PROSIMPLUS APPLICATION EXAMPLE

NATURAL GAS DEACIDIFICATION

WITH SELEXOL PROCESS

EXAMPLE PURPOSE
This example illustrates a natural gas deacidification with the Selexol process. Selexol, mixture of polyethylene glycol dimethyl ether, is used as the solvent. The deacidification is done through a contactor and the solvent regeneration needs three successive flashes. The process objective is to highly decrease the CO_2 composition of the input gas. Selexol make-up is automatically calculated with simple modules. This example is taken from [RAN76] publication which describes main features of this process.

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1. PROCESS MODELING

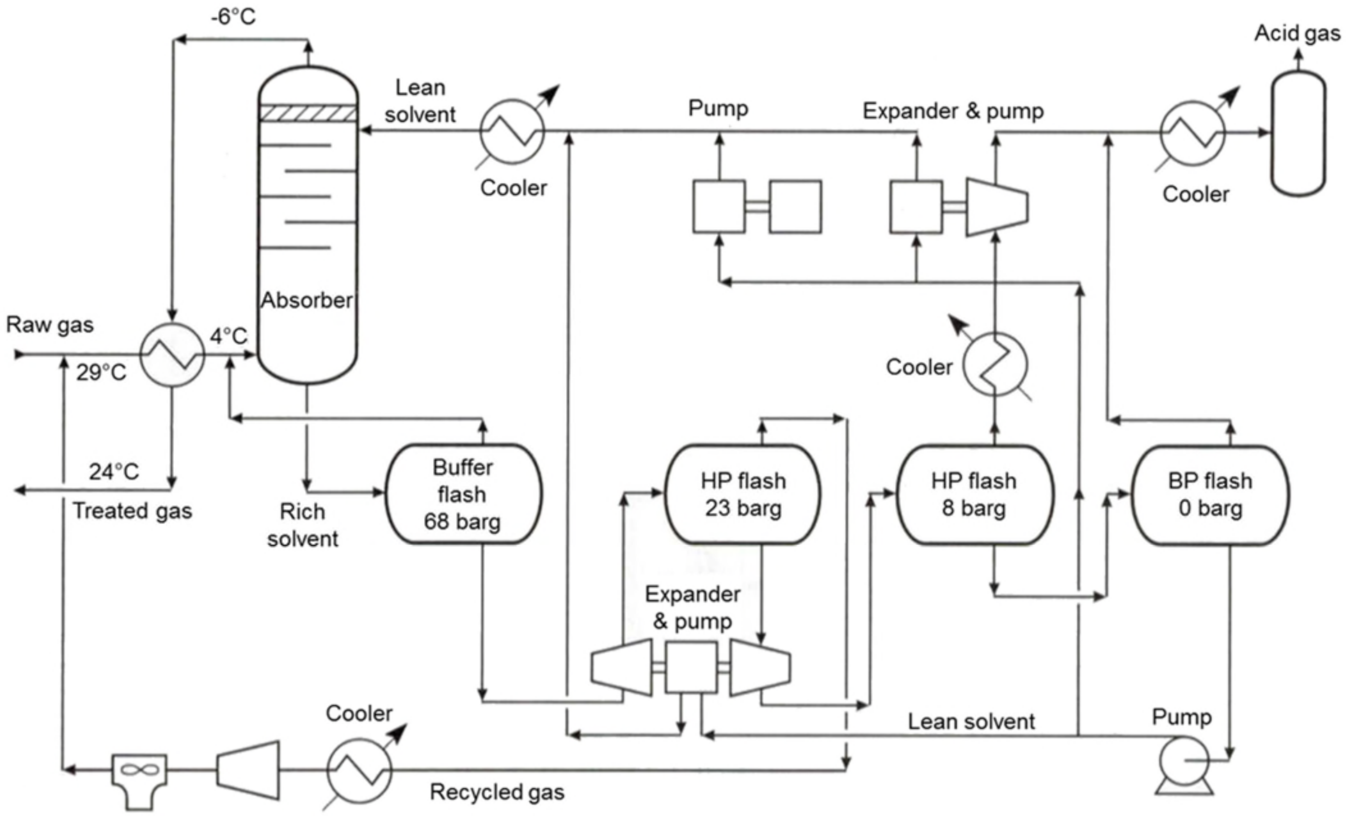
1.1. Process description

Selexol process is used to eliminate selectively or simultaneously sulfur compounds, carbon dioxide and water from a gas or an air stream (example given an H_2S rich feed for a Claus unit). Selexol, the solvent, is a mixture of polyethylene glycol dimethyl ether (PGDE). There are several applications of this process:

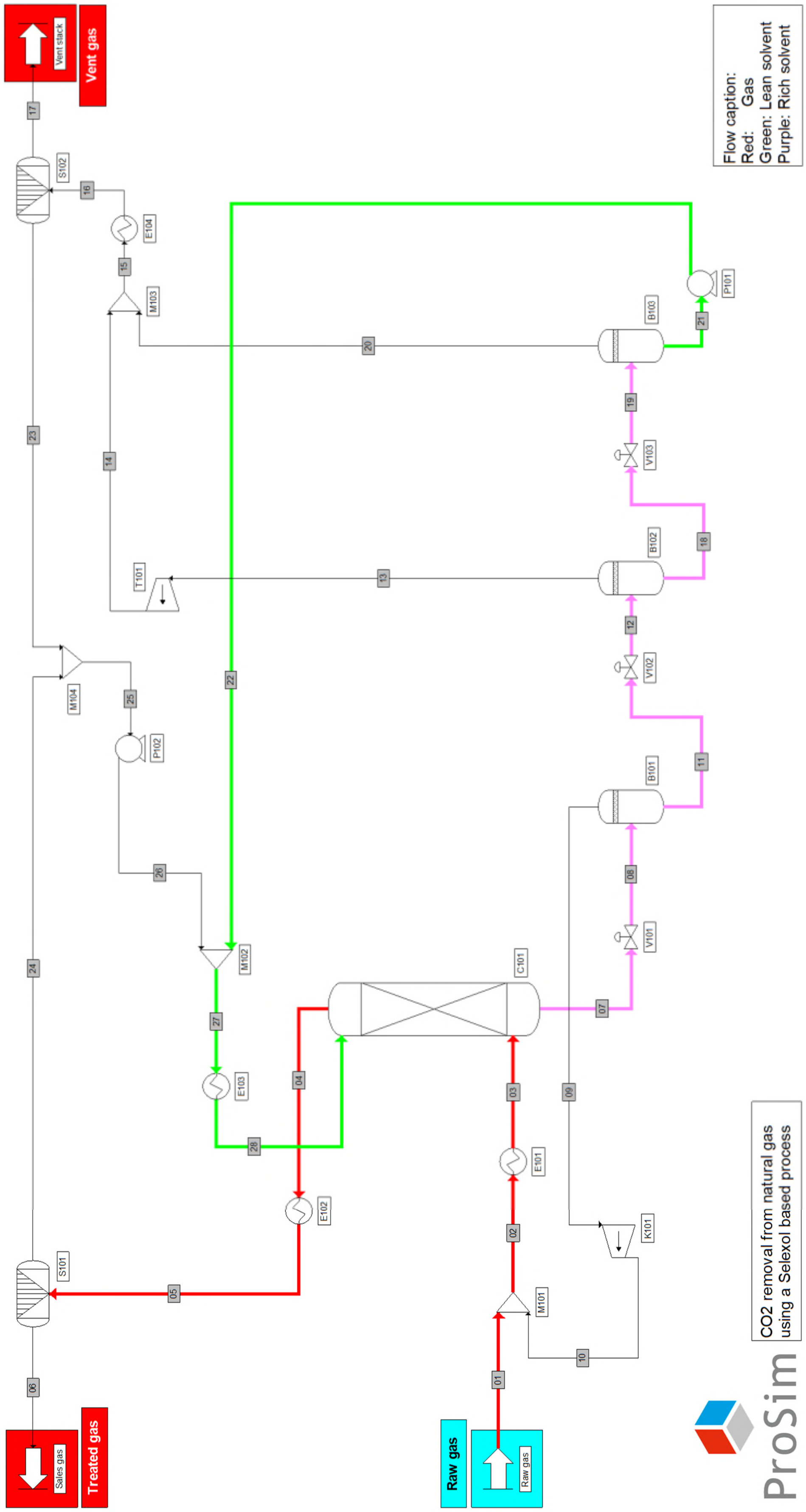
- ✓ Removal of CO_2 from ammonia production,
- ✓ Removal of CO_2 and H_2S from natural gas, syngas, gas coming from gasification,
- ✓ Purification of gas coming from biodegradation of municipal waste.

The process is described based on the process scheme of the section 1.2. The names of the equipment and the streams refer to the simulation flowsheet presented in the section 1.3. The gas to be treated (stream 01) is first cooled in the heat exchanger E101 before entering the absorber C101 at the bottom (stream 03). The regenerated solvent (stream 28) feeds the absorber C101 at the top. The treated gas leaves the absorber overhead (stream 04) and the enriched solvent with acid components and dissolved hydrocarbons leaves at the bottom (stream 07). The solvent is regenerated with three successive expansion valves (V101, V102 and V103) from operating pressure of the absorber (68 barg) to the atmospheric pressure. The vapor phase coming from the first expansion (stream 09), methane rich, is compressed and recycled at the input of the process. Vapor phases coming from the two other expansions (streams 13 and 20) are sent to the flare. Turbine T101 allows saving energy on the vapor coming from the second expansion (stream 13). Liquid phase going out of the last expansion valve (stream 21) corresponds to the regenerated solvent. Stream 26 is the Selexol make-up. The flash drum at the bottom of the absorber, only used for physical withdrawn of entrained gas (§ 1.2), it is not represented on the flowsheet (§ 1.3).

1.2. Process Scheme



1.3. Simulation flowsheet



1.4. Components

Components taken into account in the simulation, their chemical formula and CAS number are presented in the following table. Selexol is represented with one of its component, tetraethylene glycol dimethyl ether. It is the component chosen by [CLA02] to present equilibrium data of the solvent, similar to Selexol. Pure components physical properties are extracted from the ProSimPlus standard database [ROW11].

Component name	Chemical formula	CAS number
Methane	CH_4	74-82-8
Ethane	C_2H_6	74-84-0
Propane	C_3H_8	74-98-6
Nitrogen	N_2	7727-37-9
Carbon dioxide	CO_2	124-38-9
Hydrogen sulfide	H_2S	7783-06-4
Tetraethylene glycol dimethyl ether (solvent)	$C_{10}H_{22}O_5$	143-24-8

1.5. 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.

1.6. Operating conditions

✓ Process feed

	Raw Gas
Temperature (°C)	29,44
Pressure (barg)	68
Total flowrate (Nm^3/h)	110 170
Molar fraction	
Methane	0.547038
Ethane	0.005601
Propane	0.001400
Nitrogen	0.005901
Carbon dioxide	0.440000
Hydrogen sulfide	0.000060
Solvent	0

✓ Absorber C101

Operating parameters	Value
Type of column	Absorbeur
Number of theoretical stages	10
Overhead pressure (bar)	66.21
Pressure drop (barg)	0.71

✓ Valves

Operating parameters	Value
Type of valve	Expansion valve
Pressure (barg)	
V101	22.77
V102	7.95
V103	0.09

✓ Separators B101, B102 and B103

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

- ✓ Heat exchangers

Operating parameters	Value
Type of exchanger	Cooler / Heater
Outlet temperature (°C)	
E101	4.44
E102	20
E103	-6
E104	20

- ✓ Compressor K101

Operating parameters	Value
Isentropic efficiency	0.65
Mechanical efficiency	1
Exhaust pressure (barg)	68

- ✓ Expander T101

Operating parameters	Value
Isentropic efficiency	0.65
Outlet pressure (barg)	0.09

- ✓ Pumps P101 and P102

Operating parameters	Value
Type of pump	Centrifugal Pump
Volumetric efficiency	0.65
Mechanical efficiency	1
Exhaust pressure (barg)	68

- ✓ Mixers M101, M102, M103 and M104

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

✓ Separators S101 and S102

Operating parameters	**Value**
Type of separator	Component splitter
Overhead recovery ratio	
Selexol	0
Other components	1

1.7. Initialization

Selexol flowrate and purity in the recycle loop are initialized in the enriched solvent stream entering the absorber C101 (stream 28). The flowrate and the purity have been chosen to obtain less than 3% molar of CO_2 in the treated gas.

	Enriched solvent (stream 28) Initialization
Temperature (°C)	-6
Pressure (barg)	68
Total flowrate	1 038 500 kg/h
	Mass fraction
Methane	0
Ethane	0
Propane	0
Nitrogen	0
Carbon dioxide	0.015
Hydrogen sulfide	0
Solvent	0.985

1.8. "Tips and tricks"

Component splitters S101 and S102 are used for collecting the lost solvent (Selexol) in the treated gas (stream 05) and in the vapor streams sent to the vent (stream 16). This quantity of Selexol corresponds to the required solvent make-up. To respect the material balance, it is recycled in the process with the stream 25.

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		01	03	04	05	07	10
Total flow	kg/h	1.4027E005	1.9254E005	44529	44529	1.189E006	52271
Total flow	Nm3/h	1.1017E005	1.4611E005	58794	58794	1.997E005	35939
Mass fractions							
Selexol		0	6.8525E-007	3.5336E-006	3.5336E-006	0.8603	2.5241E-006
CARBON DIOXIDE		0.67855	0.70851	0.07172	0.07172	0.12716	0.78889
NITROGEN		0.0057926	0.0044366	0.018207	0.018207	3.6573E-005	0.00079777
METHANE		0.30752	0.27769	0.90675	0.90675	0.011012	0.19763
ETHANE		0.0059016	0.0072506	0.0028815	0.0028815	0.001091	0.010871
PROPANE		0.0021633	0.0020589	0.00042274	0.00042274	0.00038008	0.0017788
HYDROGEN SULFIDE		7.1655E-005	6.1451E-005	1.1432E-005	1.1432E-005	2.4362E-005	3.407E-005
Mole fractions							
Selexol		0	9.1056E-008	2.6987E-007	2.6987E-007	0.51652	3.7018E-007
CARBON DIOXIDE		0.44	0.47551	0.027665	0.027665	0.38561	0.58435
NITROGEN		0.005901	0.0046778	0.011033	0.011033	0.00017424	0.00092835
METHANE		0.54704	0.51126	0.95951	0.95951	0.091609	0.40159
ETHANE		0.005601	0.0071222	0.0016268	0.0016268	0.004842	0.011785
PROPANE		0.0014	0.0013791	0.00016275	0.00016275	0.0011503	0.001315
HYDROGEN SULFIDE		6E-005	5.3257E-005	5.6945E-006	5.6945E-006	9.5398E-005	3.2589E-005
Physical state		Vapor	Vapor	Vapor	Vapor	Liquid	Vapor
Temperature	°C	29.44	4.44	-2.4146	20	28.021	135.26
Pressure	barg	68	68	66.21	66.21	66.92	68
Enthalpic flow	kcal/h	-2.012E006	-5.0702E006	-1.5064E006	-8.6177E005	-8.7686E007	1.2582E006
Vapor molar fraction		1	1	1	1	0	1

Streams		11	14	16	18	20	21
Total flow	kg/h	1.1368E006	38924	95741	1.0978E006	56817	1.041E006
Total flow	Nm3/h	1.6376E005	22041	51376	1.4172E005	29335	1.1238E005
Mass fractions							
Selexol		0.89985	9.5575E-007	7.0627E-007	0.93176	5.3535E-007	0.98261
CARBON DIOXIDE		0.096733	0.9261	0.96079	0.067328	0.98455	0.017268
NITROGEN		1.5719E-006	4.4994E-005	1.8663E-005	3.235E-008	6.2433E-007	4.1472E-011
METHANE		0.0024311	0.061475	0.028814	0.00033767	0.006439	4.6673E-006
ETHANE		0.00064126	0.0099987	0.0073061	0.00030949	0.0054615	2.8304E-005
PROPANE		0.00031576	0.002327	0.0029727	0.00024445	0.0034151	7.1402E-005
HYDROGEN SULFIDE		2.3915E-005	4.9919E-005	9.9652E-005	2.2993E-005	0.00013372	1.695E-005
Mole fractions							
Selexol		0.62988	1.702E-007	1.3271E-007	0.72785	1.0455E-007	0.91784
CARBON DIOXIDE		0.34199	0.83295	0.91186	0.26563	0.97116	0.081466
NITROGEN		8.7306E-006	6.3576E-005	2.7827E-005	2.0051E-007	9.6749E-007	3.0738E-010
METHANE		0.023578	0.15168	0.075021	0.0036547	0.017424	6.0406E-005
ETHANE		0.0033182	0.013162	0.010149	0.0017872	0.0078849	0.00019544
PROPANE		0.0011141	0.0020888	0.0028158	0.00096256	0.0033621	0.0003362
HYDROGEN SULFIDE		0.00010918	5.7978E-005	0.00012213	0.00011715	0.00017033	0.00010326
Physical state		Liquid	Vapor	Vapor	Liquid	Vapor	Liquid
Temperature	°C	20.416	-67.14	20	10.926	-8.8254	-8.8254
Pressure	barg	22.77	0.09	0.09	7.95	0.09	0.09
Enthalpic flow	kcal/h	-8.7335E007	-7.733E005	-1.2573E005	-8.7128E007	-4.0332E005	-8.6725E007
Vapor molar fraction		0	1	1	0	1	0

Streams		26	28
Total flow	kg/h	0.22497	1.041E006
Total flow	Nm3/h	0.022685	1.1238E005
Mass fractions			
Selexol		1	0.98261
CARBON DIOXIDE		0	0.017268
NITROGEN		0	4.1472E-011
METHANE		0	4.6673E-006
ETHANE		0	2.8304E-005
PROPANE		0	7.14E-005
HYDROGEN SULFIDE		0	1.6949E-005
Mole fractions			
Selexol		1	0.91784
CARBON DIOXIDE		0	0.081466
NITROGEN		0	3.0738E-010
METHANE		0	6.0406E-005
ETHANE		0	0.00019544
PROPANE		0	0.00033619
HYDROGEN SULFIDE		0	0.00010326
Physical state		Liquid	Liquid
Temperature	°C	26.79	-6
Pressure	barg	68	68
Enthalpic flow	kcal/h	-16.133	-8.4122E007
Vapor molar fraction		0	0

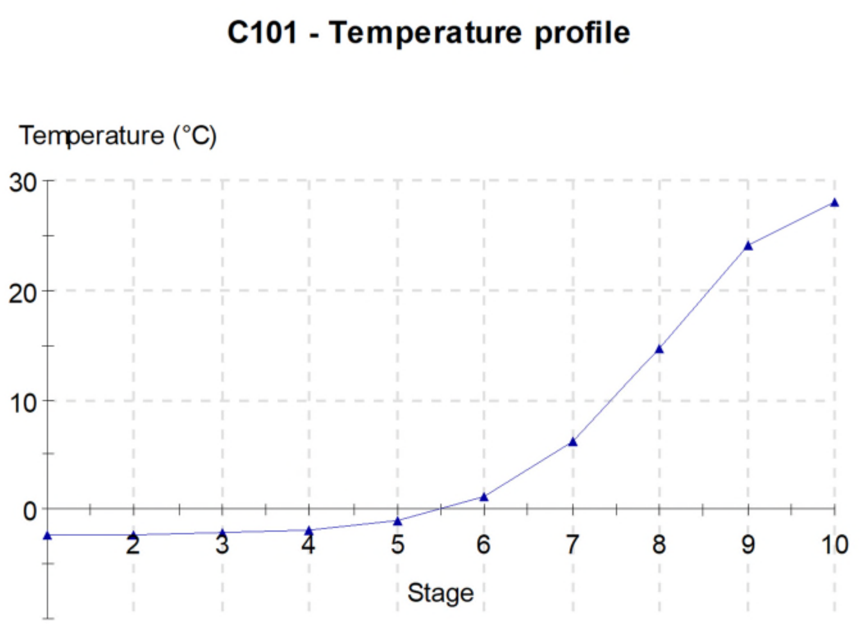
2.2. Process performance

The following table presents compositions of CO_2 and H_2S in the raw gas and in the treated syngas.

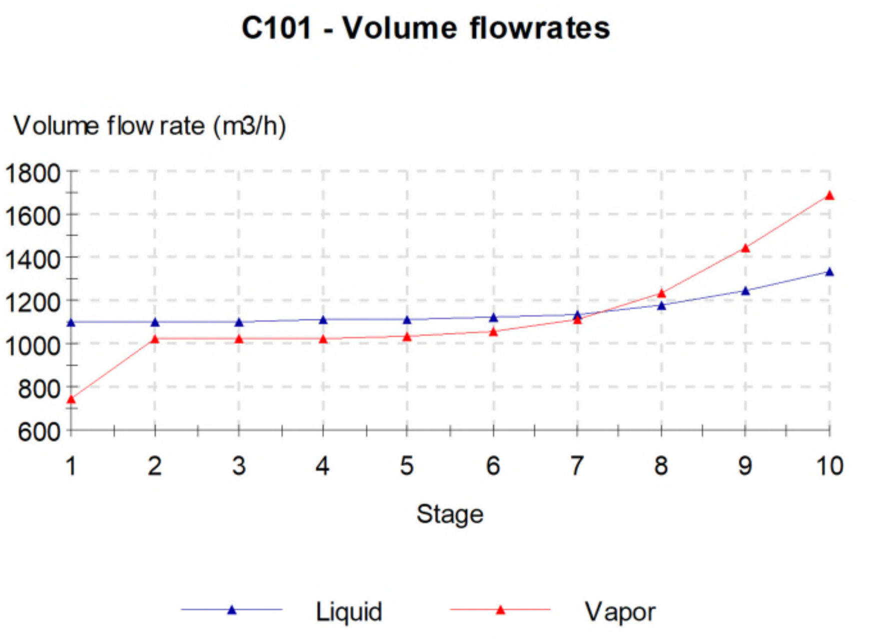
Component	Raw gas	Treated gas
CO_2	44% mol.	2.8% mol.
H_2S	60 ppm mol.	6 ppm mol.

2.3. Columns profiles

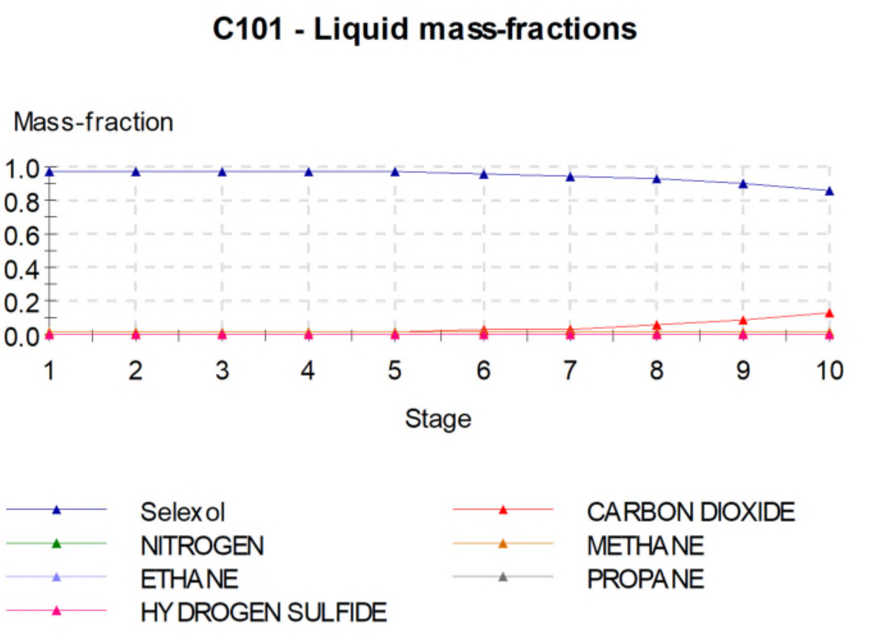
In ProSimPlus, column stages are numbered from top to bottom. The following graphs present the profiles in the absorber.



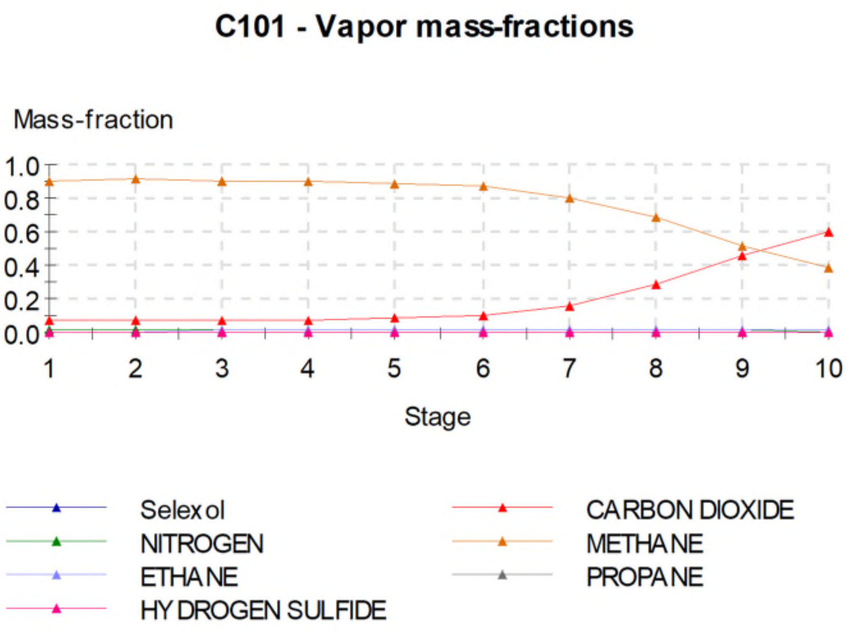
Temperature profile in the column



Volume flow rates profile in the column



Liquid mass-fractions profile in the column



Vapor mass-fractions profile in the column

3. REFERENCES

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[ROW11] ROWLEY R.L., WILDING W.V., OSCARSON J.L., GILES N.F., “DIPPR® Data Compilation of Pure Chemical Properties”, Design Institute for Physical Properties, AIChE, New York, NY (2011)

