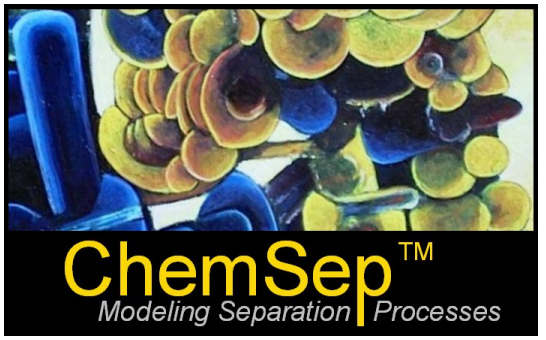
ChemSep / Cape-Open Property Packages



Harry Kooijman & Ross Taylor
ChemSep

CO-LaN AGM, Amsterdam, October 2015

Cape-Open Property Packages

Overview

Introduction

Implementation

Testing & Validation

Case stories

Conclusions & Outlook

Introduction

Business case for Cape-Open Property Packages

Leverage existing property models: do what others cannot

Cutting edge technology: from published to implemented in weeks

Use without limitations: the same packages in all simulators

LEAN = As Fast / As Efficient / As Accurate / As Simple as can be

Introduction

Can we do this with reactive electrolyte models?

→ no standards specification (yet)

→ use of true / apparent species (= potential for problems?)

Example:

at the flowsheet level: CO_2, H_2O

→

in the Property Package: CO_2, H_2O, [H^+, OH^-, HCO_3^- , CO_3^{--}]
(equilibrium changes with p,T, pH)

Introduction

Time line

2013 Q3: CO-LaN sends out RFP for Consultancy Services

2013 Q4: CO-LaN agrees to support ChemSep proposal (80 hrs)

2014: delays due to unavailability UNISIM socket & resources

Feb 2015: started implementation by Jasper van Baten

Apr 2015: alpha version available, tested in COCO

May 2015: finally test socket for UNISIM R430 available

→ Testing in target environment could finally commence

2015 Q3: CS/copp available online

2015 Q4: tests being finalized

Implementation

Approach

Fortran DLL-wrapper for existing Fortran libraries (non-reentrant)

COPP C-wrapper (*AmsterCHEM's COM CAPE-OPEN Wizard*):

- copies Fortran DLL (to enable multiple parallel calls)
- copies configuration-file (same)

Adapt ChemSep GUI to define components & property models
(configuration in existing text-format)

Auto-generate species from apparent species & set of reactions
(reactions only known inside the property package)

Ionic species after apparent species

Automatic back-conversion to apparent species

Implementation

Features:

Pure component property intrinsic data:
casRegistryNumber, chemicalFormula, structureFormula, SMILESformula, criticalTemperature, criticalPressure, ...

Temperature Dependent Properties (with derivatives):
idealGasEnthalpy

Mixture intensive properties (with derivatives):
Kvalue, FugacityCoeffient, LogKvalue, LogFugacityCoeffient, Enthalpy, EnthalpyF, Entropy, EntropyF, MolecularWeight

Mixture physical / transport properties:
Density, Volume, Viscosity, ThermalConductivity, SurfaceTension, Diffusivities

Flash types: T-p, T-VF, p-VF, p-H, p-S, p-HF (more coming)

Both Cape-Open 1.0 and 1.1 Support

Support editing & persistence (IPersistStream + IPersistPropertyBag)

Implementation

Messaging

Warnings / Errors written to logs

Debugging

Logs:

- ChemSep built in log (text dumps in temp folder)
- OATS and COLTT

Debuggers:

- GDB (not so sophisticated)

Testing & Validation

Testing

Fortran DLL: direct calls with Fortran test program

C DLL: Streams in COCO for flash and properties

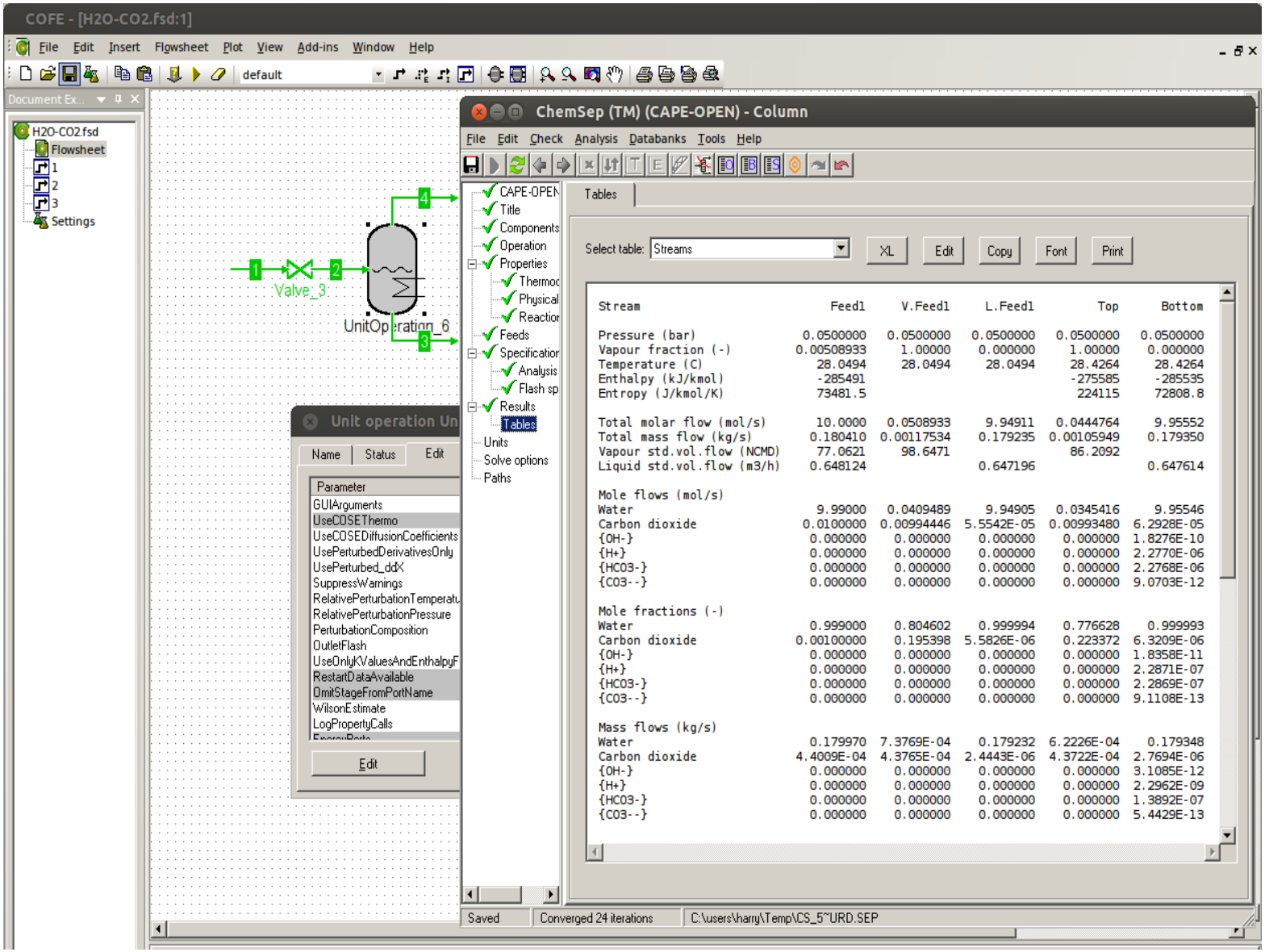
Unit Operations: Compressor, Pump, Valve, HXCH, Column in COCO

Commercial Software: PRO/II, UNISIM, …

Testing & Validation

Streams in COCO

test flash and properties



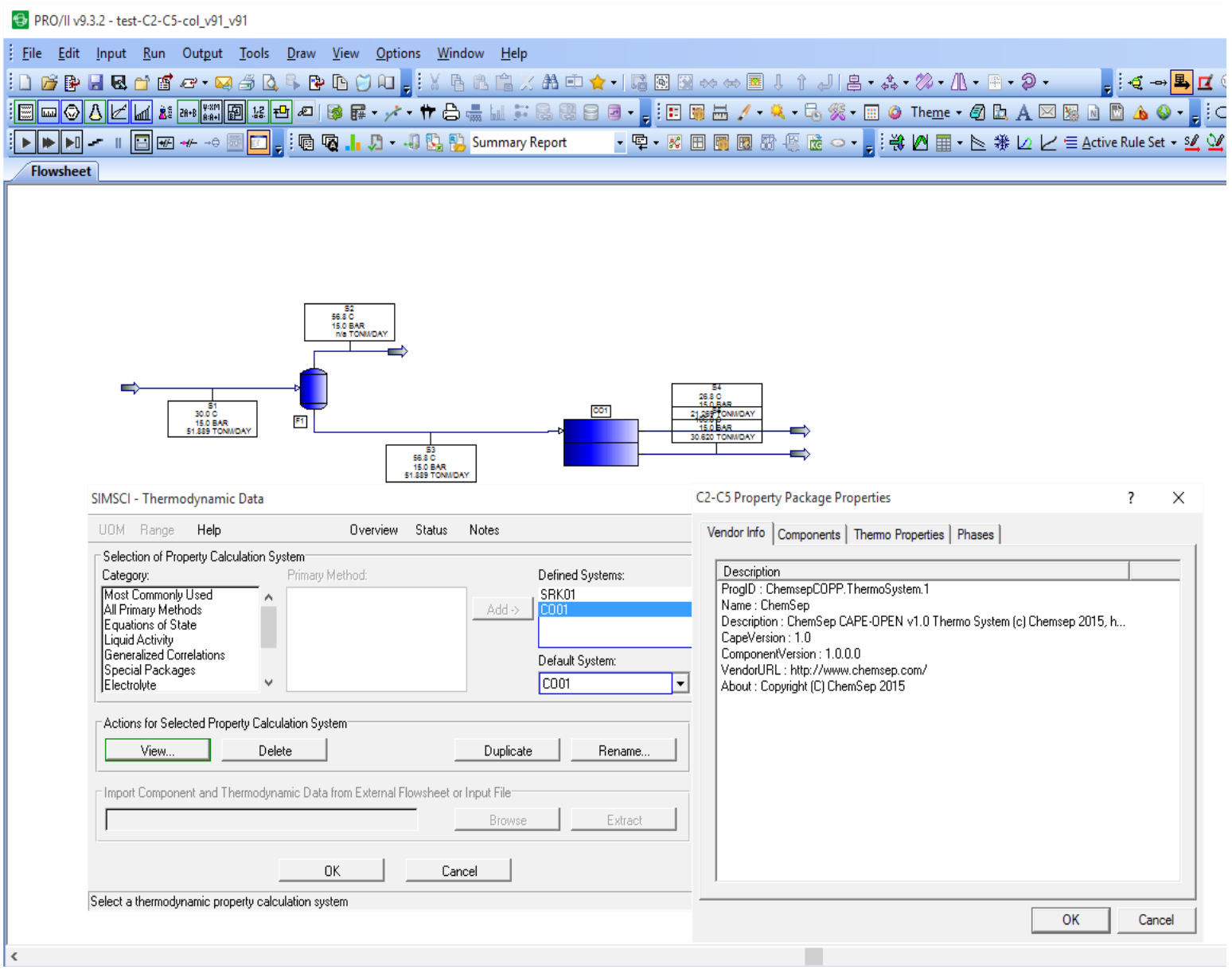
Stream	Feed1	V.Feed1	L.Feed1	Top	Bottom
Pressure (bar)	0.0500000	0.0500000	0.0500000	0.0500000	0.0500000
Vapour fraction (-)	0.00508933	1.00000	0.000000	1.00000	0.000000
Temperature (C)	28.0494	28.0494	28.0494	28.4264	28.4264
Enthalpy (kJ/kmol)	-285491			-275585	-285535
Entropy (J/kmol/K)	73481.5			224115	72808.8
Total molar flow (mol/s)	10.0000	0.0508933	9.94911	0.0444764	9.95552
Total mass flow (kg/s)	0.180410	0.00117534	0.179235	0.00105949	0.179350
Vapour std.vol.flow (NCMD)	77.0621	98.6471		86.2092	
Liquid std.vol.flow (m3/h)	0.648124		0.647196		0.647614
Mole flows (mol/s)					
Water	9.99000	0.0409489	9.94905	0.0345416	9.95546
Carbon dioxide	0.0100000	0.00994446	5.5542E-05	0.00993480	6.2928E-05
{OH-}	0.000000	0.000000	0.000000	0.000000	1.8276E-10
{H+}	0.000000	0.000000	0.000000	0.000000	2.2770E-06
{HCO3-}	0.000000	0.000000	0.000000	0.000000	2.2768E-06
{CO3--}	0.000000	0.000000	0.000000	0.000000	9.0703E-12
Mole fractions (-)					
Water	0.999000	0.804602	0.999994	0.776628	0.999993
Carbon dioxide	0.00100000	0.195398	5.5826E-06	0.223372	6.3209E-06
{OH-}	0.000000	0.000000	0.000000	0.000000	1.8358E-11
{H+}	0.000000	0.000000	0.000000	0.000000	2.2871E-07
{HCO3-}	0.000000	0.000000	0.000000	0.000000	2.2869E-07
{CO3--}	0.000000	0.000000	0.000000	0.000000	9.1108E-13
Mass flows (kg/s)					
Water	0.179970	7.3769E-04	0.179232	6.2226E-04	0.179348
Carbon dioxide	4.4009E-04	4.3765E-04	2.4443E-06	4.3722E-04	2.7694E-06
{OH-}	0.000000	0.000000	0.000000	0.000000	3.1085E-12
{H+}	0.000000	0.000000	0.000000	0.000000	2.2962E-09
{HCO3-}	0.000000	0.000000	0.000000	0.000000	1.3892E-07
{CO3--}	0.000000	0.000000	0.000000	0.000000	5.4429E-13

Testing & Validation

PRO/II

Flash + Distillation

Ethane,
Propane,
nButane,
nPentane

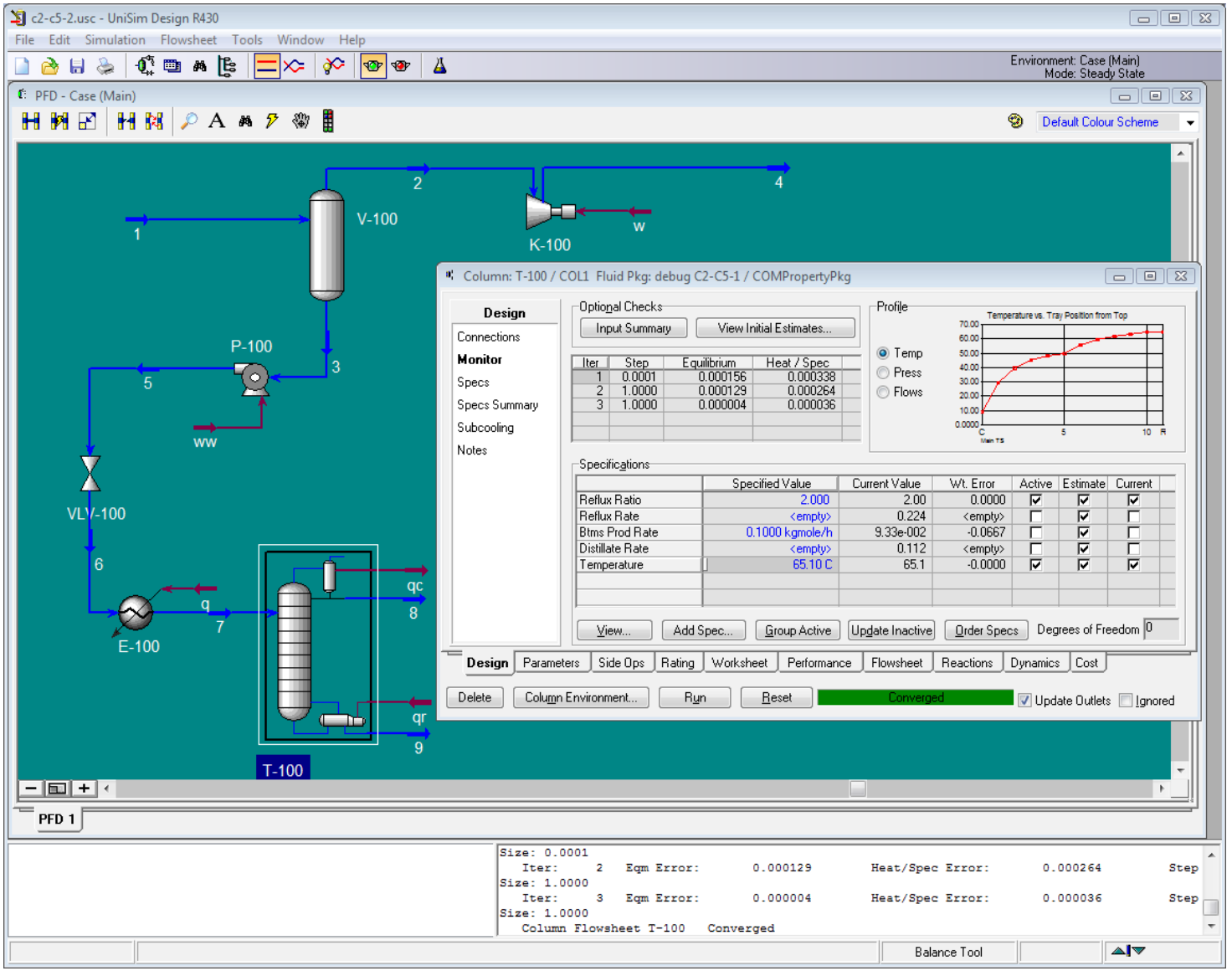


Testing & Validation

UNISIM Design

Distillation
T specification

Ethane,
Propane,
nButane,
nPentane



Case Stories

Safety in Air Separation Units / PPR78

Tracking impurities in MEG plants / PSRK

Air Separation Unit / PPR78

Safety assessments of ASU's

Failure of the adsorption Pre-Purification Units (PPU) in Shell GTL plant at Bintulu to remove light hydrocarbons from haze particle desorption:

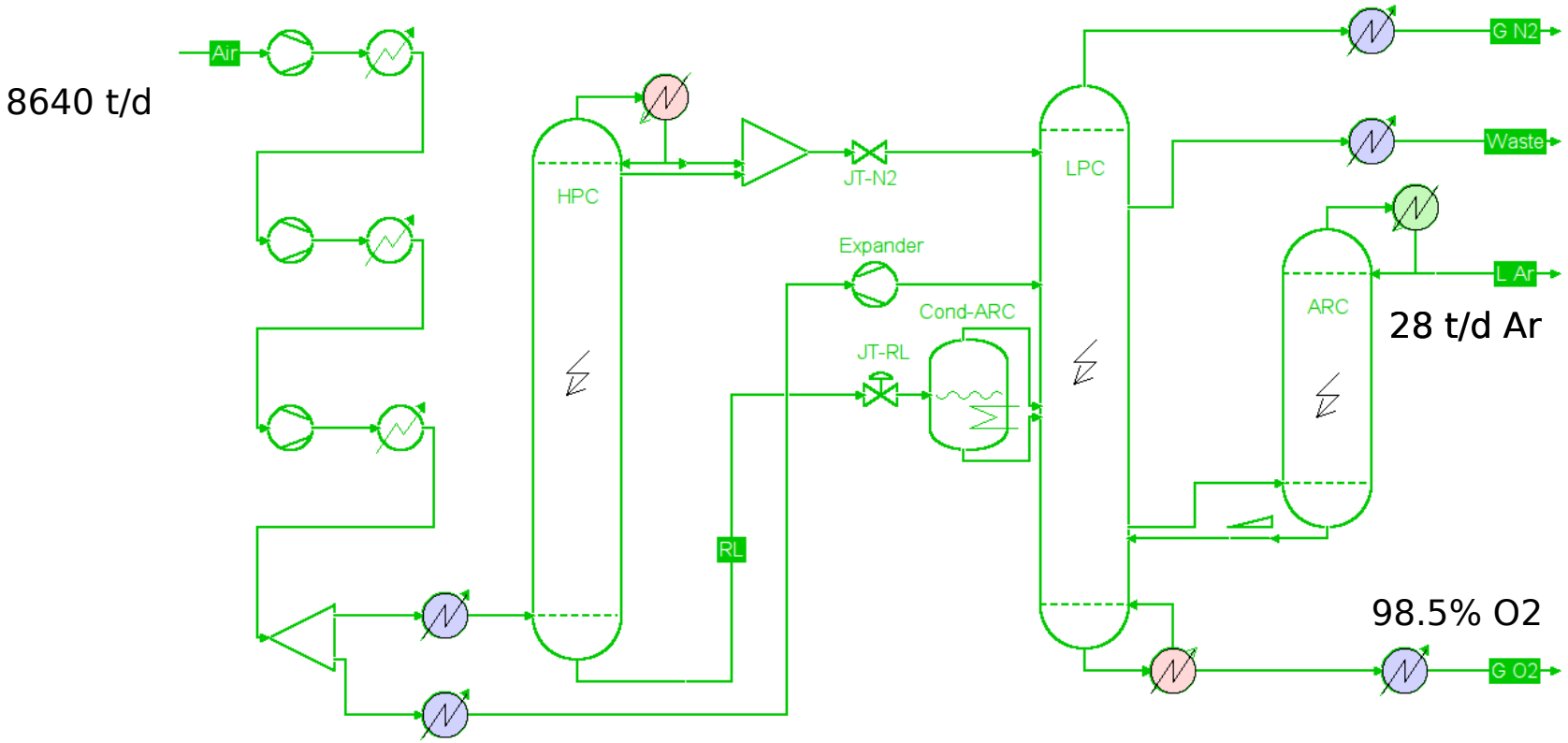
Component	Amount removed by PPU
Methane	0%
Ethane	30-70%
Ethylene	30-70%
Propane	30-70%
Nitric Oxide	30-100%

Determine intake limits on Ethane & Propane to remain below recommended 450 ppm Methane equivalent in the O_2 reboiler

Use 25 August 2015 extension of the Predictive Peng-Robinson

Air Separation Unit / PPR78

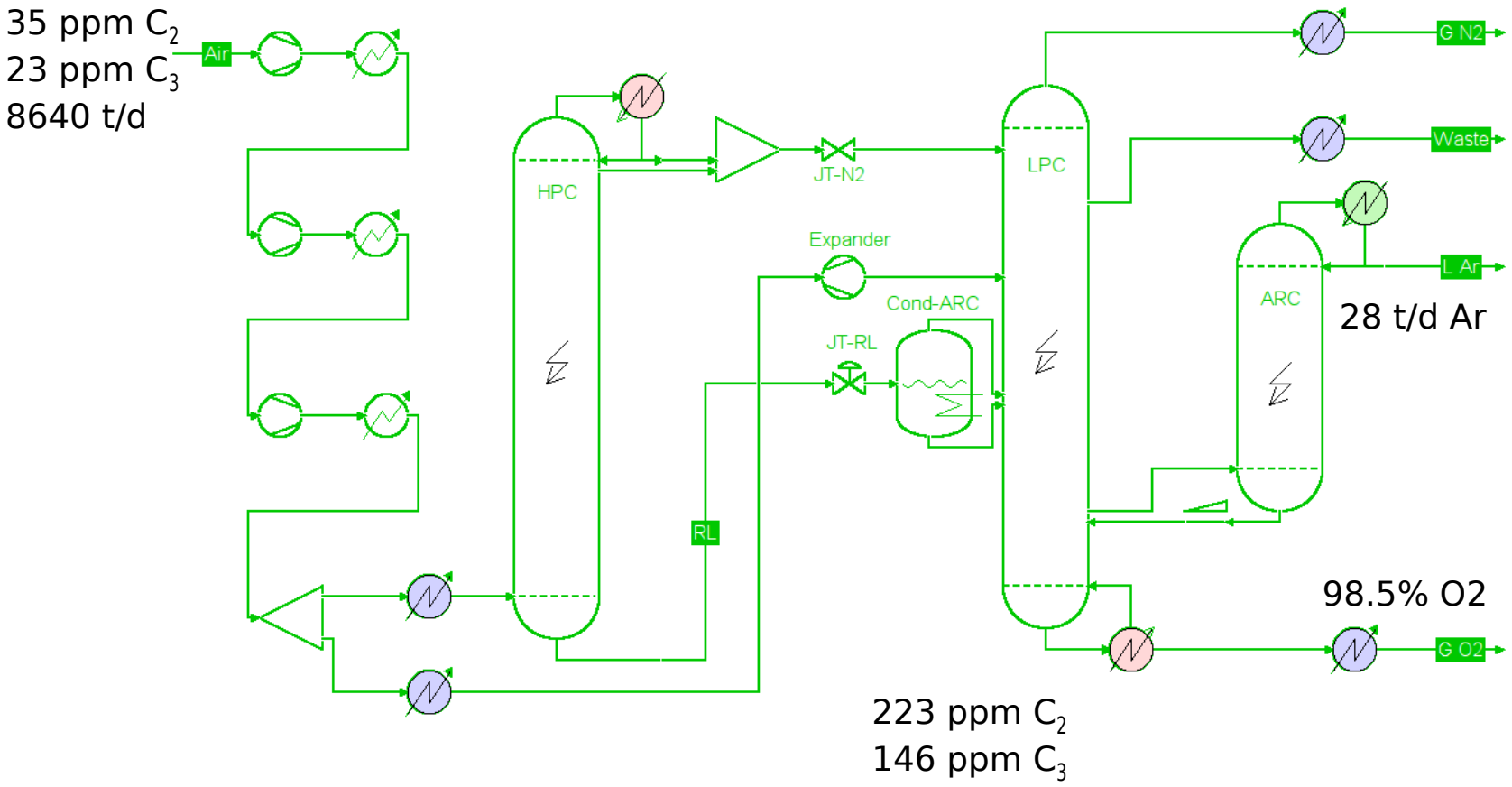
ASU simulation, replace existing property pack with CS/copp



PPR78 provides similar solution as PR with specially tuned BIP's

Air Separation Unit / PPR78

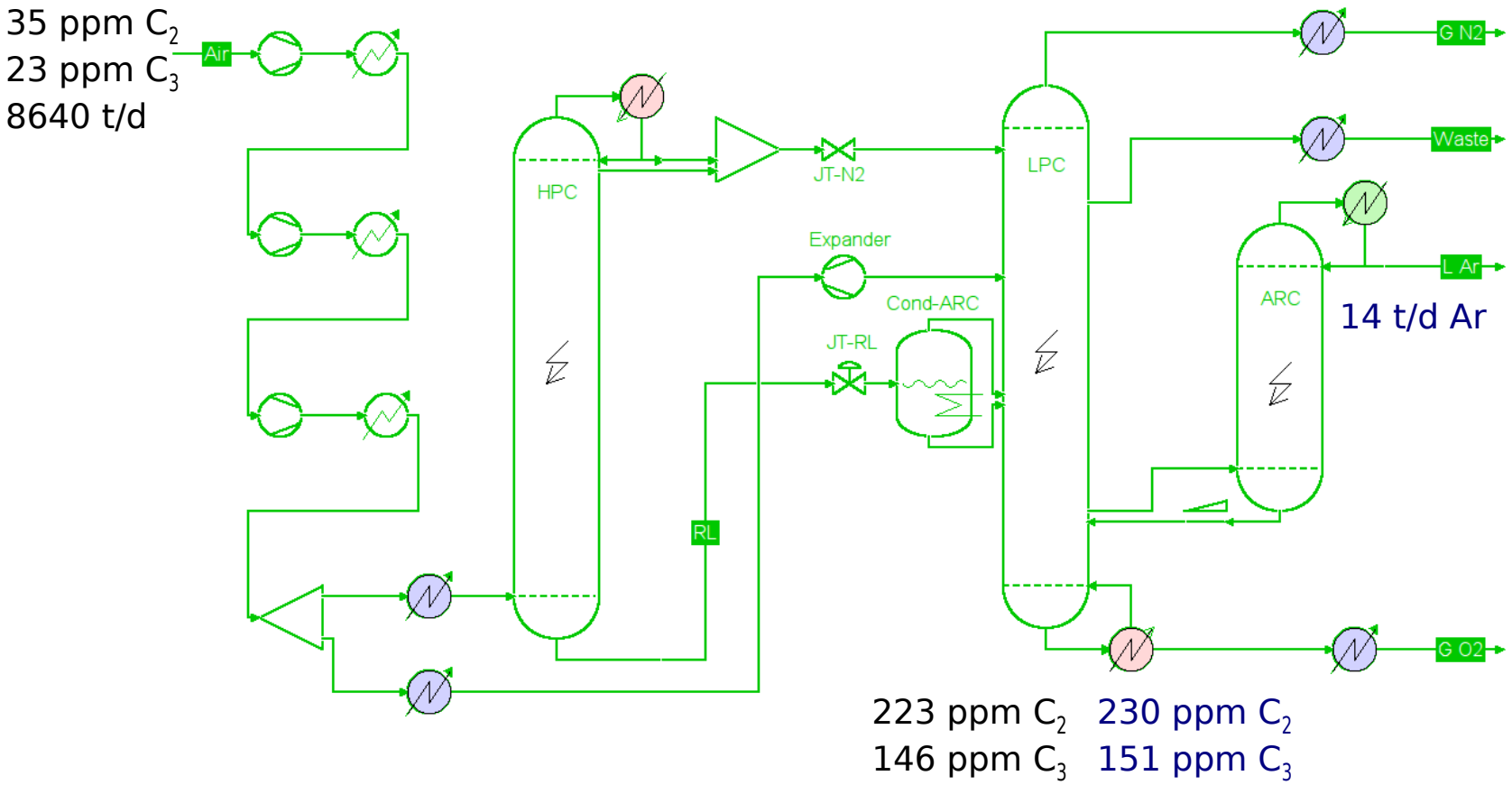
Added Ethane & Propane traces and check limit values



Considerable build-up observed

Air Separation Unit / PPR78

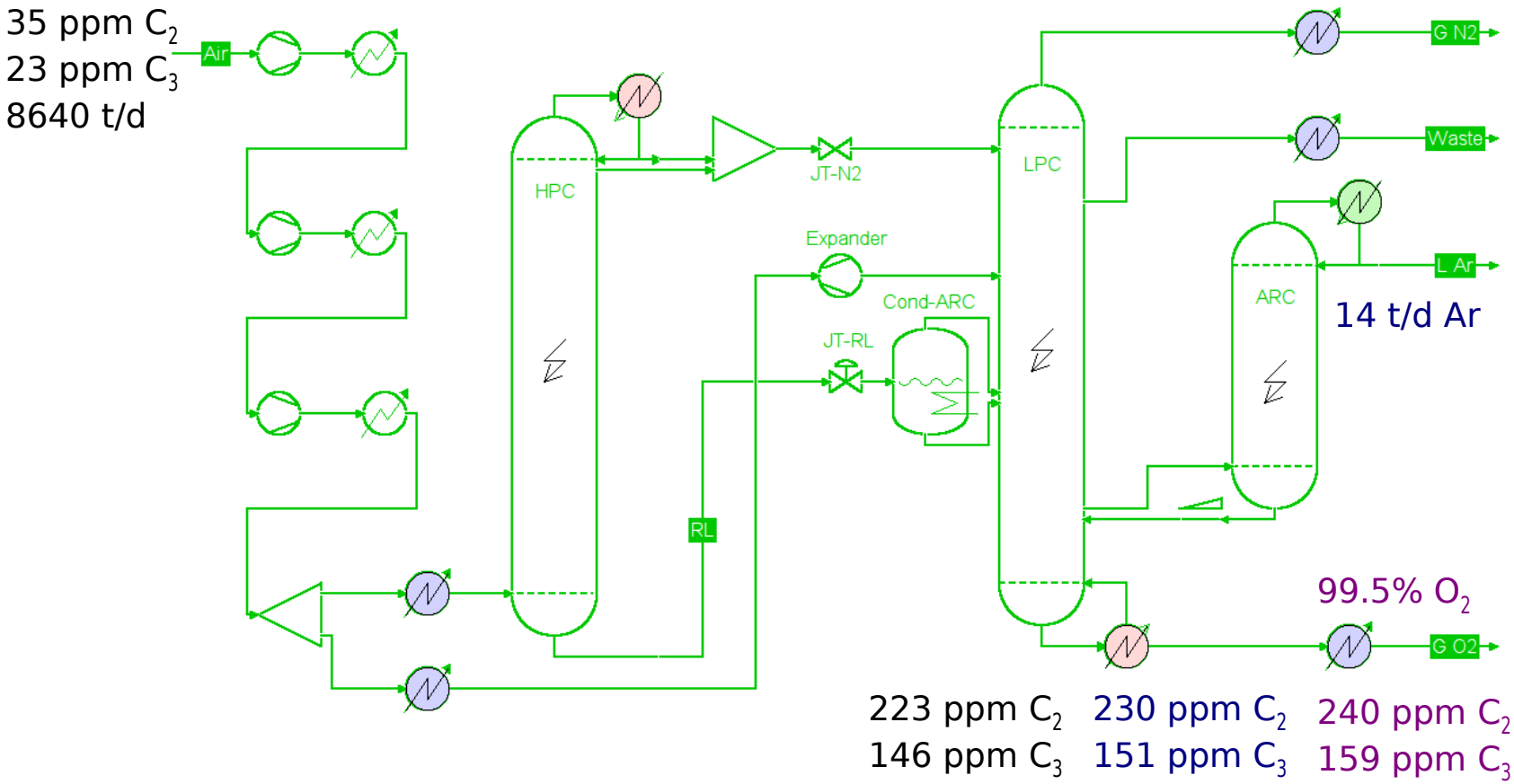
Is this build-up dependent on plant operation?



Argon production not much of influence

Air Separation Unit / PPR78

Is this build-up dependent on plant operation?



Fluctuations in Oxygen product purity can lead to higher build-up

Air Separation Unit / PPR78

Take Away

CS/copp handles compressors, expanders, HXCH, and distillation

New enhanced-PPR78 method available in matter of week(s)

Enhanced-PPR78 can describe non-ideal cryogenic O_2 / Ar

Quick assessment of light HC traces possible with e-PPR78

Note:

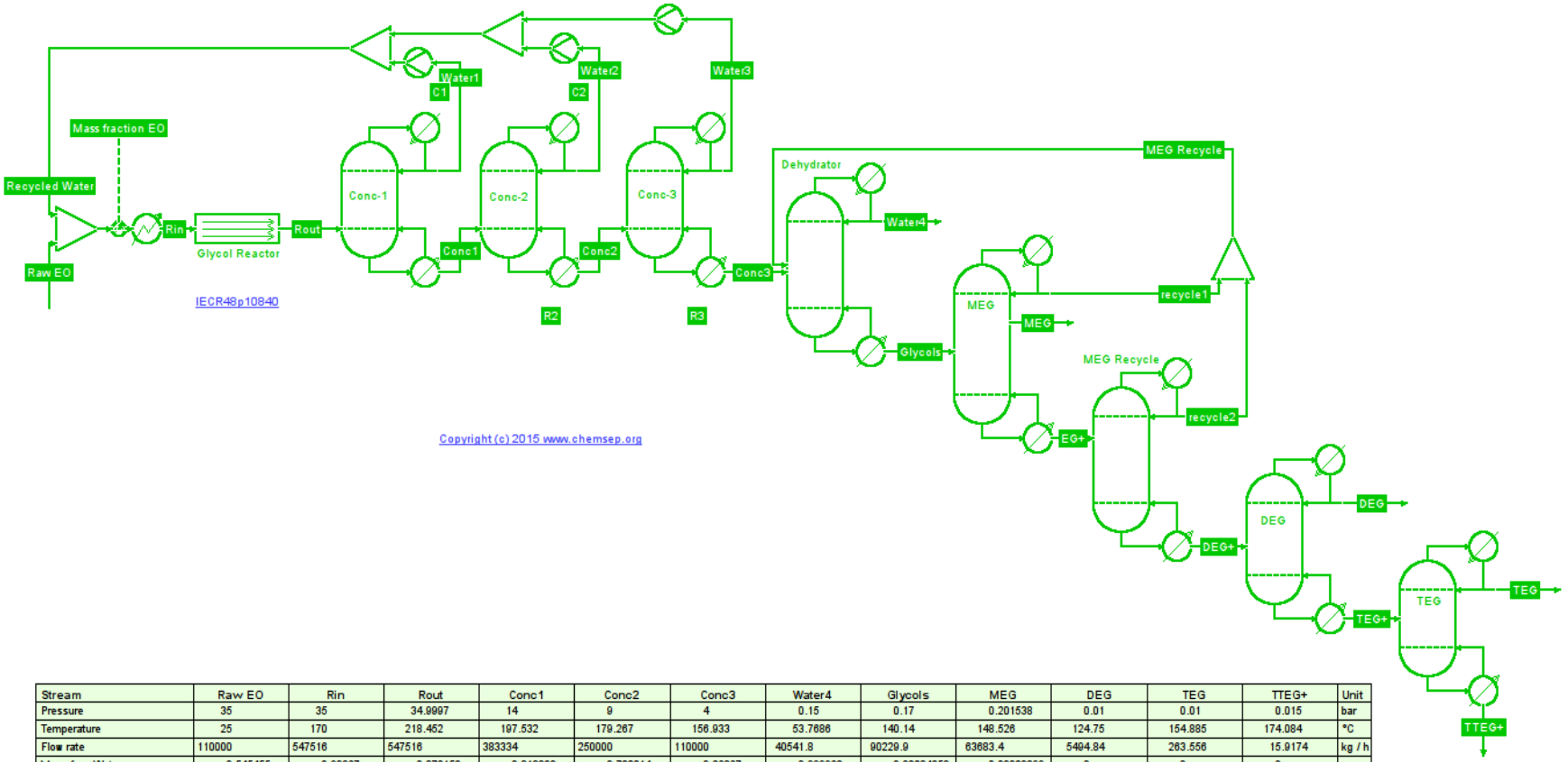
Stronger build-up when gaseous Oxygen produced

Trace levels < 1ppm with online (FTIR) measurement

Tracking impurities in MEG / PSRK

Nonideal thermo for trace impurities

Air ingress in vacuum columns oxidizes MEG to e.g. Acetic Acid

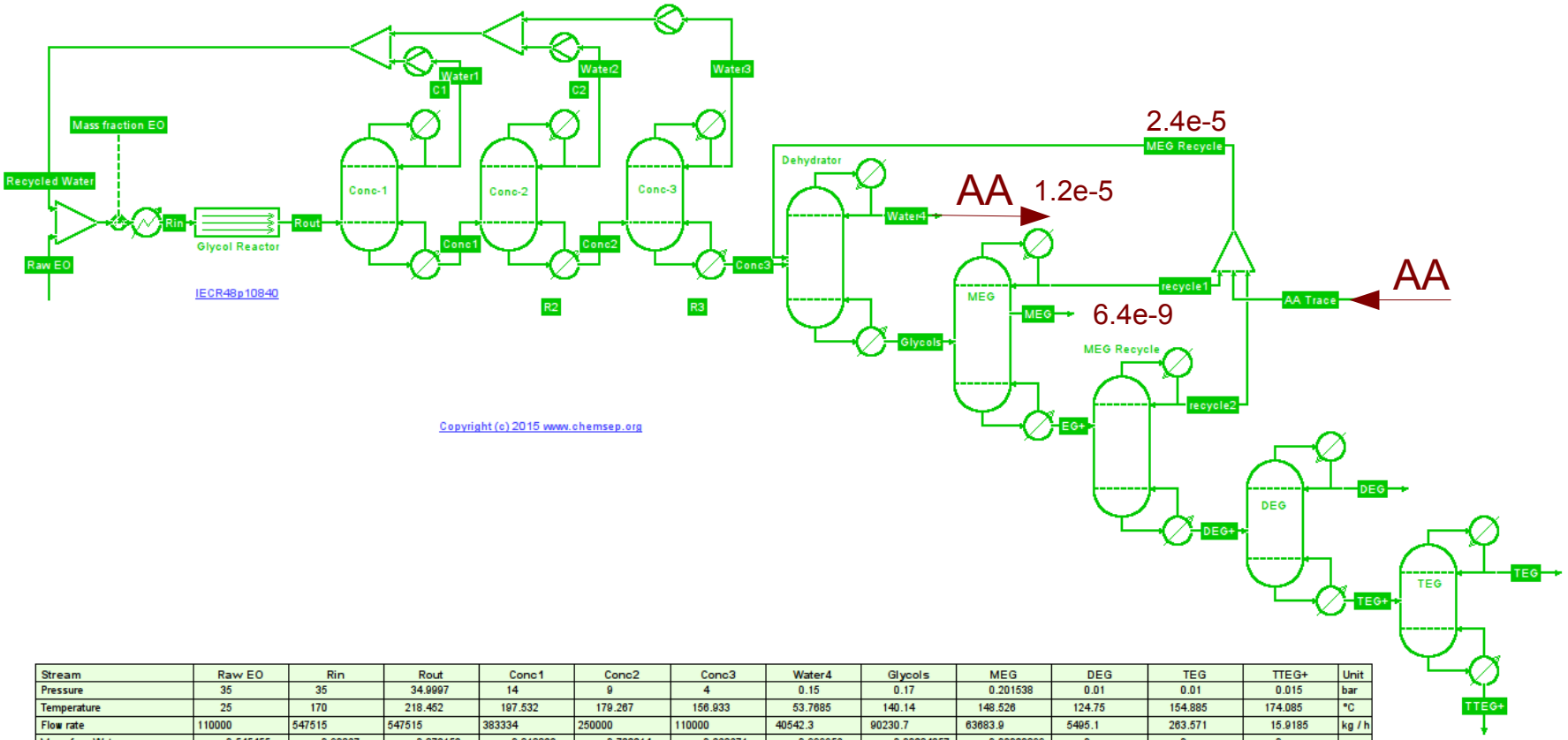


Stream	Raw EO	Rin	Rout	Conc1	Conc2	Conc3	Water4	Glycols	MEG	DEG	TEG	TTEG+	Unit
Pressure	35	35	34.9997	14	9	4	0.15	0.17	0.201538	0.01	0.01	0.015	bar
Temperature	25	170	218.452	197.532	179.267	156.933	53.7686	140.14	148.526	124.75	154.885	174.084	°C
Flow rate	110000	547516	547516	383334	250000	110000	40541.8	90229.9	63683.4	5494.84	263.556	15.9174	kg / h
Mass frac Water	0.545455	0.90867	0.873153	0.818833	0.722214	0.36867	0.999968	0.00284358	0.00020899	0	0	0	
Mass frac Monoethylene glycol	0	6.9648e-06	0.1163	0.166104	0.254689	0.578837	3.17842e-05	0.932957	0.999791	2.77055e-05	1.12504e-13	8.4135e-23	
Mass frac Diethylene glycol	0	6.59302e-13	0.010017	0.0143072	0.0219378	0.0498586	2.31788e-13	0.0607988	1.05083e-11	0.998059	0.00104047	4.40624e-08	
Mass frac Triethylene glycol	0	1.22673e-11	0.000510402	0.000729008	0.00111781	0.00254048	2.06742e-11	0.00328726	1.1638e-07	0.00191306	0.994401	0.430948	
Mass frac Tetraethylene glycol	0	1.33882e-13	1.8738e-05	2.67635e-05	4.10374e-05	9.32667e-05	2.84818e-15	0.00011371	1.83873e-16	1.15358e-08	0.00455853	0.569052	
Mass frac Acetic acid	0	0	0	0	0	0	0	0	0	0	0	0	
Mass frac Ethylene oxide	0.454545	0.0913227	1.0563e-06	7.24947e-09	2.18055e-11	6.41275e-15	1.73995e-14	4.90918e-25	0	0	0	0	
Vapor phase													
MolecularWeight											150.263	168.268	-
Liquid phase													
MolecularWeight	24.6329	19.043	19.8256	20.7173	22.5188	33.0276	18.0154	63.3533	62.0361	106.178		186.886	-

Tracking impurities in MEG / PSRK

Replaced existing package with Predictive-SRK (PSRK)

Added trace Acetic Acid (AA) and see where it builds up / leaves



Stream	Raw EO	Rin	Rout	Conc1	Conc2	Conc3	Water4	Glycols	MEG	DEG	TEG	TTEG+	Unit
Pressure	35	35	34.9997	14	9	4	0.15	0.17	0.201538	0.01	0.01	0.015	bar
Temperature	25	170	218.452	197.532	179.267	156.933	53.7685	140.14	148.526	124.75	154.885	174.085	°C
Flow rate	110000	547515	547515	383334	250000	110000	40542.3	90230.7	63683.9	5495.1	263.571	15.9185	kg / h
Mass frac Water	0.545455	0.90867	0.873153	0.818833	0.722214	0.368671	0.999956	0.00284357	0.00020899	0	0	0	
Mass frac Monoethylene glycol	0	6.96484e-06	0.1163	0.166103	0.254688	0.578834	3.17857e-05	0.932954	0.999791	2.77041e-05	1.12498e-13	7.90716e-19	
Mass frac Diethylene glycol	0	6.59344e-13	0.010017	0.0143079	0.0219389	0.049861	2.31782e-13	0.0608012	1.05087e-11	0.998059	0.00104046	4.40571e-08	
Mass frac Triethylene glycol	0	1.22685e-11	0.000510403	0.000729069	0.00111791	0.0025407	2.06745e-11	0.00328742	1.16386e-07	0.00191306	0.994401	0.430907	
Mass frac Tetraethylene glycol	0	1.33901e-13	1.8738e-05	2.6767e-05	4.10428e-05	9.32789e-05	2.8481e-15	0.000113724	1.83897e-16	1.15366e-08	0.00455855	0.569093	
Mass frac Acetic acid	0	0	0	0	0	0	1.23227e-05	6.16564e-08	6.3891e-09	0	0	0	
Mass frac Ethylene oxide	0.454545	0.0913227	1.05629e-06	7.25142e-09	2.18114e-11	6.4145e-15	1.7404e-14	1.05256e-24	0	0	0	0	
Vapor phase													
MolecularWeight											150.263	188.269	-
Liquid phase													
MolecularWeight	24.6329	19.043	19.8256	20.7173	22.5188	33.0276	18.0156	63.3534	62.0361	106.178		186.886	-

Tracking impurities in MEG / PSRK

Take Away

CS/copp handles reactors and recycles with no performance loss

PSRK allows for quick assessment of oxygenates in MEG process

Conclusions & Outlook

CS/copp:

Available in ChemSep v7 since Q3/2015

No observed performance losses

Free download in ChemSep LITE http://www.chemsep.com/
(does not include electrolytes)

Outlook:

Integration with reaction standard specification

Improve speed & robustness

More flash types

Questions?

Backup-Slide

Electrolyte specification:

- Set of species dependent on the selected apparent species AND selected set(s) of reaction packages
- Not always all species desired everywhere
- Equilibrium and rates to be stored separately / independently per reaction

Backup-Slide

Feedback: selection/definition of packages in various software (e.g. UNISIM Design) needs to be simplified