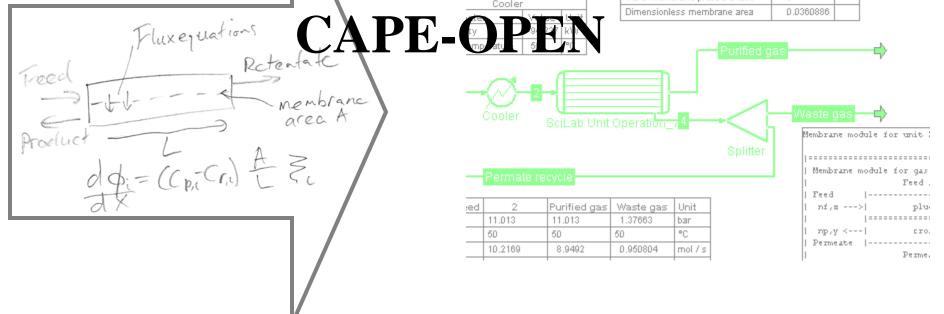


# RAPID PROTOTYPING OF UNIT OPERATION MODELS USING GENERIC TOO



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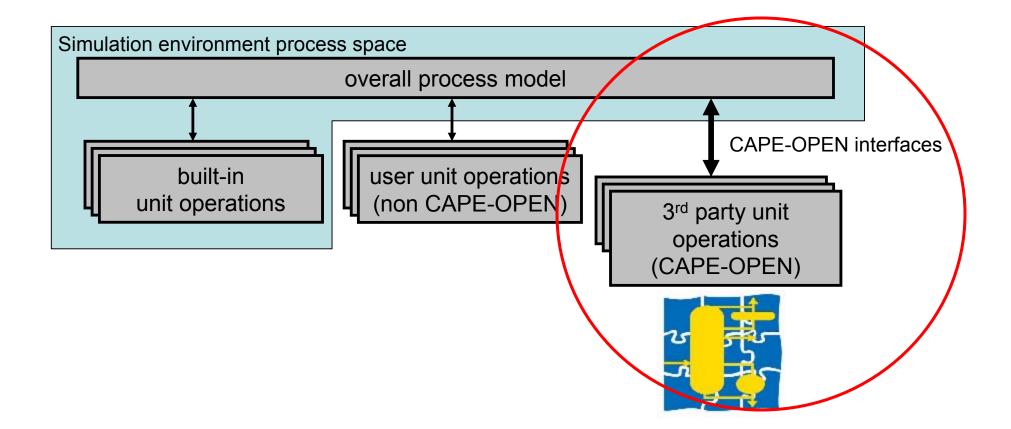


#### **Presentation outline**

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



# Why CAPE-OPEN?



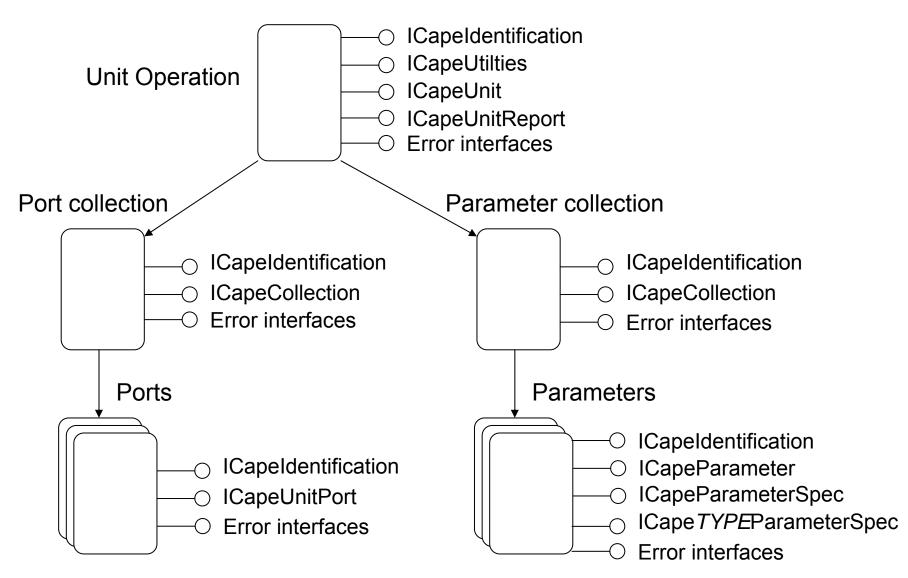


# Why CAPE-OPEN?

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

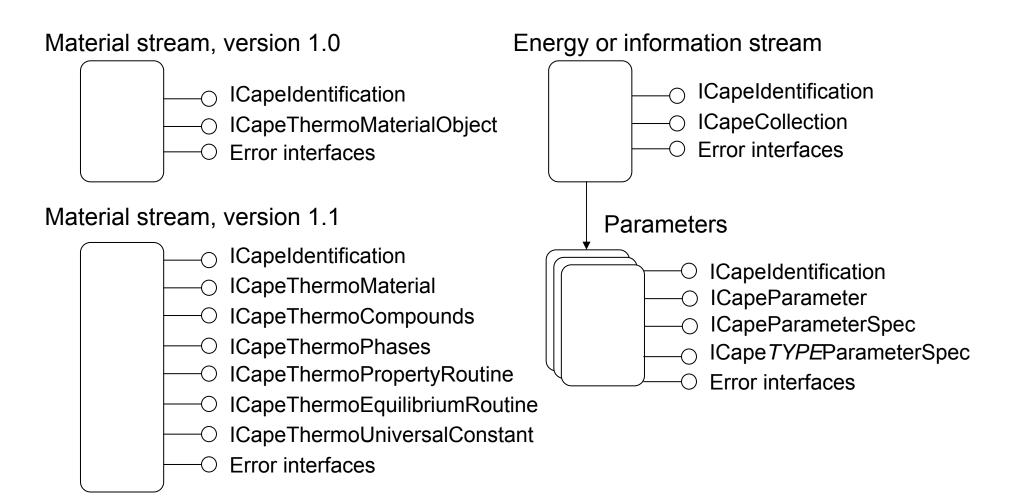


#### CAPE-OPEN: what is involved?





# CAPE-OPEN: what is involved?





### 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:

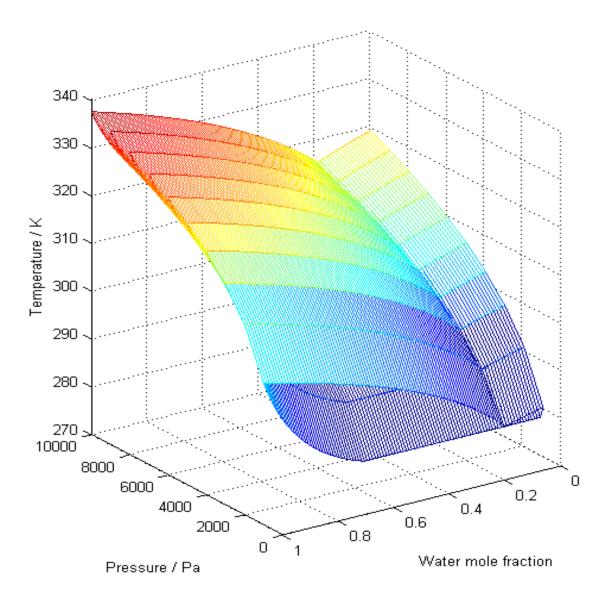
- evaluate our model equations
  - $\rightarrow$  we require access to thermodynamics
- evaluate the final process model
  - → requires running as Unit Operation inside simulation environment



#### 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





Slide 10



```
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;



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Ports Parameters Reports Matlab Additional files About										
Report: Matlab Output										
Unit operation has not yet been runMATLAB output:										
compCount =										
4										
vaporPhaseName =										
'Vapor'										
vol =										
0.0902										
dP =										
0										
·										
<u>Add</u> <u>R</u> emove										
Save model     Load model     Help										



Matlab CAPE-OPEN Unit Operation:									
Ports Parameters Reports Matlab Additional files About									
Matlab script info level: default echo									
%This is an example of an adiabatic CSTR, performing %reaction: Ethylene + Hydrogen -> Ethane %									
XThe underlying thermo system must include the three compounds, an X expose CASRegistryNumber, enthalpyF and volume									
%we presume the reaction takes place in the vapor phase									
%these we will need in our goal function global flow indexEthane indexEthylene indexHydrogen stoi_Ethane st									
CAS_Ethane='74-84-0'; CAS_Ethylene='74-85-1'; CAS_Hydrogen='1333-74-0';									
%stoichiometry stoi_Ethane=1; stoi_Ethylene=-1; stoi_Hydrogen=-1;									
Script Output									
<u>Script</u> Output									
Save model Load model Help									



#### Excel based Unit Operation:

M	Microsoft Excel - Worksheet in Excel unit operation														
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#### Excel based Unit Operation:

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#### Excel based Unit Operation:

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	A	В	C	D	E	F	G	H					
1		T/[K]	t/[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 mod	lel				
8	Hot outlet limit	681.8378622	200	28019.92	5603984			FALSE	ALSE				
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

