ChemSep, COCO and other modeling tools for versatility in custom process modeling

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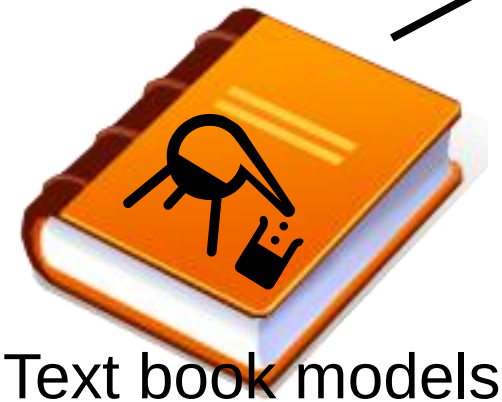
Introduction

Unit Operation

feed

?

product



Text book models

```
SUBROUTINE USERMODEL(NSTREAM,STREAMDATA,...)
INTEGER NSTREAM
DOUBLE PRECISION STREAMDATA(*)
INCLUDE 'SIMDETAILS.INC'
SET UP A REFERENCE TO PRESSURE
STREAMINDEX=PRESSURE_OFFSET_STREAM_1
```

User FORTRAN

CO-LaN

CAPE-OPEN

Presentation outline

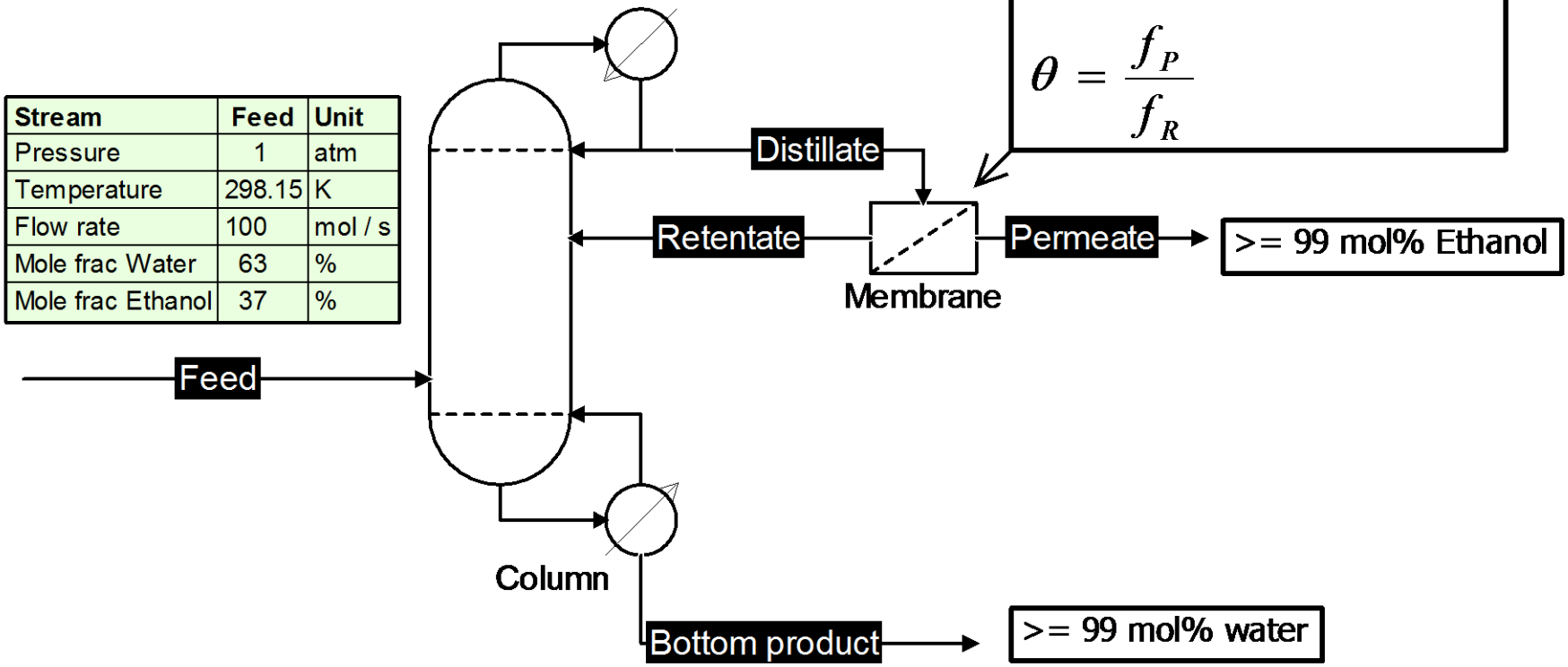
- Introduction
- Example problem specification
- Scilab Unit Operation
- Closing the loop
- Excel Unit Operation
- Conclusions

Example problem specification I

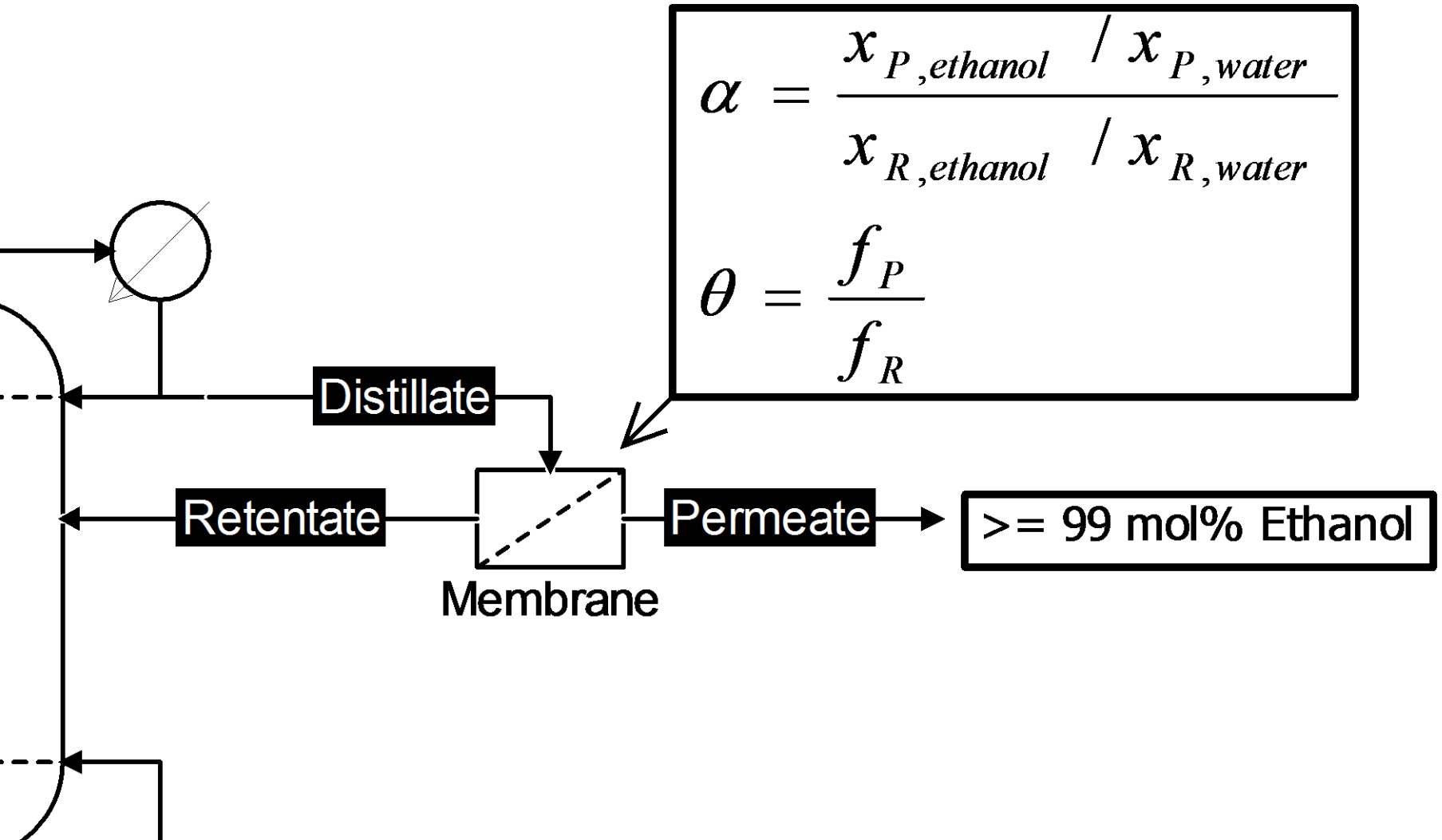
Stream	Feed	Unit
Pressure	1	atm
Temperature	298.15	K
Flow rate	100	mol / s
Mole frac Water	63	%
Mole frac Ethanol	37	%

$$\alpha = \frac{x_{P,ethanol} / x_{P,water}}{x_{R,ethanol} / x_{R,water}}$$

$$\theta = \frac{f_P}{f_R}$$



Example problem specification II



Example problem specification III

Property pack definition:

Package Mode Configure Help

Name: water-ethanol

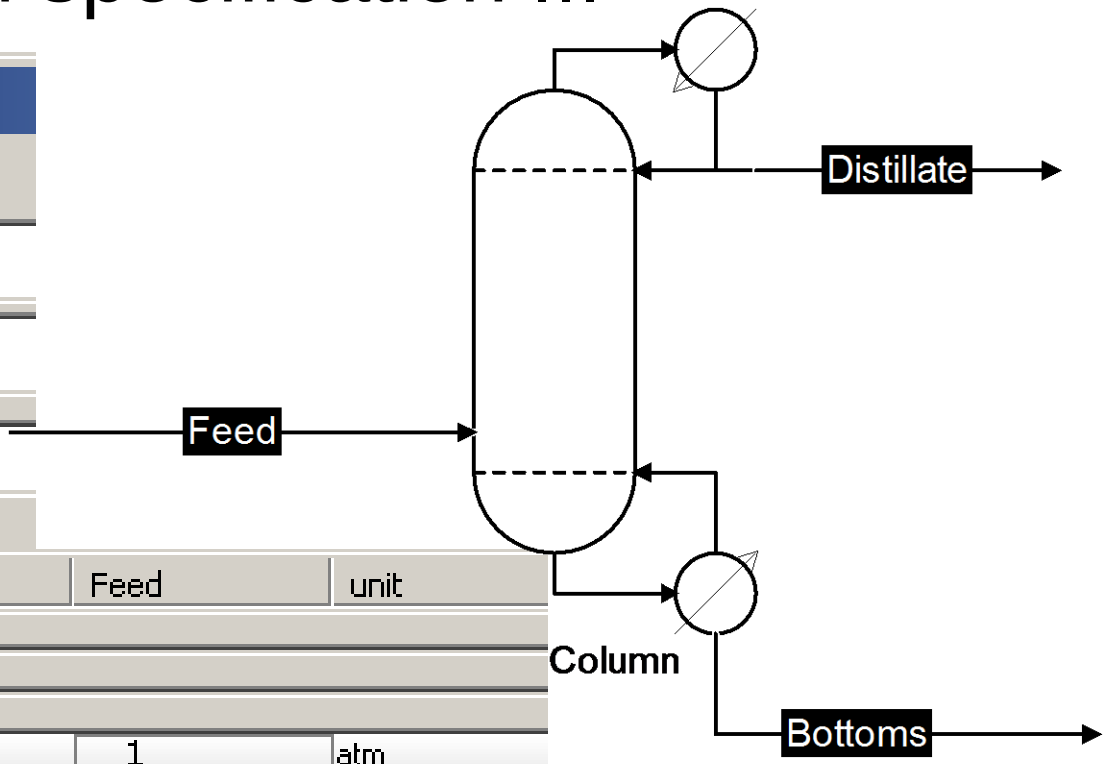
Description:

Model set: NRTL

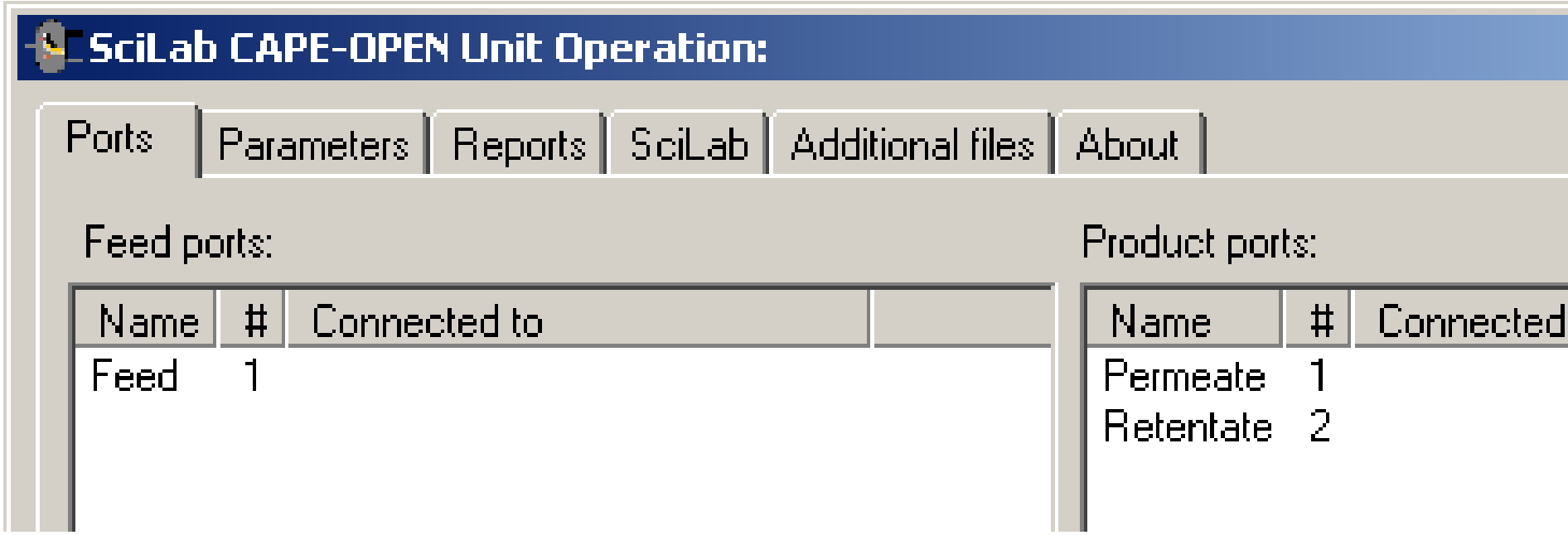
Compounds:

Water
Ethanol

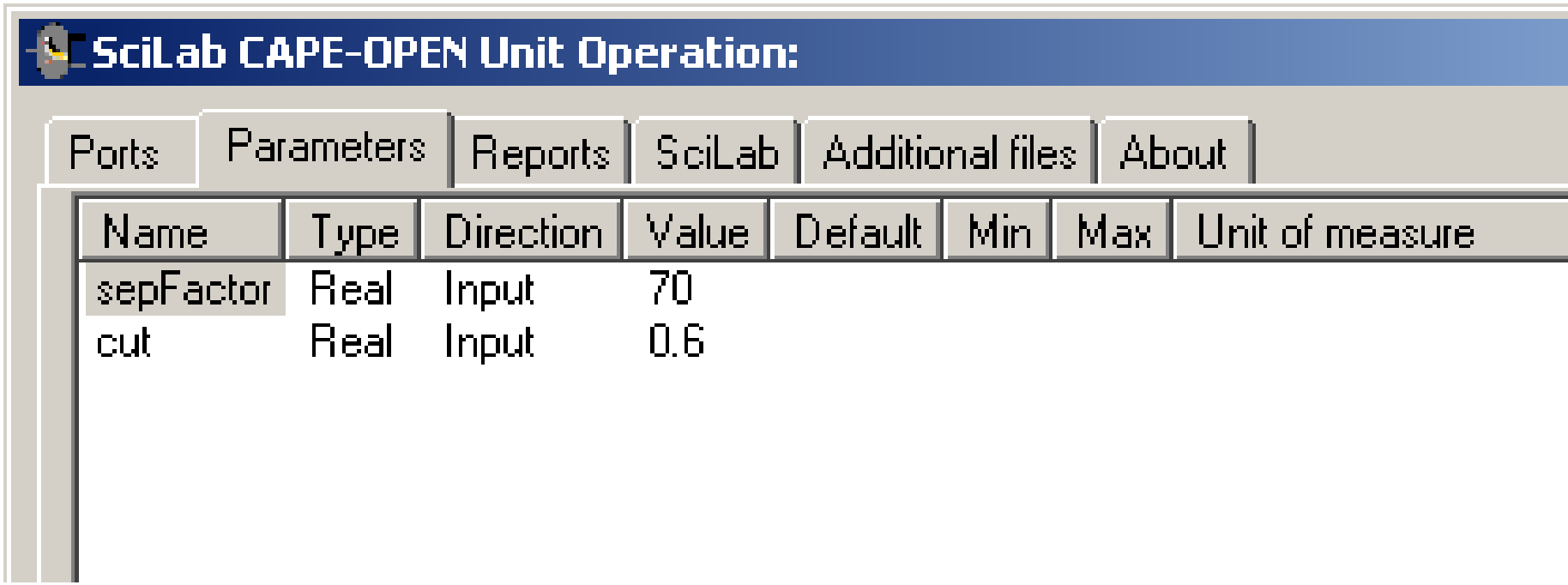
name	Feed	unit
Stream		
Connections		
Overall		
pressure	1	atm
temperature	298.15	K
mole fraction [Water]	63	%
mole fraction [Ethanol]	37	%
flow	100	mol / s
MW	28.39498	g / mol
Compound flows		
Phase Fractions		
Liquid composition		



Scilab Unit operation I



Scilab Unit operation II



Scilab Unit operation III

```
// compound indices:
water=1;
ethanol=2;

//parameter values:
alpha=getParameter('sepFactor');
theta=getParameter('cut');

//feed values
XF=getFeedProp(1,'fraction');
FF=getFeedProp(1,'totalFlow');
TF=getFeedProp(1,'temperature');
PF=getFeedProp(1,'pressure');

//product flows (explicit solution of theta=FP/FR and FF=FP+FR):
FR=FF/(theta+1);
FP=theta*FR;
```

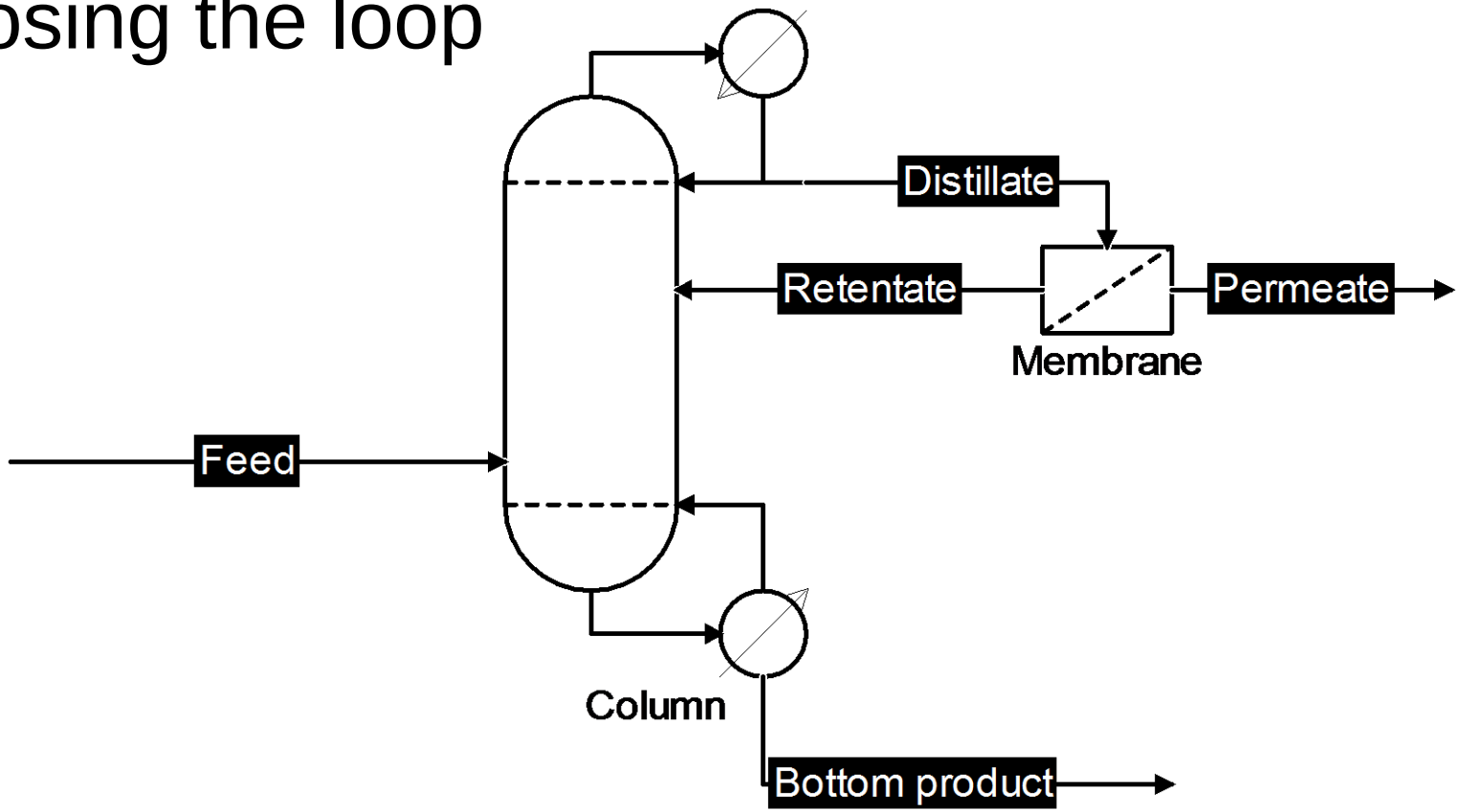
Scilab Unit operation IV

```
//function to calculate compositions from XPE:
function [XP,XR]=GetCompositions(XPE)
 XP=[1-XPE,XPE];
 XRE=(FF*XF(ethanol)-FP*XPE)/FR;
 XR=[1-XRE,XRE];
endfunction

//function to solve compositions
function errorValue=CompositionFunction(XPE)
 //get the compositions given XPE:
 [XP,XR]=GetCompositions(XPE);
 //return the error in alpha
 errorValue= (XP(ethanol)/XP(water))/(XR(ethanol)/XR(water))-alpha;
endfunction
```

Scilab Unit operation VI

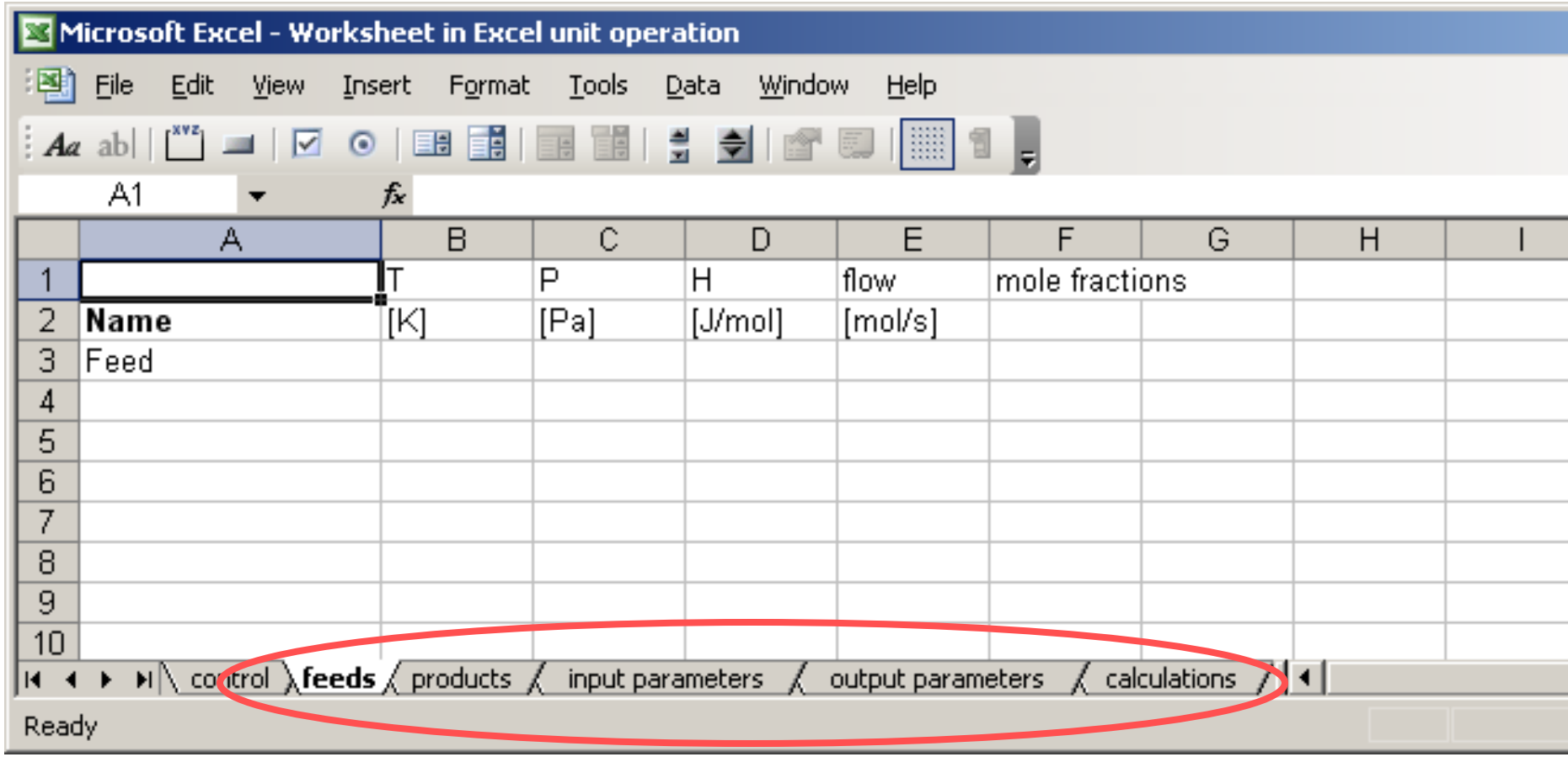
```
//solve for the compositions to match alpha:
XPE=fsolve(0.999,CompositionFunction);

//the compositions at solutions are then
[XP,XR]=GetCompositions(XPE);

//set the permeate, given FP, XP, TF, PF
setProduct(1,FP,XP,'temperature',TF,'pressure',PF);
//set the retentate, given FR, XR, TF, PF
setProduct(2,FR,XR,'temperature',TF,'pressure',PF);
```

Closing the loop



Stream	Feed	Distillate	Retentate	Permeate	Bottom product	Unit
Pressure	1	1	1	1	1	atm
Temperature	298.15	351.471	351.471	351.471	373.774	K
Flow rate	100	98.9368	61.8355	37.1013	62.8987	mol / s
Mole frac Water	63	15	23.7344	0.442615	99.9	%
Mole frac Ethanol	37	85	76.2656	99.5574	0.1	%

Excel Unit Operation I

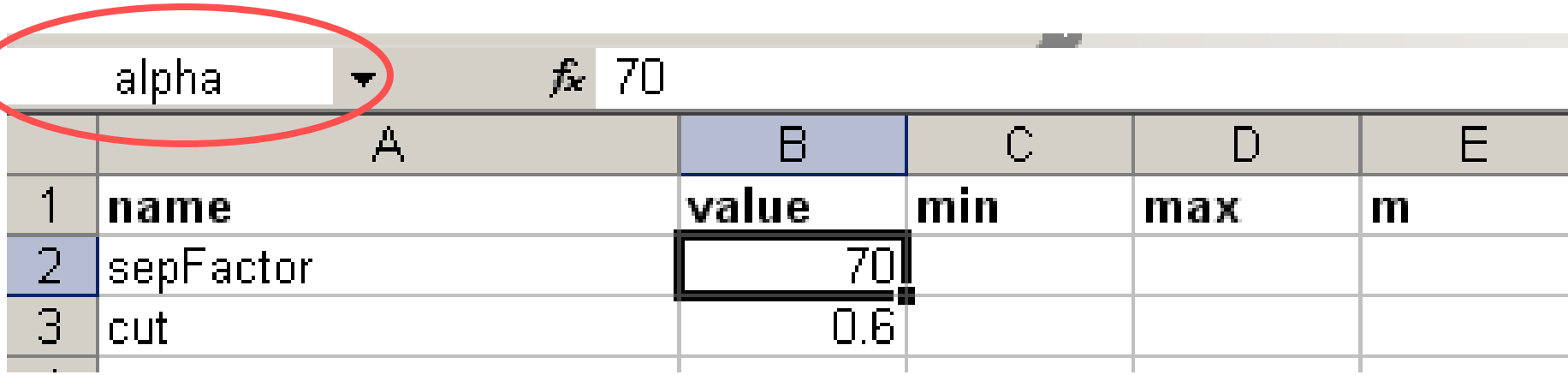


	A	B	C	D	E	F	G	H	I
1		T	P	H	flow	mole fractions			
2	**Name**	[K]	[Pa]	[J/mol]	[mol/s]				
3	Feed								
4									
5									
6									
7									
8									
9									
10									

Excel Unit Operation II

	A	B	C	D	E	F	G	H
1		T	P	H	flow	mole fractions		
2	**Name**	[K]	[Pa]	[J/mol]	[mol/s]			
3	Permeate							
4	Retentate							

Excel Unit Operation III



Excel Unit Operation IV

	A	B	C	D	E	F	G	H
1		T	P	H	flow	mole fractions		
2	**Name**	[K]	[Pa]	[J/mol]	[mol/s]	Water	Ethanol	
3	Feed	351.4708	101325	-35678.5	43.4629	0.15	0.85	
4								

Excel Unit Operation V

	A	B	C	
1	F retentate	=feeds!E3/(theta+1)	mol/s	
2	F permeate	=theta*B1	mol/s	
3				
4	X p ethanol guess	0.999	mol/mol	Initial guess f
5	X p ethanol	0.999	mol/mol	Will be solved
6	X p water	=1-B5	mol/mol	
7	X r ethanol	=(feeds!E3*feeds!G3-B2*B5)/B1	mol/mol	
8	X r water	=1-B7	mol/mol	
9				
10	alpha	=(B5/B6)/(B7/B8)		
11	error	=B10-alpha		

Excel Unit Operation VI

	A	B	C	D	E	F
1		T	P	H	flow	mole fractions
2	**Name**	[K]	[Pa]	[J/mol]	[mol/s]	Water
3	Permeate	=feeds!B3	=feeds!C3		=calculations!B2	=calculations!B6
4	Retentate	=feeds!B3	=feeds!C3		=calculations!B1	=calculations!B8
5						

Conclusions:

- Need for custom models
- Only enter model equations
- Use existing solvers
- Solutions: Scilab, Matlab, Excel
- Context: CAPE-OPEN
- Simulation environment: COCO / ChemSep
- Suitable for research and teaching

- Download COCO: http://www.cocosimulator.org/
- ChemSep: http://www.chemsep.com/

- CAPE-OPEN standards: http://www.colan.org/
- Matlab, Scilab, Excel Unit Operations: http://www.amsterchem.com/

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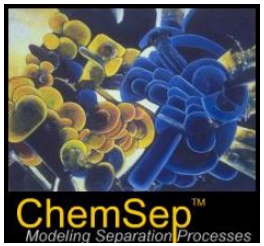

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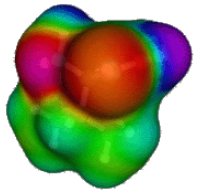
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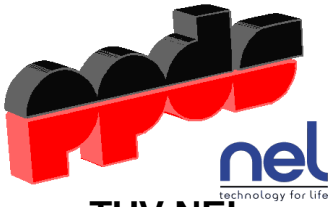

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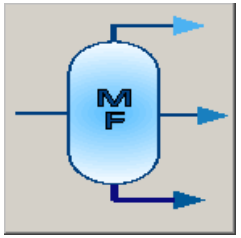

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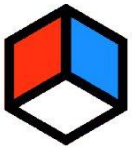
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Adding solids to the flowsheet

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