ProSim

ProSimPlus Application Example

Syngas Deacidification

with Rectisol Process

Example purpose
This example illustrates a syngas deacidification with the Rectisol process. Methanol is used as the solvent. The deacidification is done through a contactor and the solvent regeneration needs several columns and flashes. The process objective is to refine a syngas of CO_2 and H_2S in order to have a satisfactory purity in CO_2 allowing its storage and a stream of H_2S able to be treated in a Claus unit. Methanol make-up is automatically calculated with simple modules. This example is taken from [KOH97] publication which describes main features of this process.

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Corresponding ProSimPlus files	*PSPS_EX_EN-Rectisol-Process.pmp3*

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1. PROCESS MODELING

1.1. Process description

Rectisol process uses methanol as solvent. Its main application is purification of syngas coming from gasification of heavy oils or coal instead of natural gas treatment. Rectisol process can selectively remove acid gas. Purity with very low composition in sulfur compounds can be achieved (less than 0.1 ppmv). This process is very flexible and several schemes exist depending on the objective.

The process is described based on the simulation flowsheet of the section 1.2.

This process can be divided in four steps:

1. Purification of syngas by absorption of CO_2 and H_2S,
2. Recovery of CO and H_2 from methanol stream,
3. Recovery of CO_2 purified from methanol stream,
4. Regeneration of methanol.

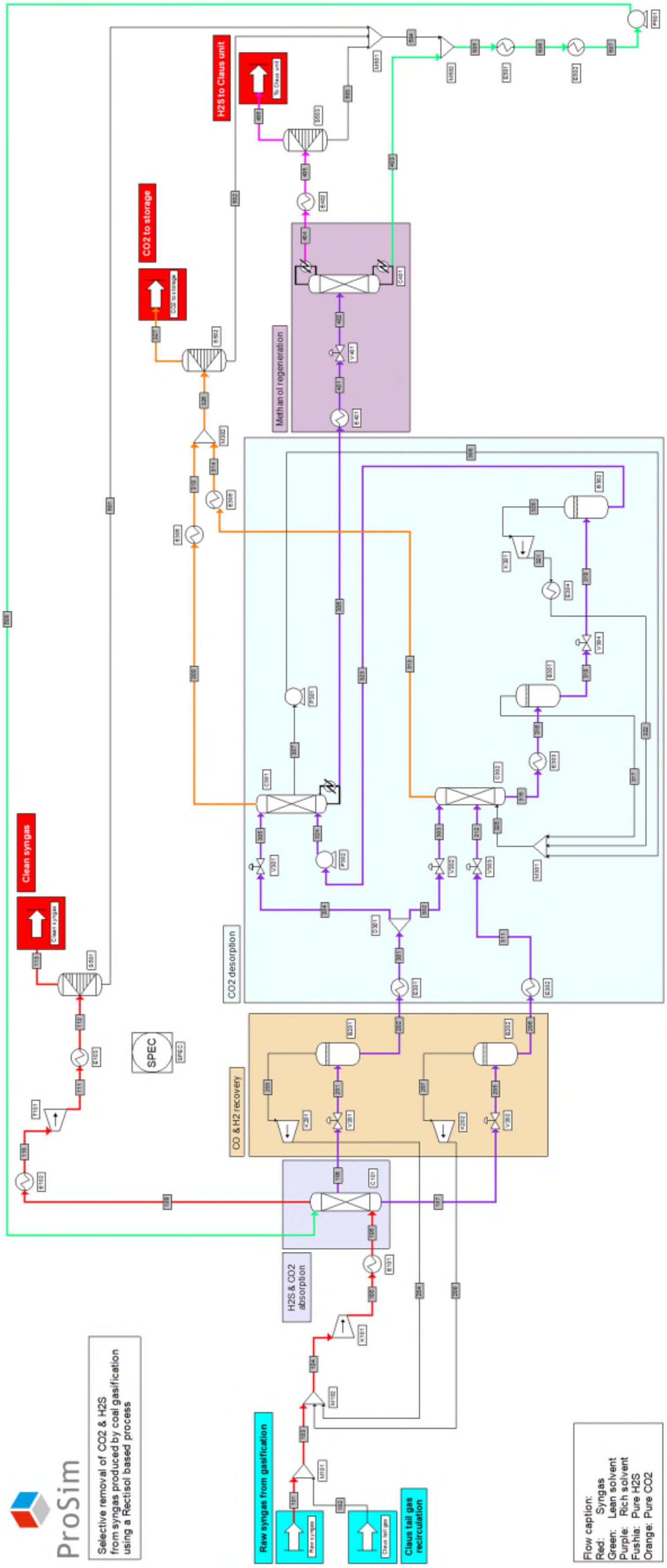
The syngas to be treated is fed through the stream 101. A tail gas recycle from Claus unit (stream 102) is also treated by the process. After compression and cooling, these streams feed the absorber C101 at the bottom. Regenerated methanol is introduced at the top of this absorber (stream 508). Syngas exits the process at the top of the absorber C101 (stream 109) and after heating and expansion. Two methanol streams are extracted from the absorber C101: one at the bottom (stream 107) and another one in a side stream (stream 108). The absorber C101 has also a side cooler that allows eliminating the heat of absorption of CO_2 and H_2S in the solvent (methanol).

The C101 absorber outlet methanol streams (streams 107 and 108) are expanded (valves V201 and V202) to recover CO and H_2 contained therein. The B201 and B202 separator outlet vapor streams (streams 203 and 207) are compressed and recycled at the input of the process (mixer M102).

Liquid streams coming from the flash drums B201 and B202 (streams 202 and 206) are expanded (valves V301, V302 and V303) to feed the low pressure column C301 and the high pressure column C302. The objective of these two columns is to desorb and purify CO_2 contained in the methanol. Overhead vapor streams of these two columns (streams 309 and 313) form purified CO_2 stream that is going to storage. Bottom liquid outlet of the column C302 (stream 315) passes through two successive flashes (B301 and B302) to feed the C301 column bottom (stream 324). Gas phases of these two flashes (streams 317 and 320) and the side stream of the column C301 (stream 307) feed the C302 column bottom (stream 325).

The C301 column bottom containing the methanol (stream 306) is expanded at atmospheric pressure (valve V401) before feeding the distillation column with partial condenser C401. The regenerated methanol is the liquid residue (stream 403). After cooling and pressurizing, the regenerated methanol feeds the absorber C101 (stream 508). The vapor distillate (stream 404) is a stream of CO_2 and H_2S that is sent to the Claus unit input.
Methanol make-up required for the process is the stream 504.

1.2. Simulation flowsheet



1.3. Components

Components taken into account in the simulation, their chemical formula and CAS numbers are presented in the following table. Pure components physical properties are extracted from the ProSimPlus standard database [ROW11].

Component name	Chemical formula	CAS number
Methanol (solvent)	CH_4O	67-56-1
Carbon dioxide	CO_2	124-38-9
Hydrogen sulfide	H_2S	7783-06-4
Carbon monoxide	CO	630-08-0
Nitrogen	N_2	7727-37-9
Hydrogen	H_2	1333-74-0

1.4. Thermodynamic model

Considering the temperature and pressure conditions of this process and that polar components are also present (particularly the solvent), a combined model, PSRK [HOL91], [GME95], [CHE02], has been chosen. This model is a predictive model based on group contributions.

1.5. Operating conditions

1.5.1. Process feeds

	Syngas	Tail gas from Claus unit
Temperature (°C)	30	30
Pressure (bar)	35	35
Total flowrate (t/h)	396.612	45.108
Molar fraction		
Methanol (solvent)	0	0
Carbon dioxide	0.280	0.968849
Hydrogen sulfide	0.013	0.002408
Carbon monoxide	0.234	0.015236
Nitrogen	0.004	0.001796
Hydrogen	0.469	0.011711

1.5.2. Acid gas absorption

✓ Absorber C101

Operating parameters	Value
Type of column	Absorber
Number of theoretical stages	18
Liquid side stream at stage 8 (t/h)	500.796
Overhead pressure (bar)	60
Thermal losses at stage 4 (MW) (initial value)	0.73

Objectives / Constraints:

Specification	Value
Temperature at stage 4 (°C)	-25.15
Action variable	**Value**
Intermediate cooling at stage 4	

✓ Heat exchangers

Operating parameters	Value
Type of exchanger	Cooler / Heater
Outlet temperature (°C)	
E101	-15
E102	20
E103	20

- ✓ Compressor K101

Operating parameters	Value
Isentropic efficiency	0.82
Mechanical efficiency	0.92
Exhaust pressure (bar)	60

- ✓ Expander T101

Operating parameters	Value
Isentropic efficiency	0.88
Outlet pressure (bar)	30

- ✓ Mixers M101 and M102

Operating parameters	Value
Type of mixer	Other mixer
Outlet pressure	Equal to the lowest of the feeds

- ✓ Separator S501

Operating parameters	Value
Type of separator	Component splitter
Overhead recovery ratio	
Methanol (solvent)	0
Other components	1

1.5.3. Recovery of CO and H_2

- ✓ Valves V201 and V202

Operating parameters	Value
Type of valve	Expansion valve
Pressure (bar)	23

- ✓ Separators B101 and B102

Operating parameters	Value
Type of separator	Diphasic V-L separator
Type of flash	Constant pressure and enthalpy flash
Heat duty exchanged	Adiabatic
Pressure	The lowest of the feed streams

✓ Compressor K201 and K202

Operating parameters	Value
Exhaust pressure (bar)	35
Isentropic efficiency	
K201	0.51
K202	0.62
Mechanical efficiency	0.92

1.5.4. Recovery of CO_2

✓ Column C301

Operating parameters	Value
Type of column	Absorber with a reboiler
Number of theoretical stages	15
Feed	Stage 14
Liquid side stream at stage 4 (kmol/h)	1 080
Overhead vapor flowrate (t/h)	17.388
Overhead pressure (bar)	2.7

✓ Column C302

Operating parameters	Value
Type of column	Absorber
Number of theoretical stages	20
Feed	Stage 19
Overhead pressure (bar)	6

✓ Valves

Operating parameters	Value
Type of valve	Expansion valve
Pressure (bar)	
V301	2.7
V302	6
V303	6
V304	2.3

✓ Heat exchangers

Operating parameters	Value
Type of exchanger	Cooler / Heater
Outlet temperature (°C)	
E301	-43
E302	10
E303	-17
E304	20
E305	20
E306	20

✓ Separators B301 and B302

Operating parameters	Value
Type of separator	Diphasic V-L separator
Type of flash	Constant pressure and enthalpy flash
Heat duty exchanged	Adiabatic
Pressure	The lowest of the feed streams

✓ Compressor K301

Operating parameters	Value
Isentropic efficiency	0.84
Mechanical efficiency	0.92
Exhaust pressure (bar)	6

✓ Pumps P301 and P302

Operating parameters	Value
Type of pump	Centrifugal pump
Isentropic efficiency	0.78
Mechanical efficiency	0.92
Exhaust pressure (bar)	
P301	6
P302	2.7

✓ Splitter D101

Operating parameters	Value
Type of splitter	Stream splitter
Splitting ratio of stream 302	0.90

✓ Mixers M301 and M302

Operating parameters	Value
Type of mixer	Other mixer
Outlet pressure	Equal to the lowest of the feeds

✓ Separator S502

Operating parameters	Value
Type of separator	Component splitter
Overhead recovery ratio	
Methanol (solvent)	0
Other components	1

1.5.5. Recovery of methanol (solvent)

✓ Column C401

Operating parameters	Value
Type of column	Distillation column with partial condenser
Number of theoretical stages	10
Feed	Stage 5
Vapor distillate flowrate (kmol/h) (initial value)	1 282
Reflux flowrate (kmol/h)	5.04
Overhead pressure (bar)	1.2

Objectives / Constraints:

Specification	Value
Purity of methanol in vapor distillate (molar)	0.002
Action variable	**Value**
Vapor distillate flowrate	

✓ Valve V401

Operating parameters	Value
Type of valve	Expansion valve
Pressure (bar)	1.2

✓ Heat exchangers

Operating parameters	Value
Type of exchanger	Cooler / Heater
Outlet temperature (°C)	
E401	-42
E402	20
E501	0
E502	-50

✓ Pump P501

Operating parameters	Value
Type of pump	Centrifugal pump
Isentropic efficiency	0,78
Mechanical efficiency	0,92
Exhaust pressure (bar)	60
Fixed liquid physical state	

✓ Mixers M501 and M502

Operating parameters	Value
Type of mixer	Other mixer
Outlet pressure	Equal to the lowest of the feeds

✓ Separator S503

Operating parameters	Value
Type of separator	Component splitter
Overhead recovery ratio	
Methanol (solvent)	0
Other components	1

1.6. Initialization

Methanol flowrate and purity in the recycle loop are initialized in the inlet stream of the absorber C101 (stream 508). The flowrate and the purity have been chosen to obtain less than 2.5% molar of CO_2 in the treated gas.

The flash vapor phase recycles in the upstream columns need the initialization of two complementary streams: the bottom vapor feeds of absorbers C101 (stream 106) and C302 (stream 325).

	Regenerated Solvent (stream 508) Initialization	Bottom vapor feed of C101 (stream 106) Initialization	Bottom vapor feed of C302 (stream 325) Initialization
Temperature (°C)	-50	-20	-21
Pressure (bar)	60	60	6
Total flowrate (t/h)	750	469	146
Molar fraction			
Methanol (solvent)	1	0	0.25
Carbon dioxide	0	0.33	0.72
Hydrogen sulfide	0	0.01	0.03
Carbon monoxide	0	0.22	0
Nitrogen	0	0	0
Hydrogen	0	0.44	0

1.7. "Tips and tricks"

Component splitters S501, S502 and S503 are used for collecting the lost methanol in the treated syngas (stream 109), the CO_2 sent to storage (stream 326) and the gas sent to the Claus unit (stream 405). This quantity of methanol corresponds to the required solvent make-up. To respect the material balance, it is recycled in the process with the stream 504.

The regenerated methanol (stream 508) is almost pure. As this stream is also a tear stream, convergence difficulty can occur. To avoid this, the following elements are taken into account:

- ✓ Fixed liquid physical state for the pump P501,
- ✓ A « Constraints and recycles » module is added in the flowsheet to select the « enthalpies » and not the « temperatures » as « tear streams iterative variables ».

2. RESULTS

2.1. Mass and energy balance

This document presents only the most relevant stream results. In ProSimPlus, mass and energy balances are provided for every stream. Results are also available at the unit operation level ("report" tab in the configuration window).

Streams		101	102	106	107	108	109	202
Total flow	t/h	396.61	45.108	468.82	566.73	500.8	150.88	488.79
Total flow	kmol/h	19463	1043.7	21324	16366	14558	13794	14192
Mass fractions								
METHANOL		0	0	7.9879E-005	0.68586	0.72066	0.00015526	0.73833
CARBON DIOXIDE		0.60472	0.98652	0.65515	0.29331	0.27424	0.023713	0.26027
HYDROGEN SULFIDE		0.021742	0.0018988	0.019041	0.015716	3.9586E-005	4.4748E-008	3.9607E-005
CARBON MONOXIDE		0.32165	0.0098739	0.28088	0.004697	0.0046461	0.8397	0.0012863
NITROGEN		0.0054989	0.0011641	0.004863	5.4933E-005	5.4853E-005	0.014722	1.1991E-005
HYDROGEN		0.046396	0.00054621	0.039985	0.00035627	0.00035974	0.12171	6.1987E-005
Mole fractions								
METHANOL		0	0	5.4809E-005	0.74124	0.77369	5.3002E-005	0.79362
CARBON DIOXIDE		0.28	0.96885	0.32729	0.2308	0.21436	0.0058935	0.20368
HYDROGEN SULFIDE		0.013	0.002408	0.012283	0.015969	3.9956E-005	1.4362E-008	4.0026E-005
CARBON MONOXIDE		0.234	0.015236	0.22047	0.0058069	0.005706	0.3279	0.0015816
NITROGEN		0.004	0.001796	0.0038166	6.7906E-005	6.7357E-005	0.0057483	1.4742E-005
HYDROGEN		0.469	0.011711	0.43609	0.0061201	0.0061388	0.6604	0.001059
Physical state		Vapor	Vapor	Vapor	Liquid	Liquid	Vapor	Liquid
Temperature	°C	30	30	-15	-6.7711	-5.953	-45.5	-6.5767
Pressure	bar	35	35	60	60	60	60	23
Enthalpic flow	kW	109.48	-389.02	-11556	-1.5554E005	-1.4143E005	-8370.7	-1.4126E005
Vapor molar fraction		1	1	1	0	0	1	0

Streams		203	206	207	303	305	306	307
Total flow	t/h	12.01	551.64	15.087	439.91	48.879	803.51	36.655
Total flow	kmol/h	366.31	15915	450.75	12773	1419.2	24676	1080
Mass fractions								
METHANOL		0.0014714	0.70458	0.001311	0.73833	0.73833	0.93278	0.78881
CARBON DIOXIDE		0.84283	0.27834	0.84084	0.26027	0.26027	0.056394	0.20403
HYDROGEN SULFIDE		3.8719E-005	0.015752	0.014399	3.9607E-005	3.9607E-005	0.010823	0.0071648
CARBON MONOXIDE		0.14138	0.0012552	0.13054	0.0012863	0.0012863	0	0
NITROGEN		0.0017992	1.1476E-005	0.0016439	1.1991E-005	1.1991E-005	0	0
HYDROGEN		0.012477	5.7895E-005	0.011266	6.1987E-005	6.1987E-005	0	0
Mole fractions								
METHANOL		0.0015056	0.76219	0.0013694	0.79362	0.79362	0.94793	0.83552
CARBON DIOXIDE		0.62792	0.21922	0.63947	0.20368	0.20368	0.041726	0.15734
HYDROGEN SULFIDE		3.725E-005	0.016021	0.014141	4.0026E-005	4.0026E-005	0.01034	0.0071351
CARBON MONOXIDE		0.16549	0.0015533	0.15599	0.0015816	0.0015816	0	0
NITROGEN		0.0021058	1.42E-005	0.0019641	1.4742E-005	1.4742E-005	0	0
HYDROGEN		0.20294	0.00099547	0.18706	0.001059	0.001059	0	0
Physical state		Vapor	Liquid	Vapor	Liq./Vap.	Liq./Vap.	Liquid	Liquid
Temperature	°C	-6.5767	-7.7572	-7.7572	-43.28	-51.913	-14.489	-50.543
Pressure	bar	23	23	23	6	2.7	2.7	2.7
Enthalpic flow	kW	-169.87	-1.5532E005	-220.45	-1.3807E005	-15341	-2.7913E005	-12242
Vapor molar fraction		1	0	1	0.0080513	0.055557	0	0

Streams		309	312	313	315	317	318	322
Total flow	t/h	17.388	551.64	219.53	919.86	40.82	879.04	70.373
Total flow	kmol/h	397.41	15915	5033.4	27286	934.45	26351	1617
Mass fractions								
METHANOL		0.00015711	0.70458	0.00028295	0.8072	0.00156	0.84461	0.0017194
CARBON DIOXIDE		0.99575	0.27834	0.99363	0.17923	0.97477	0.14229	0.96192
HYDROGEN SULFIDE		0.00026588	0.015752	3.6659E-005	0.013574	0.023665	0.013105	0.036358
CARBON MONOXIDE		0.0036158	0.0012552	0.0057315	2.018E-007	4.2896E-006	1.1975E-008	1.4791E-007
NITROGEN		3.3706E-005	1.1476E-005	5.2864E-005	1.0956E-009	2.3581E-008	5.1471E-011	6.371E-010
HYDROGEN		0.00017425	5.7895E-005	0.00026969	2.4757E-009	5.3982E-008	8.3898E-011	1.0415E-009
Mole fractions								
METHANOL		0.00021454	0.76219	0.00038514	0.84928	0.0021267	0.87932	0.0023353
CARBON DIOXIDE		0.98996	0.21922	0.98473	0.13729	0.96753	0.10785	0.95124
HYDROGEN SULFIDE		0.00034133	0.016021	4.6914E-005	0.013427	0.030332	0.012828	0.046428
CARBON MONOXIDE		0.0056481	0.0015533	0.0089247	2.4288E-007	6.6898E-006	1.4262E-008	2.2982E-007
NITROGEN		5.2645E-005	1.42E-005	8.2307E-005	1.3185E-009	3.6771E-008	6.1292E-011	9.8978E-010
HYDROGEN		0.003782	0.00099547	0.005835	4.1402E-008	1.1698E-006	1.3883E-009	2.2485E-008
Physical state		Vapor	Liq./Vap.	Vapor	Liquid	Vapor	Liquid	Vapor
Temperature	°C	-51.269	-11.313	-37.227	-24.372	-17	-17	20
Pressure	bar	2.7	6	6	6	6	6	6
Enthalpic flow	kW	-314.82	-1.4778E005	-3585.7	-2.9518E005	-475.88	-2.8632E005	-198.17
Vapor molar fraction		1	0.15195	1	0	1	0	1

Streams		324	325	403	404	504	508
Total flow	t/h	808.67	147.85	749.42	54.092	0.17077	749.59
Total flow	kmol/h	24734	3631.5	23389	1287.4	5.3296	23394
Mass fractions							
METHANOL		0.91796	0.19681	1	0.0015252	1	1
CARBON DIOXIDE		0.070961	0.77757	4.3343E-010	0.83771	0	4.3333E-010
HYDROGEN SULFIDE		0.011082	0.025615	1.0379E-007	0.16077	0	1.0377E-007
CARBON MONOXIDE		1.4553E-010	1.2547E-006	0	0	0	0
NITROGEN		5.0708E-013	6.8136E-009	0	0	0	0
HYDROGEN		5.6502E-013	1.54E-008	0	0	0	0
Mole fractions							
METHANOL		0.93665	0.25007	1	0.002	1	1
CARBON DIOXIDE		0.052717	0.71933	3.1557E-010	0.7998	0	3.155E-010
HYDROGEN SULFIDE		0.010631	0.0306	9.7582E-008	0.1982	0	9.7557E-008
CARBON MONOXIDE		1.6986E-010	1.8238E-006	0	0	0	0
NITROGEN		5.9182E-013	9.9024E-009	0	0	0	0
HYDROGEN		9.1638E-012	3.1102E-007	0	0	0	0
Physical state		Liquid	Liq./Vap.	Liquid	Vapor	Liquid	Liquid
Temperature	°C	-27.609	-22.548	68.759	-36.719	18.889	-48.452
Pressure	bar	2.7	6	1.2	1.2	1.2	60
Enthalpic flow	kW	-2.854E005	-12910	-2.2442E005	-803.39	-57.998	-2.9055E005
Vapor molar fraction		0	0.70826	0	1	0	0

2.2. Process performance

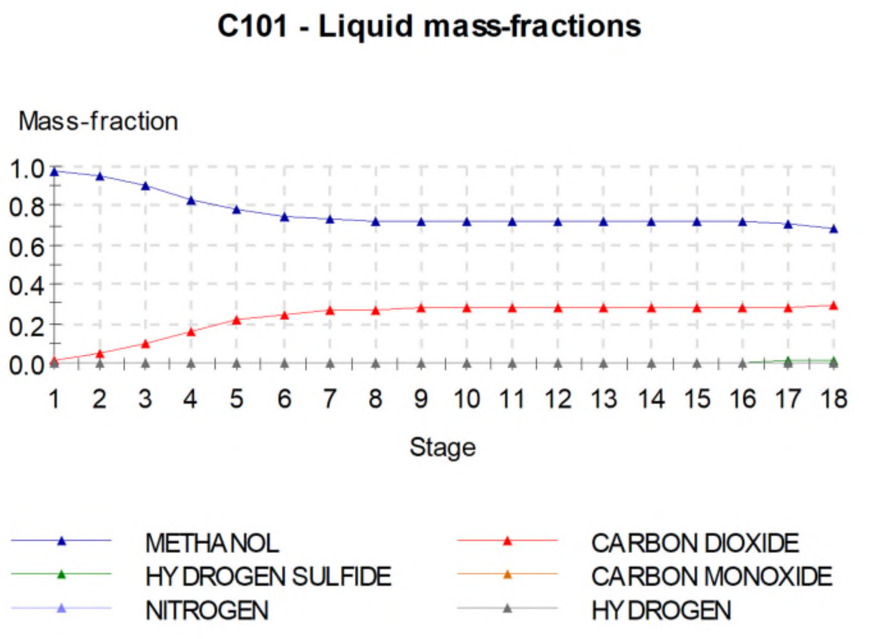
The following table presents compositions of H_2, CO_2 and H_2S in the raw syngas, the treated syngas, the CO_2 sent to storage and the H_2S sent to Claus unit.

Component	Raw syngas	Treated syngas	CO_2 in the storage	H_2S to Claus unit
H_2	46.9% mol.	66.0% mol.	0.6% mol.	traces
H_2S	1.3% mol.	traces	0.01% mol.	19.8% mol.
CO_2	28.0% mol.	0.6% mol.	98.5% mol.	80.0% mol.

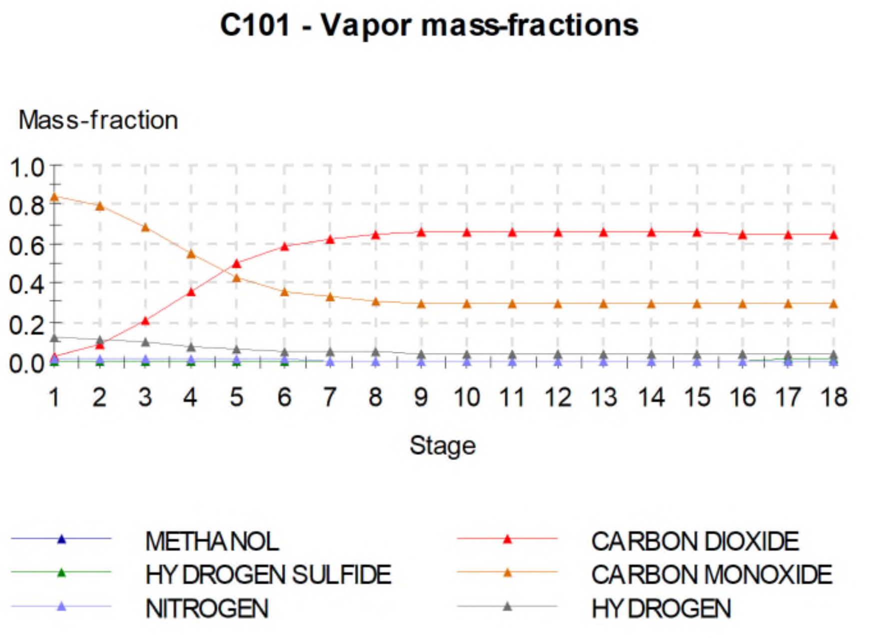
2.3. Columns profiles

In ProSimPlus, column stages are numbered from top to bottom (first stage corresponds to the condenser if present and the last stage to the reboiler if present).

2.3.1. Absorber C101

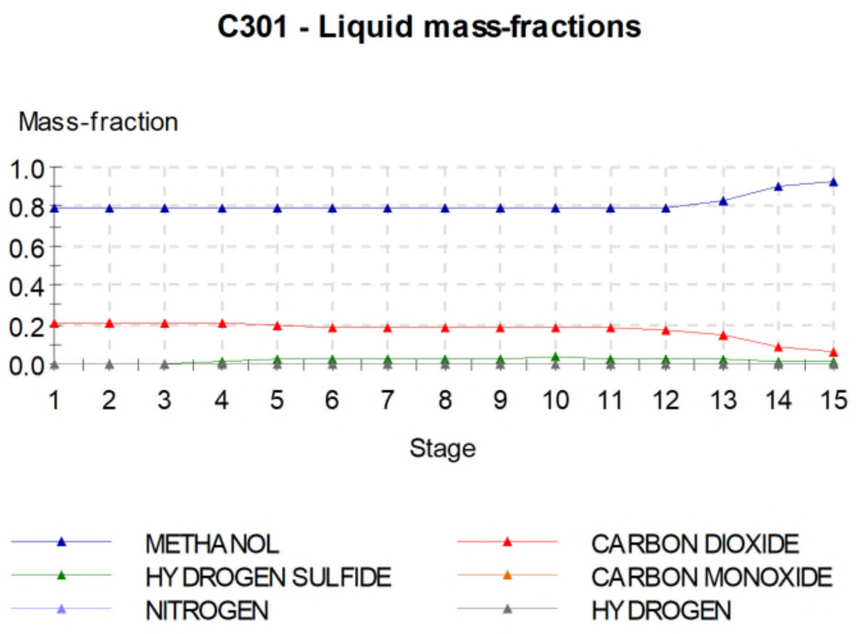


Liquid mass-fractions profile in the column

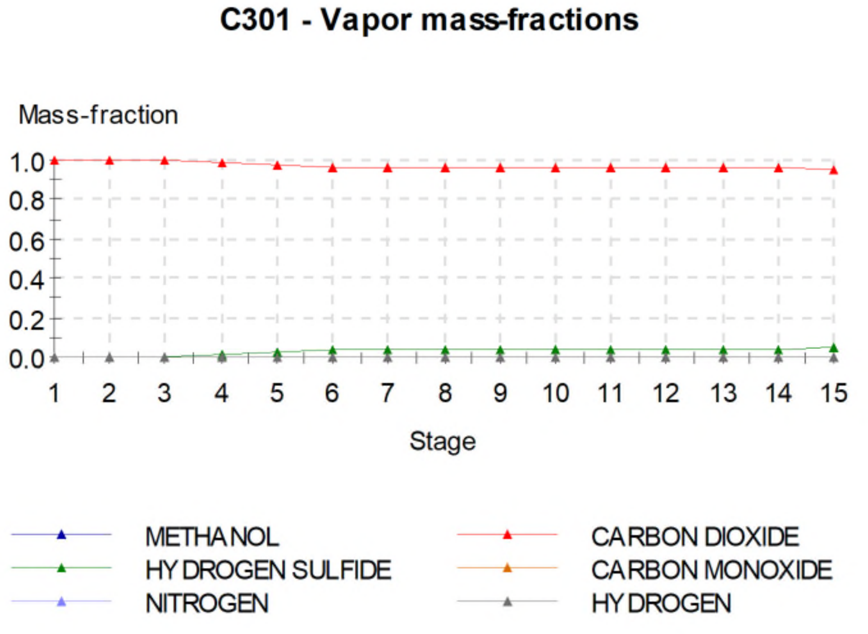


Vapor mass-fractions profile in the column

2.3.2. Column C301

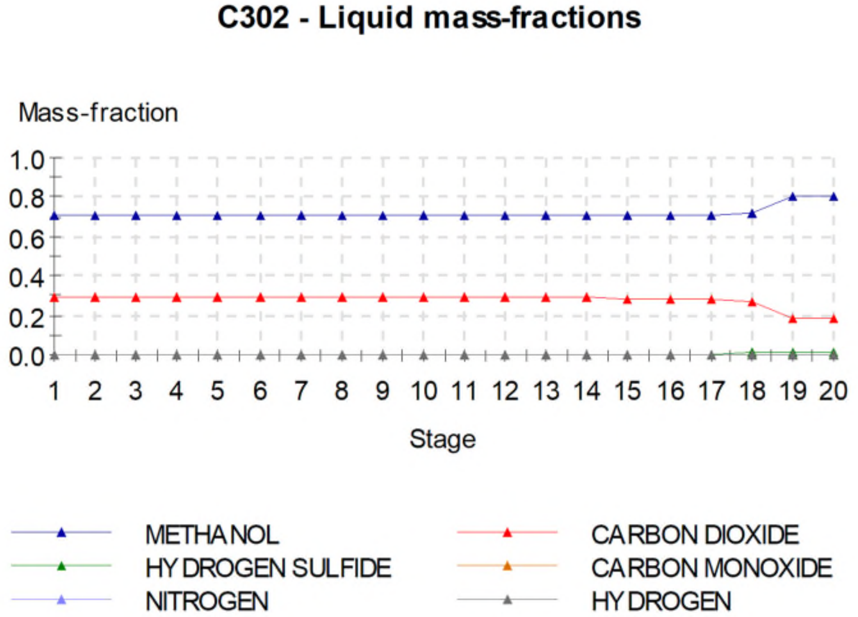


Liquid mass-fractions profile in the column

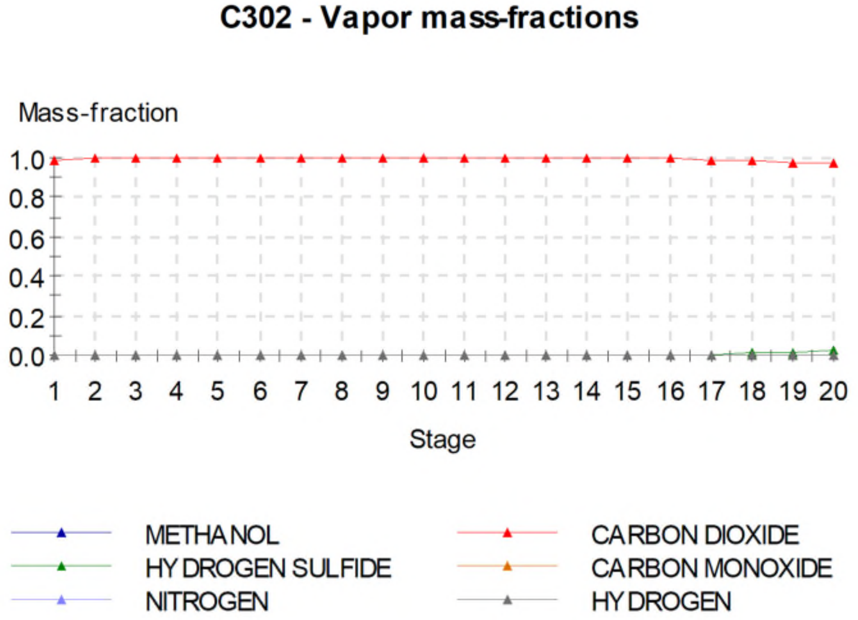


Vapor mass-fractions profile in the column

2.3.3. Column C302

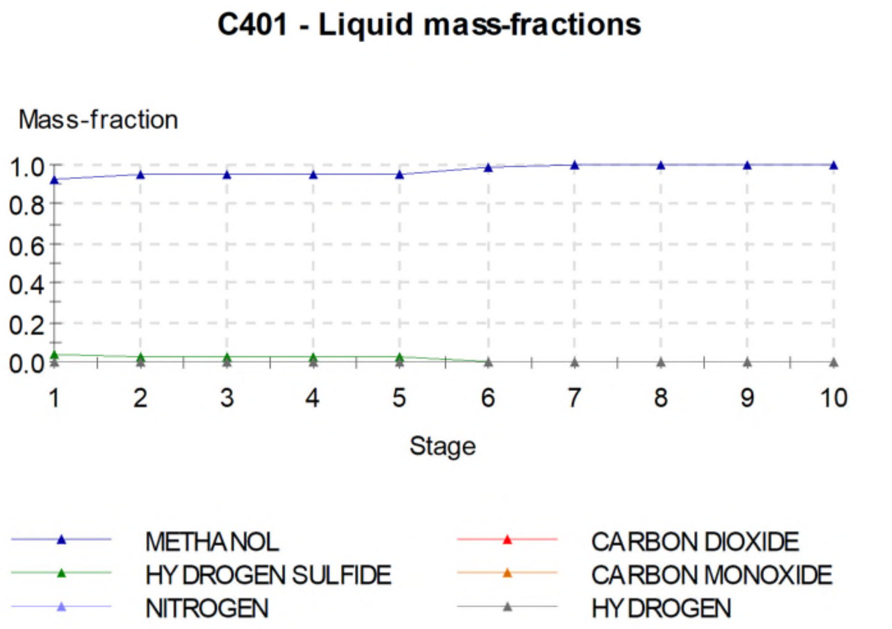


Liquid mass-fractions profile in the column

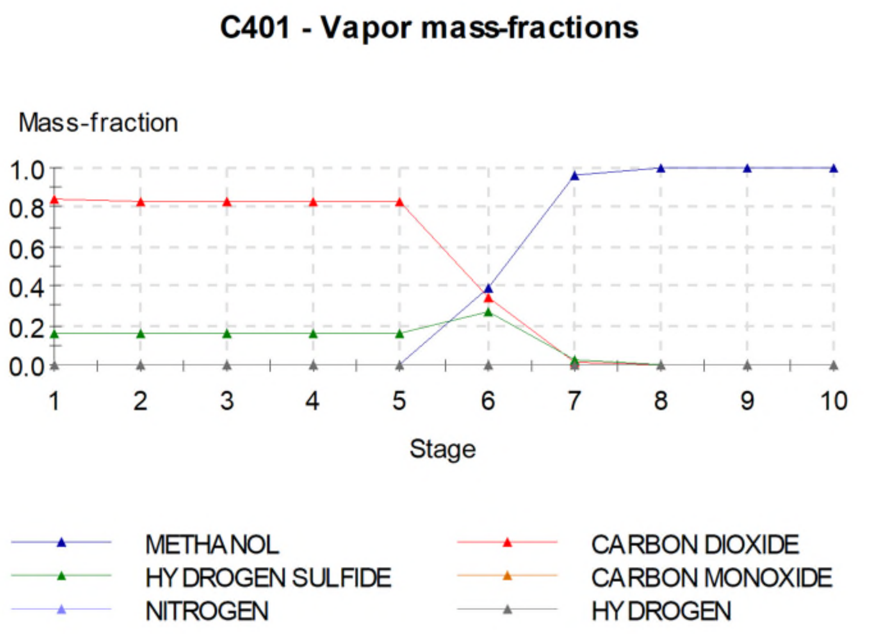


Vapor mass-fractions profile in the column

2.3.4. Column C401



Liquid mass-fractions profile in the column



Vapor mass-fractions profile in the column

3. REFERENCES

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