

An introduction to



COCO

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Introduction

- Overview of COCO software components
- Overview of how this fits in to CAPE-OPEN framework
- Some details on implemented algorithms
- Interoperability demonstration
- Benefits of having COCO on *your* computer

CAPE-OPEN to CAPE-OPEN (COCO):



Simulation environment (COFE)



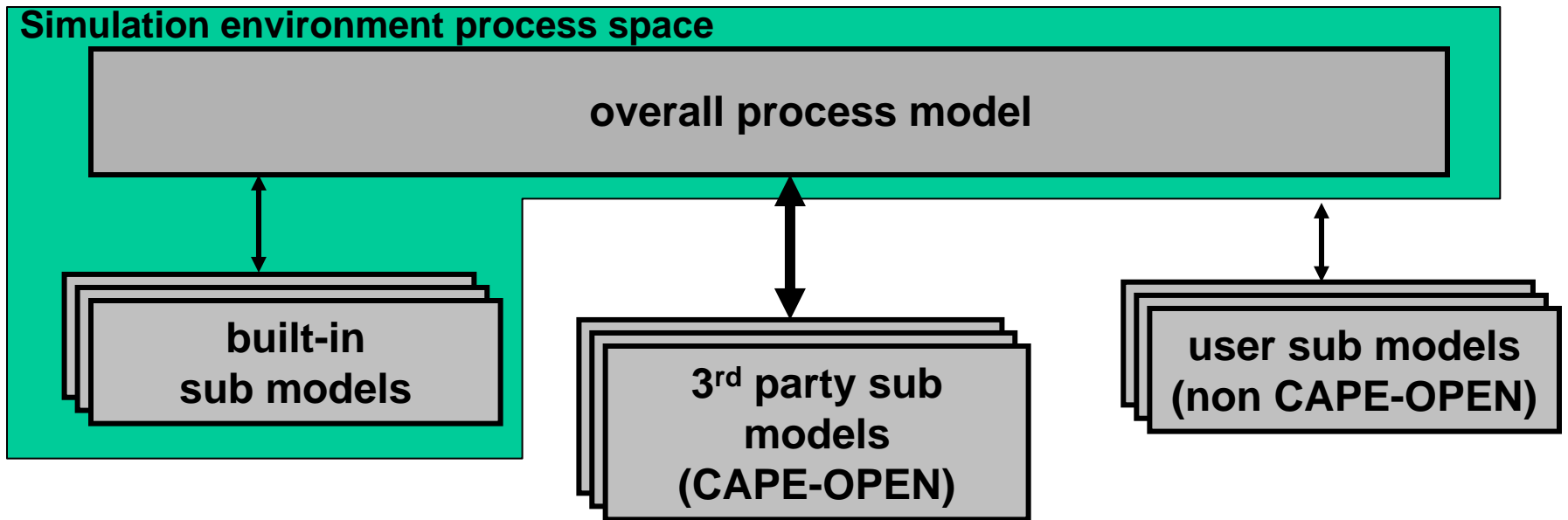
Thermodynamic property package (TEA)

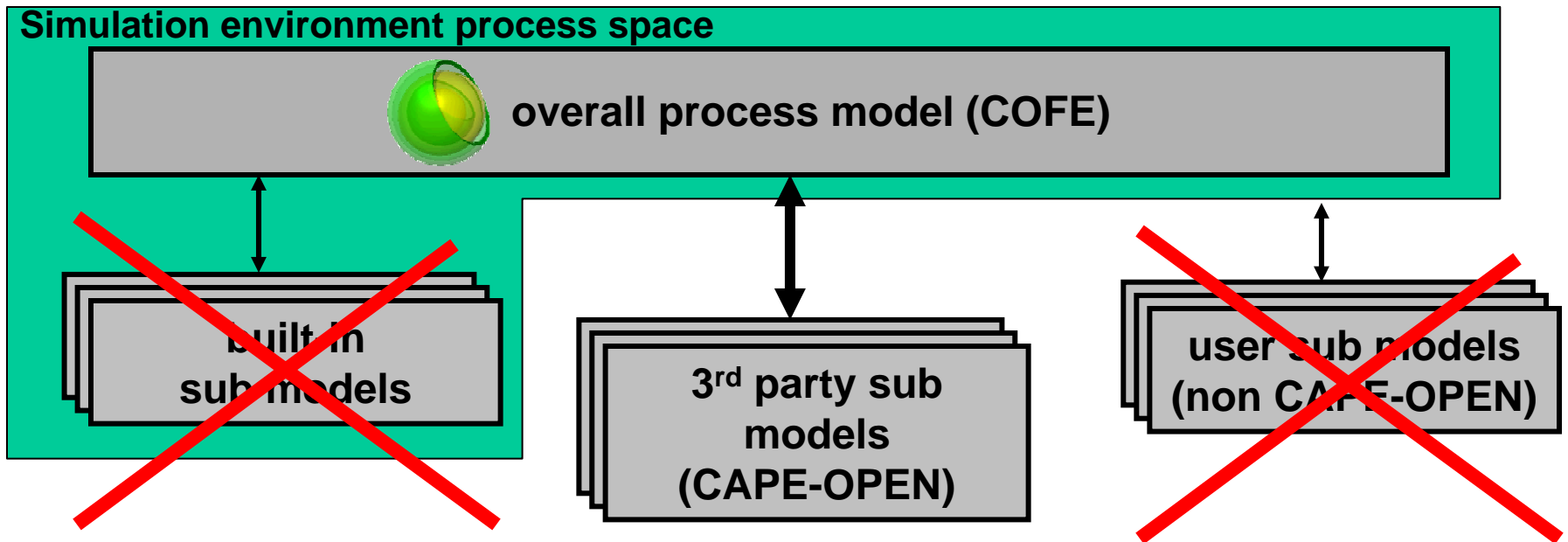


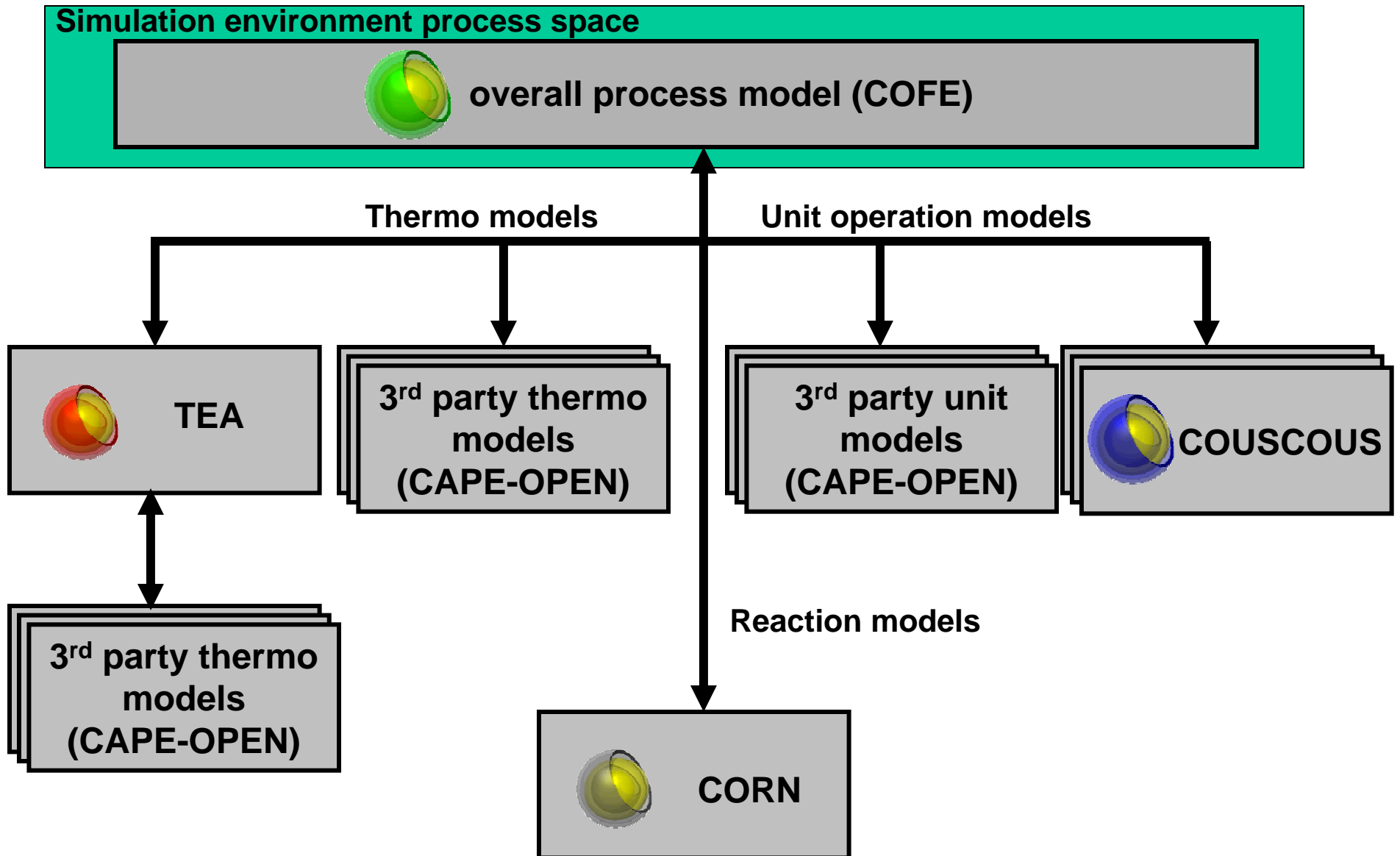
Collection of unit operations (COUSCOUS)



Reaction package (CORN)









COFE: CAPE-OPEN Flowsheeting Environment

Graphical flowsheeting

The screenshot displays the COFE software interface with three main windows:

- Graphical flowsheeting:** Shows a process flowsheet with units like 'Pump_470', 'MO1', 'reactor', and 'Comp'. Streams are labeled with numbers like 15, 24, 50, and 12.
- Graphing:** A composition plot titled 'sample3packs.fsd:2 [Composition Plot Ethane/Methane]'. The y-axis is 'Temperature /K' (110 to 190) and the x-axis is 'molar phaseFraction [Liquid]' (0 to 1). The plot shows bubble point and dew point curves for three streams: TEA_IN, MF_IN, and PPDS_IN.
- Streams view:** A table showing stream properties for TEA_OUT, PPDS_OUT, and MF_OUT.

name	TEA_OUT	PPDS_OUT	MF_OUT	unit
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	

Multiple models

Logging

Streams view

warning: Material object error in SetProp: invalid phase for temperature in SetProp
 warning: Material object error in SetProp: invalid phase for pressure in SetProp
 (last 2 messages repeated 1 time)
 solving HEATER_MF
 Solve finished in 109ms



COFE: CAPE-OPEN Flowsheeting Environment

- Breaking recycles by automatic tearing
- Solving recycles by hybrid Newton / Wegstein approach, using reparameterization
- Support for multiple material types, with selection for thermo and sub-set of compounds
- Material, energy and information streams



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 and external equilibrium servers

The image shows two overlapping dialog boxes from the software. The top one is titled 'Property pack definition:' and has tabs for 'Property Calculations', 'Interaction Parameters', and 'Group Contributions'. Under 'Property Calculations', there are sub-tabs for 'General', 'Compounds', 'Equilibrium', and 'External Routines'. The 'Compounds' tab is active, showing a table of compounds with columns for Name, Formula, MW, and CAS. The bottom one 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



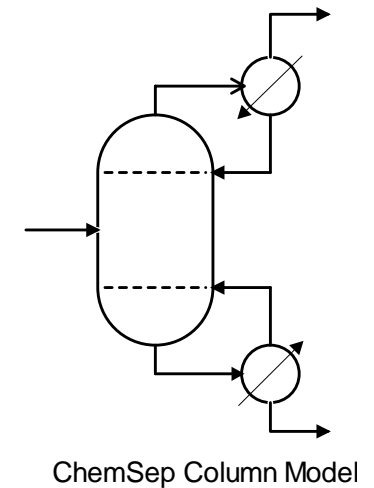
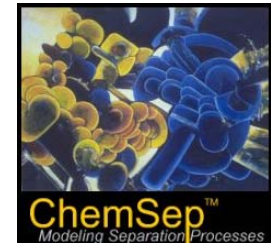
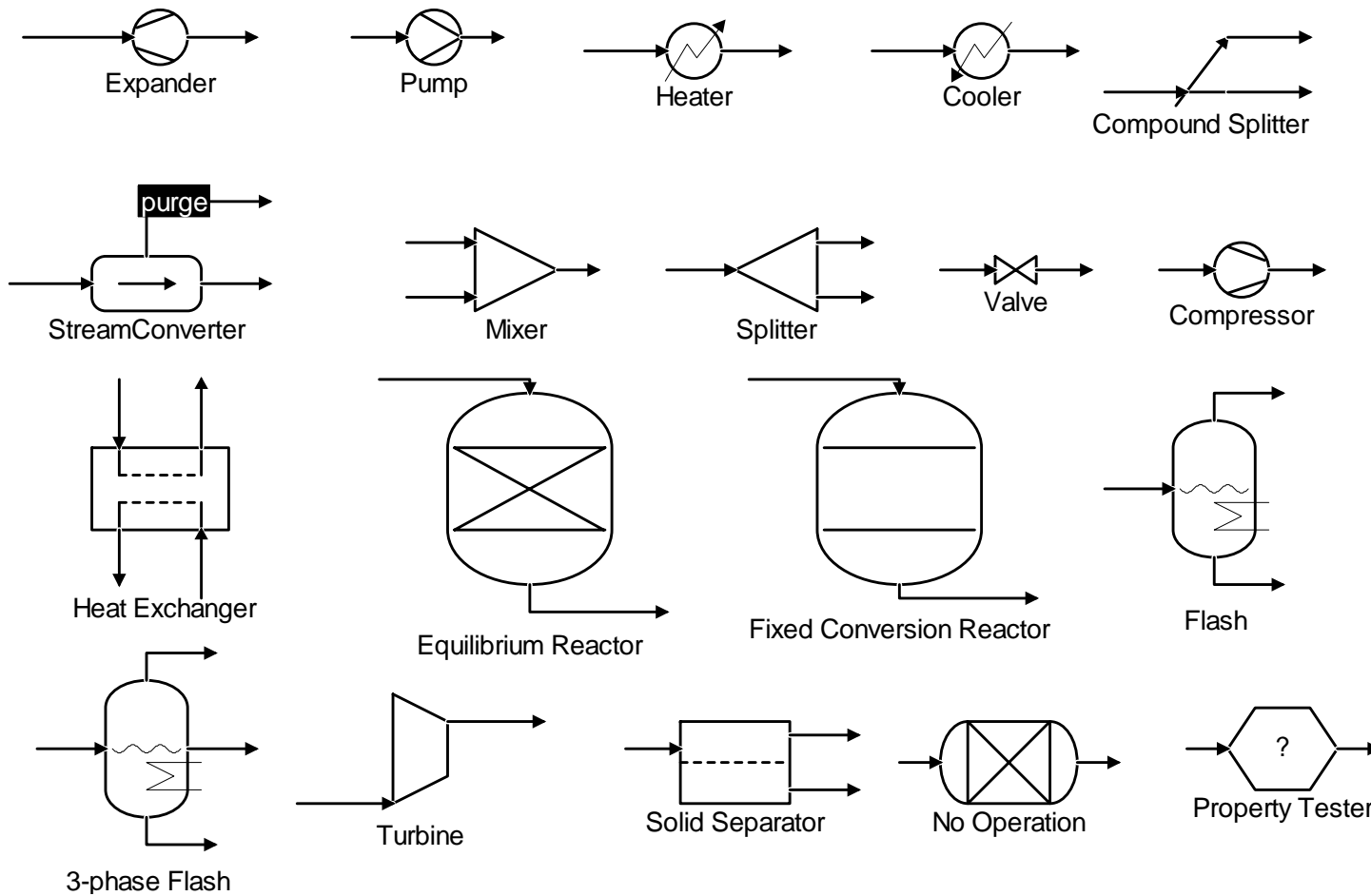
TEA: Thermodynamics for Engineering Applications

VLE equilibrium calculations

- Large diversity of supported flash specifications
- Inside-out approach
- Post-checking of solution (since version 1.09)
- Back-up full Newton approach



COUSCOUS: Simple unit operations





COFE: OLE and Excel

EXCEL

Enthalpy

Ideal

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

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

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

ONLINE HELP



COFE: OLE and Excel

EXCEL

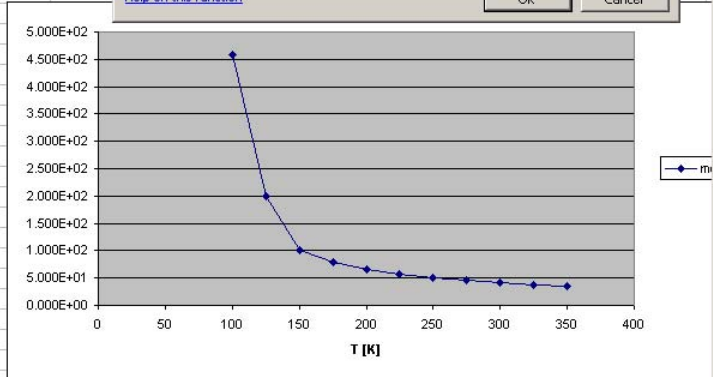
FORMULA WIZARD

The spreadsheet contains the following data:

composition for property calculation below			
default compound count:	5	basis:	mole
default compounds:	Hydrogen		0.2
	Methane		0.2
	Benzene		0.2
	Toluene		0.2
	Biphenyl		0.2

property calculations:			
<i>(the example shows a scalar property; fugacity for example will return for a list of properties, see the 'Properties' page when choosing Conf</i>			
phase	vapor		
basis	mole		
property	density		
P/Pa	T/K	mol / m ³	
1.00E+05	100	4.590E+02	
1.00E+05	125	1.991E+02	
1.00E+05	150	1.019E+02	
1.00E+05	175	7.940E+01	
1.00E+05	200	6.629E+01	
1.00E+05	225	5.732E+01	
1.00E+05	250	5.068E+01	
1.00E+05	275	4.552E+01	
1.00E+05	300	4.137E+01	
1.00E+05	325	3.795E+01	
1.00E+05	350	re", \$C\$29)	

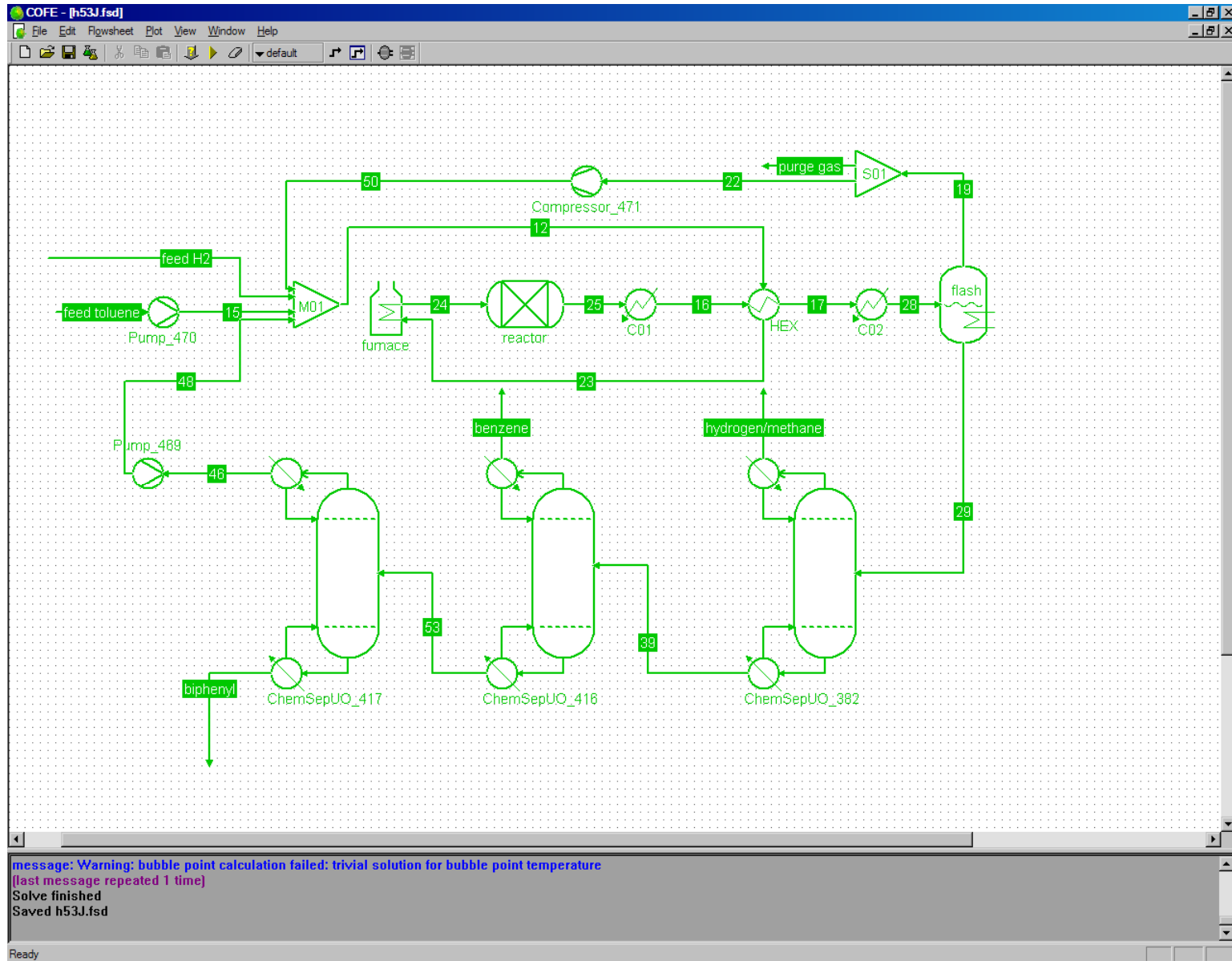
compound constant example:				
<i>(for a list of available compound constants, see CAPE OPEN thermodynamic specification)</i>				
name	molecularWeight	criticalPressure	criticalTemperature	
compound	Hydrogen	Hydrogen	Methane	
value	2.01588	1313000	190.56	
dimension	-	Pa	K	





COCO: CAPE-OPEN interface support

- Full support for thermodynamic standard versions 1.0 and 1.1 in all components
- Unit operation sockets & plugs (steady state)
- Reaction package sockets & plugs
- Full support for all COSE interfaces
- All common interfaces (identification, error handling, utilities, parameters with dimensionality, persistence, ...)



COCO stand-alone

The screenshot displays the Aspen Plus 2004.1 interface. The main window shows a process flowsheet with a central reactor block (B1) and four streams (1, 2, 3, 4). The 'Block B1 (Flash3) Stream Results - Data Browser' window is open, showing a table of stream results for four streams (1, 2, 3, 4).

	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

Three-phase AspenPlus flash using TEA + CosmoTherm

PRO/II with PROVISION - CStest1

File Edit Input Output Tools Draw View Options Window Help

Summary Report

Flowsheet

Stream Name		S1	S2	S3
Thermodynamic system		SRK01	SRK01	SRK01
Phase		Liquid	Liquid	Liquid
Temperature	F	100.000	100.000	97.050
Pressure	PSIA	100.000	100.000	100.000
Flowrate	LB-MOL/HR	50.000	50.000	100.000
Total Enthalpy	MM BTU/HR	0.116	0.128	0.244
Total Molar Comp. Fractions				
NC4		1.0000	0.0000	0.5000
NC5		0.0000	1.0000	0.5000

Stream Name		S1MIX	S2MIX	S3MIX
Thermodynamic system		SRK01	SRK01	SRK01
Phase		Liquid	Liquid	Liquid
Temperature	F	100.000	100.000	97.050
Pressure	PSIA	100.000	100.000	100.000
Flowrate	LB-MOL/HR	50.000	50.000	100.000
Total Enthalpy	MM BTU/HR	0.116	0.128	0.244
Total Molar Comp. Fractions				
NC4		1.0000	0.0000	0.5000
NC5		0.0000	1.0000	0.5000

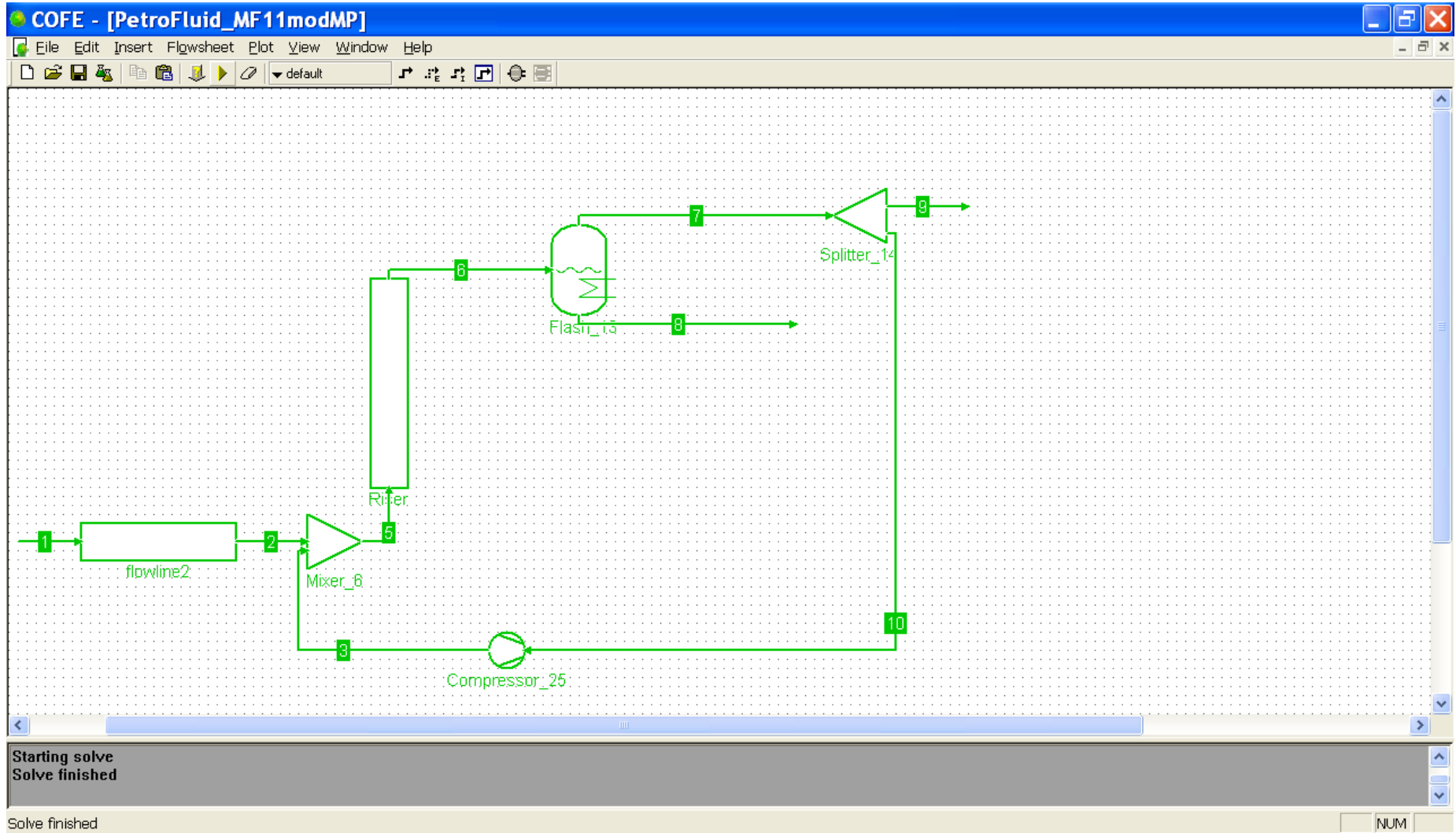
Pro/II showing internal and COUSCOUS mixer

The screenshot shows the 'SIMSCI - Thermodynamic Data' interface. In the 'Selection of Property Calculation System' section, the 'Category' is set to 'CAPE-OPEN'. The 'Defined Systems' list contains 'SRK01' and 'CO01', with 'SRK01' selected as the 'Default System'. An 'Add ->' button is visible. Below this, there are 'View...' and 'Delete' buttons for the selected system. A 'PRO/II - Select Property Package' dialog box is open, displaying a tree view of 'CAPE-OPEN Thermo Systems'. The selected package is 'COCO_TEA.ThermoPack.1'. Other packages listed include 'PPDS.CapeThermoSystem.1', 'MFCOThermoSys.MFCOSys', 'ATCOProperties.COPropertySystem.4', and 'VMGThermoCO.ThermoSystem.1'. The dialog has 'OK' and 'Cancel' buttons.

In the background, a data table is partially visible, showing stream properties:

Stream Name	Thermodynamic system	Phase	Temperature	Pressure	Flowrate	Total Enthalpy	Total Molar Comp. Fractions
						MM BTU/HR	
							0.116 0.128 0.244
							1.0000 0.0000 0.5000
							0.0000 1.0000 0.5000

Pro/II using TEA

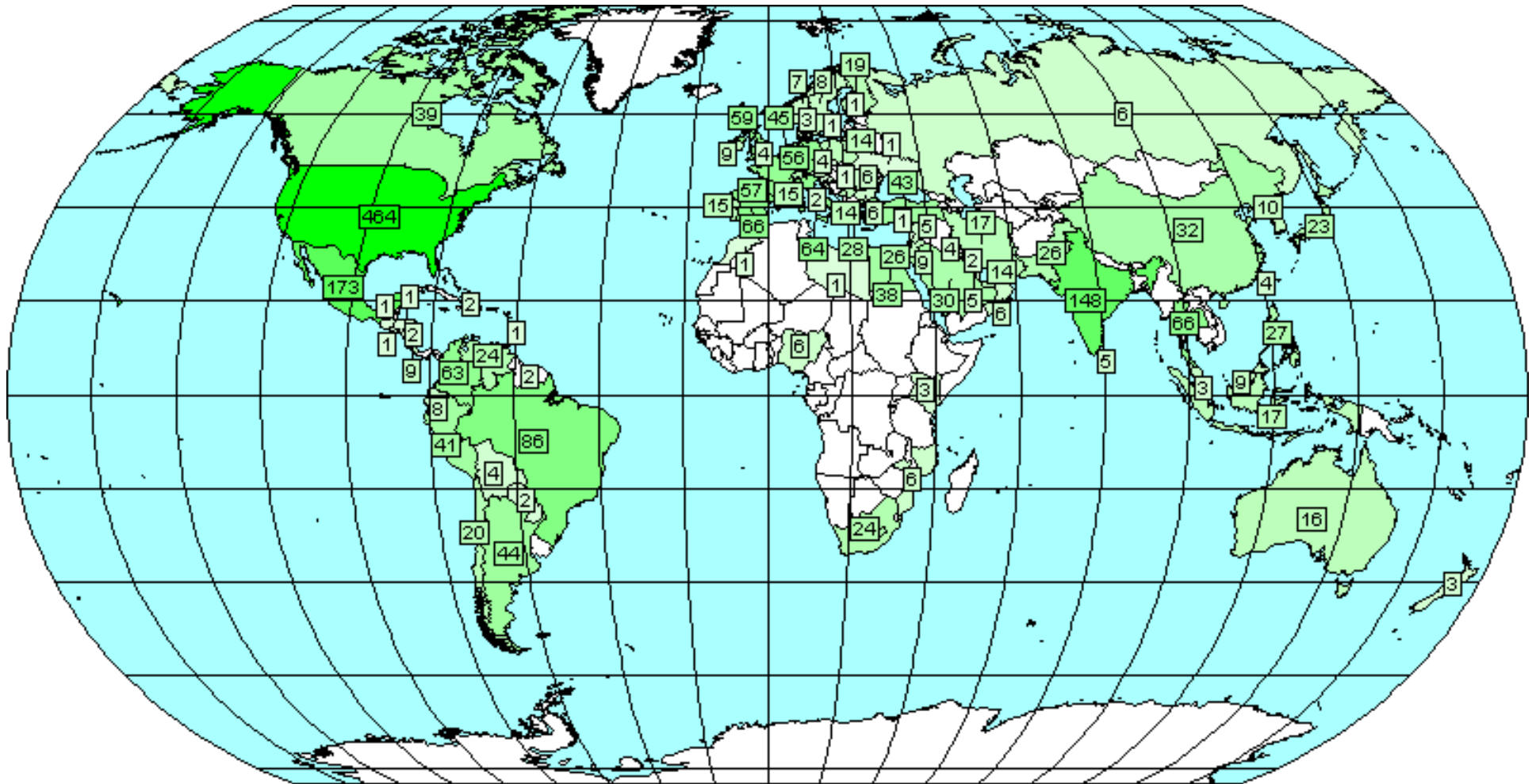


IFP/TOTAL TINA pipe model running in COFE

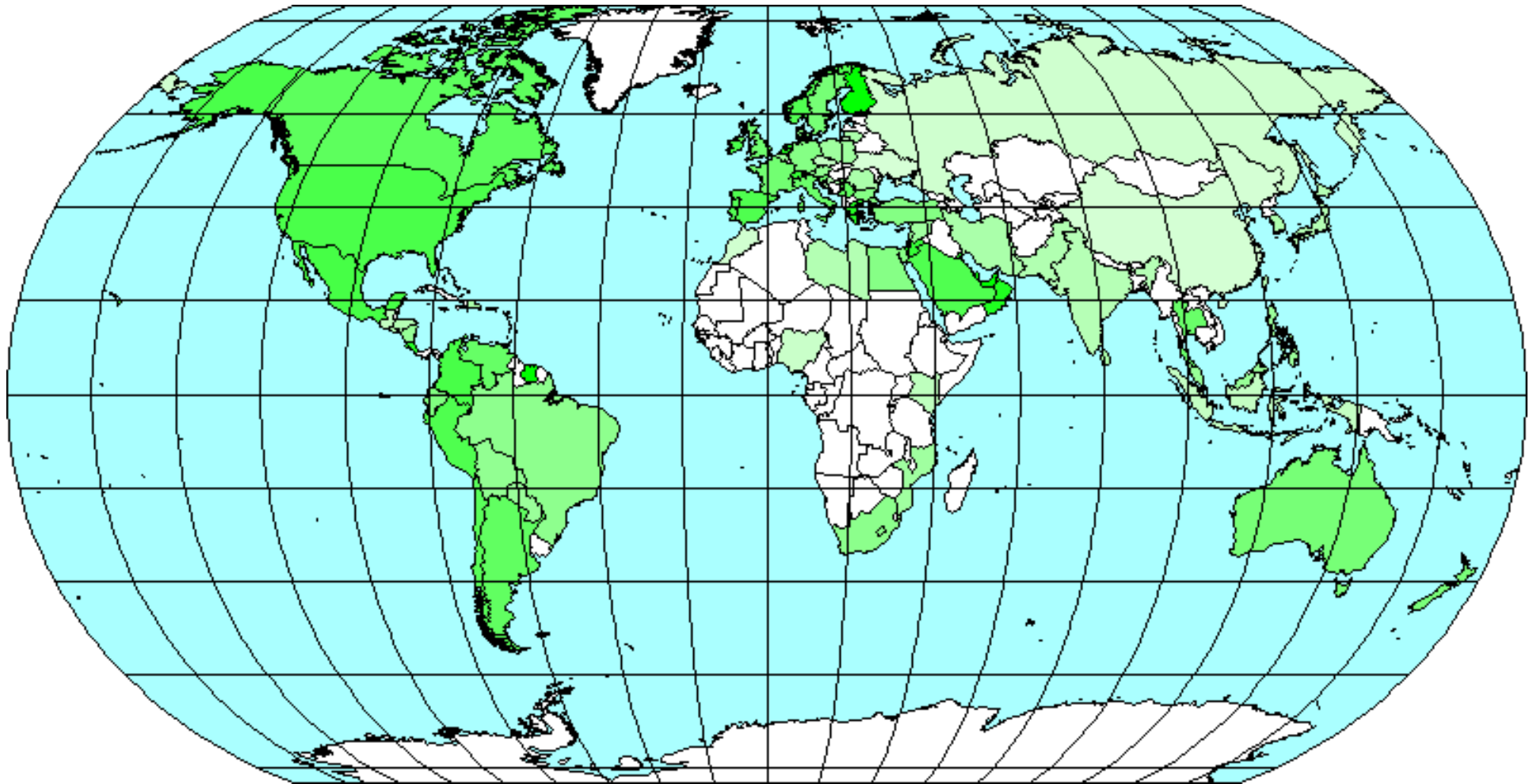


Why COCO?

- COCO integrates a useful set of thermodynamic property calculations, compound information and unit operation models
- COCO has been awarded the CO-LaN CAPE-OPEN award 2006
- COCO is widely regarded as the CAPE-OPEN interoperability testing platform
- COCO is available free of charge
- COCO is used world-wide



COCO downloads



COCO downloads per capita

- Download COCO: <http://www.cocosimulator.org/>
(or ask for a copy during the workshop)
- Contact amster**CHEM** for CAPE-OPEN consulting
- Interoperability testing program:
http://www.cocosimulator.org/index_compliance.html

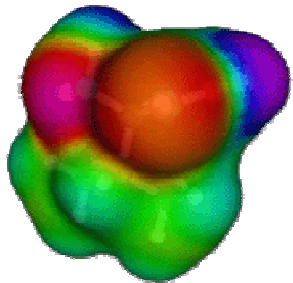
Acknowledgements:

- Richard Baur
- ChemSep: Ross Taylor, Harry Kooijman
- Cosmo*THERM*: Frank Eckert
- Michel Pons

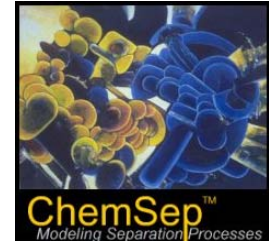
Many Thanks for CAPE OPEN testing licenses:



AspenTech: AspenPlus 2004.1

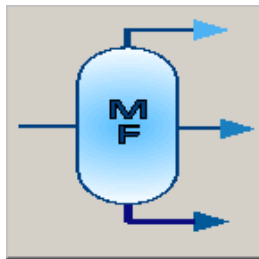


ChemSep: ChemSep 6.05



CosmoLogic: Cosmotherm C21

HTRI: Xchanger Suite 5.0



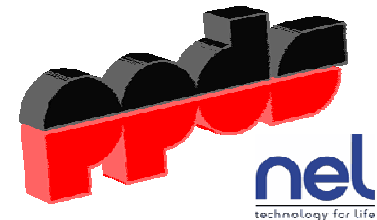
Infochem: Multiflash 3.6

PSE: gPROMS 3.0.3



Simsci-Esscor: PRO/II 8.1

TUV-NEL: PPDS v4.1.0.0



VMG: VMGThermo 5.0