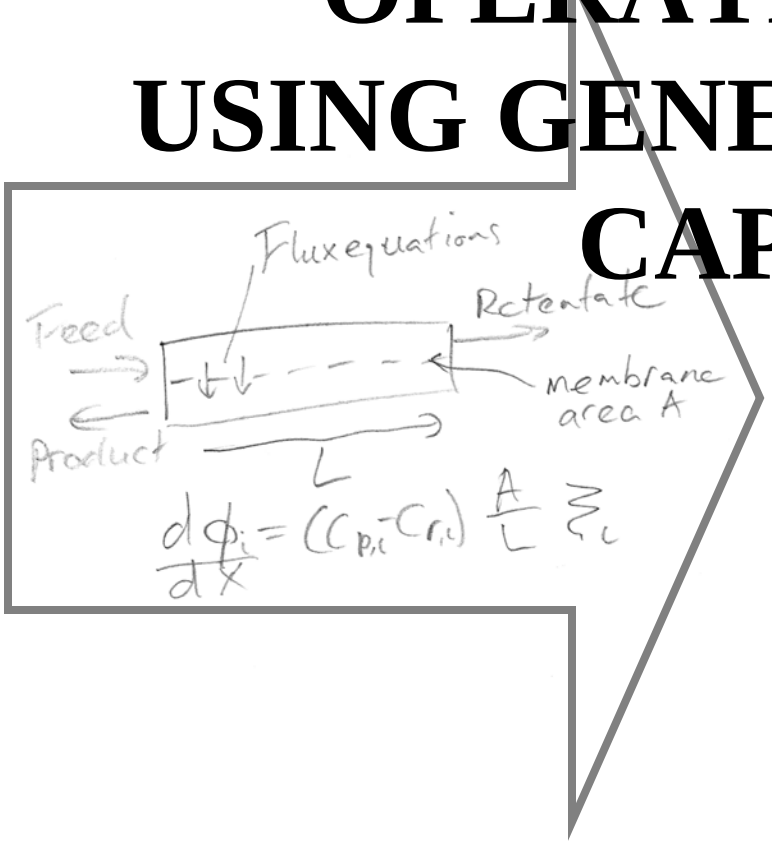
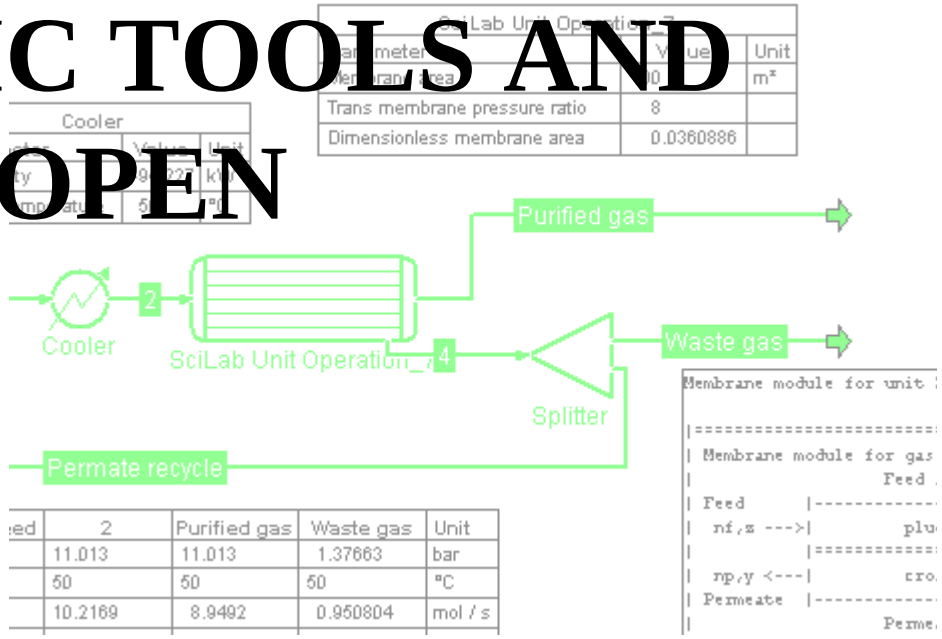
RAPID PROTOTYPING OF UNIT OPERATION MODELS USING GENERIC TOOLS AND CAPE-OPEN





	2	Purified gas	Waste gas	Unit
	11.013	11.013	1.37663	bar
	50	50	50	°C
	10.2169	8.9492	0.950804	mol / s

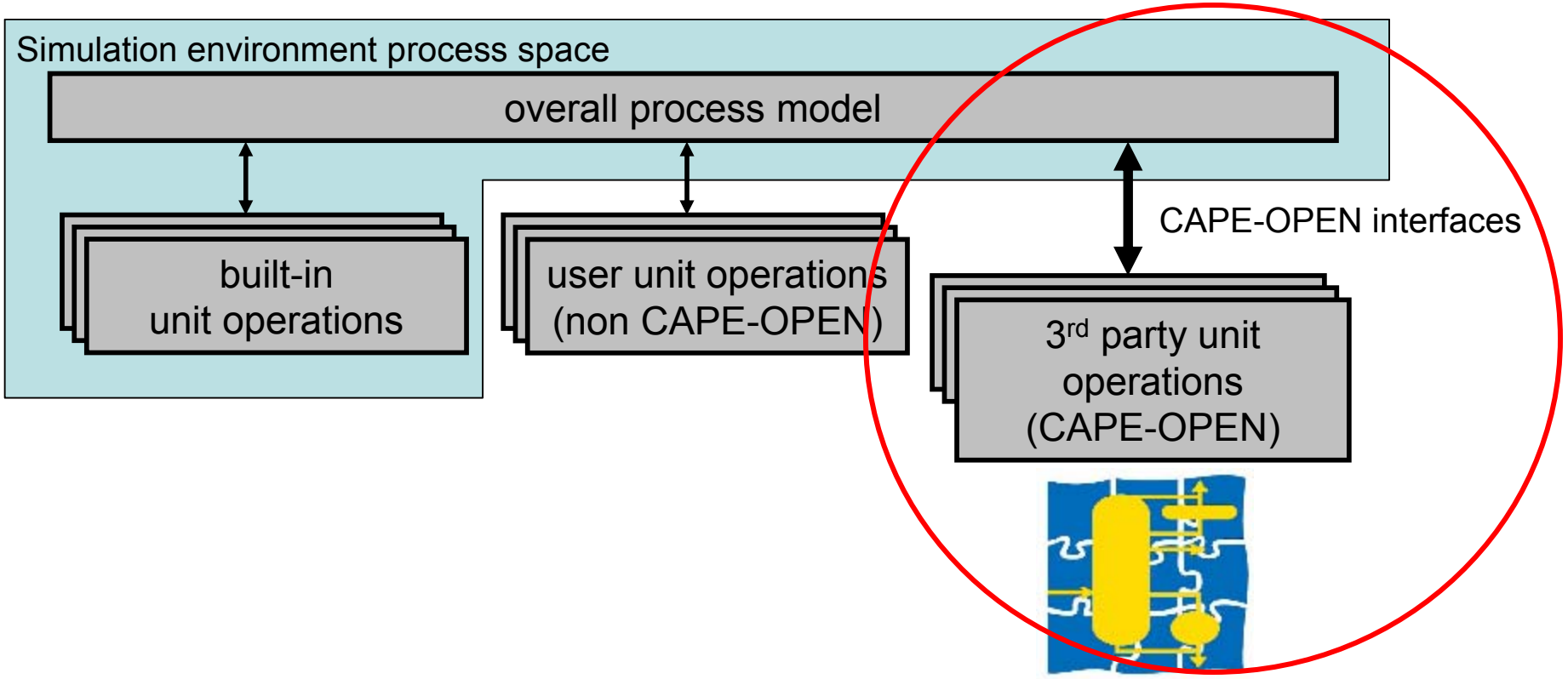
Jasper van Baten, AmsterCHEM

Michel Pons, CO-LaN

Presentation outline

- Why custom models?
- Why CAPE-OPEN?
- What is involved?
- Short-cut: Matlab and Scilab
- Short-cut: Excel Unit Operation
- Current status

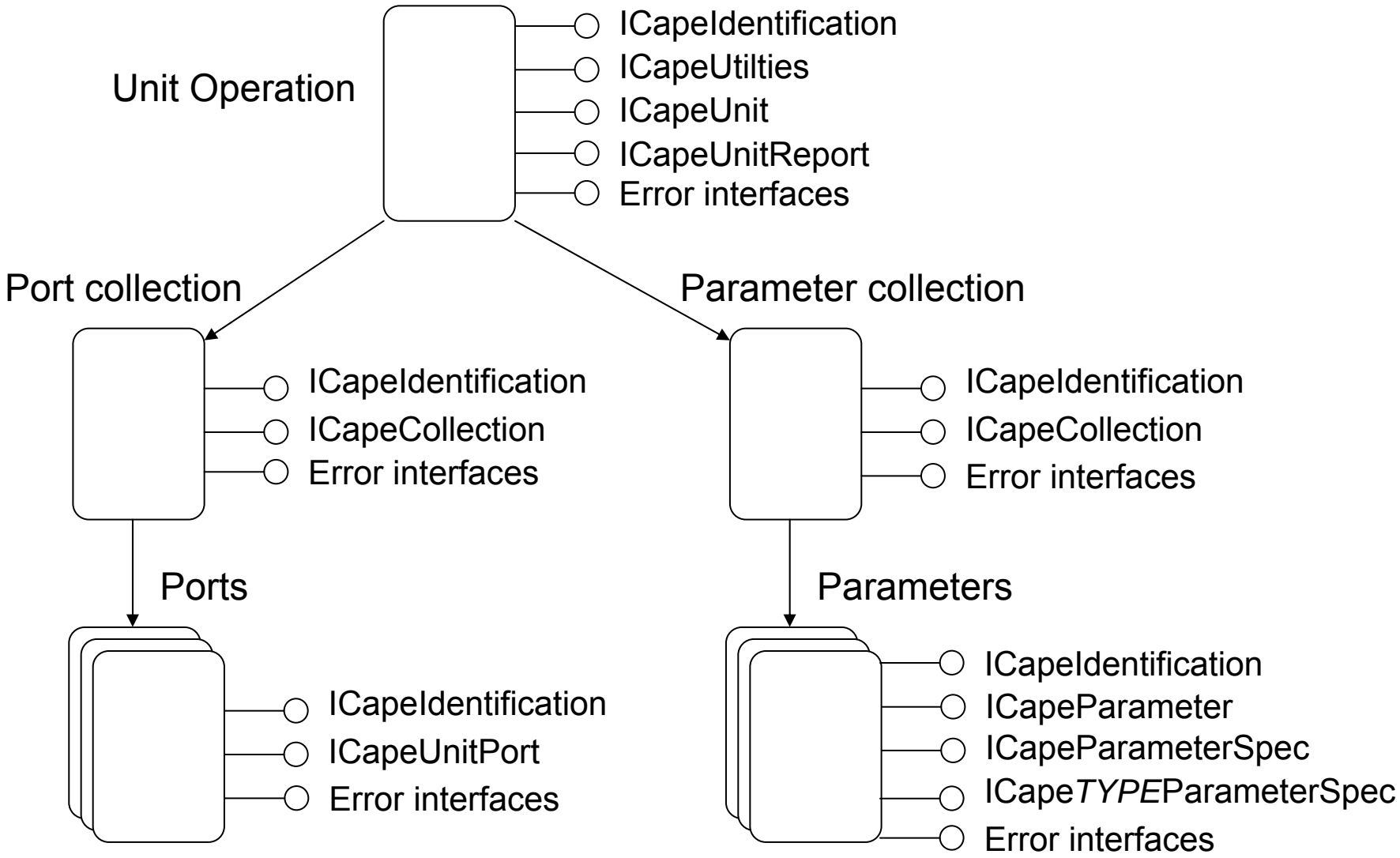
Why CAPE-OPEN?



Why CAPE-OPEN?

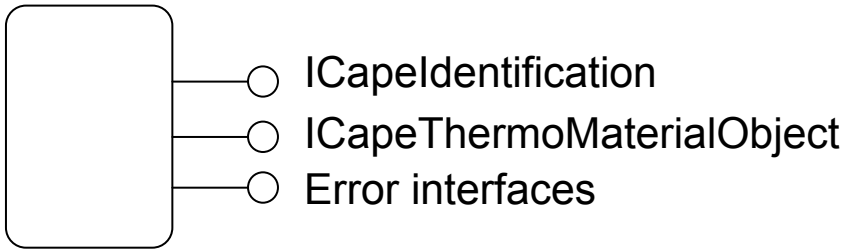
- Use of multiple simulation environment in company
- Validation of simulation results
- Bargaining position with respect to simulation vendor
- Model distribution

CAPE-OPEN: what is involved?

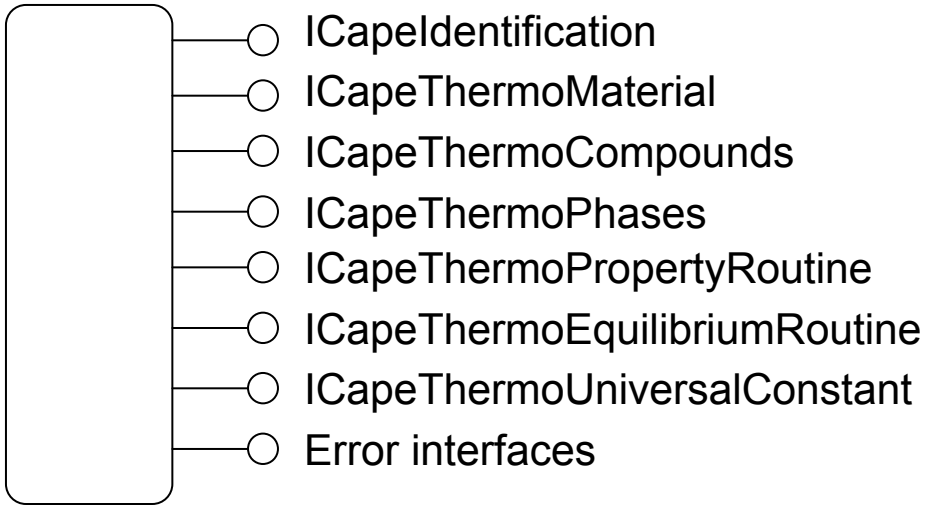


CAPE-OPEN: what is involved?

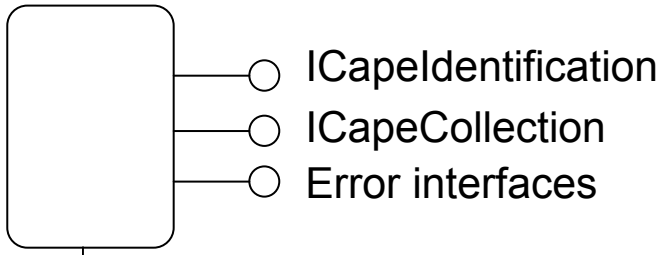
Material stream, version 1.0



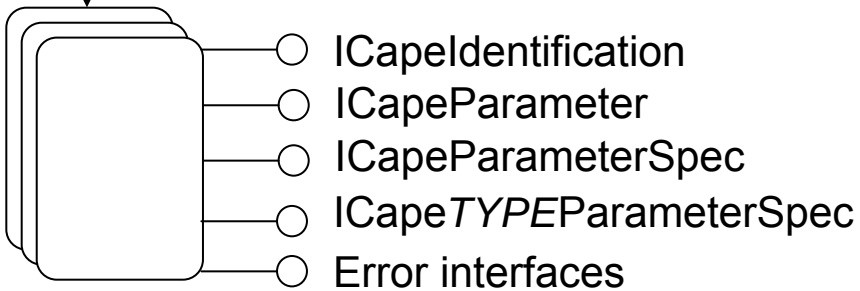
Material stream, version 1.1



Energy or information stream



Parameters



CAPE-OPEN: what is involved?

- COM server
- Implementation of the Unit Operation objects
- Deal with CAPE-OPEN interfaces exposed by streams
- Solution routines
- All in an efficient manner

A shortcut to model prototyping and testing is welcome

Two-step development:

- evaluate our model equations

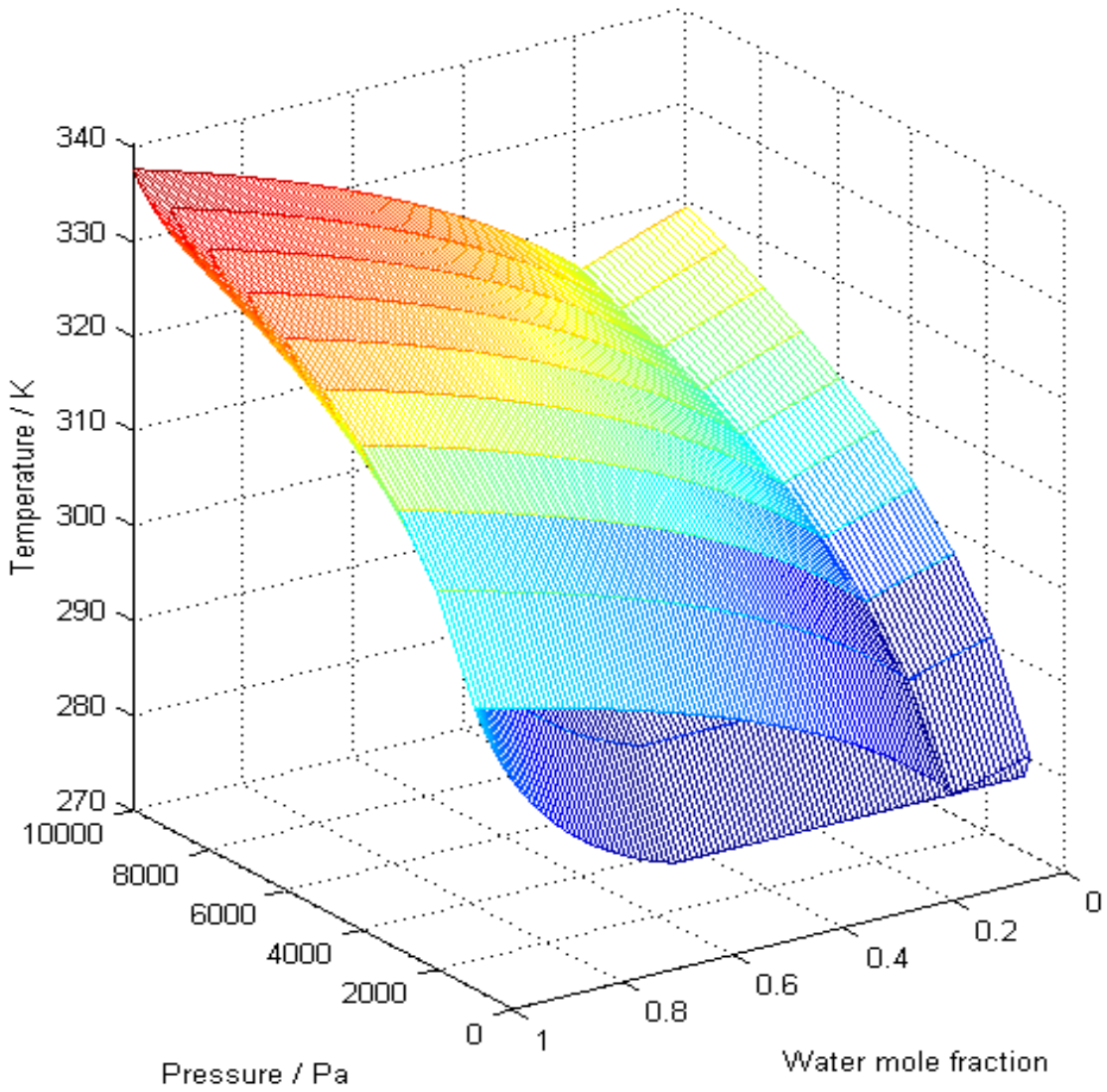
  → we require access to thermodynamics

- evaluate the final process model

  → requires running as Unit Operation inside simulation environment

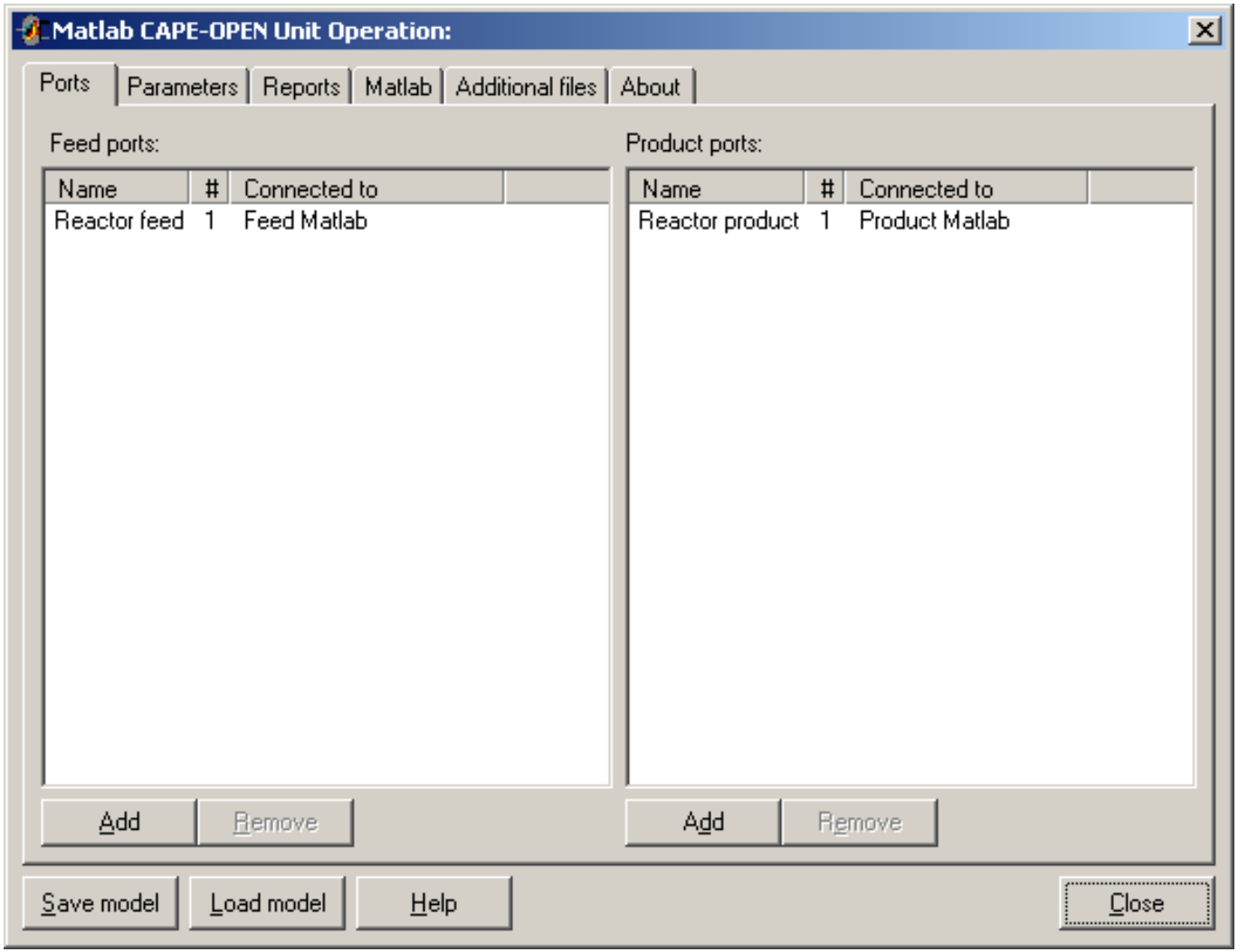
Interactive thermodynamic access:

- Matlab or Scilab: script based
- Interactive or batch script processing
- Load third party thermodynamics
- Access to:
  - ❖ Compounds and compound data
  - ❖ Phases and phase descriptions
  - ❖ Thermodynamic property calculations
  - ❖ Thermodynamic equilibrium (Flash) calculations

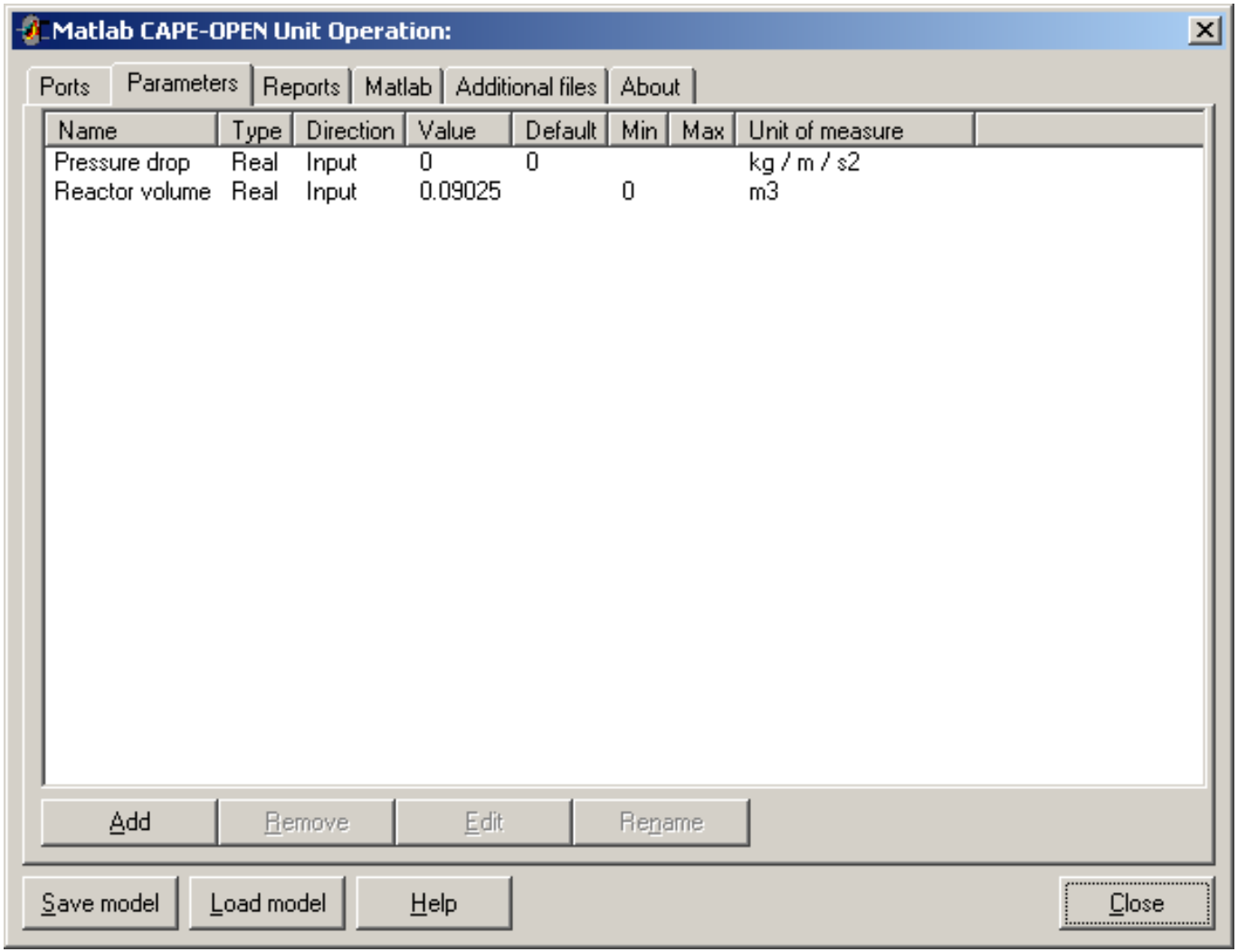

340
330
320
310
300
290
280
270
Temperature / K
10000
8000
6000
4000
2000
0
Pressure / Pa
0
0.2
0.4
0.6
0.8
1
Water mole fraction

```
handle=capeOpenGetPackage …
('Multiflash Property Package Manager','WATER-N-BUTANOL');

frac=(0:0.01:1)';
X=[frac 1-frac];
P=[1e3:1e3:1e4];
tbub=[];
tdew=[];

for p=P

 tbub=[tbub capeOpenEquilibriumProp(handle,'temperature', ...
     X,'pressure',p,'vaporFraction',0)];
 tdew=[tdew capeOpenEquilibriumProp(handle,'temperature', ...
     X,'pressure', p,'vaporFraction',1)];

end;
```

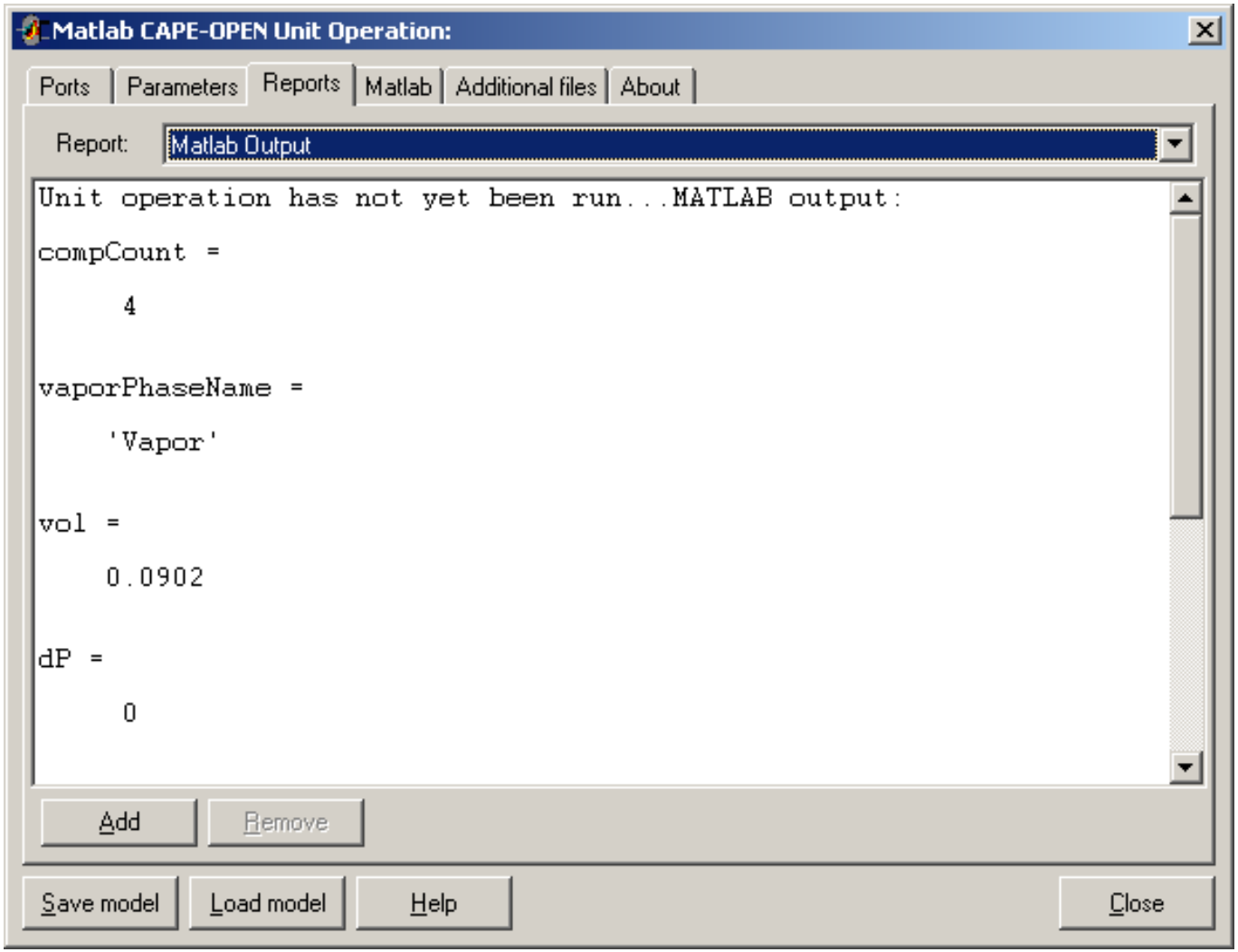
Implementation as a Unit Operation:



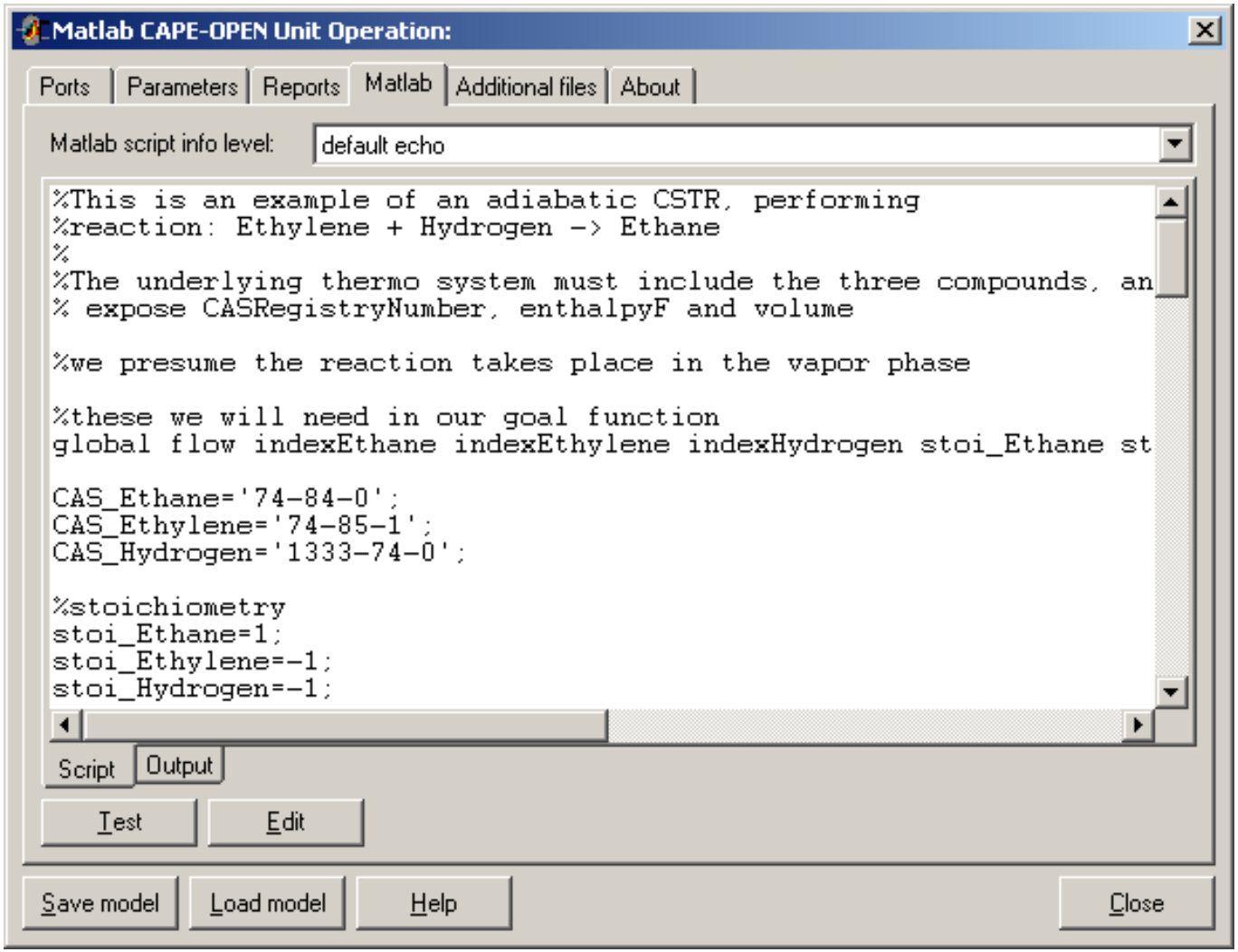
Implementation as a Unit Operation:



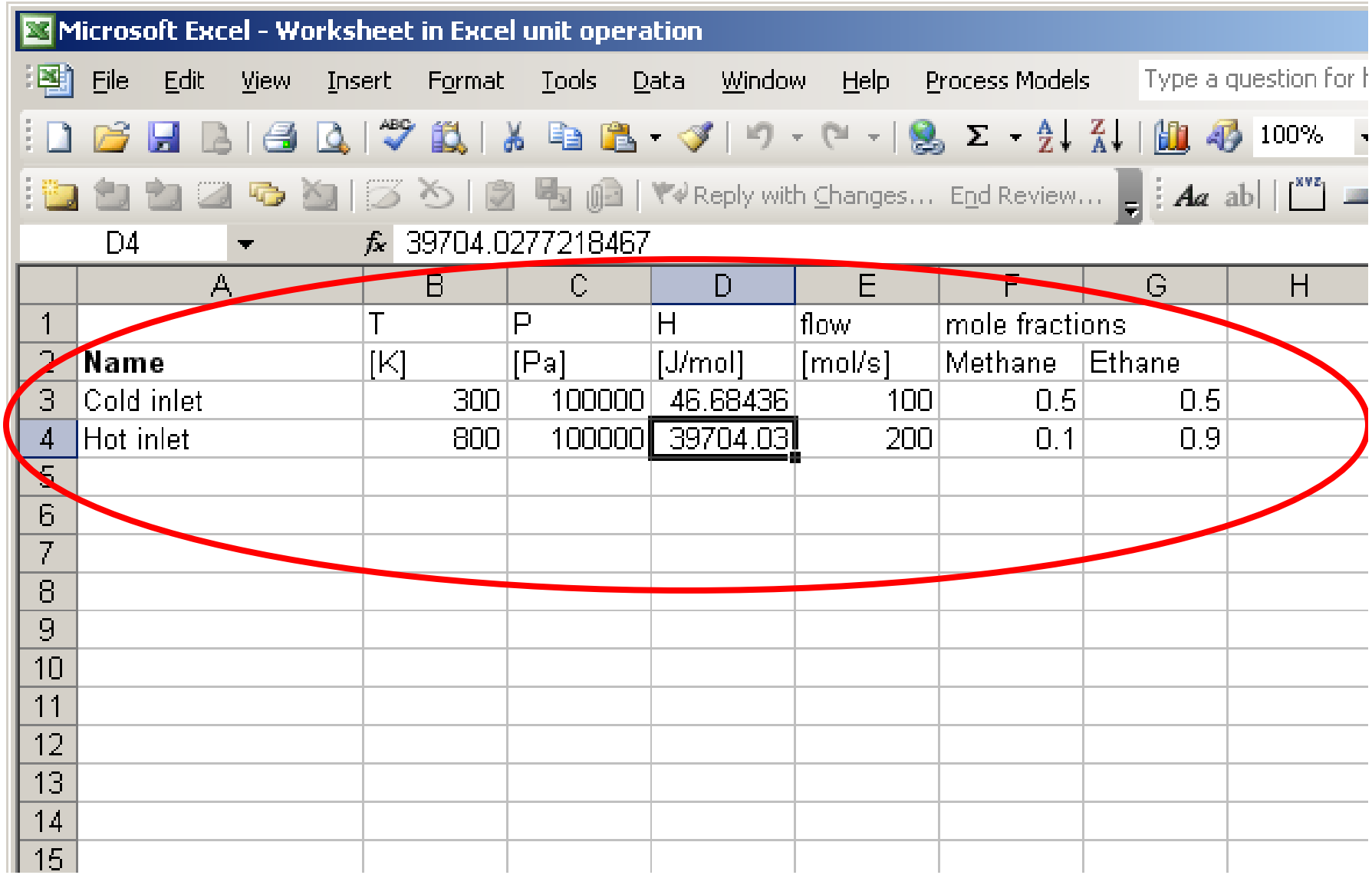
Implementation as a Unit Operation:



Implementation as a Unit Operation:

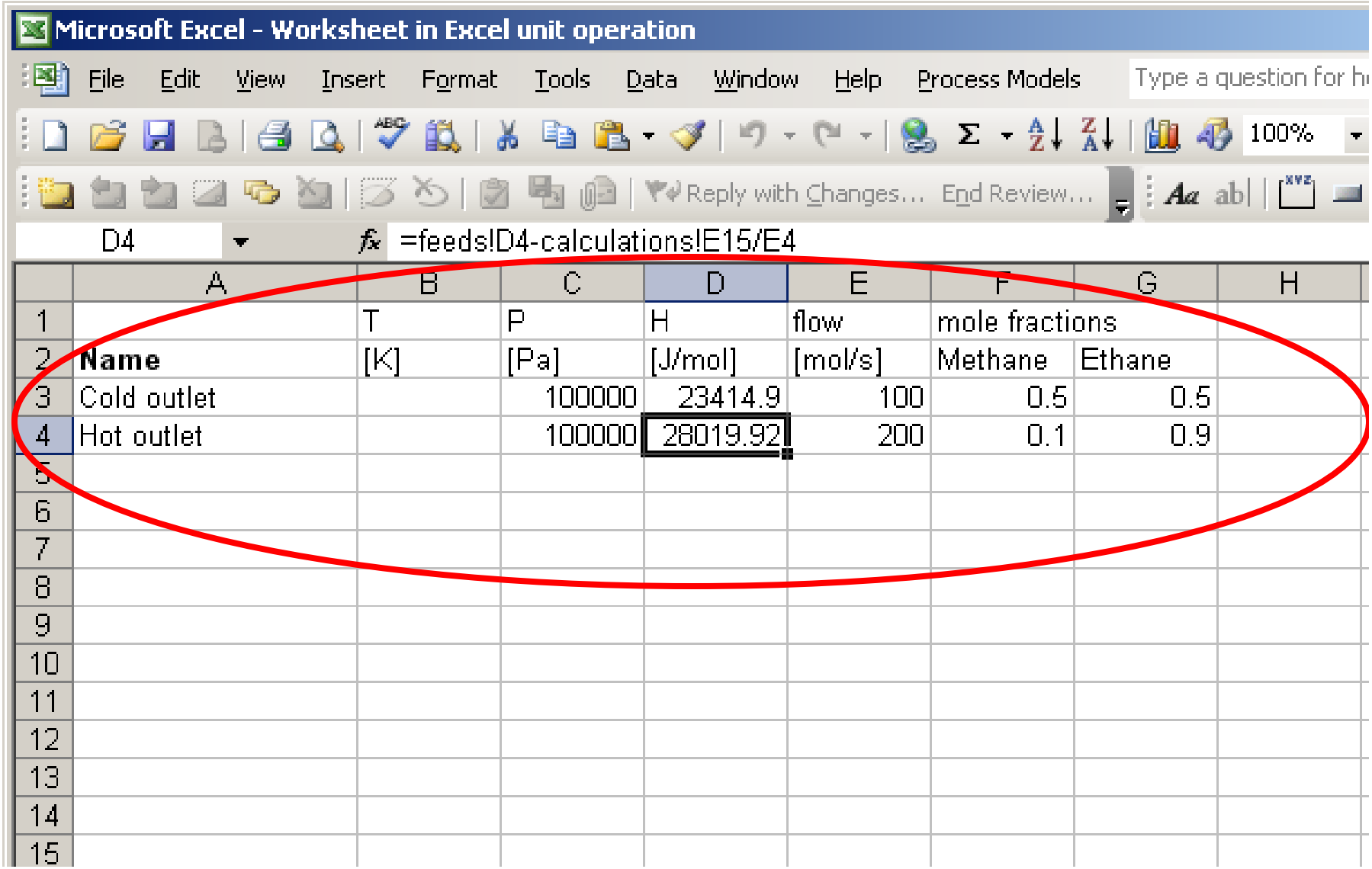


Excel based Unit Operation:



	A	B	C	D	E	F	G	H
1		T	P	H	flow	mole fractions		
2	**Name**	[K]	[Pa]	[J/mol]	[mol/s]	Methane	Ethane	
3	Cold inlet	300	100000	46.68436	100	0.5	0.5	
4	Hot inlet	800	100000	39704.03	200	0.1	0.9	
5								
6								
7								
8								
9								
10								
11								
12								
13								
14								
15								

Excel based Unit Operation:



	A	B	C	D	E	F	G	H
1		T	P	H	flow	mole fractions		
2	**Name**	[K]	[Pa]	[J/mol]	[mol/s]	Methane	Ethane	
3	Cold outlet		100000	23414.9	100	0.5	0.5	
4	Hot outlet		100000	28019.92	200	0.1	0.9	
5								
6								
7								
8								
9								
10								
11								
12								
13								
14								
15								

Excel based Unit Operation:

Microsoft Excel - Worksheet in Excel unit operation

File Edit View Insert Format Tools Data Window Help Process Models Type a question for help

100%

Reply with Changes... End Review...

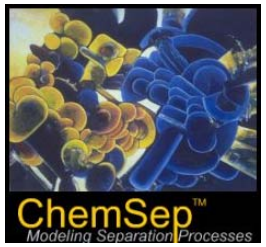
D7 =capeOverallProperty("enthalpy","temperature",B7,"pressure",feeds!C3,feeds!F3:G3)

	A	B	C	D	E	F	G	H	I
1		T/[K]	f/[mol/s]	h/[j/mol]	H/[j/s]				
2	Cold inlet	300	100	46.68436	4668.436				
3	Hot inlet	800	200	39704.03	7940806				
4									
5	Temperature guess	633.3333333							
6	limiting temperature	681.8378622							
7	Cold outlet limit	681.8378622	100	23414.9	2341490			Solver model	
8	Hot outlet limit	681.8378622	200	28019.92	5603984			FALSE	
9								1	
10	Heat duty cold				2336822			100	
11	Heat duty hot				2336822				
12	Difference				-1.8E-07				
13									
14	Efficiency				1				
15	Heat transferred				2336822				
16									
17									

Current status:

- Matlab and Scilab Thermo Import utilities
- Matlab and Scilab Unit Operation utilities
- Excel Unit Operation utility
- Available free-of-charge for non-commercial use
- All use CAPE-OPEN thermo version 1.1
- Thermo tested with TEA / Multiflash / Simulis
- Unit operations tested in COFE / ProSimPlus
- Example are available online and in help
- http://www.amsterchem.com/

- Download COCO: http://www.cocosimulator.org/
- Forum: http://capeopen.19.forumer.com/
- Interoperability testing program: http://www.cocosimulator.org/index_compliancy.html



ChemSep 6.24

HTRI

Xchanger Suite 5.0

EPA WAR / .NET libraries

SolidSim 1.1

VMG Thermo 5.0

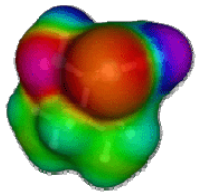
COMSOL Multiphysics 3.5

PSE gPROMS 3.1.3

TUV-NEL PPDS v4.1.0.0

AixCAPE Props 1.0

ANSYS Fluent 6.3.26 APECS

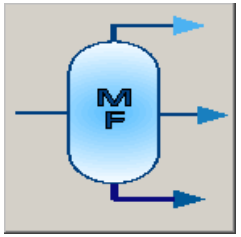


CosmoLogic CosmoTherm C21

ProSim

ProSimPlus 2.1 / Simulis 1.3

Simsci-Esscor Pro/II 8.3



Infochem Multiflash 3.8

DIGITEO Scilab 5.1.1