePointTemperature	Mixture	No	No	No	°C
density	No	Mixture	Mixture	No	mol / m ³
density.DmolFraction	No	No	No	No	mol / m ³
density.Dpressure	No	No	No	No	mol / Pa m ³
density.Dtemperature	No	No	No	No	mol / m ³ K
dewPointTemperature	Mixture	No	No	No	°C
enthalpy	Mixture	Mixture	Mixture	No	J / mol
enthalpy.DmolFraction	No	No	No	No	J / mol
enthalpy.Dpressure	No	No	No	No	J / Pa mol
enthalpy.Dtemperature	No	No	No	No	J / Pa mol K
entropy	No	Mixture	Mixture	No	J / mol K
entropy.DmolFraction	No	No	No	No	J / mol K
entropy.Dpressure	No	No	No	No	J / Pa mol K
entropy.Dtemperature	No	No	No	No	J / mol K ²
fugacity	No	Mixture	Mixture	No	bar
fugacity.DmolFraction	No	No	No	No	bar
fugacity.Dpressure	No	No	No	No	-
fugacity.Dtemperature	No	No	No	No	Pa / K
fugacityCoefficient	No	Mixture	Mixture	No	-
fugacityCoefficient.DmolFraction	No	No	No	No	-
fugacityCoefficient.Dpressure	No	No	No	No	1 / Pa
fugacityCoefficient.Dtemperature	No	No	No	No	1 / K
heatOfVaporization	No	No	Mixture	No	J / mol
heatOfVaporization.DmolFraction	No	No	No	No	1 / mol

Thermodynamic models and compounds from ChemSep



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 (ICapeThermoCalculationRoutines)**

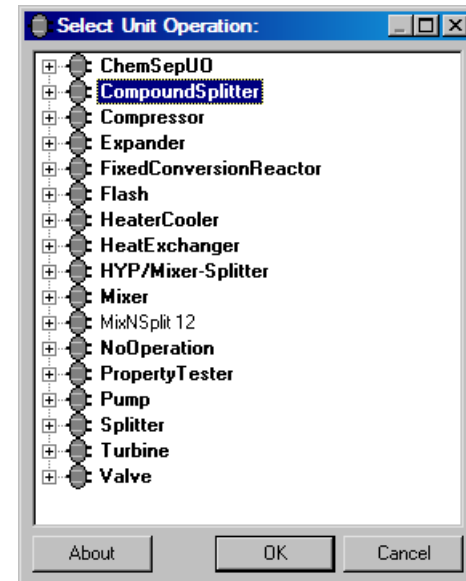


Thermodynamic models and compounds from ChemSep



COUS-COUS: Simple unit operations

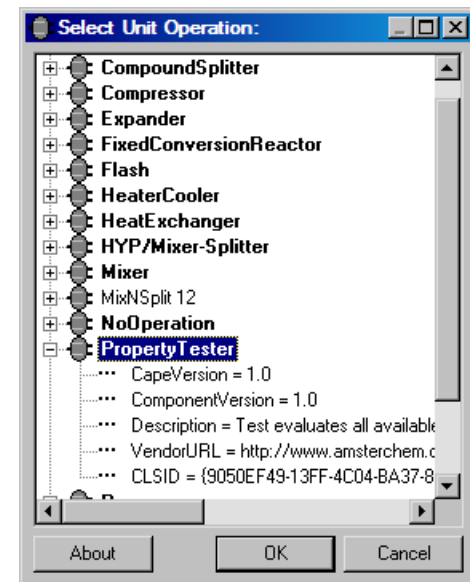
- **General purpose unit operations (mixer, splitter, heat exchanger...)**
- Property tester for thermodynamic properties
- Distillation column of ChemSep LITE





COUS-COUS: Simple unit operations

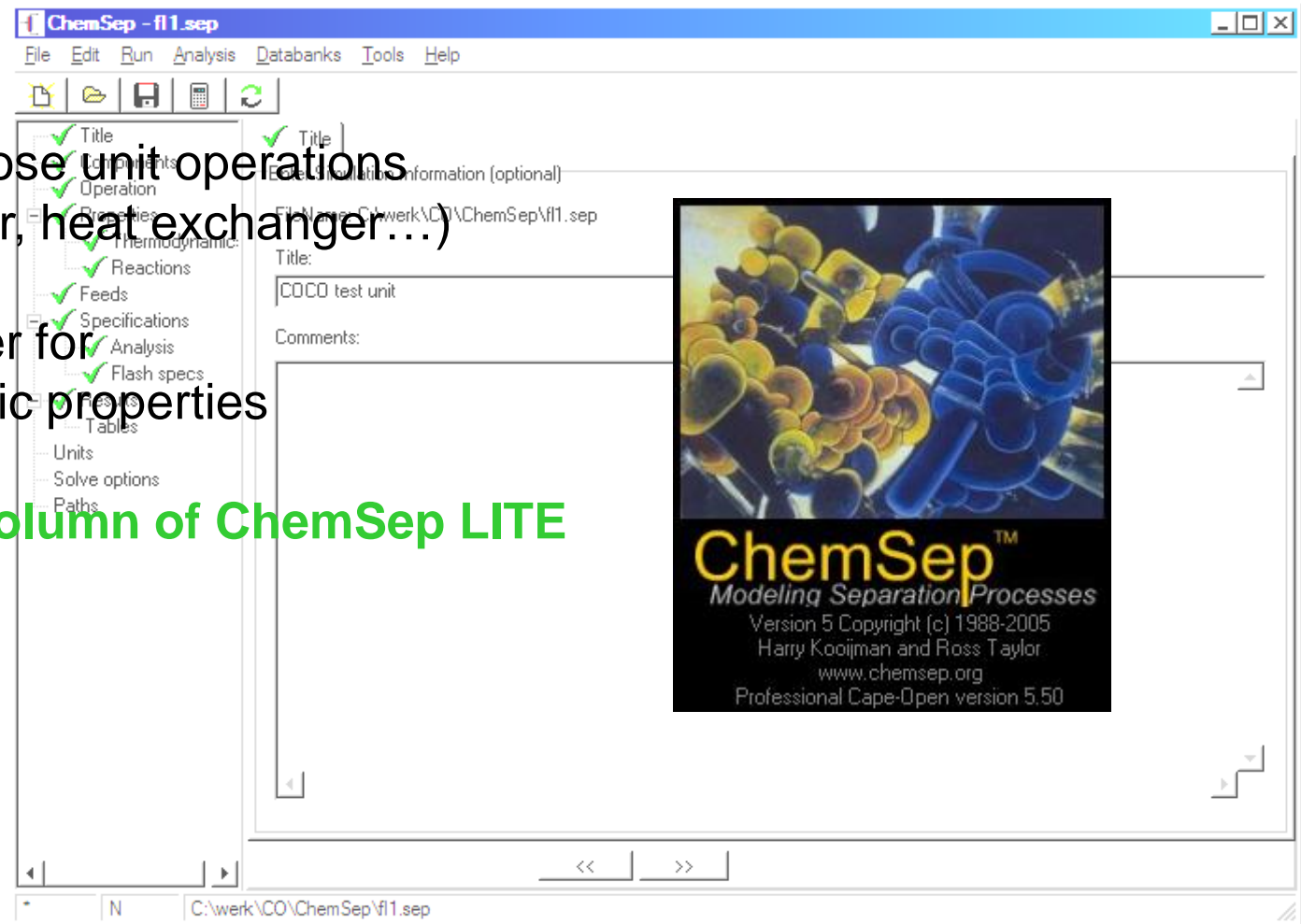
- General purpose unit operations (mixer, splitter, heat exchanger...)
- **Property tester for thermodynamic properties**
- Distillation column of ChemSep LITE





COUS-COUS: Simple unit operations

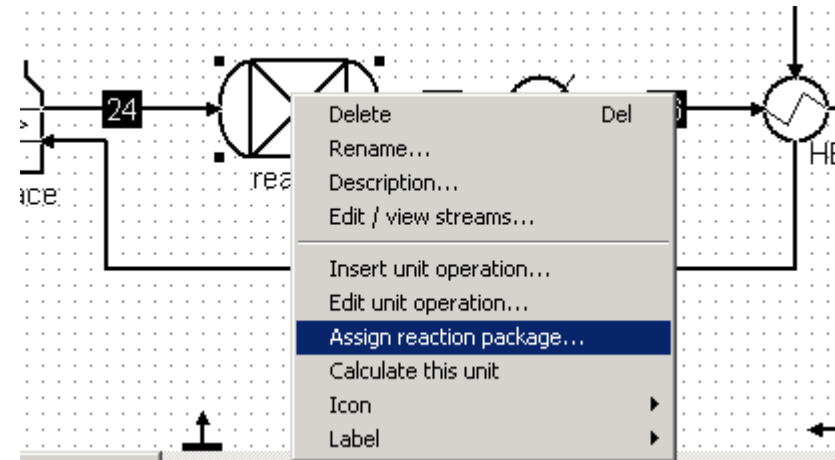
- General purpose unit operations (mixer, splitter, heat exchanger...)
- Property tester for thermodynamic properties
- **Distillation column of ChemSep LITE**





CORN: CAPE-OPEN Reaction Numerics

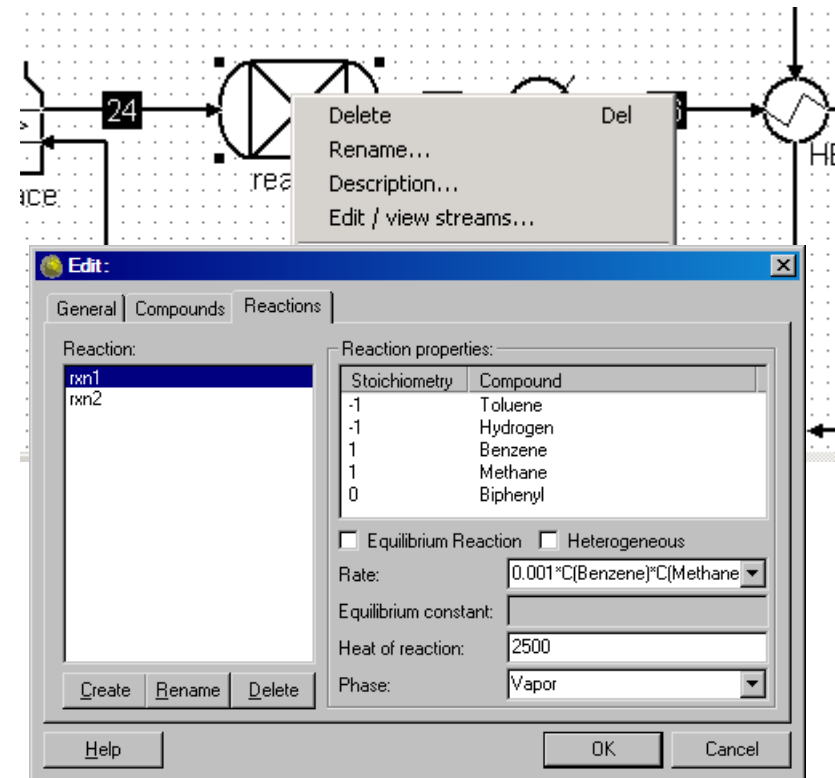
- **Currently the only reaction package manager around**
- Kinetic and equilibrium reactions
- Formula interpreter for rates, equilibrium constants, and heats of reaction
- COFE and COUS support reaction packages, i.e. CORN





CORN: CAPE-OPEN Reaction Numerics

- Currently the only reaction package manager around
- **Kinetic and equilibrium reactions**
- Formula interpreter for rates, equilibrium constants, and heats of reaction
- COFE and COUS support reaction packages, i.e. CORN





CORN: CAPE-OPEN Reaction Numerics

- Currently the only reaction package manager around
- Kinetic and equilibrium reactions
- **Formula interpreter for rates, equilibrium constants, and heats of reaction**
- COFE and COUS support reaction packages, i.e. CORN

The screenshot shows a process flow diagram with a reactor unit. A context menu is open over the reactor, listing options: Delete, Rename..., Description..., and Edit / view streams... The 'Edit' window is open, showing the 'Reactions' tab. The 'Reaction' list contains 'rxn1' and 'rxn2'. The 'Reaction properties' section shows a table of stoichiometry and compounds:

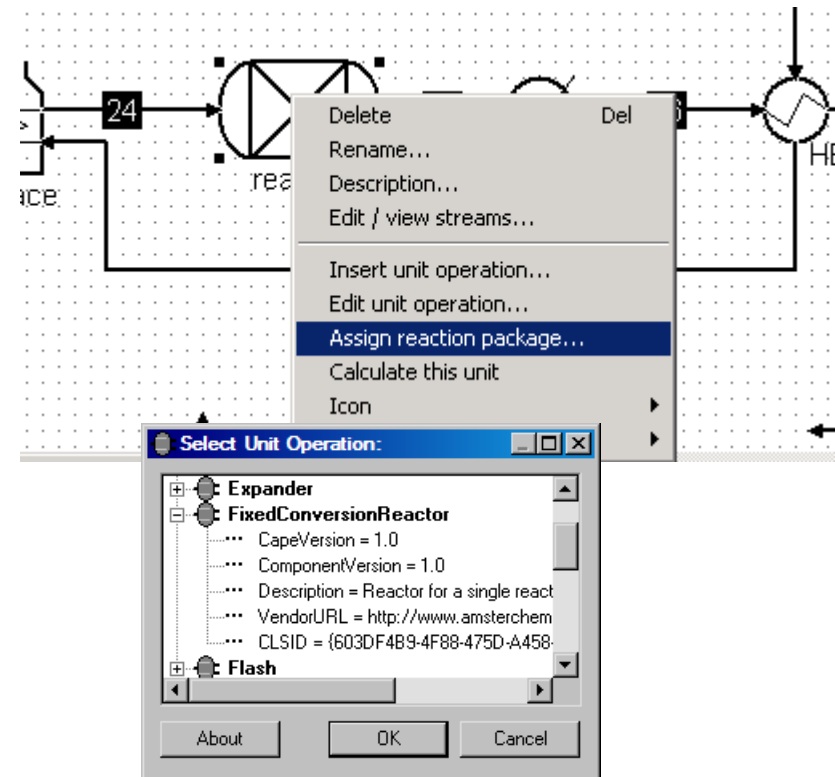
Stoichiometry	Compound
-1	Toluene
-1	Hydrogen
1	Benzene
1	Methane
0	Biphenyl

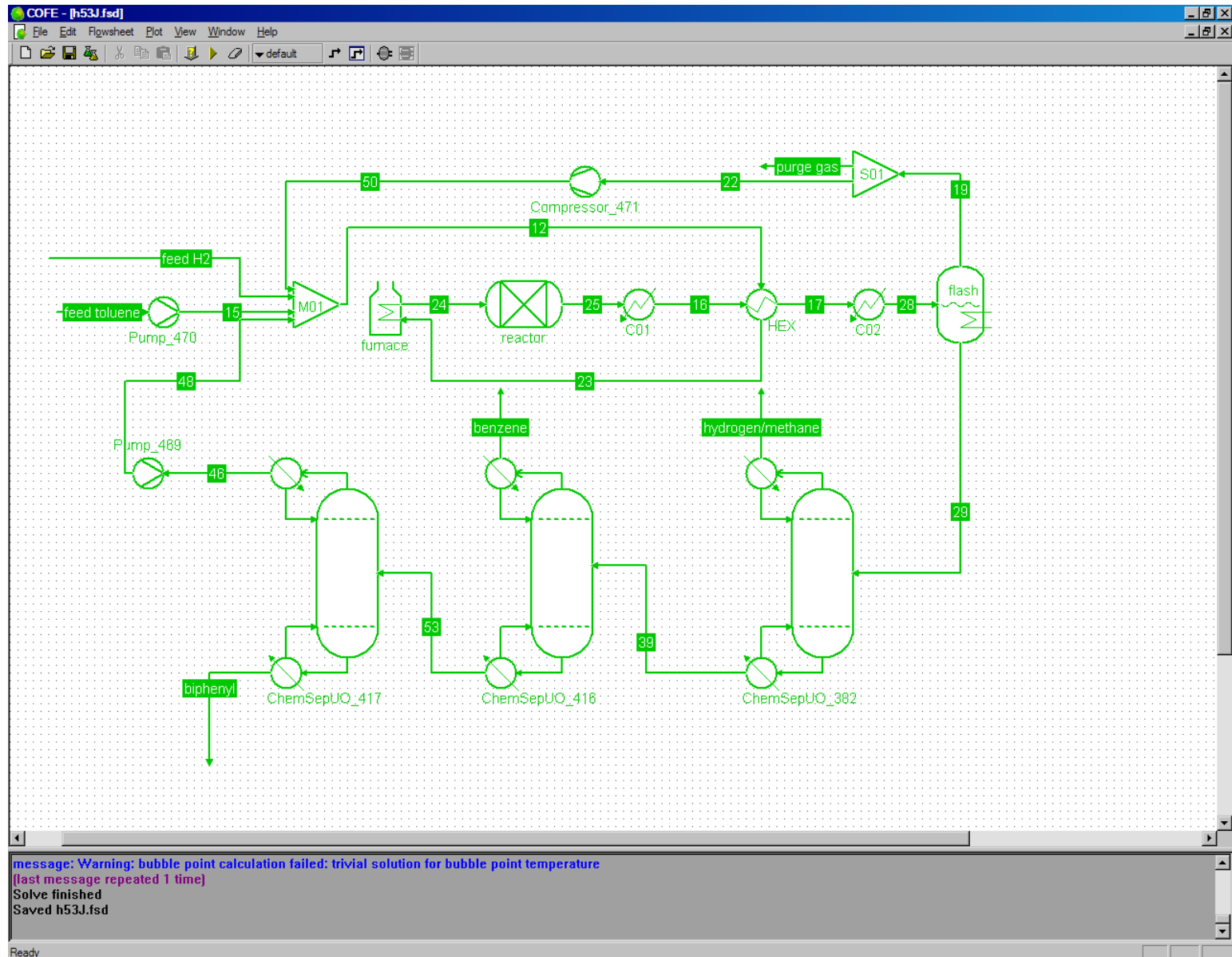
Below the table, there are checkboxes for 'Equilibrium Reaction' and 'Heterogeneous'. The 'Rate' is set to $0.001 * C(\text{Benzene}) * C(\text{Methane})$. The 'Equilibrium constant' is empty. The 'Heat of reaction' is 2500. The 'Phase' is set to 'Vapor'. Buttons for 'Create', 'Rename', 'Delete', 'Help', 'OK', and 'Cancel' are visible at the bottom of the dialog.



CORN: CAPE-OPEN Reaction Numerics

- Currently the only reaction package manager around
- Kinetic and equilibrium reactions
- Formula interpreter for rates, equilibrium constants, and heats of reaction
- **COFE and COUS support reaction packages, i.e. CORN**





Thermodynamics Interoperability tests:

	TEA ¹⁾	Aspen thermo	Simulis
COFE	✓	✓ ✗ ²⁾	✓
Aspen Plus	✓		
Pro/II	✗ ³⁾		
Simulis	✓		

- 1) TEA is currently the only support for ICapeThermoCalculationRoutines (e.g. CosmoTherm)
- 2) Equilibrium calculations ok, properties fail. Problem with compound IDs, being looked into by Aspen
- 3) Problem with resolving compound IDs inside Pro/II

Unit-operation Interoperability tests:

	COUS	ChemSep	Aspen Mixer
COFE	✓	✓	✗ ¹⁾
Aspen Plus	✓ ✗ ²⁾		
Pro/II	✓ ✗ ³⁾		

- 1) Overall enthalpy calculations fail
- 2) Enthalpy is requested without calcType (mixture or pure)
- 3) Equilibrium calculations fail for specified enthalpy

Simu1.apw - Aspen Plus 2004.1 - aspenONE - [Process Flowsheet Window]

File Edit View Data Tools Run Flowsheet Library Window Help

Grid 0.1

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Ch

Material STREAMS Mixer FSplit SSplit

Running simulation. C:\...nDocs\Cosmo_Water_Buta

Simu1.apw - Aspen Plus 2004.1 - aspenONE - [Block B1 (Flash3) Stream Results - Data Browser]

File Edit View Data Tools Run Plot Library Window Help

Stream Results

- Setup
- Components
- Properties
- Flowsheet
- Streams
- Utilities
- Blocks
 - B1
 - Input
 - Hcurves
 - Dynamic
 - Block Options
 - Results
 - EO Variables
 - EO Input
 - Spec Groups
 - Ports
 - Stream Results**
 - Reactions
 - Convergence
 - Flowsheeting Options
 - Model Analysis Tools
 - EO Configuration
 - Results Summary

Material Heat Load Vol.%Curves Wt.%Curves Petro.Curves Poly.Curves

Display: Streams Format: FULL Stream Table

	1	2	3	4
WATER	.7000000	0.0	.2134422	.4865578
N-BU-1	.3000000	0.0	.2793066	.0206934
Total Flow kmol/sec	1.000000	0.0	.4927488	.5072512
Total Flow kg/sec	34.84754	0.0	24.54821	10.29933
Total Flow cum/sec	.0365687	0.0	.0301741	.0110802
Temperature K	333.1500		333.1500	333.1500
Pressure N/sqm	1.00000E+5	1.00000E+5	1.00000E+5	1.00000E+5
Vapor Frac	0.0		0.0	0.0
Liquid Frac	1.000000		1.000000	1.000000
Solid Frac	0.0		0.0	0.0
Enthalpy J/kmol	-4.1611E+7		-3.0447E+8	-2.8534E+8
Enthalpy J/kg	-1.1941E+6		-6.1116E+6	-1.4053E+7
Enthalpy Watt	-4.1611E+7		-1.5003E+8	-1.4474E+8
Entropy J/kmol-K	1.16881E+5		-3.6773E+5	-1.7179E+5
Entropy J/kg-K	3354.066		-7381.353	-8460.652
Density kmol/cum	27.34577		16.33015	45.77983

Results Available

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids

Material STREAMS Mixer FSplit SSplit

For Help, press F1 C:\...nDocs\Cosmo_Water_Butanol Results Available

COCO serves you with:

- CAPE-OPEN based flowsheet solver
- Good interoperability; mix in any unit you like
- All flavors of thermodynamic and physical properties
- Support for external property calculation routines
- The ultimate tester for CAPE-OPEN compatibility

Still on the stove:

- CAPE-OPEN version 1.1 thermodynamics
- Excel interface to COFE
- Petroleum fractions
- Additional unit operations
- External equilibrium routines (currently disabled)
- In-/export of numeric interfaces
- ...

- Download COCO: <http://www.amsterchem.com/>
(or ask for a copy during the workshop)
- Contact AmsterCHEM for CAPE-OPEN consulting

Acknowledgements:

- Richard Baur
- ChemSep: Harry Kooijman, Ross Taylor
- Michel Pons
- CosmoLogic: Andreas Klamt, Frank Eckert
- Aspen Technology