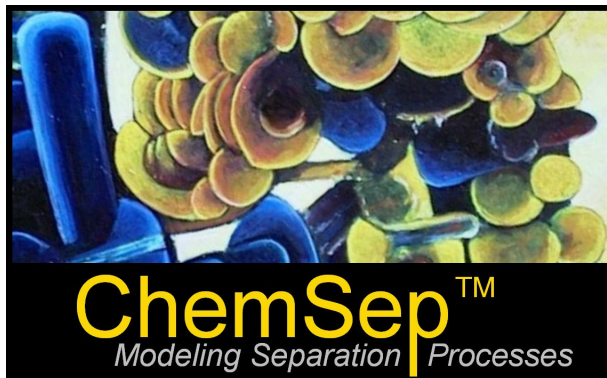


ChemSep in Motion

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 ($T_c, p_c, V_c, \omega, M_w, \dots$)

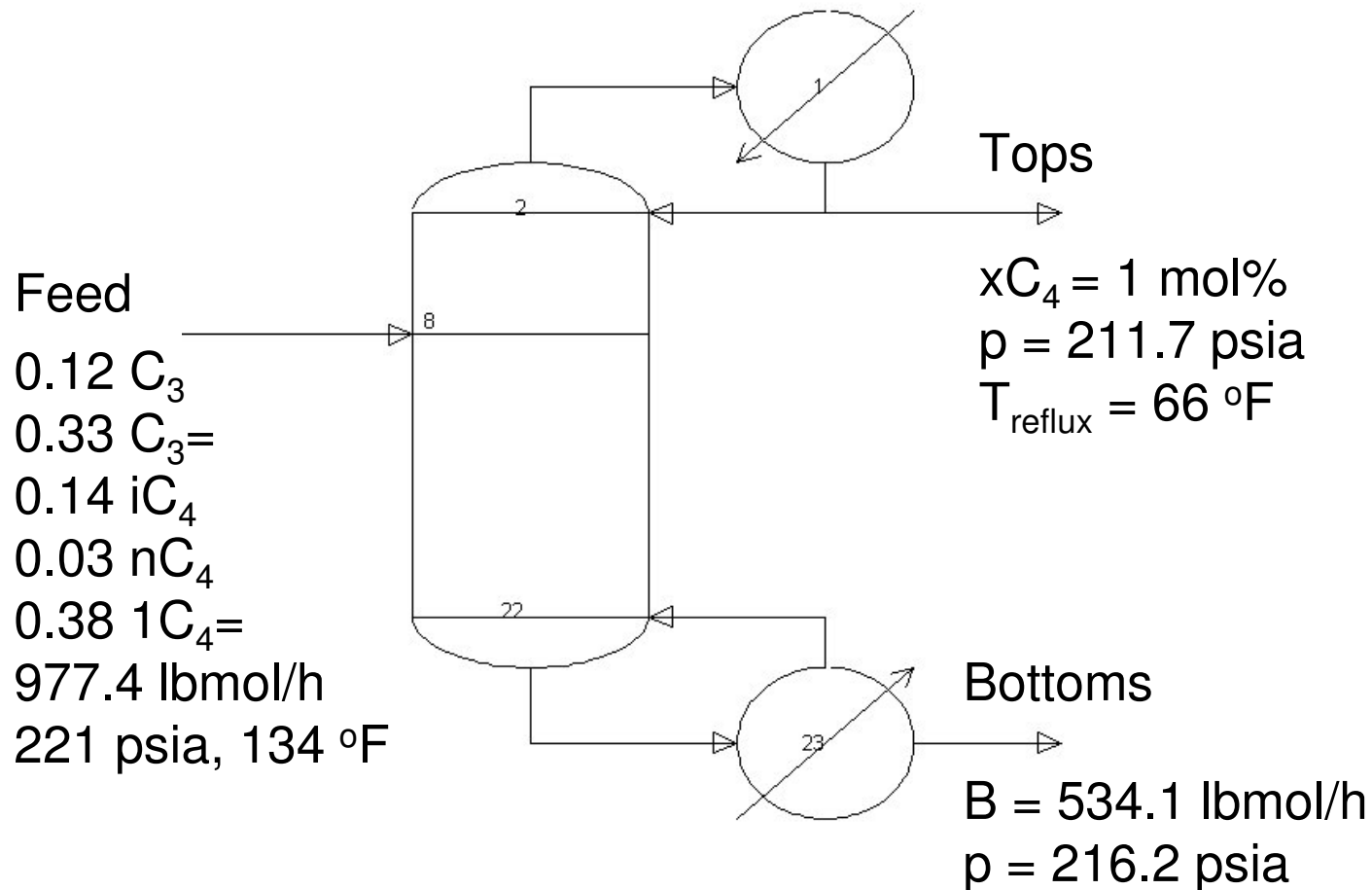
Interoperability through Flexibility

The figure displays six screenshots of the ChemSep GUI, arranged in a 2x3 grid, illustrating the software's flexibility through interoperability. Each window is titled "ChemSep Unit 'ChemSepUO_1':" and features a menu bar with "Perturbation", "Flash", "Ports", and "About".

- Top-Left:** "Status & Reports" tab. Shows "Status:" with a list: "1 Converged", "1 Iterations". A "Report:" dropdown is set to "Output" with a "Show" button.
- Top-Middle:** "Unit Operation" tab. Shows "Name:" as "ChemSepUO_1". "Sep File:" options include "Start with new sep file", "Import existing sep file", "Edit current sep file", and "Export current sep file". "Additional command line arguments for ChemSep-GUI:" is set to "/kpld".
- Top-Right:** "Options" tab. Shows checked options: "Use Cape-Open thermodynamic properties", "Use Wilson ideal solution model to initialize equilibrium calculations". Other options include "Only use K-values and enthalpies", "Only use perturbation derivatives", "Only use perturbation for molar derivatives", and "Suppress warnings". Buttons for "Clear Log" and "Clear initial guess" are present.
- Bottom-Left:** "Perturbation" tab. Shows "Perturbation distances for numerical derivatives:" with input fields for "Relative temperature perturbation: 0.001", "Relative pressure perturbation: 0.001", and "Composition perturbation: 0.001".
- Bottom-Middle:** "Flash" tab. Shows "Select flash method:" with a dropdown menu containing "TP", "PVF", and "PH". "Re-flash of inlet streams:" is set to "<none>" and "Flash of outlet streams:" is set to "PVF".
- Bottom-Right:** "Ports" tab. Shows a table of port connections:

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

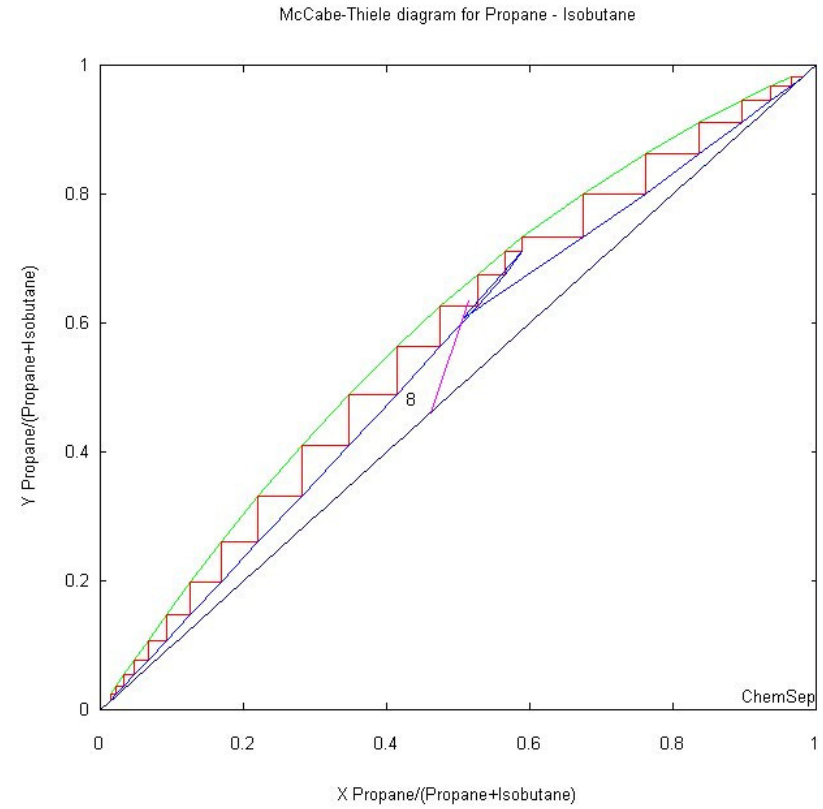
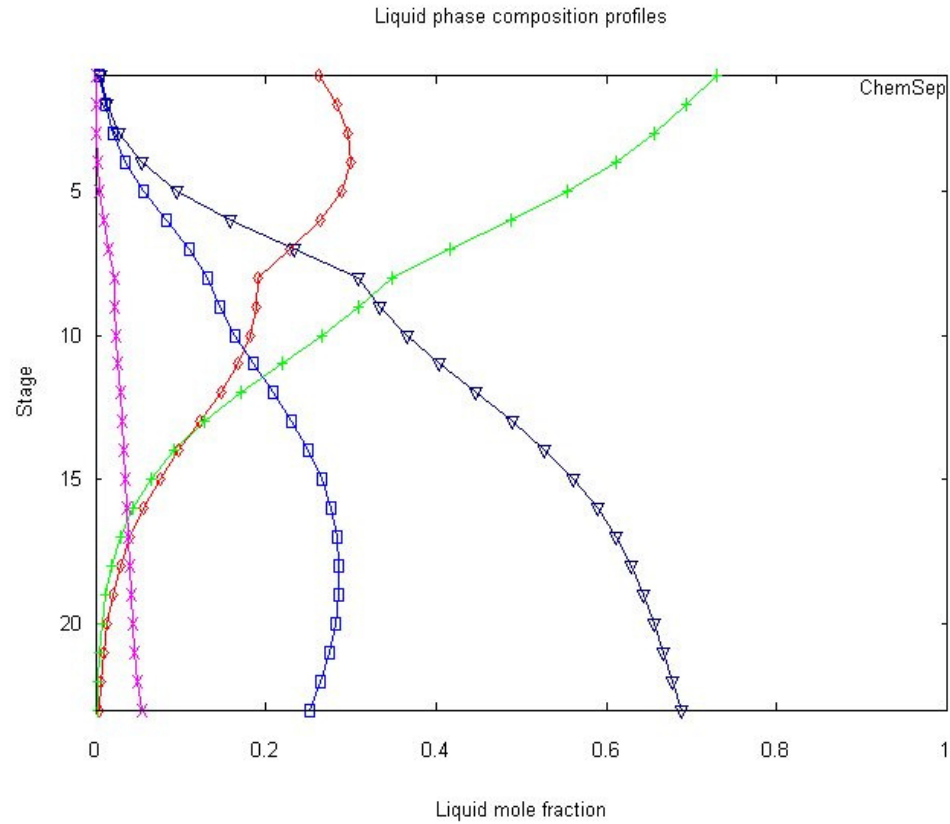
Interoperability Test Case: C₃/C₄ Splitter



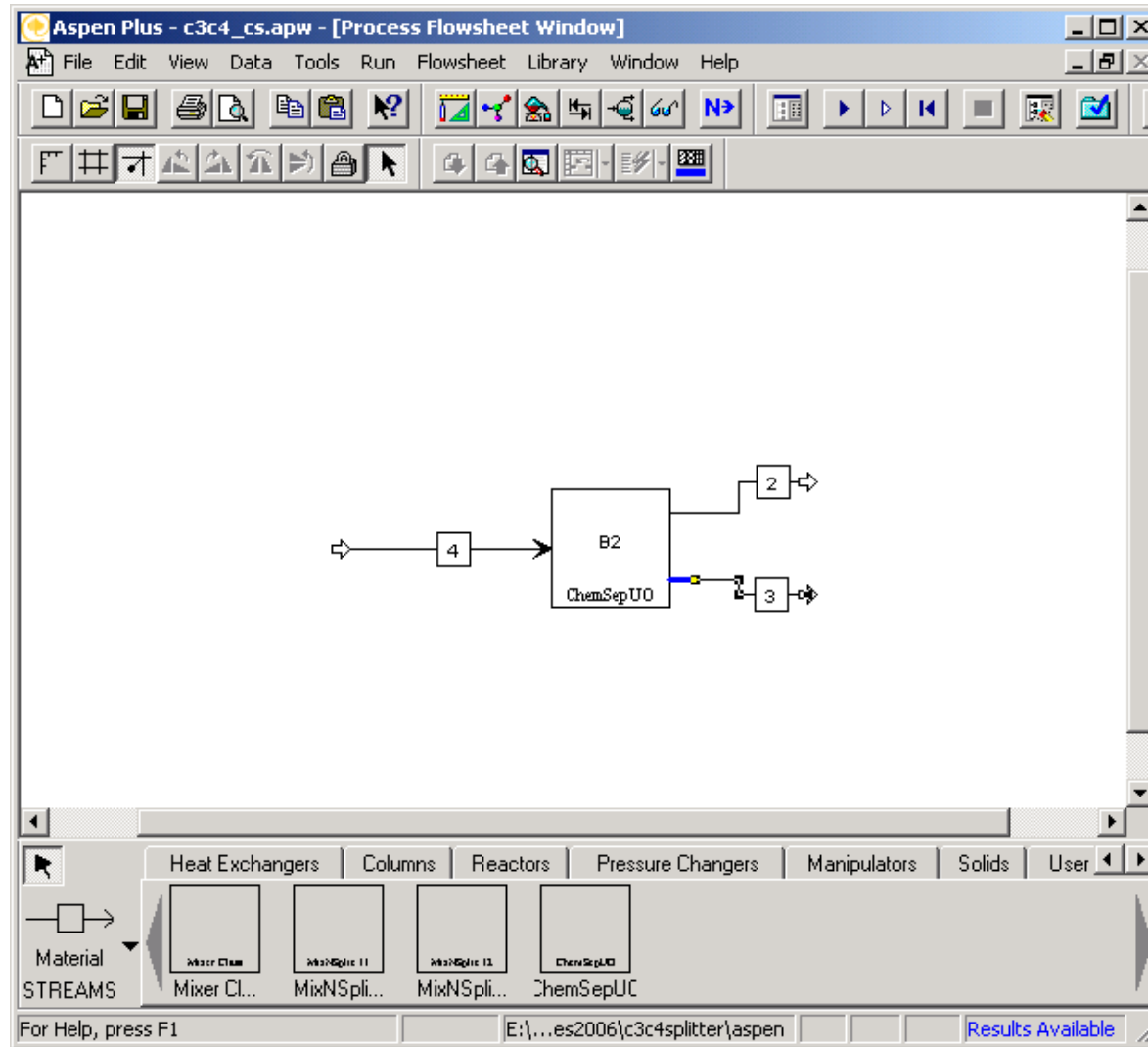
VLE = Soave-RK

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Results



C₃/C₄ Splitter in Aspen Plus v12.1.8



C₃/C₄ Splitter in COCO

The image displays the COFE software interface for a C₃/C₄ 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:

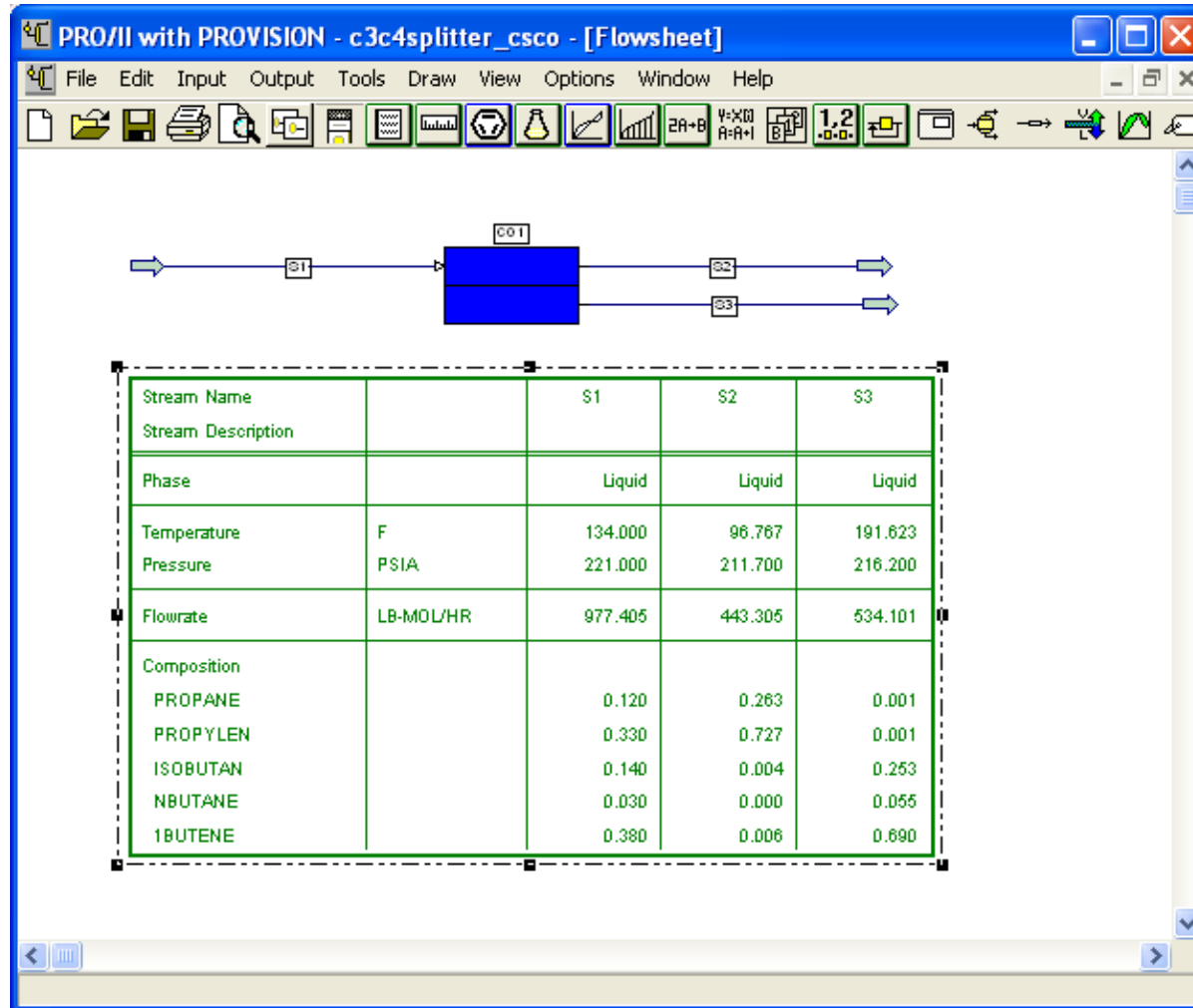
Parameter	Value	Unit
GUIArguments	/kpld	
UseCOSEThermo	TRUE	
UseCOSEDiffusionCoefficients	FALSE	
UsePerturbedDerivativesOnly	FALSE	
UsePerturbed_ddX	FALSE	
SuppressWarnings	FALSE	
RelativePerturbationTemperature	0.001	
RelativePerturbationPressure	0.001	
PerturbationComposition	0.001	
InletReflash	<none>	
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 0th element

C₃/C₄ 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 ProII 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 ProII 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

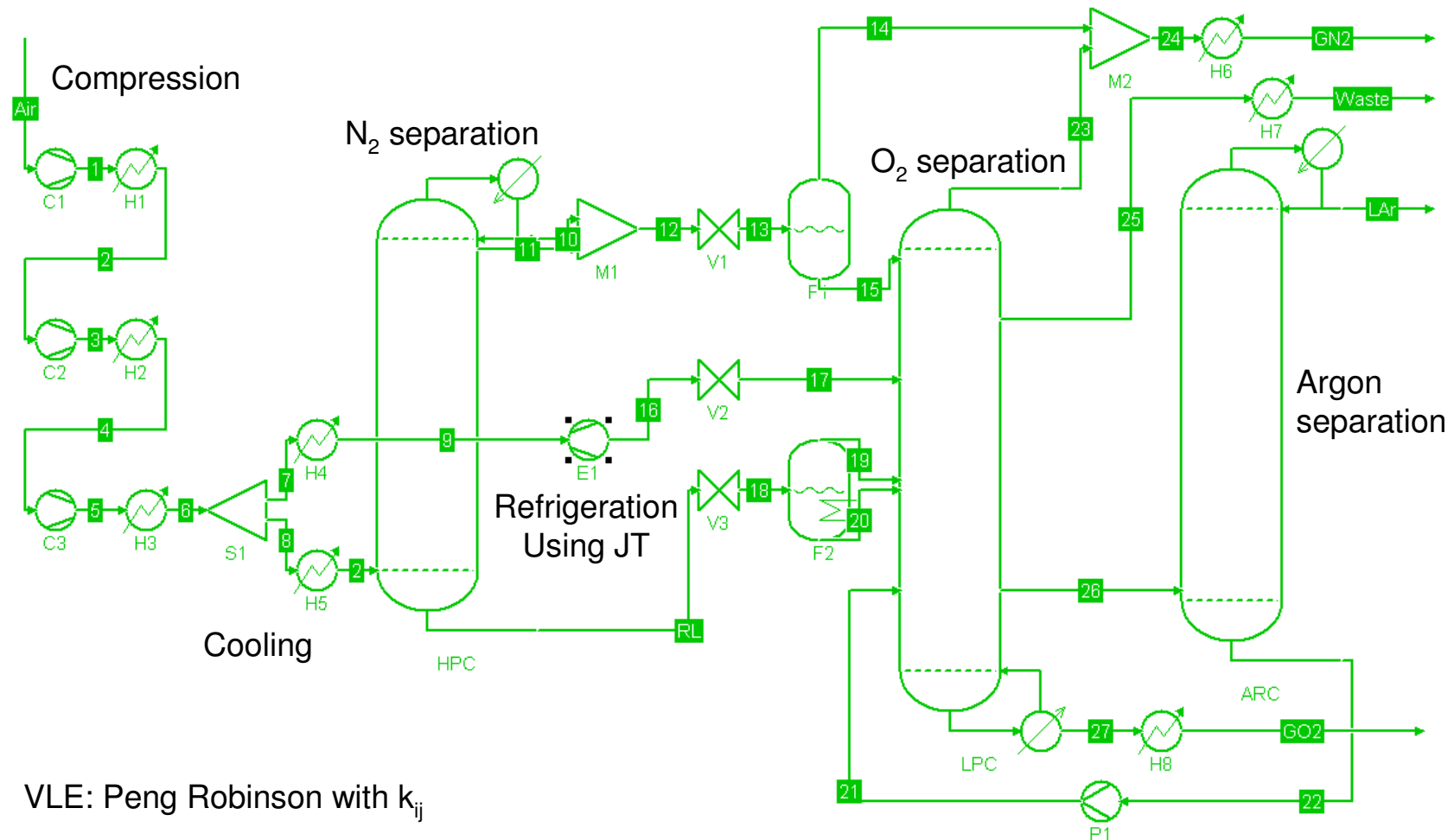
ChemSep-LITE is CAPE-OPEN

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

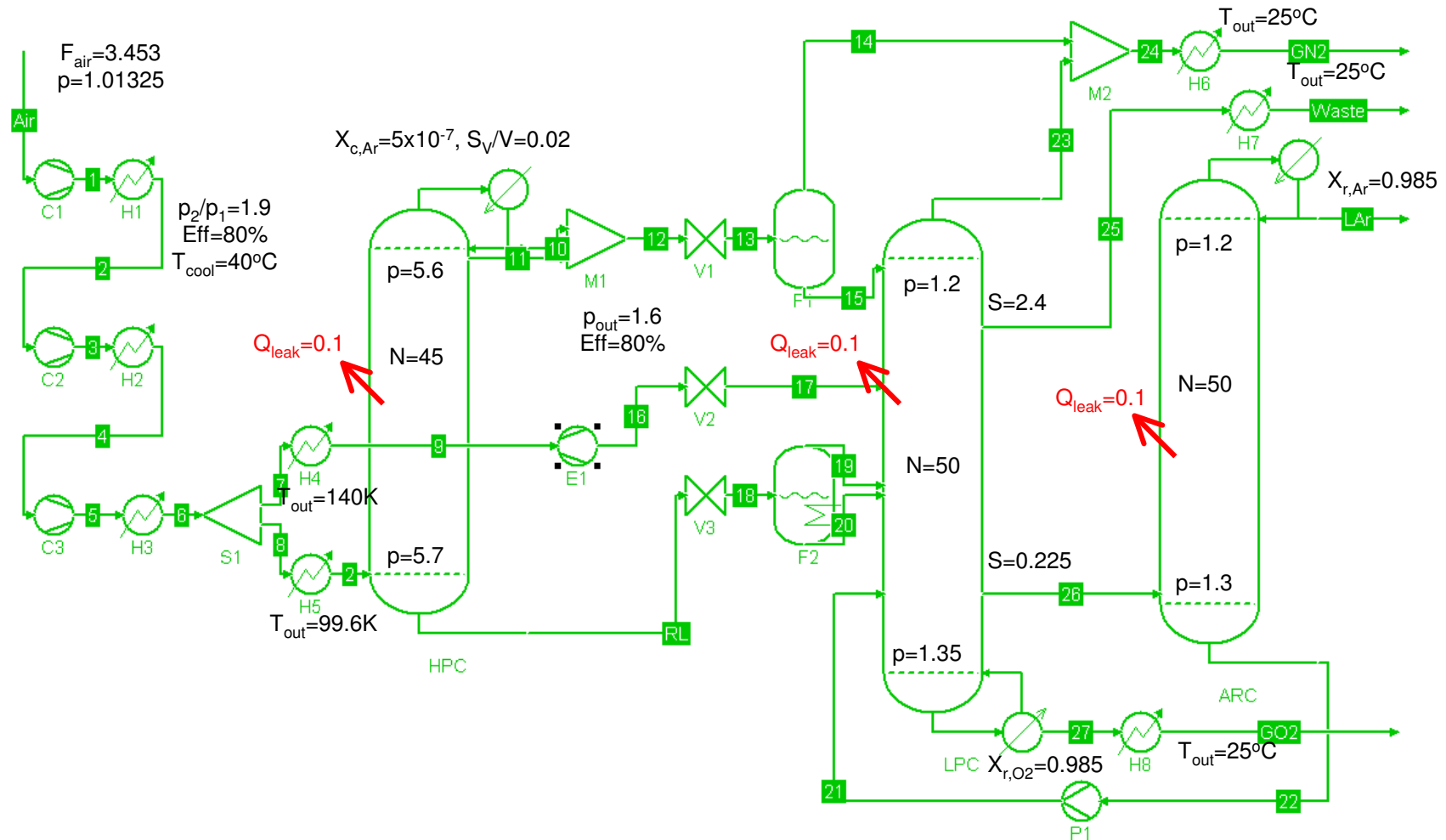
Example: Air Separation Unit using COCO
(www.amsterchem.com)

Air Separation Unit with Argon Production

With COCO: 5 iterations using stream estimate for stream 22

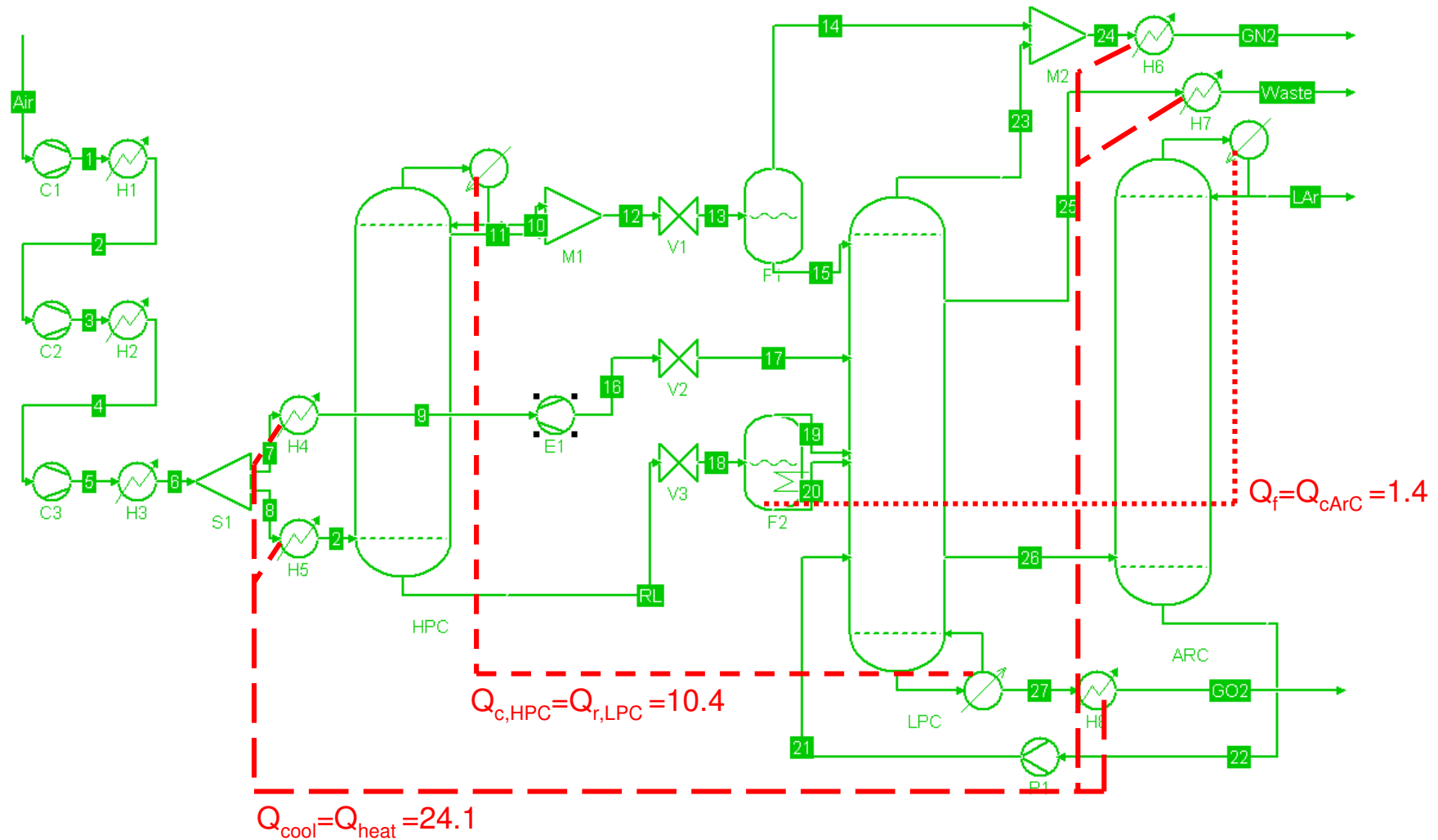


Air Separation Unit: Specifications



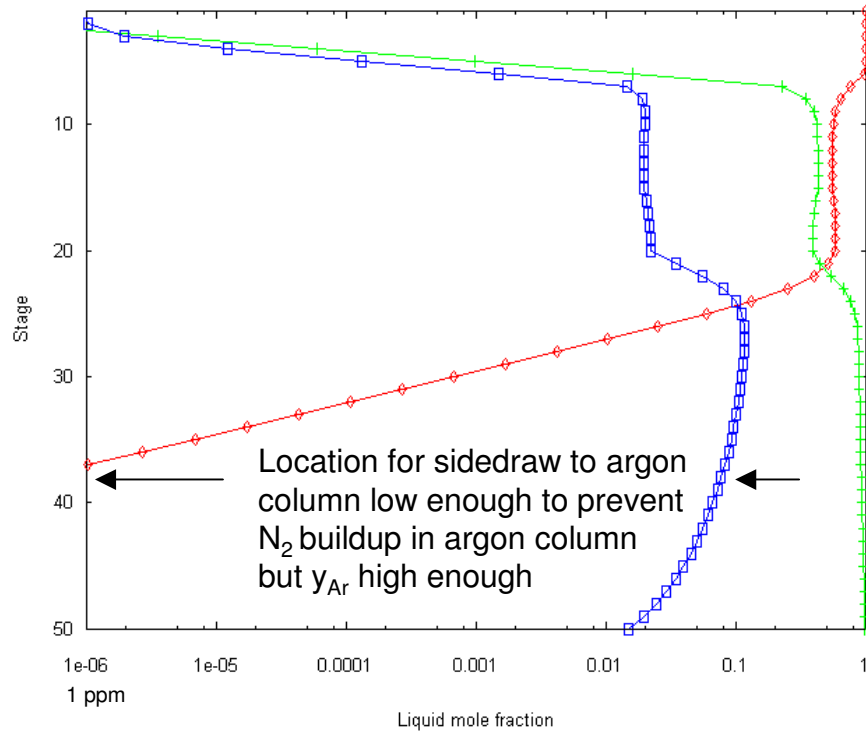
O_2 and Ar purities specified at 98.5%; Recoveries $\approx 75\%$, respectively $\approx 85\%$.
 Better recoveries and purities can be obtained with more stages!

Air Separation Unit: Heat Integration



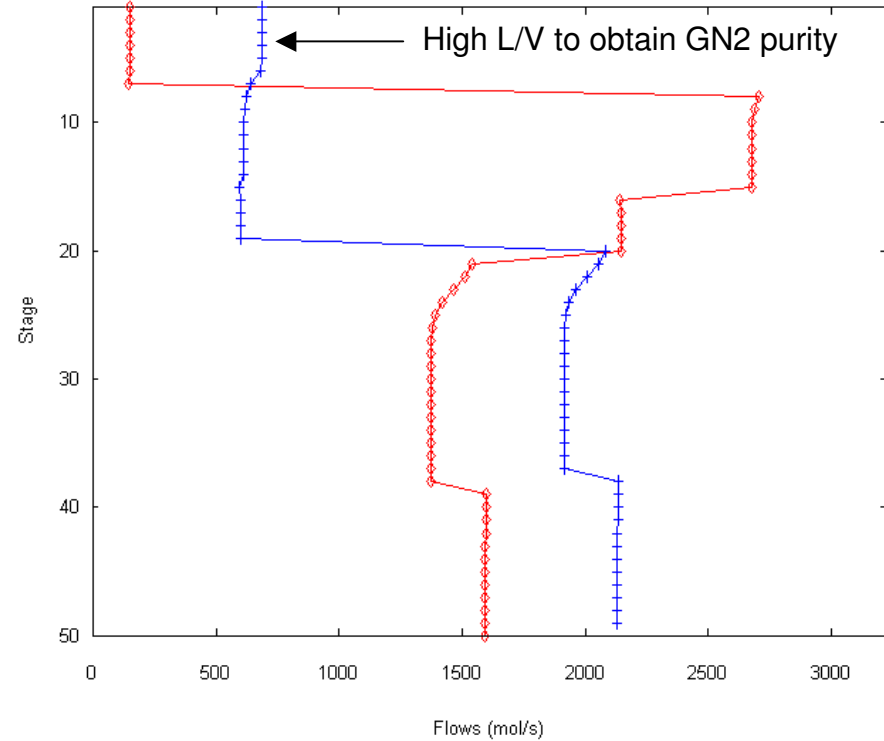
Air Separation Unit: Low Pressure Column

Liquid phase composition profiles



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

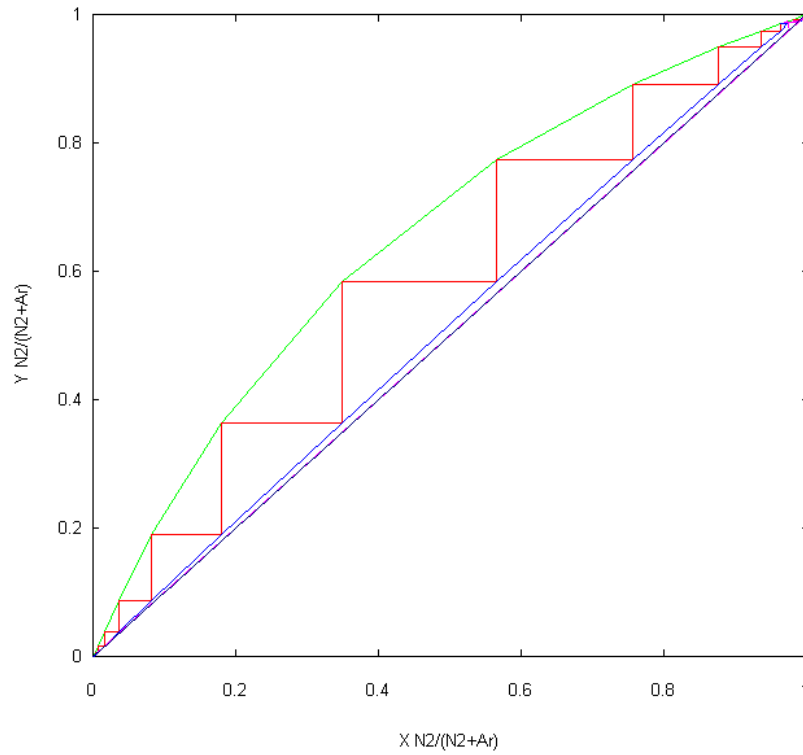
Flow profiles



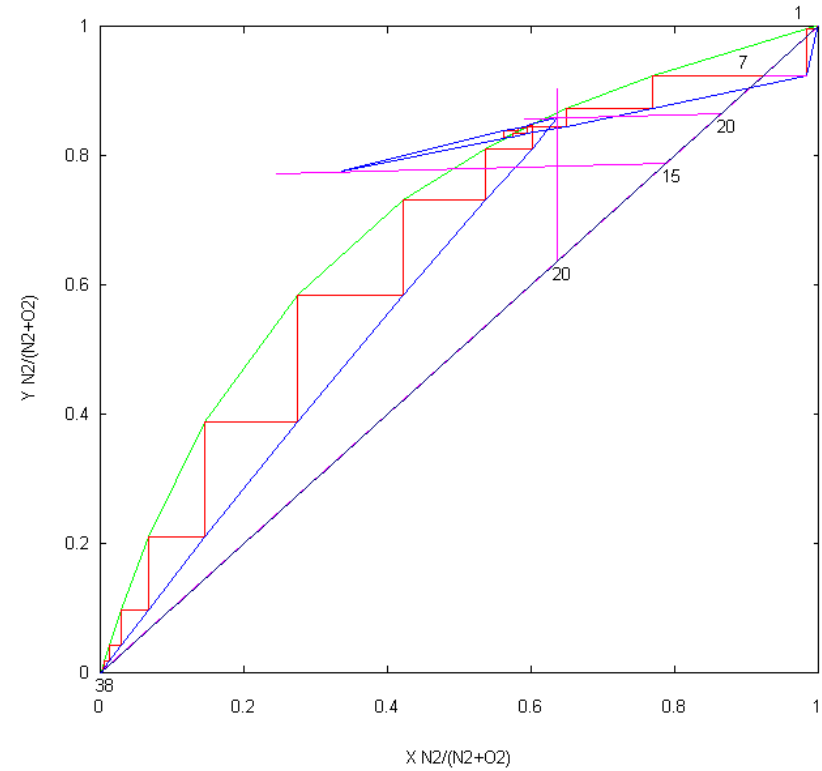
V —◇— L —+—

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)

Supplemental Slides

Binary Interaction Parameters

C_3/C_4 Splitter:

$$C_3/C_{3=} 0.0083, C_3/iC_4 -0.01, C_{3=}/iC_4 -0.0144, \\ C_{3=}/1C_{4=} 0.0011, nC_4/1C_{4=} -0.0048$$

Air Separation Unit:

$$N_2/O_2 -0.0133, N_2/Ar -0.0026, O_2/Ar 0.0089$$

ChemSep Nonequilibrium Model

- Can display profile of any physical property or mass transfer/hydraulic parameter
- Tens of MTC models for packings and trays
- More accurate liquid diffusivity models
- Dispersed liquid flow model
- Simultaneous column internal design allows nonequilibrium simulation of new columns
- 15+ years experience with MTC modeling
- Licensed to 70+ universities worldwide
- Total Reflux column simulation