# 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)

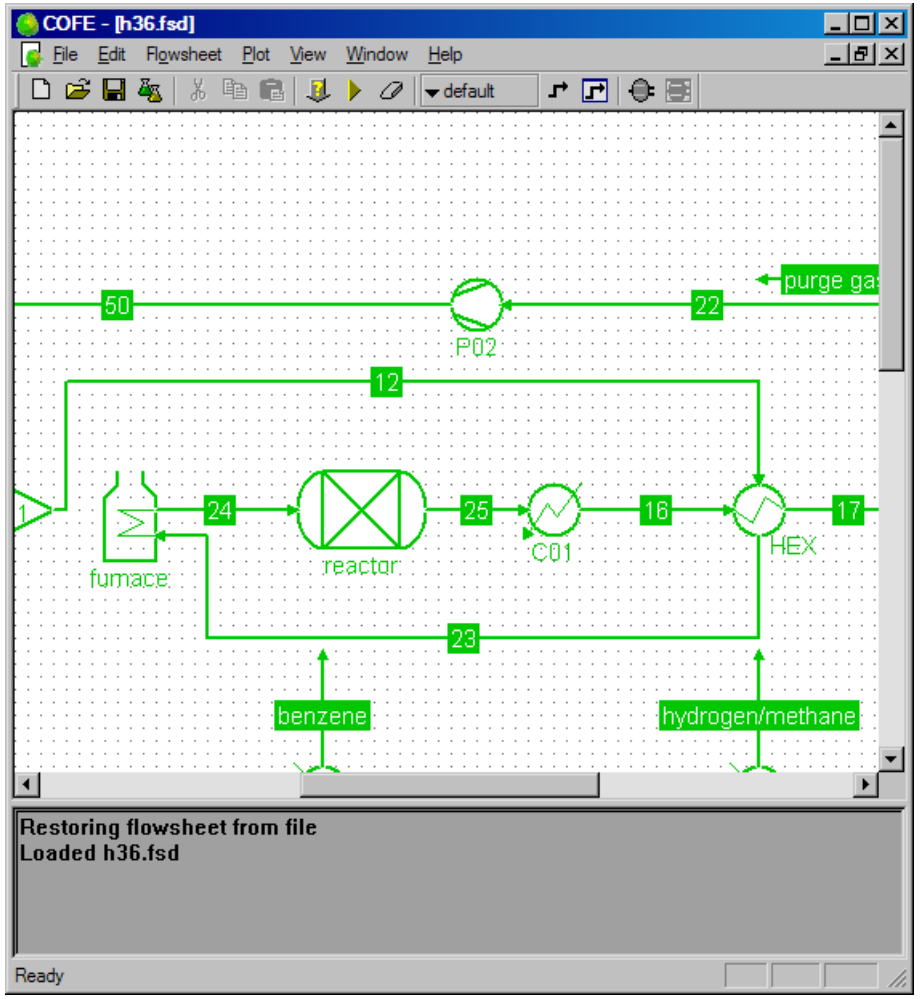
# COFE: CAPE-OPEN Flowsheeting Environment

**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



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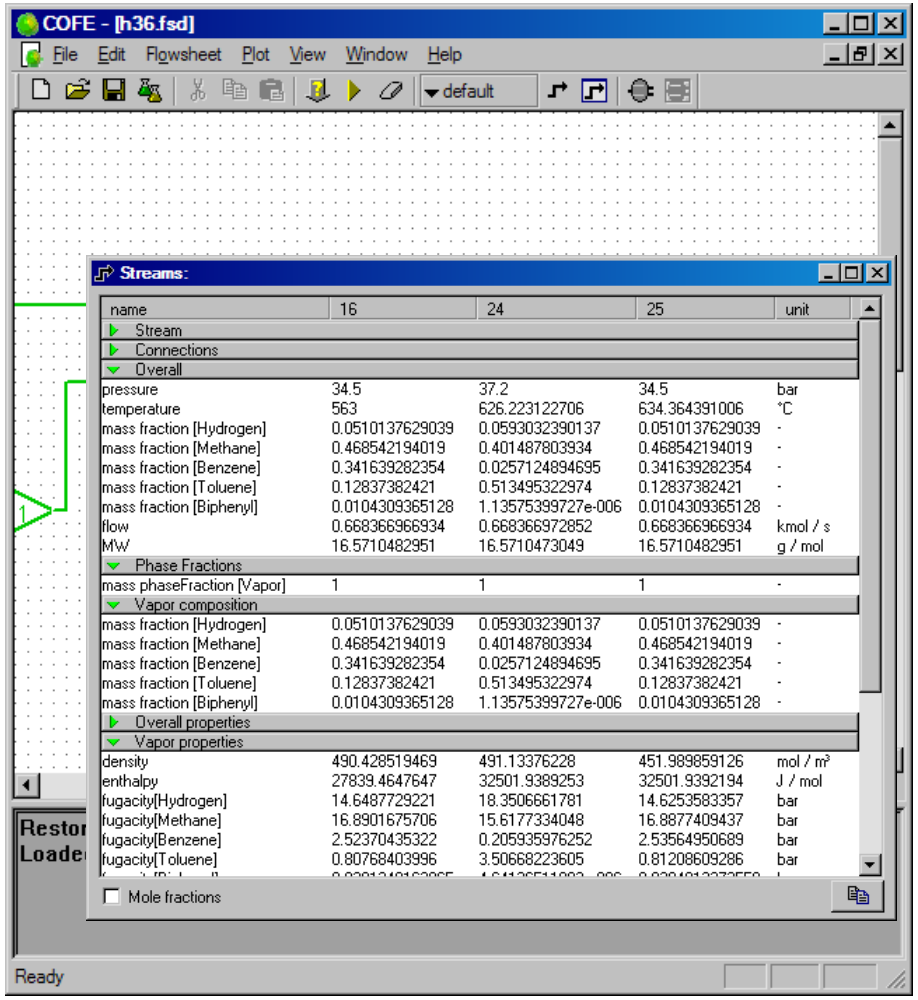

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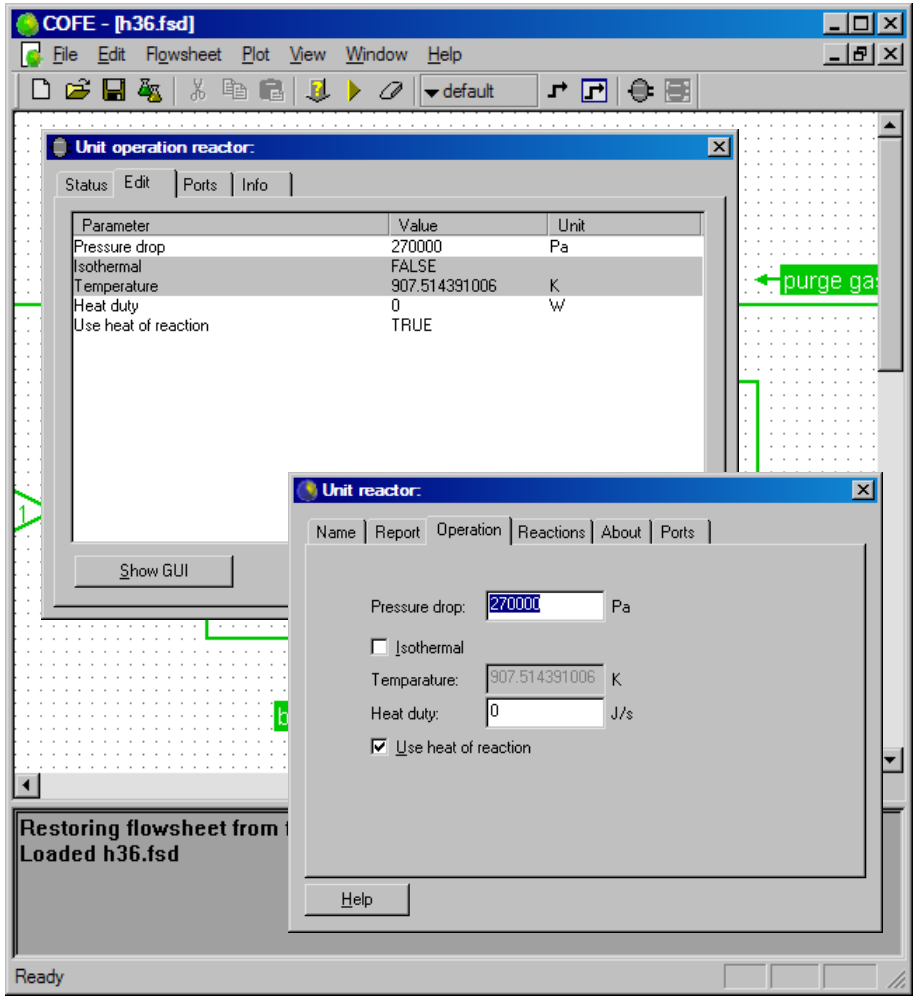

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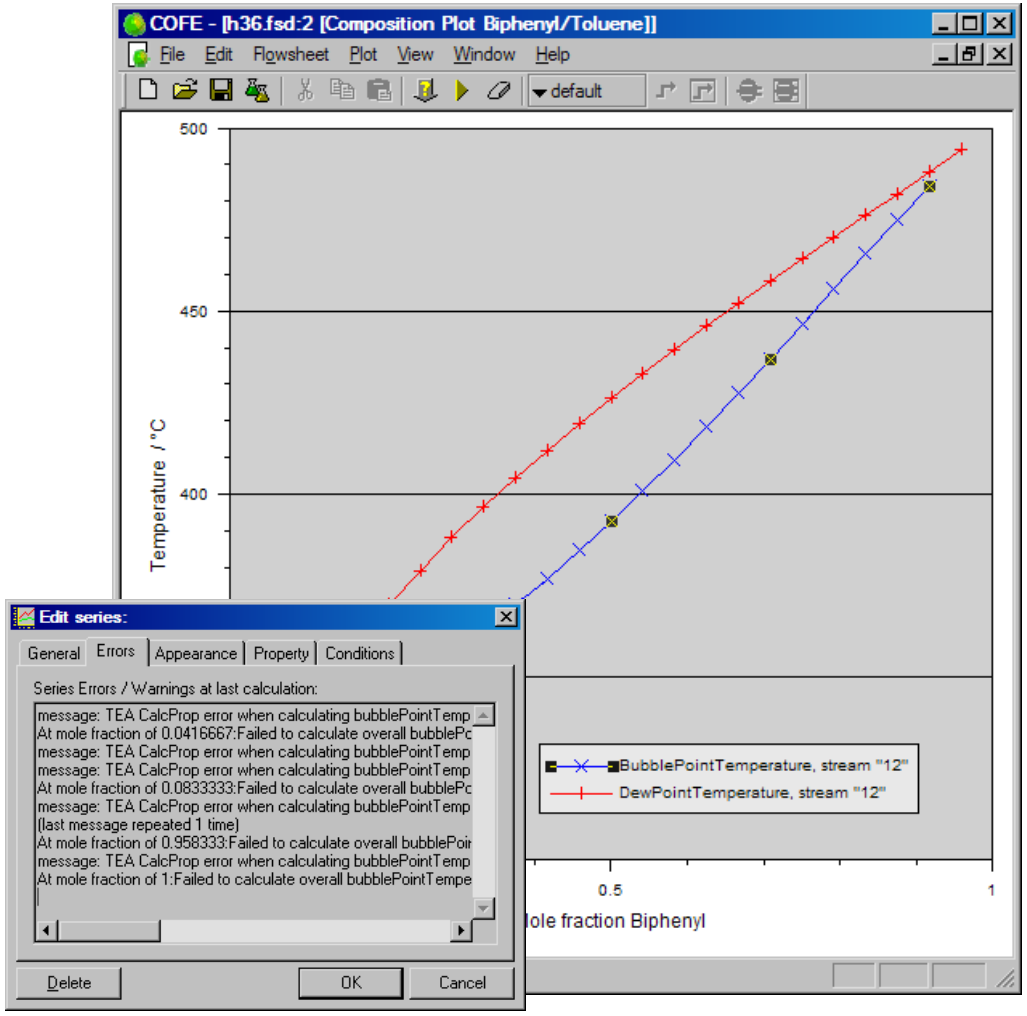

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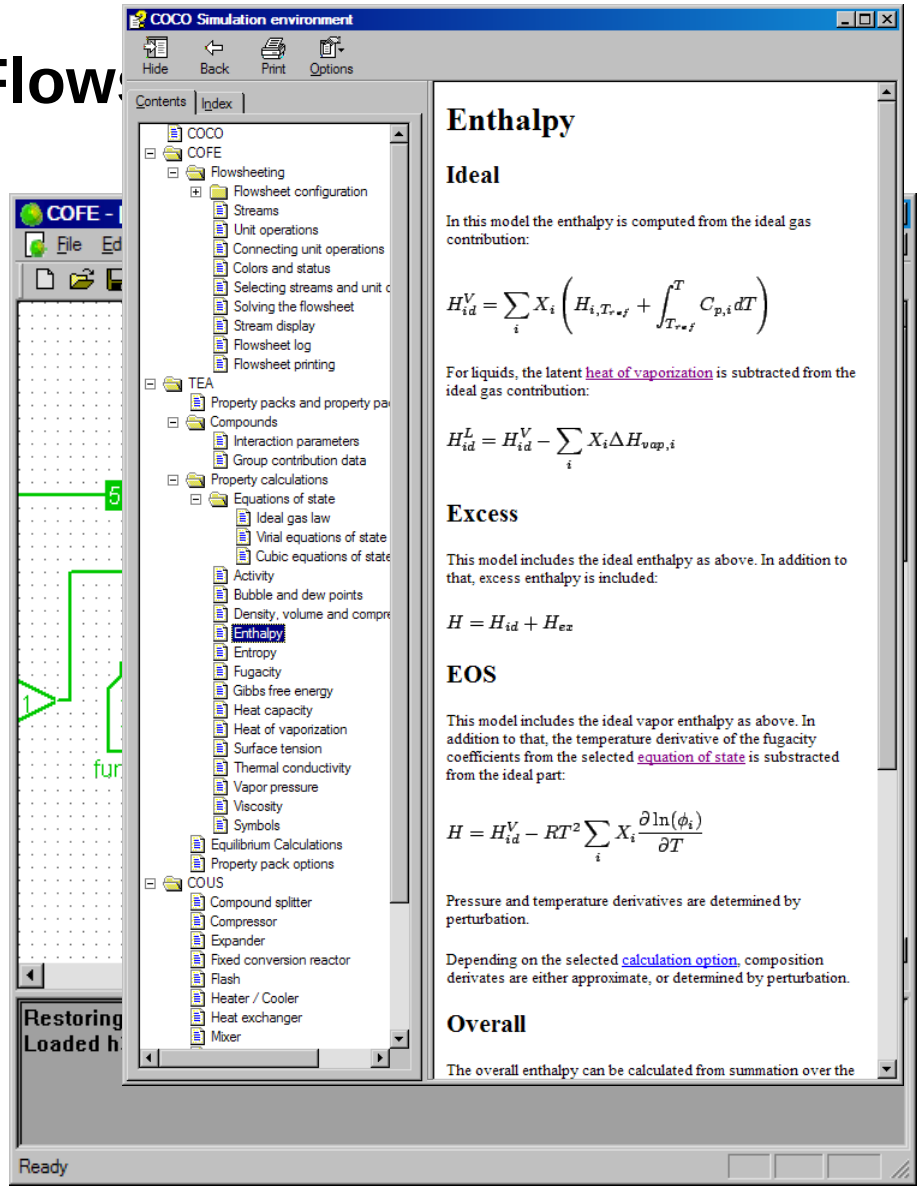

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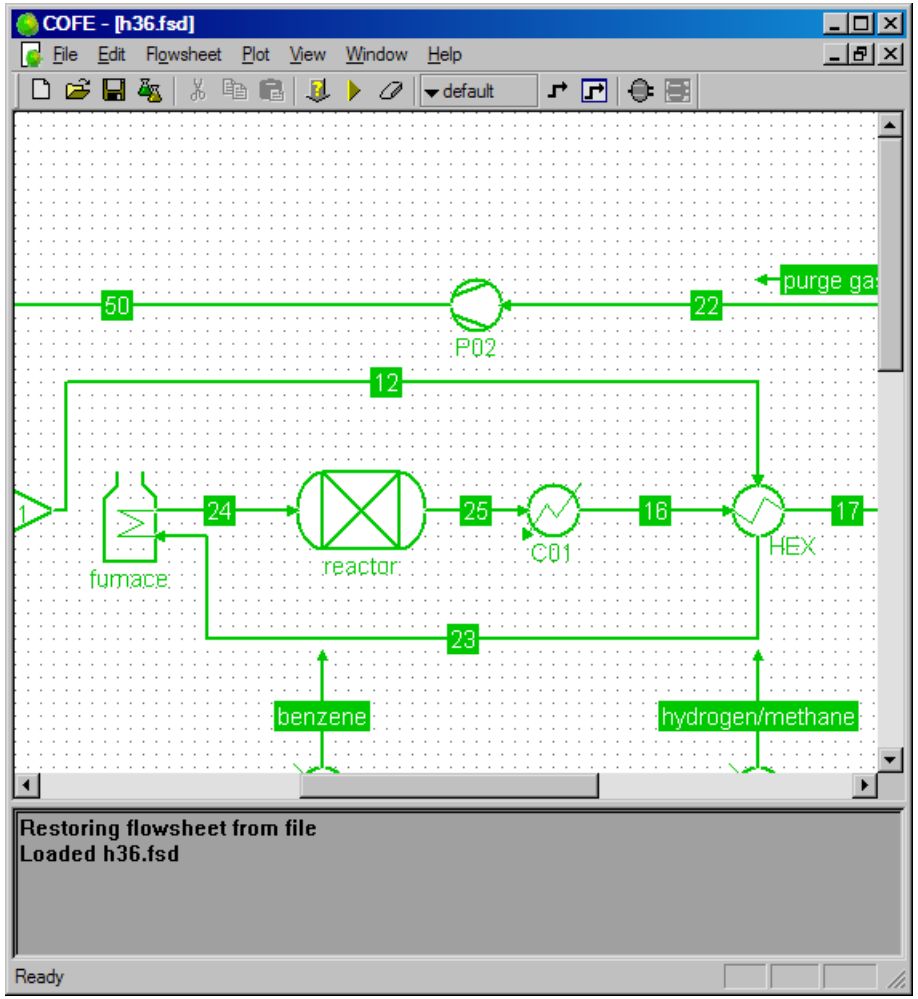
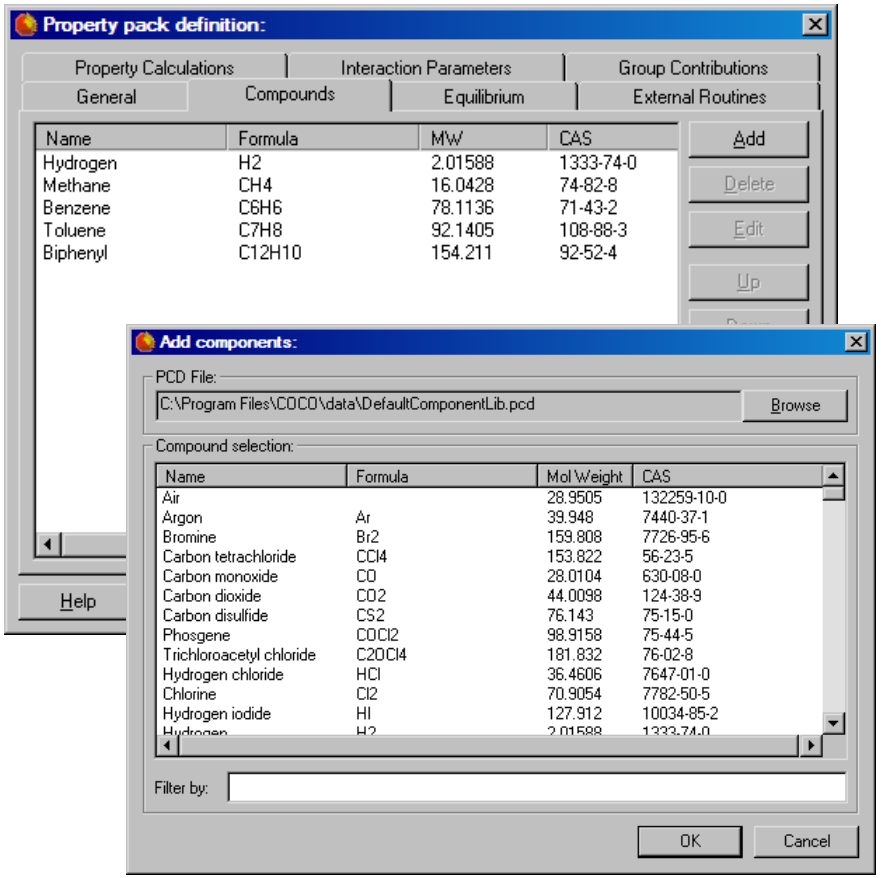


# TEA: Thermodynamics for Engineering Applications

- **Pure compound data library (extendible, or use DIPPR)**
- 100+ Property calculation methods (> 25 different properties)
- Property derivatives
- Support of external property calculation routines (ICapeThermoCalculationRoutines)




Thermodynamic models and compounds from ChemSep

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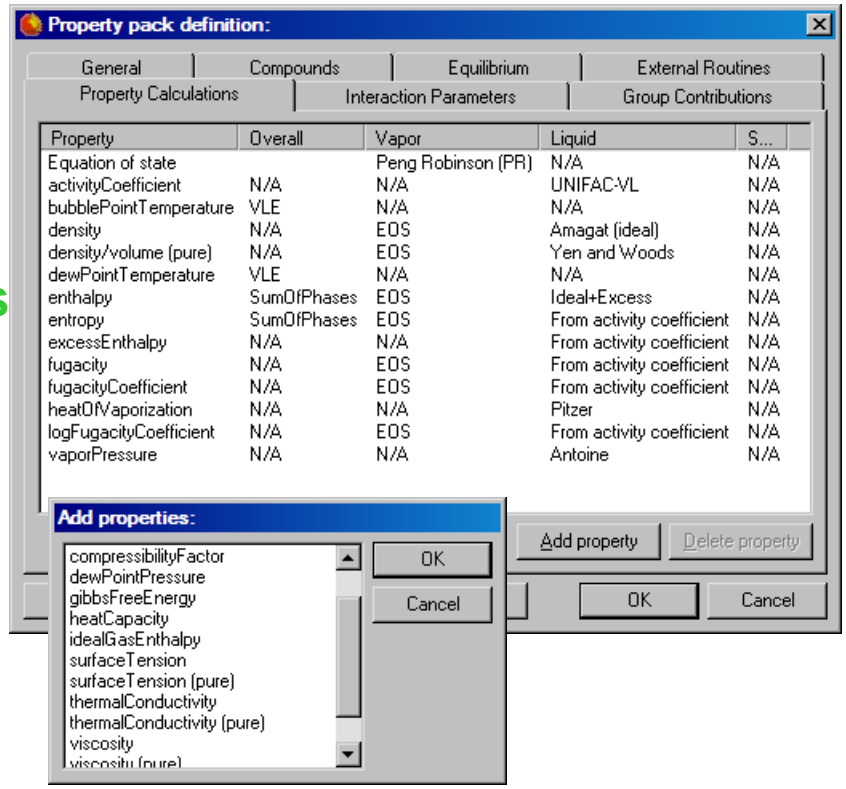


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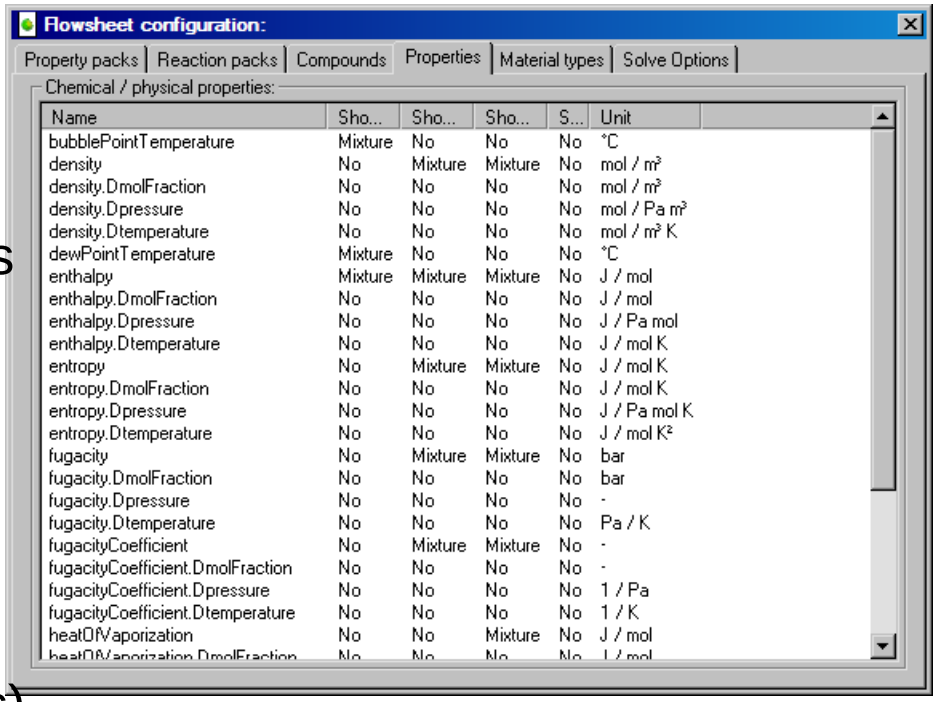


| Name | Sho... | Sho... | Sho... | S... | Unit |
|---|---|---|---|---|---|
| bubblePointTemperature | Mixture | No | No | No | °C |
| density | No | Mixture | Mixture | No | mol / m³ |
| density.DmolFraction | No | No | No | No | mol / m³ |
| density.Dpressure | No | No | No | No | mol / Pa m³ |
| density.Dtemperature | No | No | No | No | mol / m³ 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 / 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 K² |
| 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 | J / mol |

Thermodynamic models and compounds from ChemSep

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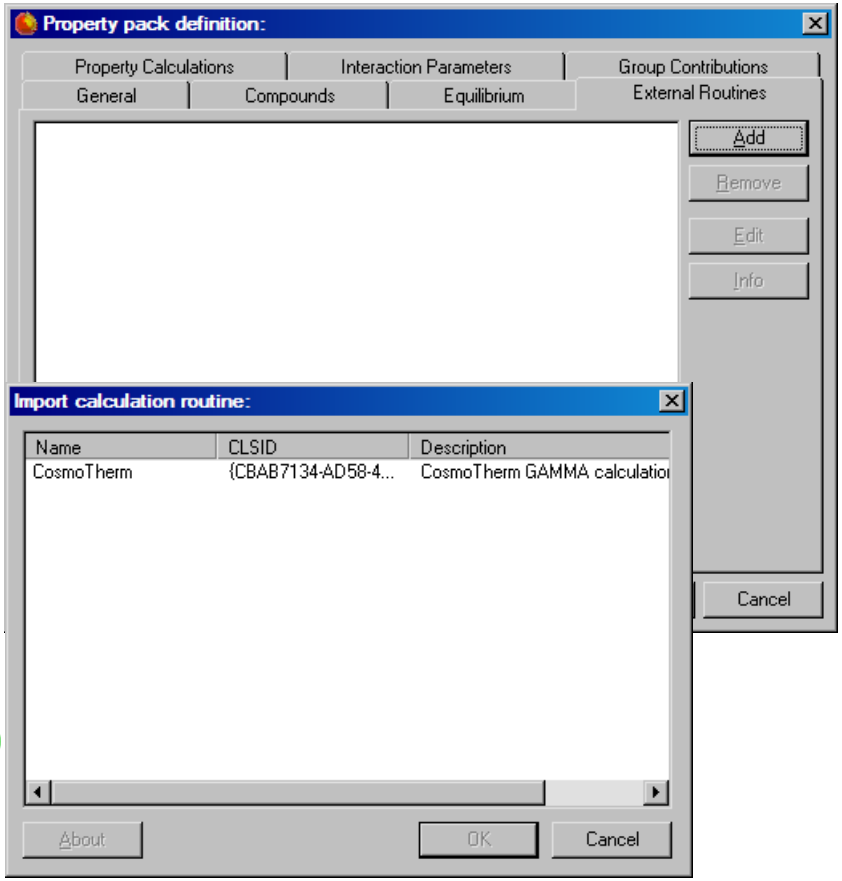


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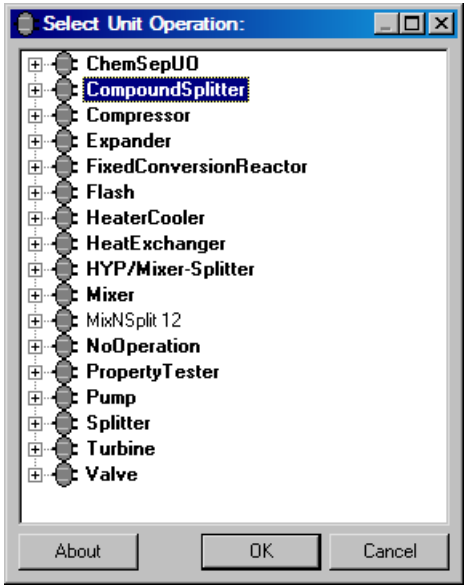
# COUS-COUS: Simple unit operations

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



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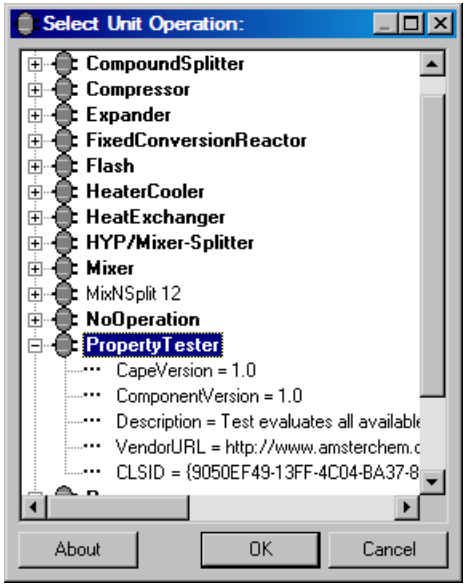

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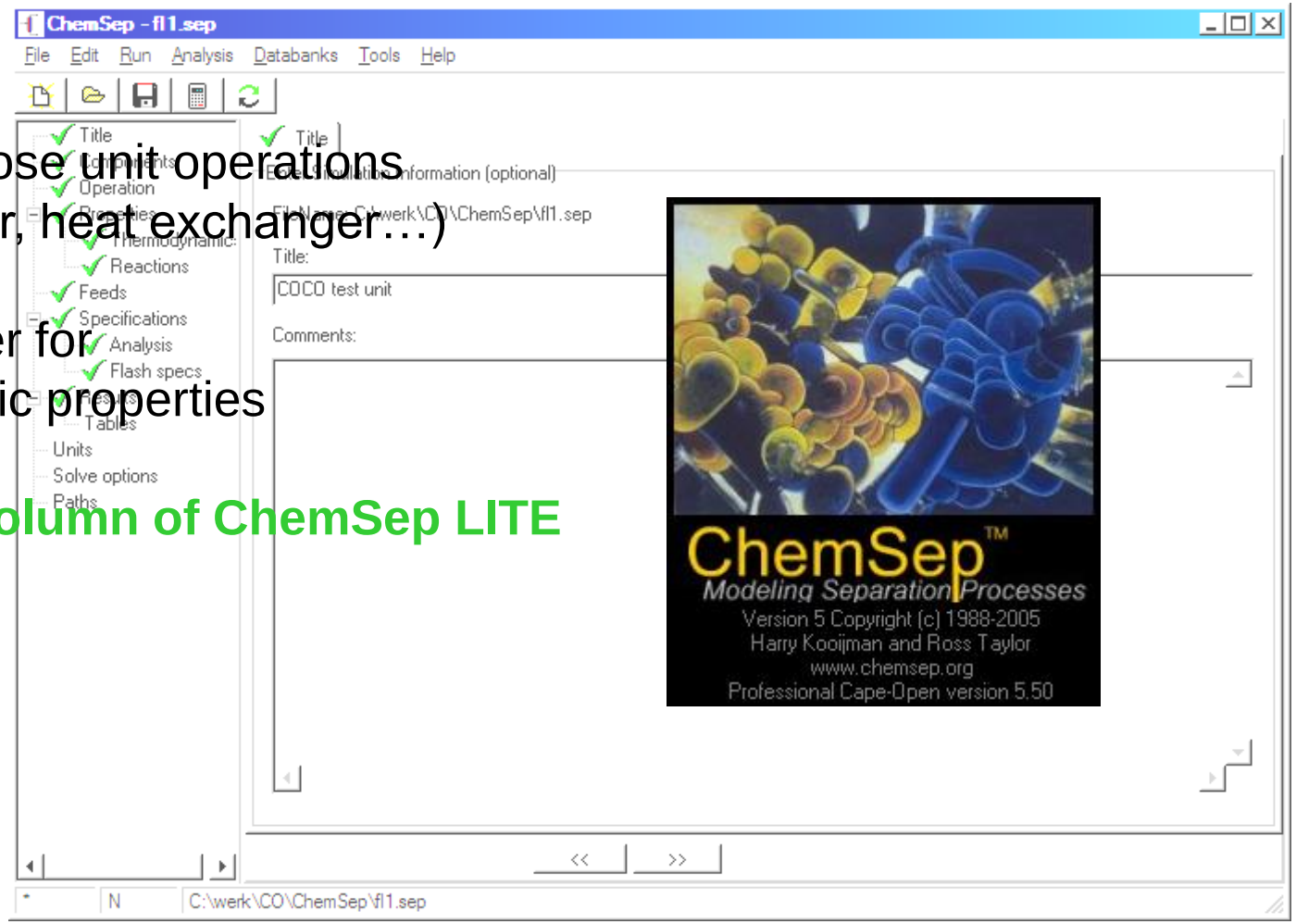
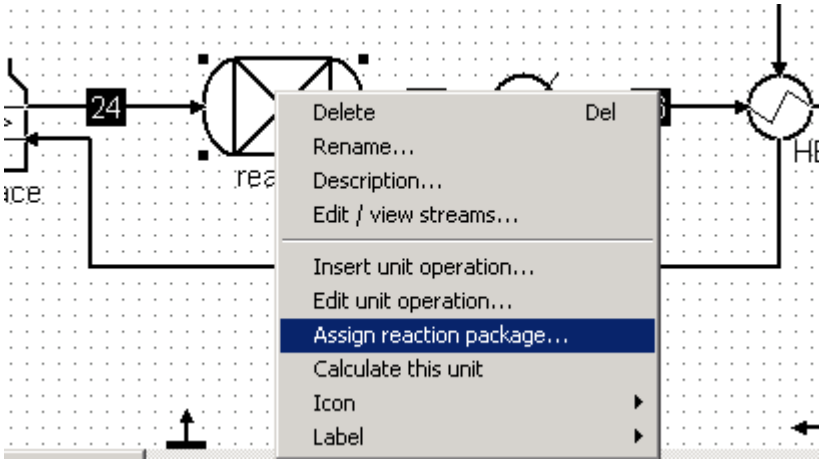


# CORN: CAPE-OPEN Reaction Numerics

- **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



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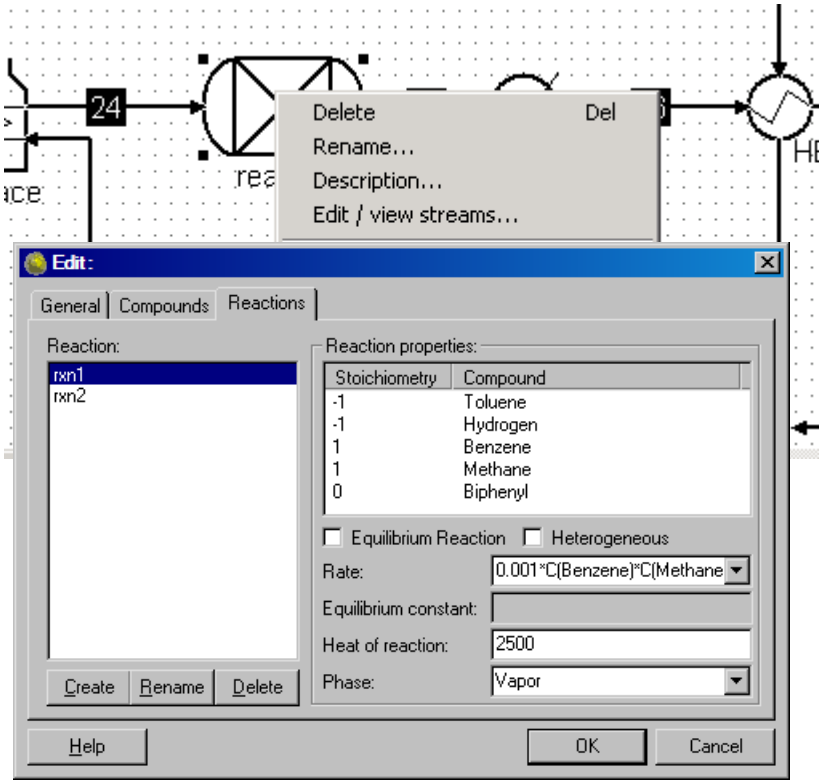

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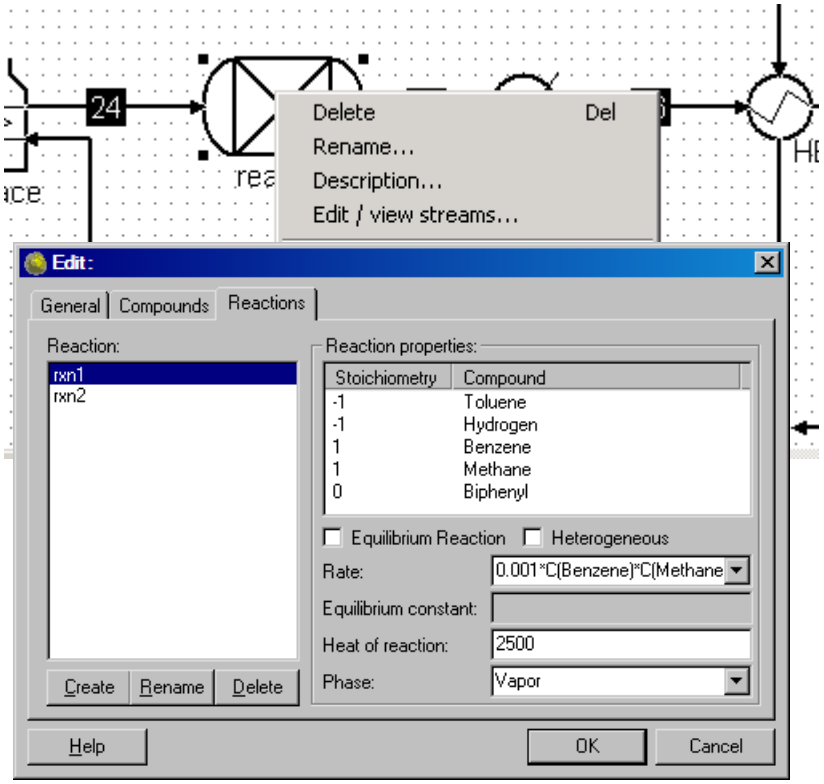

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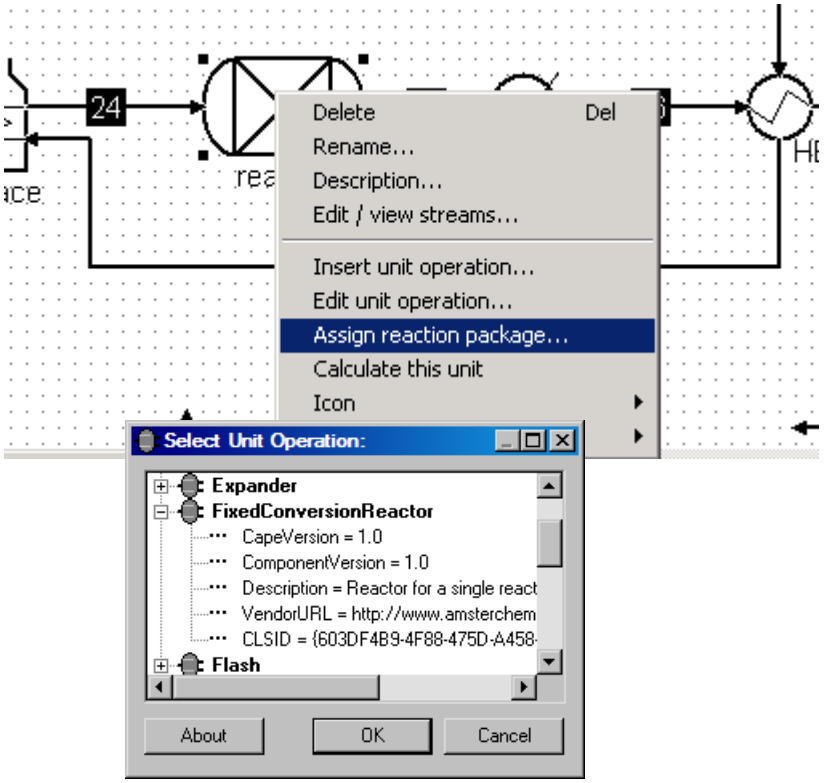
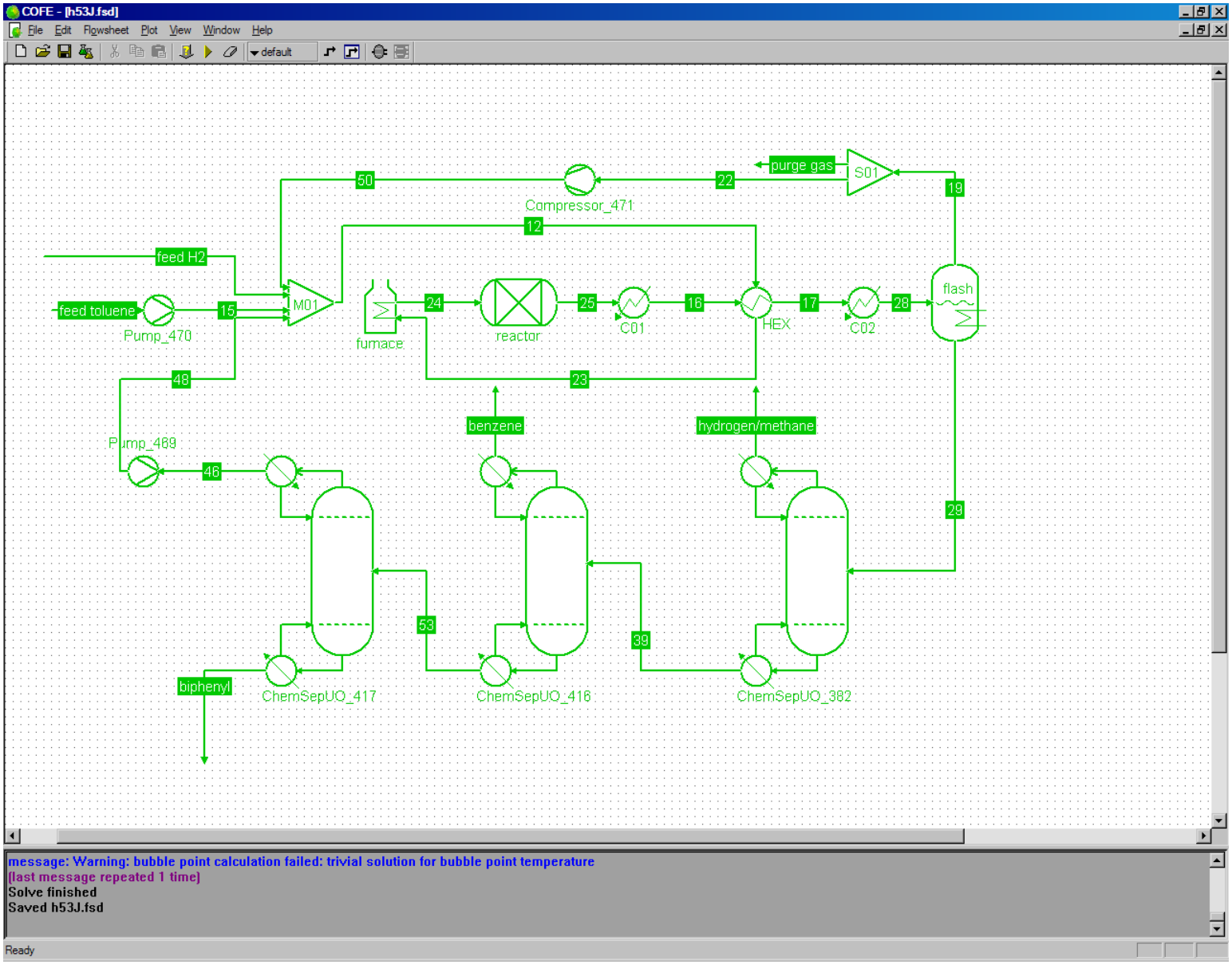



COFE - [h53J.fsd]
File Edit Flowsheet Plot View Window Help
default
purge gas
S01
19
50
22
Compressor_471
12
feed H2
feed toluene
15
Pump_470
M01
furnace
24
reactor
25
C01
16
HEX
17
C02
28
flash
48
23
benzene
hydrogen/methane
Pump_469
46
29
53
39
biphenyl
ChemSepUO_417
ChemSepUO_416
ChemSepUO_382
message: Warning: bubble point calculation failed: trivial solution for bubble point temperature
(last message repeated 1 time)
Solve finished
Saved h53J.fsd
Ready

# 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

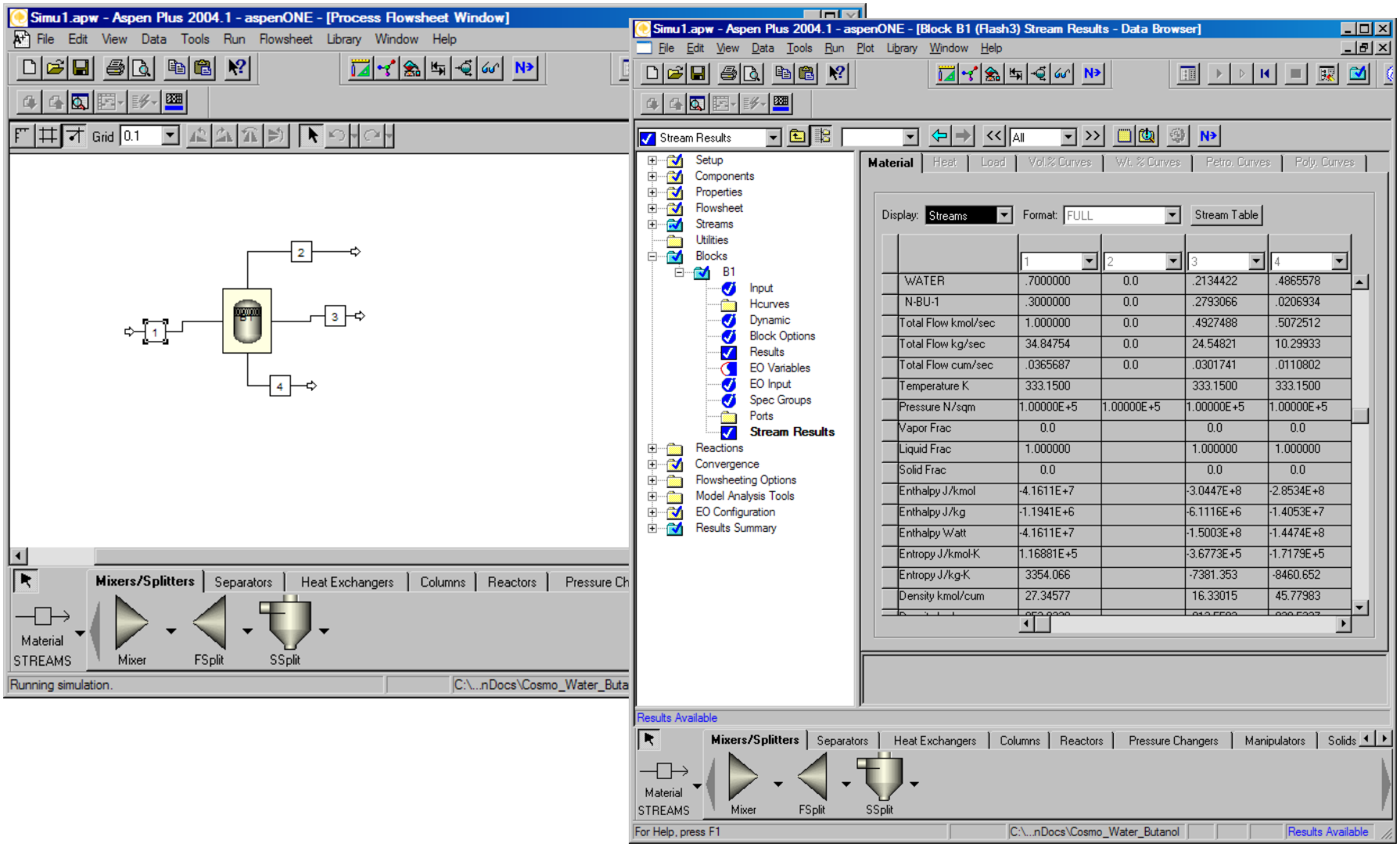
# Unit-operation Interoperability tests:

| | 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
1
2
3
4
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