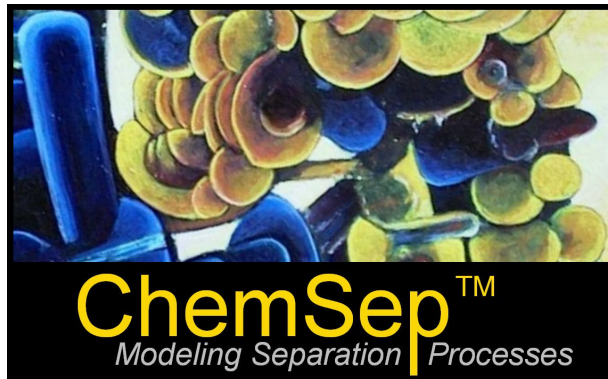


# ChemSep in Motion

Cannes, March 2006,  
Harry Kooijman & Ross Taylor



# Overview

- Where we were: Como 2005
- Interoperability status ChemSep:  
Aspen Plus, PRO/II, Aspen HYSYS, COCO
- ChemSep-LITE & flowsheet examples
- Conclusions & outlook

# Status of ChemSep-CO at Como 2005

- CAPE-OPEN ChemSep Unit Operation
- Equilibrium & nonequilibrium columns solved in
  - Aspen Plus
  - Aspen HYSYSusing ChemSep thermo & physical properties
- PRO/II crashed:
  - assumed that the Unit Operation has predefined in- and outputs whereas ChemSepUO has none by default

# Interoperability with COSE

- Running using ChemSep thermo & physical properties
- Availability of COSE thermo & properties not at VLE conditions (i.e.  $m\{p,T,x\}$  and  $m\{p,T,y\}$  @  $T < T_b$  or  $T > T_d$ )
- Availability of derivatives ( $\partial m / \partial n$ ) of the COSE thermo properties → Quadratic Newton convergence
- Possibility to add/remove/rename Ports
- Availability of pure component data (PCD) needed for calculation of (user) properties ( $T_c, p_c, V_c, \omega, M_w, \dots$ )

# Interoperability through Flexibility

ChemSep Unit "ChemSepU0\_1":

Perturbation | Flash | Ports | About  
 Status & Reports | Unit Operation | Options

Status:

1 Converged  
 1 Iterations

Report:  
 Output Show

ChemSep Interface Close

ChemSep Unit "ChemSepU0\_1":

Perturbation | Flash | Ports | About  
 Status & Reports | Unit Operation | Options

Name: ChemSepU0\_1

Sep File:  
 Start with new sep file  
 Import existing sep file  
 Edit current sep file  
 Export current sep file

Additional command line arguments for ChemSep-GUI:  
 /kpld

ChemSep Interface Close

ChemSep Unit "ChemSepU0\_1":

Perturbation | Flash | Ports | About  
 Status & Reports | Unit Operation | Options

Use Cape-Open thermodynamic properties

Only use K-values and enthalpies  
 Only use perturbation derivatives  
 Only use perturbation for molar derivatives  
 Use Wilson ideal solution model to initialize equilibrium calculations

Suppress warnings

Clear Log Clear initial guess

ChemSep Interface Close

ChemSep Unit "ChemSepU0\_1":

Status & Reports | Unit Operation | Options  
 Perturbation | Flash | Ports | About

Perturbation distances for numerical derivatives:

Relative temperature perturbation: 0.001

Relative pressure perturbation: 0.001

Composition perturbation: 0.001

ChemSep Interface Close

ChemSep Unit "ChemSepU0\_1":

Status & Reports | Unit Operation | Options  
 Perturbation | Flash | Ports | About

Select flash method:

Re-flash of inlet streams: <none>

Flash of outlet streams: PVF

TP  
 PVF  
 PH

ChemSep Interface Close

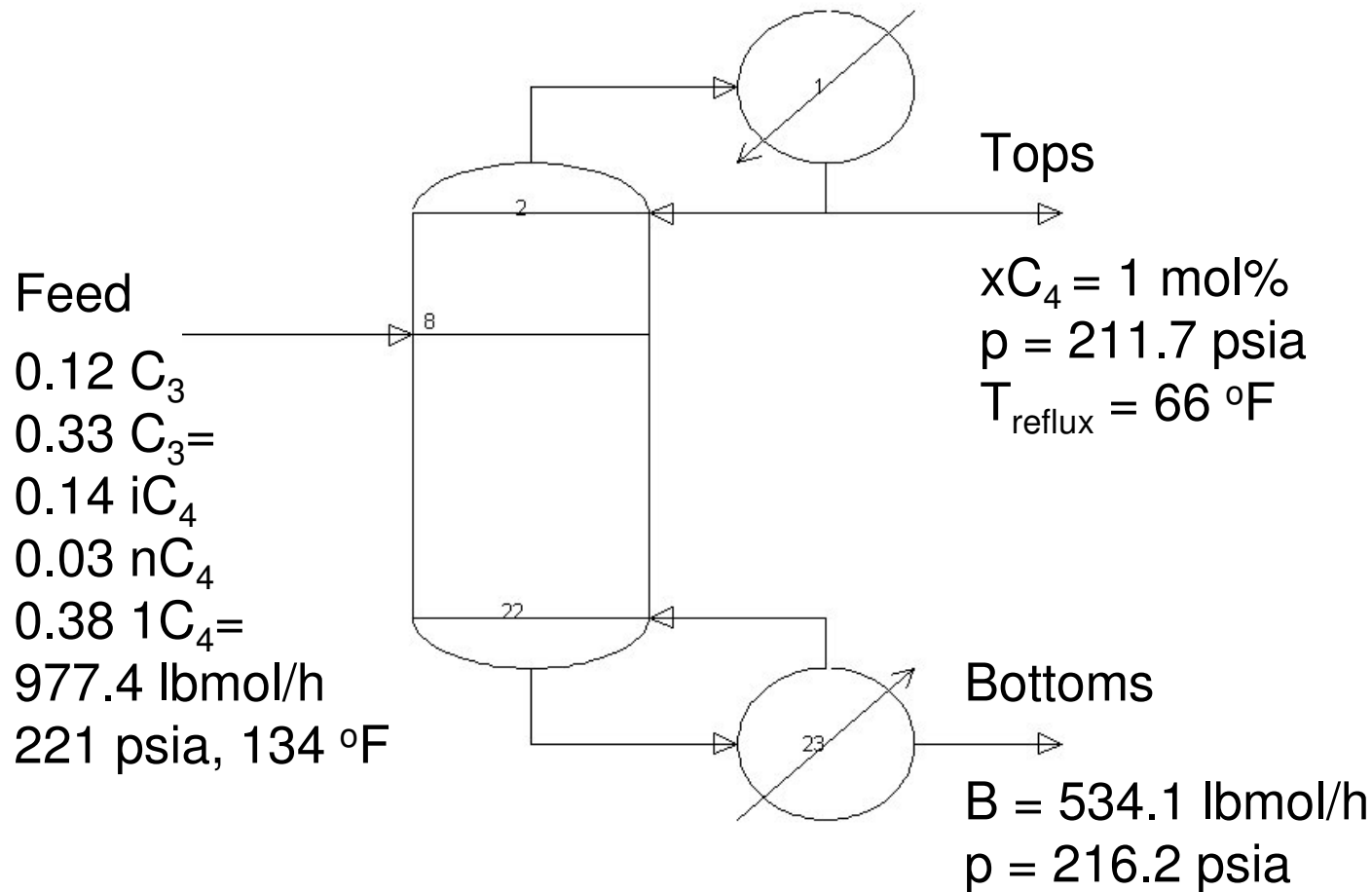
ChemSep Unit "ChemSepU0\_1":

Status & Reports | Unit Operation | Options  
 Perturbation | Flash | Ports | About

Port	Dir...	Stage	Connected to
Feed1_stage8	in	8	1
TopProduct	out	top	2
BottomProduct	out	bottom	3

ChemSep Interface Close

# Interoperability Test Case: C<sub>3</sub>/C<sub>4</sub> Splitter

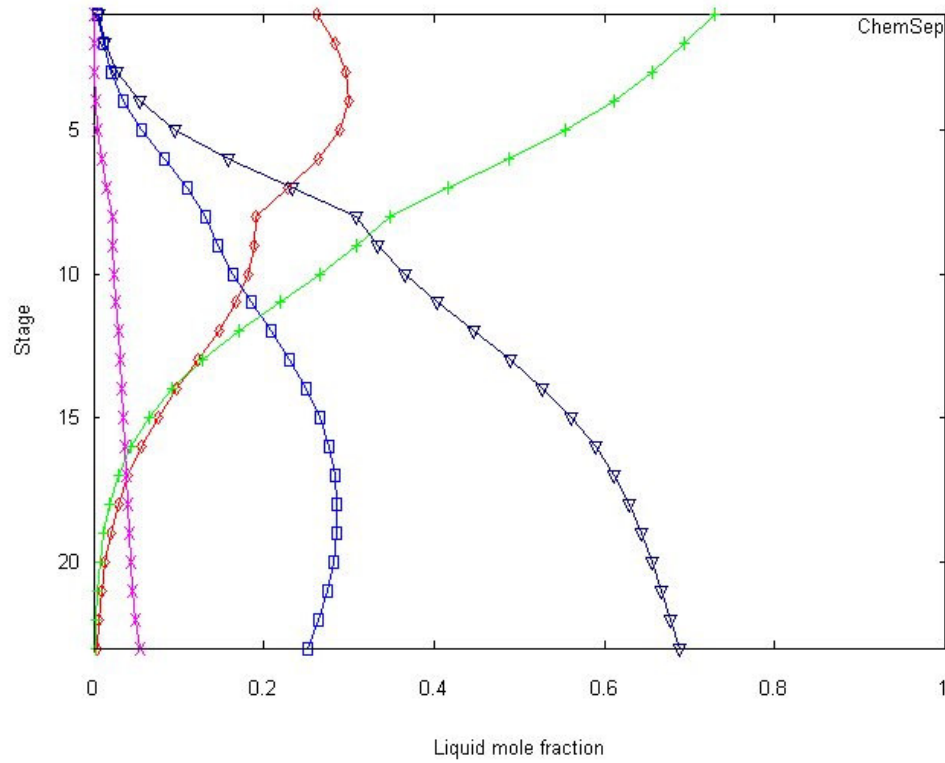


VLE = Soave-RK

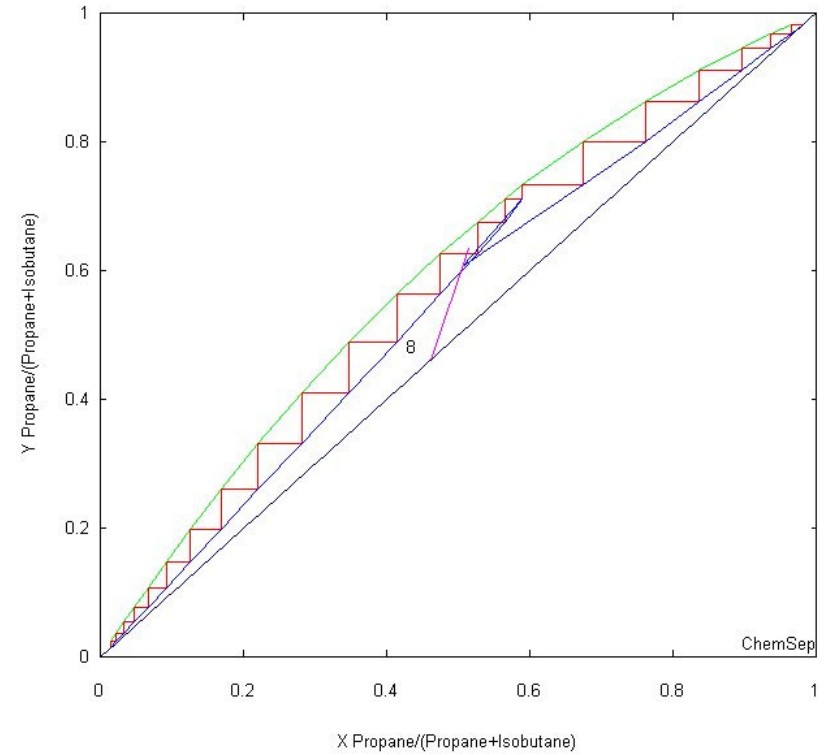
*Chem.Eng.Res.Des.* Vol. 83 p. 508

# Results

Liquid phase composition profiles

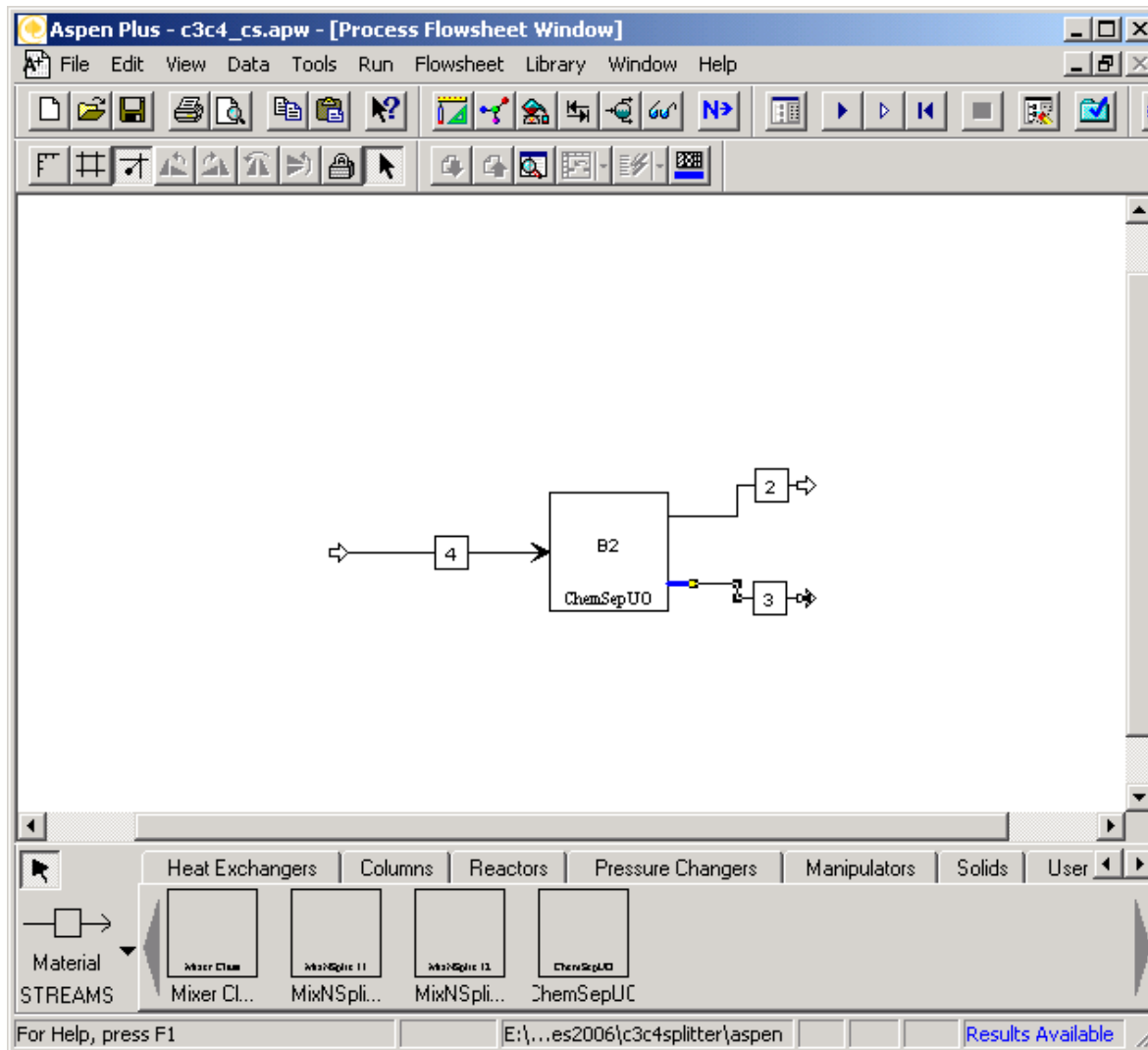


McCabe-Thiele diagram for Propane - Isobutane



- X Propane —◆—
- X Propylene —+—
- X Isobutane —□—
- X N-butane —×—
- X 1-butene —▽—

# C<sub>3</sub>/C<sub>4</sub> Splitter in Aspen Plus v12.1.8



# C<sub>3</sub>/C<sub>4</sub> Splitter in COCO

The image displays the COFE software interface for a C<sub>3</sub>/C<sub>4</sub> splitter. The main window shows a process flow diagram with a central vertical column labeled 'ChemSepUO\_1'. An inlet stream '1' enters from the left. Two outlet streams, '2' and '3', exit from the top and bottom respectively. A status window at the bottom left shows the following text:

```
Solve finished
Starting solve
solving ChemSepUO_1
Solve finished
Solve finished
```

An 'Unit operation ChemSepUO\_1' dialog box is open, showing the following parameters:

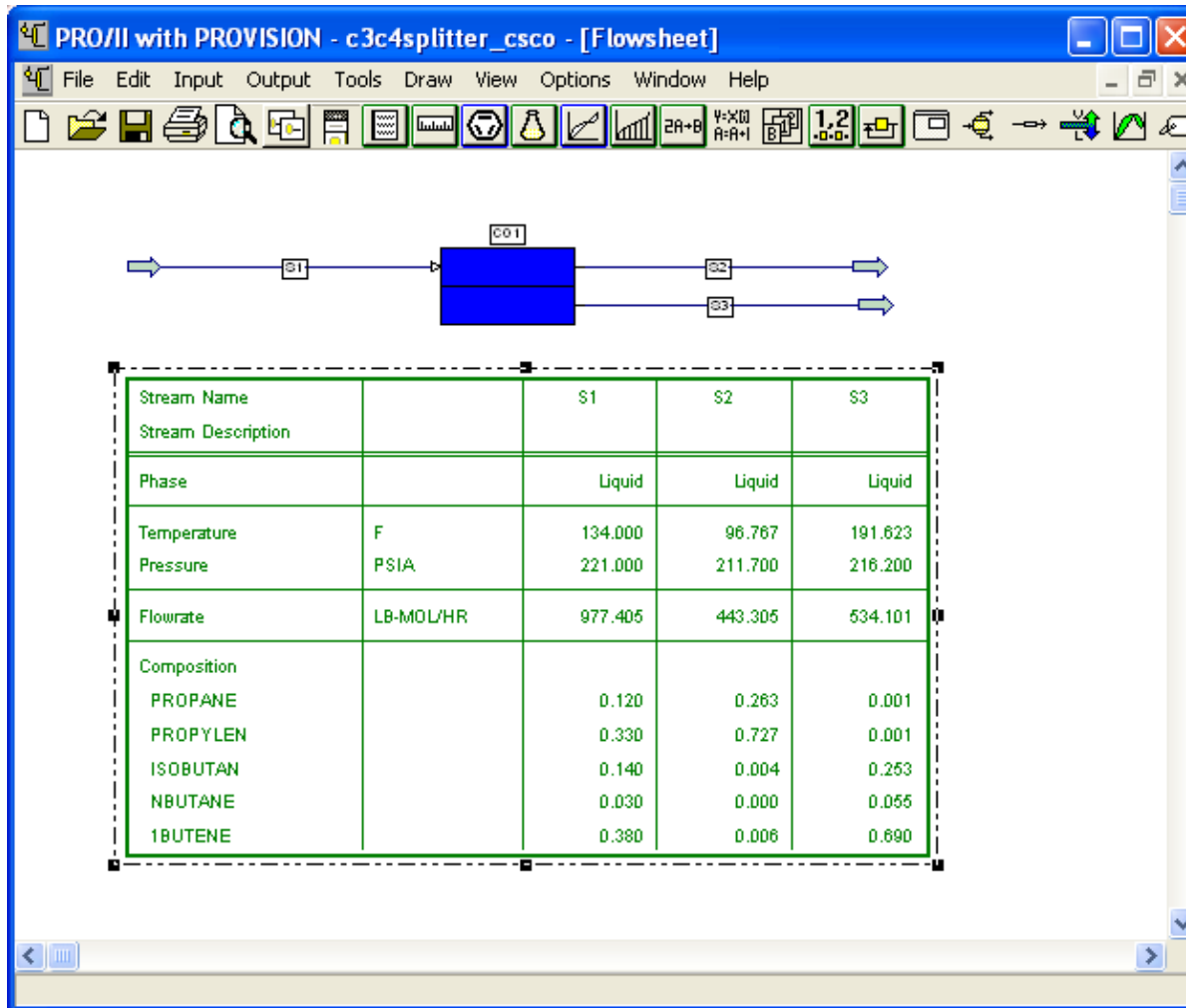
Parameter	Value	Unit
GUIArguments	/kpld	
UseCOSEThermo	TRUE	
UseCOSEDiffusionCoefficients	FALSE	
UsePerturbedDerivativesOnly	FALSE	
UsePerturbed_ddK	FALSE	
SuppressWarnings	FALSE	
RelativePerturbationTemperature	0.001	
RelativePerturbationPressure	0.001	
PerturbationComposition	0.001	
InletReflash	<none>	
OutletFlash	PVF	
UseOnlyKValuesAndEnthalpyFromCOSE	FALSE	
TryUsingRestartData	TRUE	
OmitStageFromPortName	FALSE	
WilsonEstimate	TRUE	

A 'Show GUI' button is located at the bottom of the dialog box.

# Interoperability: PRO/II v7.1 Workarounds

1. ChemSepUO with automatic port assignment:
  - Windows registry entry
  - UO has always one feed and two outlets (normally none)
2. Error in size of return result of GetComponentDescription inquiring CAS number
  - Check if executable is ProII.exe
  - Ignore error, assume CAS number is returned in 0<sup>th</sup> element

# C<sub>3</sub>/C<sub>4</sub> Splitter in PRO/II v7.1



# CAPE-OPEN Interoperability ChemSepUO

COSE	ChemSep thermo	COSE thermo	$\partial m/\partial n$	Ports	PCD	Comments
Aspen+ 12.1.8	✓	✓	✓	✓	✓	“Done”
COCO 0.9	✓	✓	✓	✓	✓	“Done”
PRO/II 7.1	✓	✗	✗	✗	✗	Saving not ok
HYSYS	✓	✗	✗	✓	✗	No response
...						Contact us!

# CAPE-OPEN Interoperability ChemSepUO

COSE	D lbmol/h	$X_{d,C3}$	$X_{d,C3=}$	$X_{d,iC4}$ $10^{-4}$	$X_{d,nC4}$ $10^{-4}$	$X_{d,1C4=}$ $10^{-4}$
RadFrac Aspen+ 12.1.8	443.300	0.2631	0.7269	36.5	1.4	62.1
ChemSepUO Aspen+ 12.1.8	443.300	0.2631	0.7269	36.5	1.4	62.1
Distill PRO/II 7.1	443.305	0.2632	0.7268	39.6	1.5	59.0
ChemSepUO PRO/II 7.1 *	443.305	0.2631	0.7269	37.8	1.4	60.8
COCO 0.9 **	443.305	0.2631	0.7269	37.8	1.4	60.8

\* ChemSepUO in Proll was set to use the ChemSep property routines

\*\* COCO/TEA uses reimplemented thermodynamic and pure component data libraries of ChemSep

All comparisons done with the same SRK binary interaction coefficients

# CAPE-OPEN Interoperability ChemSepUO

COSE	$T_b$ F	$X_{b,C3}$ $10^{-4}$	$X_{b,C3=}$ $10^{-4}$	$X_{b,iC4}$	$X_{b,nC4}$	$X_{b,1C4=}$
RadFrac Aspen+ 12.1.8	191.74	12.5	5.5	0.2532	0.0548	0.6902
ChemSepUO Aspen+ 12.1.8	191.74	12.5	5.5	0.2532	0.0548	0.6902
Distill PRO/II 7.1	191.62	11.8	6.1	0.2529	0.0548	0.6905
ChemSepUO PRO/II 7.1 *	191.37	12.6	5.4	0.2531	0.0548	0.6904
COCO 0.9 **	191.37	12.6	5.4	0.2531	0.0548	0.6904

\* ChemSepUO in Proll was set to use the ChemSep property routines

\*\* COCO/TEA uses reimplemented thermodynamic and pure component data libraries of ChemSep

All comparisons done with the same SRK binary interaction coefficients

# ChemSep-LITE is CAPE-OPEN

- Equilibrium column simulator
- Maximum 5 compounds and 50 stages
- 55 component library (extendable)
- Download *free* from [www.chemsep.com](http://www.chemsep.com)

Example: Air Separation Unit using COCO  
([www.amsterchem.com](http://www.amsterchem.com))



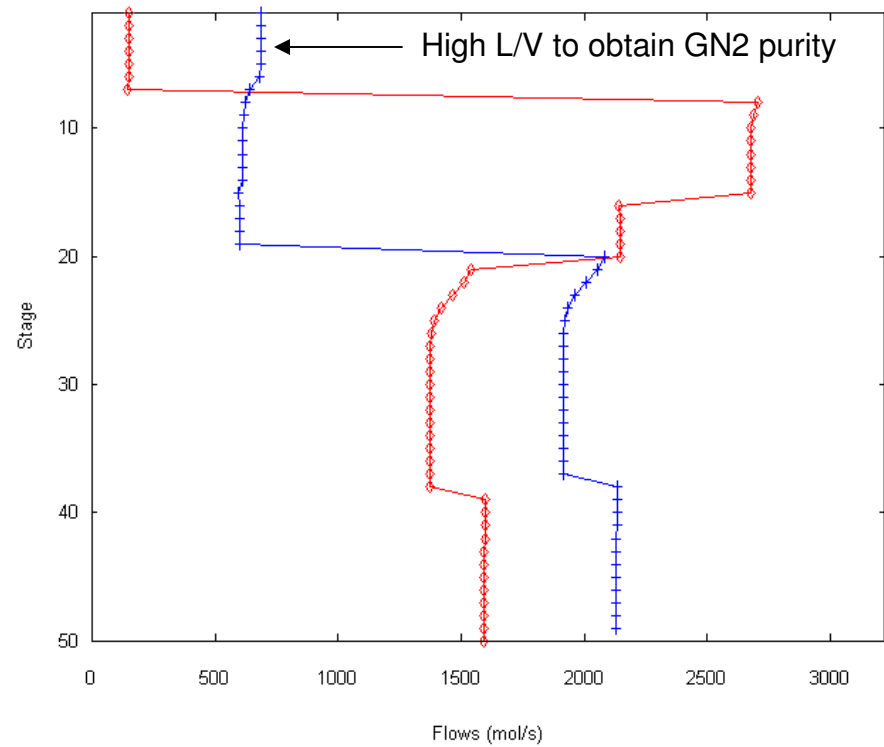
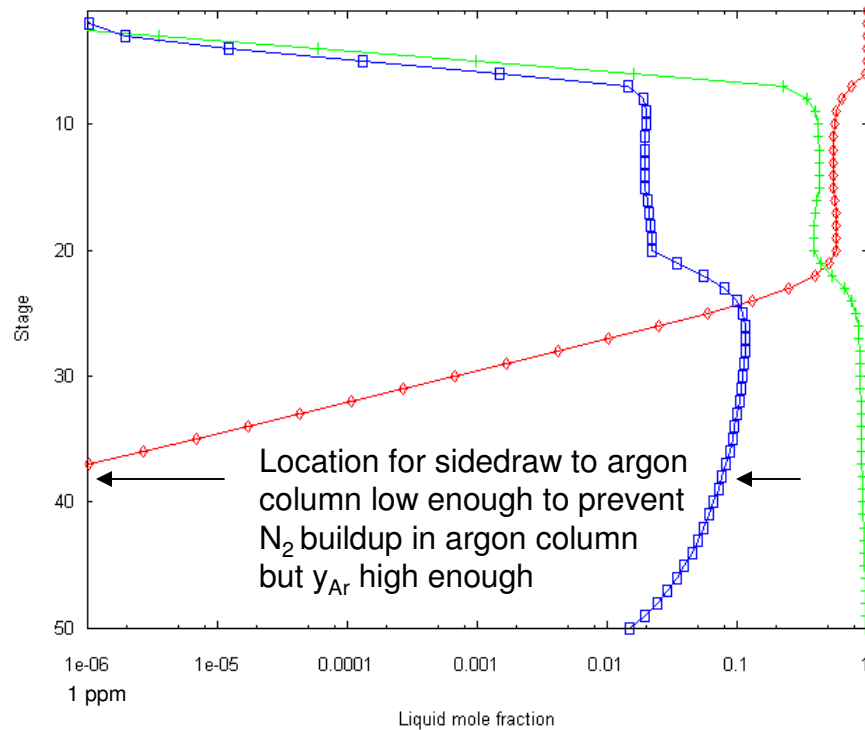




# Air Separation Unit: Low Pressure Column

Liquid phase composition profiles

Flow profiles

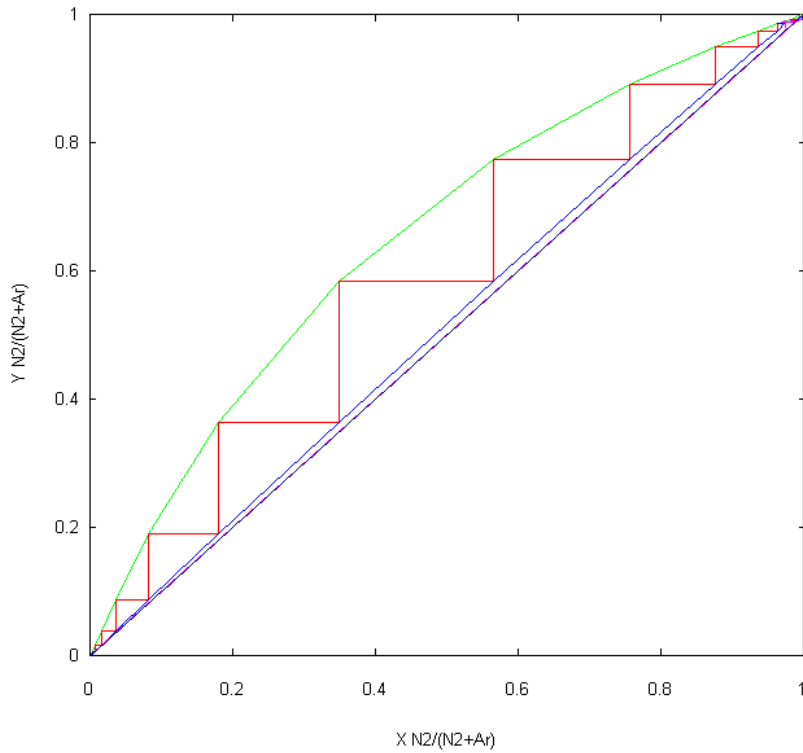


X Nitrogen —◇—      X Oxygen —+—      X Argon —□—

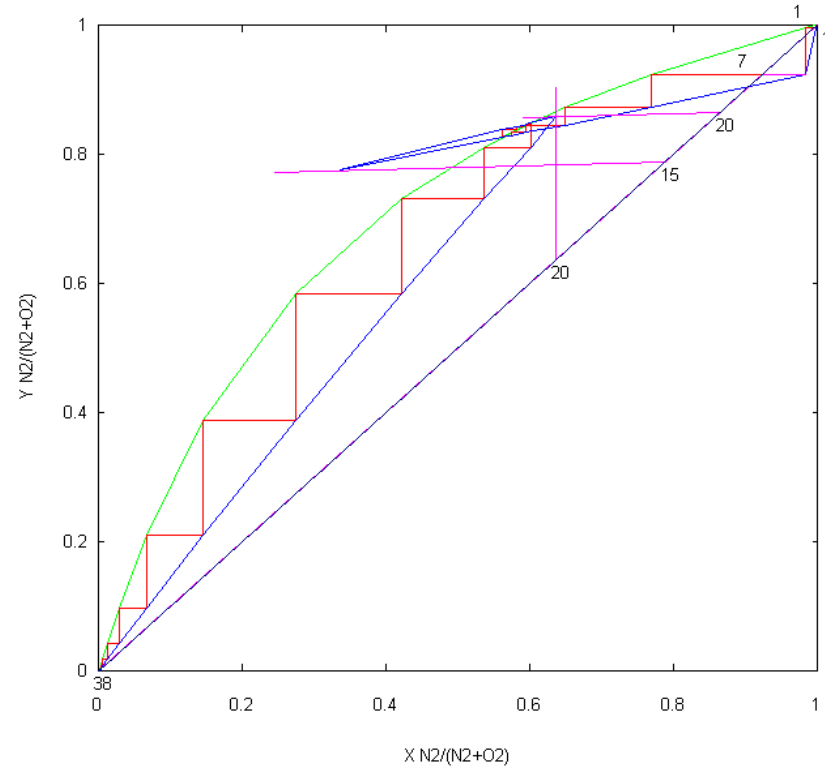
V ◇ —      L + —

# Air Separation Unit: Low Pressure Column

McCabe-Thiele diagram for Nitrogen - Argon



McCabe-Thiele diagram for Nitrogen - Oxygen



# Conclusions & Outlook

- Aspen Plus v12+ and COCO fully support ChemSepUO
- ChemSepUO runs in PRO/II v7.1 (with workarounds)
- No further progress with Aspen HYSYS
- COCO is our development tool for ChemSepUO
- *free* CAPE-OPEN version of ChemSep-LITE
  
- Test support of other COSE's (gPROMS, ProSim, ...)
- Extend our set of available column specifications
- Upgrade existing RD, LLX, & VLL models to Cape-Open  
(see <http://www.chemsep.com/chemsep/program/development.html>)

# Areas for Development

- Access to ***all*** pure component properties for user block internal property calculations
- Flowsheet reinitialisation: resetting of intermediate unit operation results or not?
- Handling of flowsheet icons/representations for unit operations (only COCO can do this)