A look into the CAPE-OPEN kitchen of

COCO

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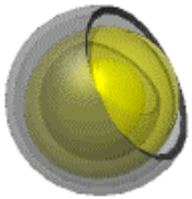
CAPE-OPEN to CAPE-OPEN (COCO):

Simulation environment (COFE)

Thermodynamic property package (TEA)

Collection of unit operations (COUS)



Reaction package (CORN)

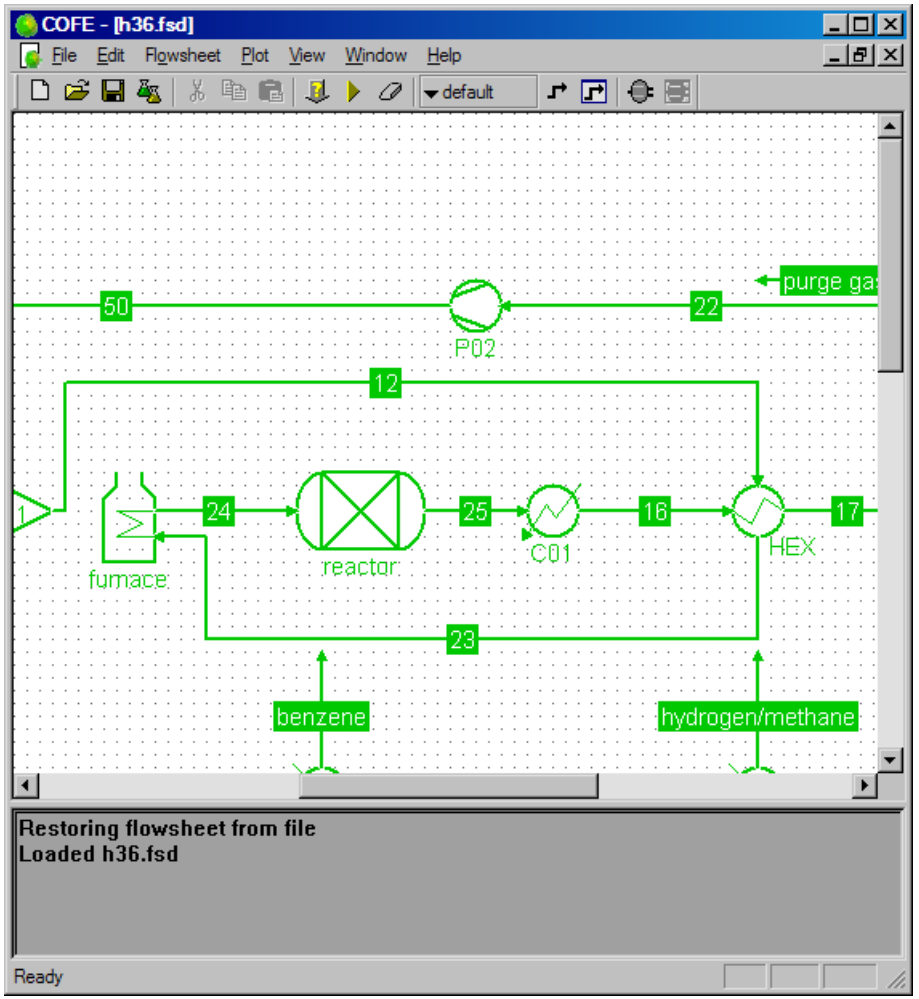
COFE: CAPE-OPEN Flowsheeting Environment

GUI:

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

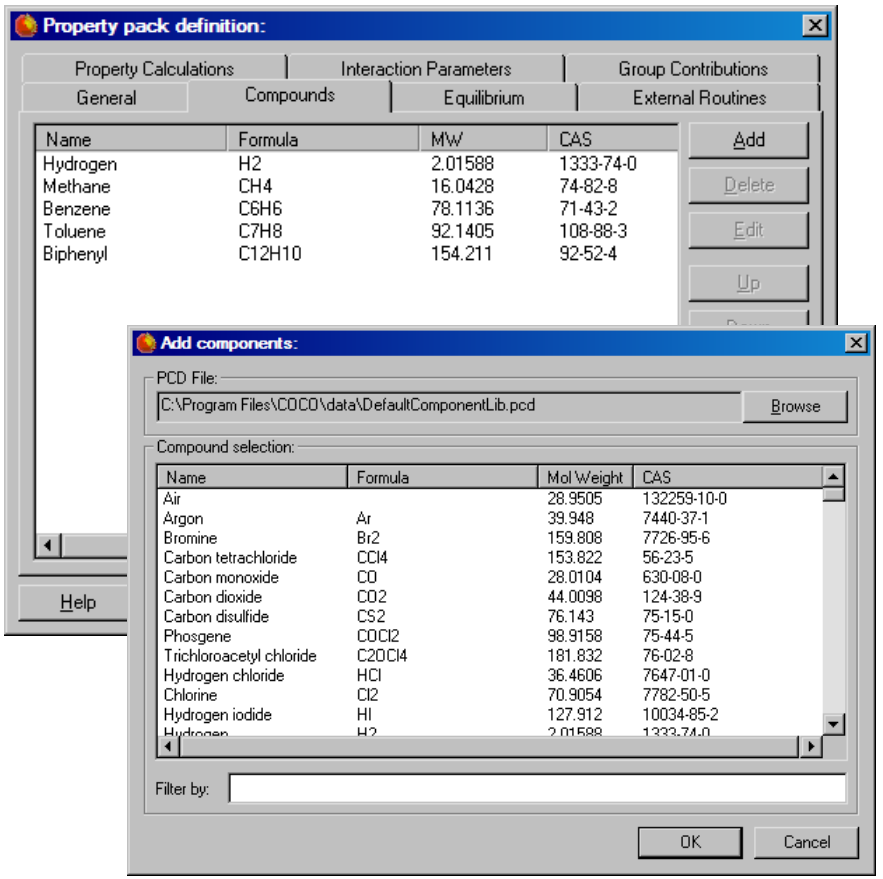
Flowsheeting:

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



TEA: Thermodynamics for Engineering Applications

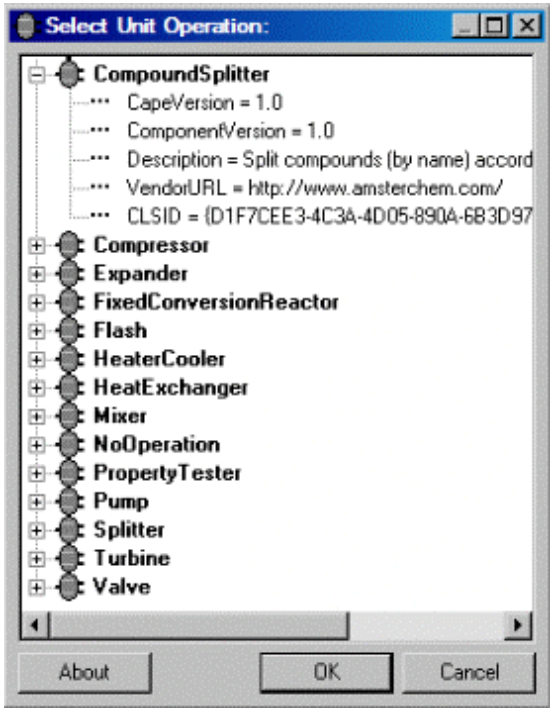
- Pure compound data library (extendible, or use DIPPR)
- 100+ Property calculation methods (> 25 different properties)
- Property derivatives
- Support of external property calculation routines (ICapeThermoCalculationRoutines)



Thermodynamic models and compounds from ChemSep

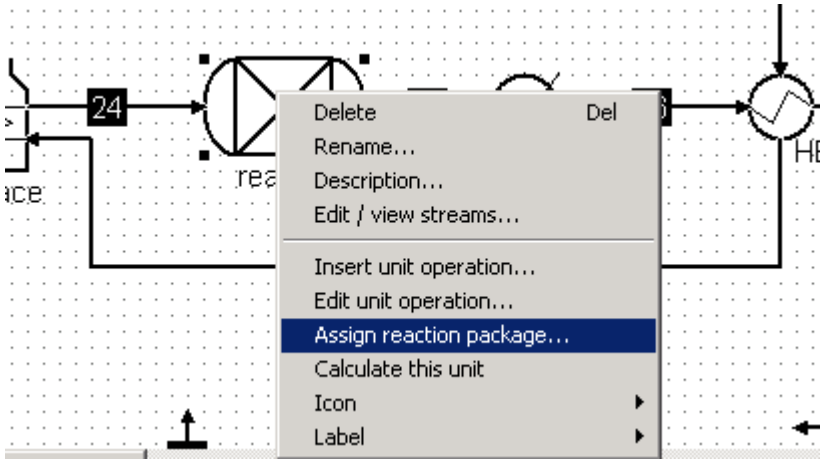
COUS-COUS: Simple unit operations

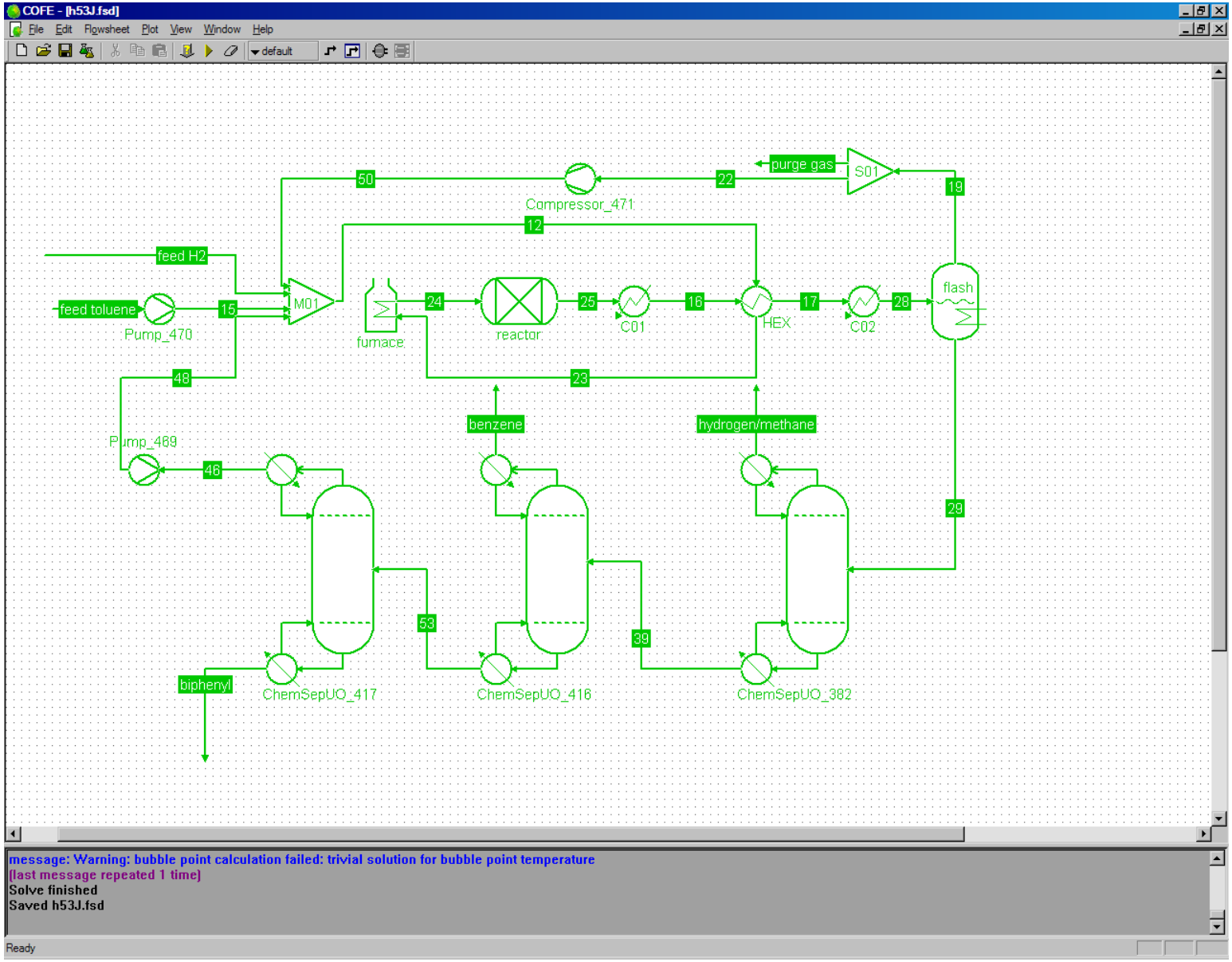
- General purpose unit operations (mixer, splitter, heat exchanger…)
- Property tester for thermodynamic properties
- Distillation column of ChemSep LITE



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





HDA case study

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

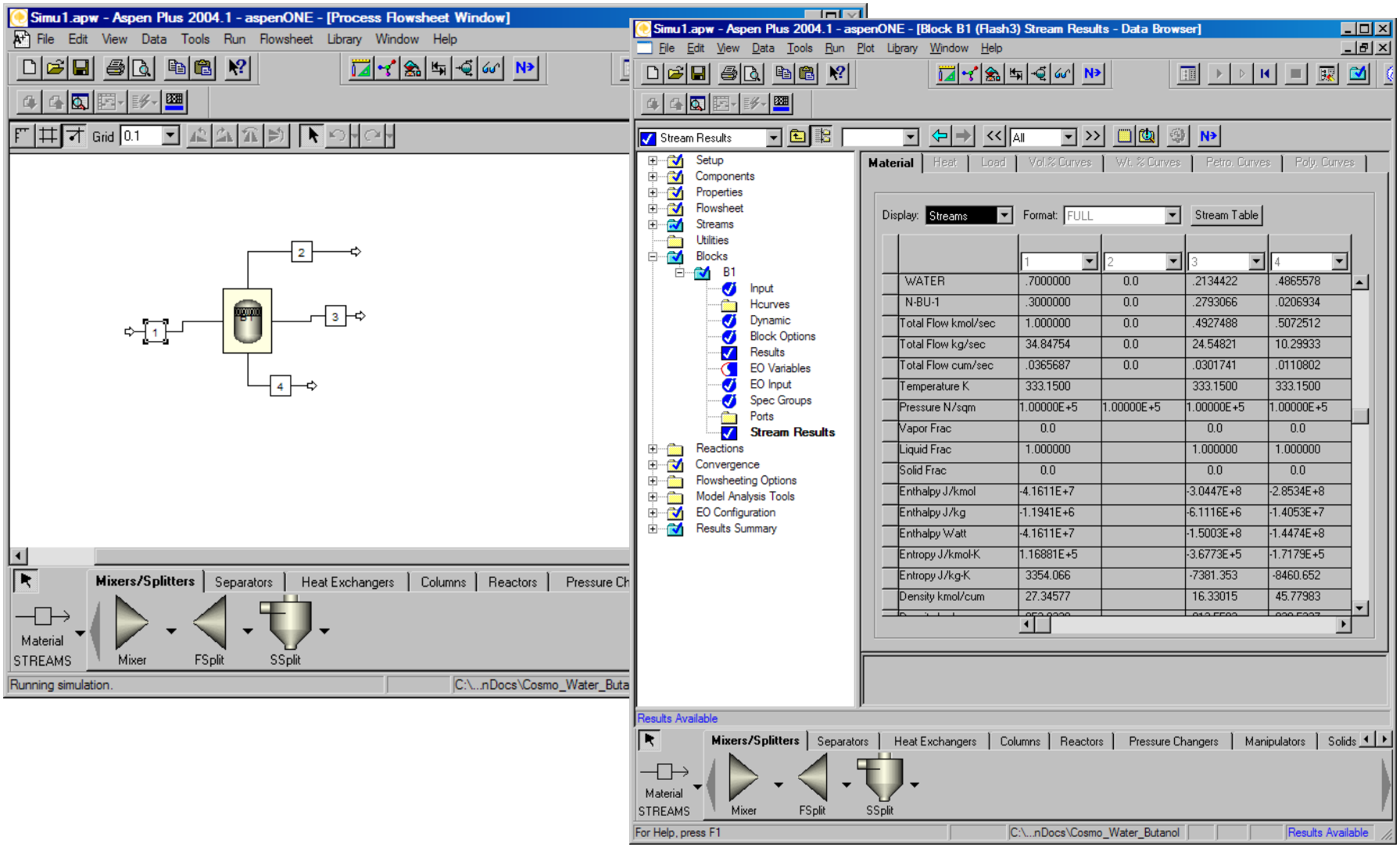
Unit-operation Interoperability tests:

	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



TEA using CosmoTherm in AspenPlus 2004.1

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
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- Aspen Technology