PROSIMPLUS APPLICATION EXAMPLE

GAS DEACIDIFICATION

WITH PURISOL PROCESS

EXAMPLE PURPOSE
This example illustrates a gas deacidification of a hydrogen stream with the Purisol process. N-Methyl-2-Pyrrolidone (NMP) 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. NMP make-up is automatically calculated with simple modules. This example is taken from [KOH97] publication which describes main features of this process.

ACCESS	☑ Free Internet	☐ Restricted to clients	☐ Restricted	☐ Confidential

CORRESPONDING PROSIMPLUS FILES	*PSPS_EX_EN-Purisol-Process.pmp3*

Reader is reminded that this use case is only an example and should not be used for other purposes. Although this example is based on actual case it may not be considered as typical nor are the data used always the most accurate available. Fives ProSim shall have no responsibility or liability for damages arising out of or related to the use of the results of calculations based on this example.

Energy

Fives ProSim

Siège social : Immeuble Stratège A - 51 rue Ampère - 31670 Labège - FRANCE

Tél. : +33 (0)5 62 88 24 30

S.A.S. au capital de 147 800 € - 350 476 487 R.C.S. Toulouse - Siret 350 476 487 00037 - APE 5829C - N° TVA FR 10 350 476 487

www.fivesgroup.com / www.fives-prosim.com

TABLE OF CONTENTS

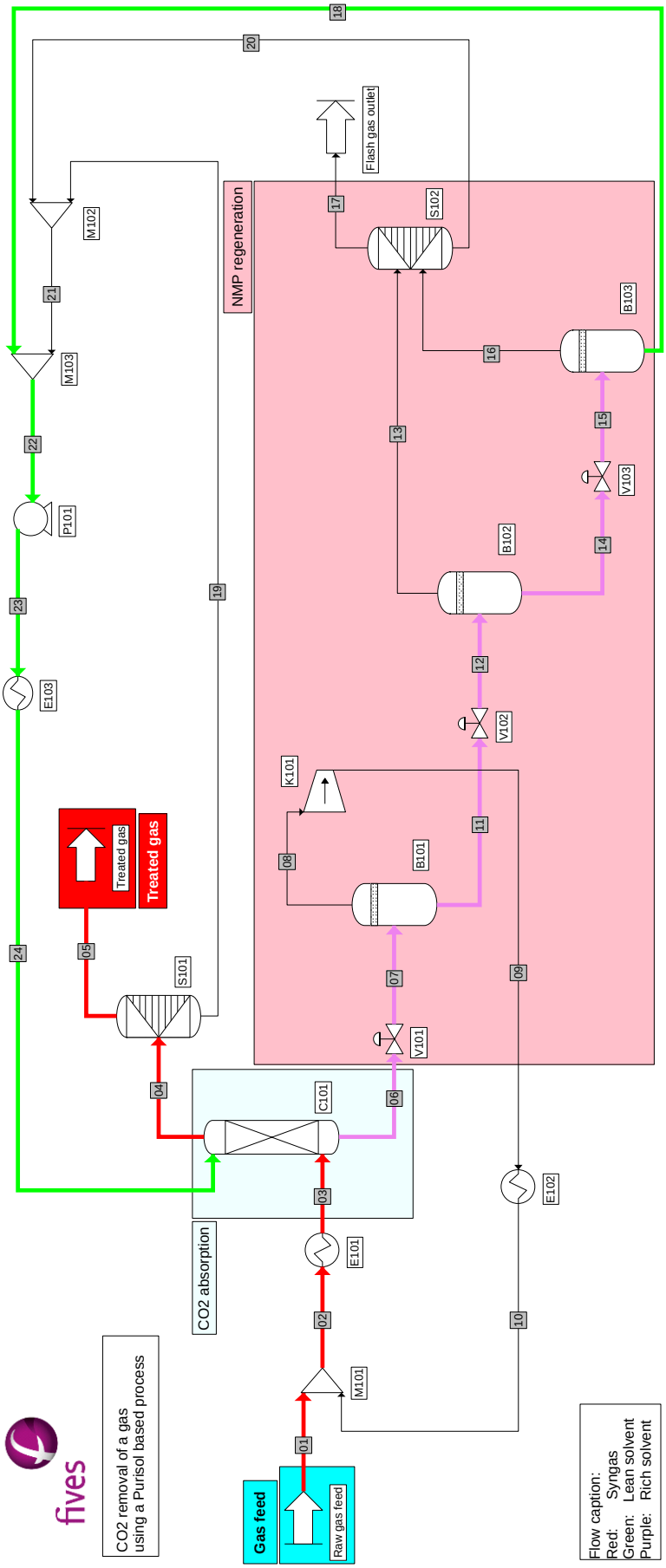
1. PROCESS MODELING

1.1. Process description

Purisol process uses N-Methyl-2-Pyrrolidone (NMP) as solvent. This process is particularly adapted for syngas purification at high pressure and high content of CO_2 for turbines of Integrated Gasification Combined Cycle (IGCC) due to its high selectivity with respect to H_2S. Purisol process also allows eliminating the COS impurity.

The process is described based on the simulation flowsheet of the section 1.2. The gas to be treated (stream 01) is first cooled in the heat exchanger E101 before entering the bottom of the absorber C101 (stream 03). The regenerated solvent (stream 24) is fed at the top of the absorber C101. The treated gas leaves the absorber overhead (stream 04) and the solvent enriched with acid components and dissolved hydrocarbons leaves at the bottom (stream 06). Solvent is regenerated with three successive expansion valves (V101, V102, V103) from operating pressure of the absorber (32 bars) to the atmospheric pressure. The vapor phase coming from the first expansion (stream 08), hydrogen rich, is compressed and recycled at the input of the process. Vapor phases coming from the two other expansions (streams 13 and 16) leave the process. Liquid phase going out of the last expansion valve (stream 18) corresponds to the regenerated solvent. Stream 21 is the NMP make-up.

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
Hydrogen	H_2	1333-74-0
Nitrogen	N_2	7727-37-9
Carbon monoxide	CO	630-08-0
Methane	CH_4	74-82-8
Carbon dioxide	CO_2	124-38-9
N-methyl-2-pyrrolidone (solvent)	C_5H_9NO	872-50-4

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

✓ Process feed

	Raw Gas
Temperature (°C)	40
Pressure (bar)	32
Total flowrate (Nm^3/h)	110 000
Molar fraction	
Hydrogen	0.6453
Nitrogen	0.0038
Carbon monoxide	0.0150
Methane	0.0044
Carbon dioxide	0.3315
Solvent	0

✓ Absorber C101

Operating parameters	Value
Type of column	Absorber
Number of theoretical stages	10
Overhead pressure (bar)	32

✓ Valves

Operating parameters	Value
Type of valve	Expansion valve
Pressure (bar)	
V101	11
V102	5
V103	1.1

✓ 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 E101, E102 and E103

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

✓ Compressor K101

Operating parameters	Value
Isentropic efficiency	0.84
Mechanical efficiency	1
Exhaust pressure (bar)	32

✓ Pump P101

Operating parameters	Value
Type of pump	Centrifugal Pump
Volumetric efficiency	0.65
Mechanical efficiency	1
Exhaust pressure (bar)	32

✓ Mixers M101, M102 and M103

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	
N-methyl-2-pyrrolidone (solvent)	0
Other components	1

1.6. Initialization

N-methyl-2-pyrrolidone flowrate and purity in the recycle loop are initialized in the enriched solvent stream leaving the absorber C101 (stream 06). The flowrate and the purity have been chosen to obtain less than 4% molar of CO_2 in the treated gas.

	Enriched solvent (stream 06) Initialization
Temperature (°C)	-2
Pressure (bar)	32
Partial mass flowrate (kg/h)	
Hydrogen	0
Nitrogen	0
Carbon monoxide	0
Methane	0
Carbon dioxide	83 541
Solvant	700 000

1.7. "Tips and tricks"

Component splitters S101 and S102 are used for collecting the lost solvent (NMP) in the treated gas (stream 04) and in the vapor streams coming from the flashes (streams 13 and 16). This quantity of NMP corresponds to the required solvent make-up. To respect the material balance, it is recycled in the process with the stream 21.

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	06	09	10	11
Total flow	kg/h	80914	83401	14951	7.8208E005	2487.1	2487.1	7.796E005
Total flow	Nm3/h	1.1E005	1.1172E005	76324	2.0061E005	1719.8	1719.8	1.9889E005
Mass fractions								
HYDROGEN		0.078901	0.077039	0.42659	6.032E-005	0.016471	0.016471	7.9684E-006
NITROGEN		0.0064566	0.0063283	0.034847	8.6814E-006	0.0021555	0.0021555	1.8326E-006
CARBON MONOXIDE		0.025484	0.025064	0.13721	4.9771E-005	0.011414	0.011414	1.3518E-005
METHANE		0.0042813	0.0042715	0.022271	2.977E-005	0.0039522	0.0039522	1.7257E-005
CARBON DIOXIDE		0.88488	0.8873	0.37907	0.10481	0.96599	0.96599	0.10206
N-METHYL-2-PYRROLIDONE		0	4.1324E-007	1.1961E-005	0.89504	1.3858E-005	1.3858E-005	0.8979
Mole fractions								
HYDROGEN		0.6453	0.63944	0.92912	0.0026146	0.26484	0.26484	0.00034728
NITROGEN		0.0038	0.0037799	0.0054617	2.7079E-005	0.0024941	0.0024941	5.7473E-006
CARBON MONOXIDE		0.015	0.014972	0.021508	0.00015527	0.013208	0.013208	4.2399E-005
METHANE		0.0044	0.0044552	0.0060953	0.00016215	0.0079853	0.0079853	9.4505E-005
CARBON DIOXIDE		0.3315	0.33735	0.037817	0.20809	0.71147	0.71147	0.20374
N-METHYL-2-PYRROLIDONE		0	6.9751E-008	5.2975E-007	0.78895	4.5311E-006	4.5311E-006	0.79577
Physical state		Vapor	Vapor	Vapor	Liquid	Vapor	Liq./Vap.	Liquid
Temperature	°C	40	-15	-15.031	-1.92	83.4	-15	-1.3307
Pressure	bar	32	32	32	32	32	32	11
Enthalpic flow	kcal/h	5.3545E005	-1.7951E006	-9.3776E005	-1.1437E008	35228	-43626	-1.1435E008
Vapor molar fraction		1	1	1	0	1	0.99997	0

Streams		13	14	16	18	21	23	24
Total flow	kg/h	24900	7.547E005	41064	7.1363E005	1.2923	7.1363E005	7.1363E005
Total flow	Nm3/h	12761	1.8613E005	20915	1.6522E005	0.2922	1.6522E005	1.6522E005
Mass fractions								
HYDROGEN		0.00024749	6.5852E-008	1.2093E-006	5.7272E-011	0	5.7272E-011	5.7272E-011
NITROGEN		5.6579E-005	2.6279E-008	4.8229E-007	3.9248E-011	0	3.9248E-011	3.9248E-011
CARBON MONOXIDE		0.00041518	2.6518E-007	4.8644E-006	5.3298E-010	0	5.3298E-010	5.3298E-010
METHANE		0.00050035	1.3175E-006	2.3984E-005	1.3211E-008	0	1.3211E-008	1.3211E-008
CARBON DIOXIDE		0.99877	0.072475	0.99995	0.019106	0	0.019106	0.019106
N-METHYL-2-PYRROLIDONE		1.216E-005	0.92752	1.9742E-005	0.98089	1	0.98089	0.98089
Mole fractions								
HYDROGEN		0.0053692	2.9687E-006	2.6398E-005	2.7505E-009	0	2.7505E-009	2.7505E-009
NITROGEN		8.8331E-005	8.5254E-008	7.5764E-007	1.3564E-010	0	1.3564E-010	1.3564E-010
CARBON MONOXIDE		0.00064825	8.604E-007	7.6425E-006	1.8422E-009	0	1.8422E-009	1.8422E-009
METHANE		0.001364	7.4635E-006	6.5791E-005	7.9729E-008	0	7.9729E-008	7.9729E-008
CARBON DIOXIDE		0.99252	0.14966	0.99989	0.04203	0	0.04203	0.04203
N-METHYL-2-PYRROLIDONE		5.3645E-006	0.85033	8.7639E-006	0.95797	1	0.95797	0.95797
Physical state		Vapor	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid
Temperature	°C	-5.985	-5.985	-14.366	-14.366	-7.0431	-13.862	-15
Pressure	bar	5	5	1.1	1.1	1.1	32	32
Enthalpic flow	kcal/h	-1.8615E005	-1.1416E008	-3.3002E005	-1.1383E008	-202.58	-1.1306E008	-1.1351E008
Vapor molar fraction		1	0	1	0	0	0	0

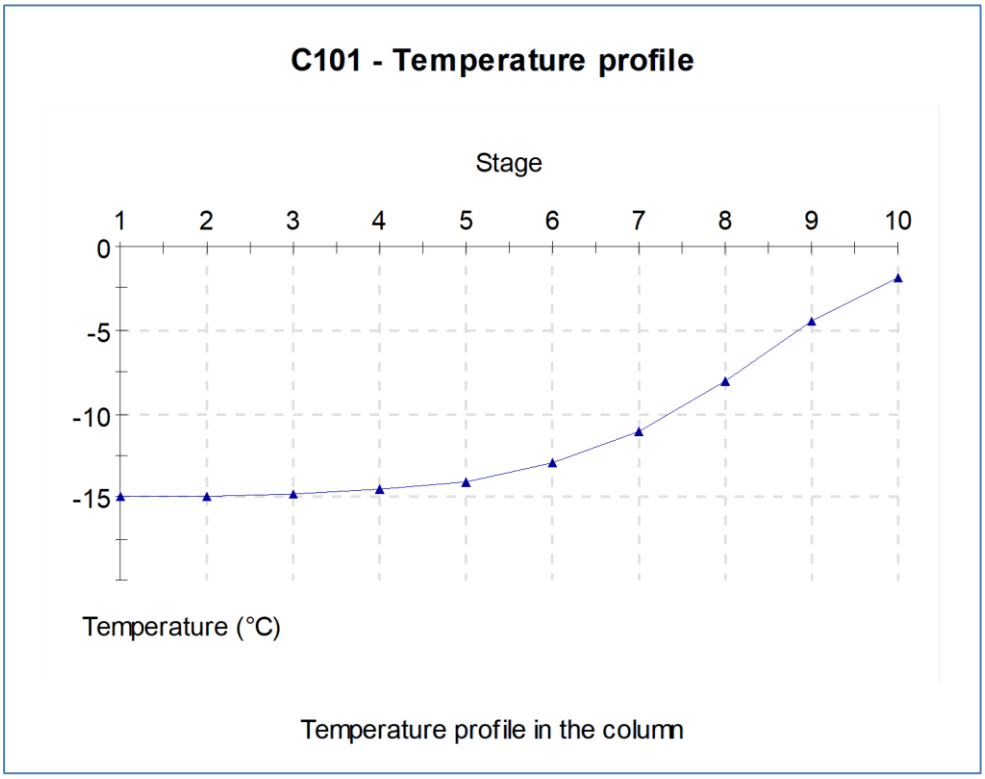
2.2. Process performance

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

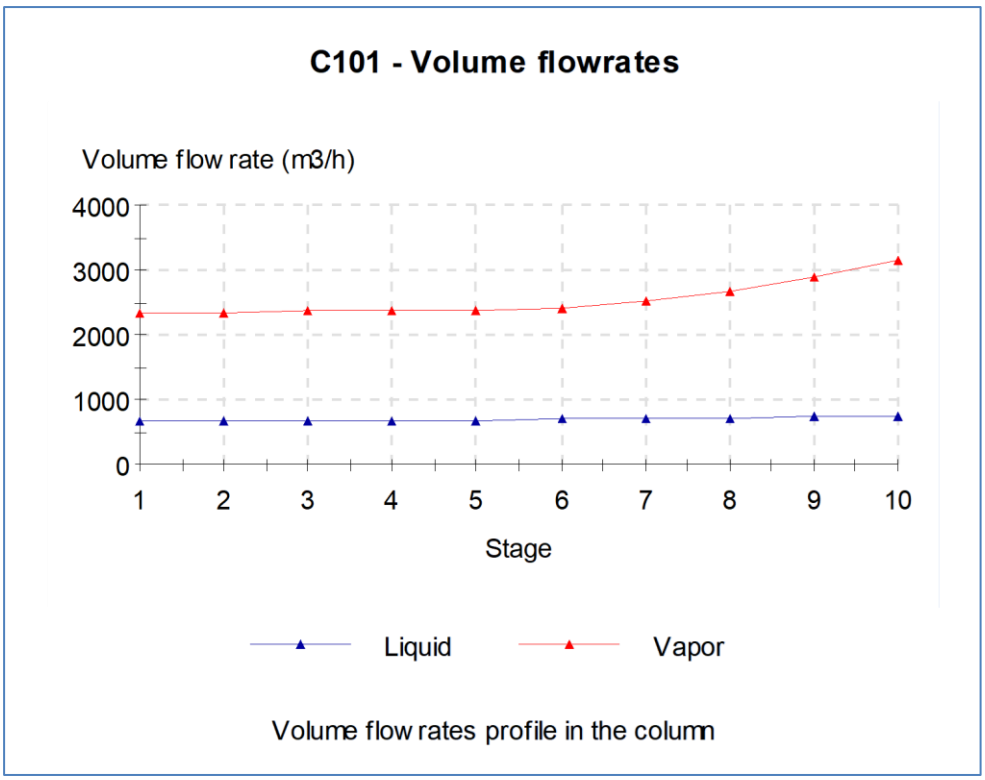
Component	Raw gas	Treated gas
CO_2	33.15% mol.	3.78% mol.

2.3. Columns profiles

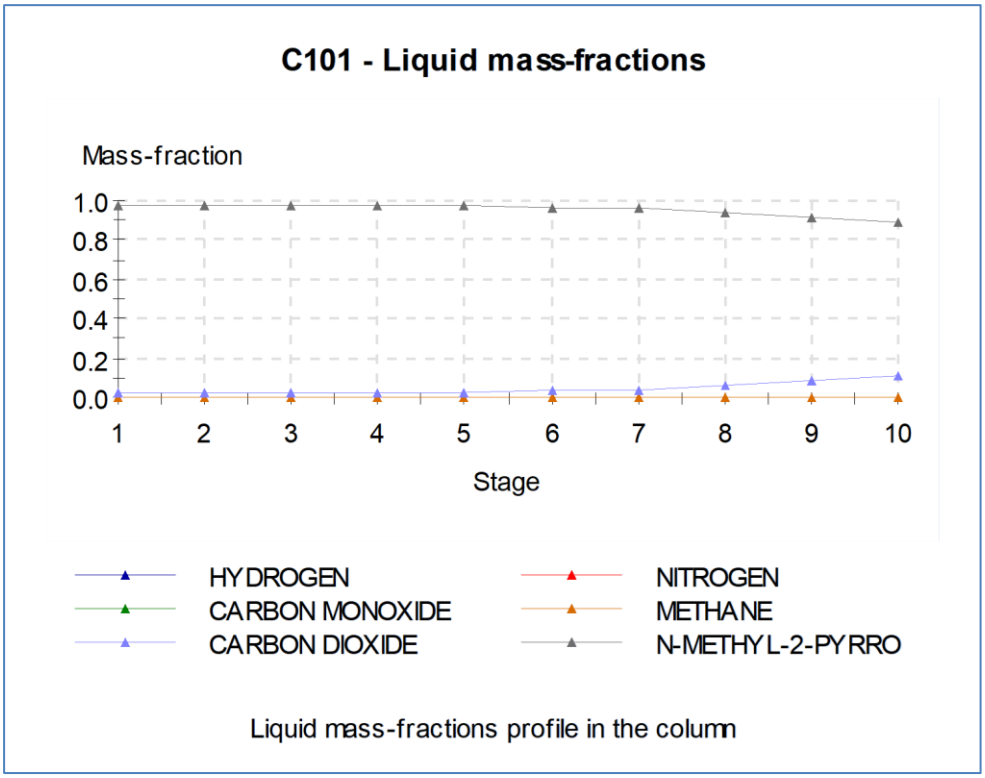
In ProSimPlus, column stages are numbered from top to bottom. The following graphs present the profiles in the absorber.



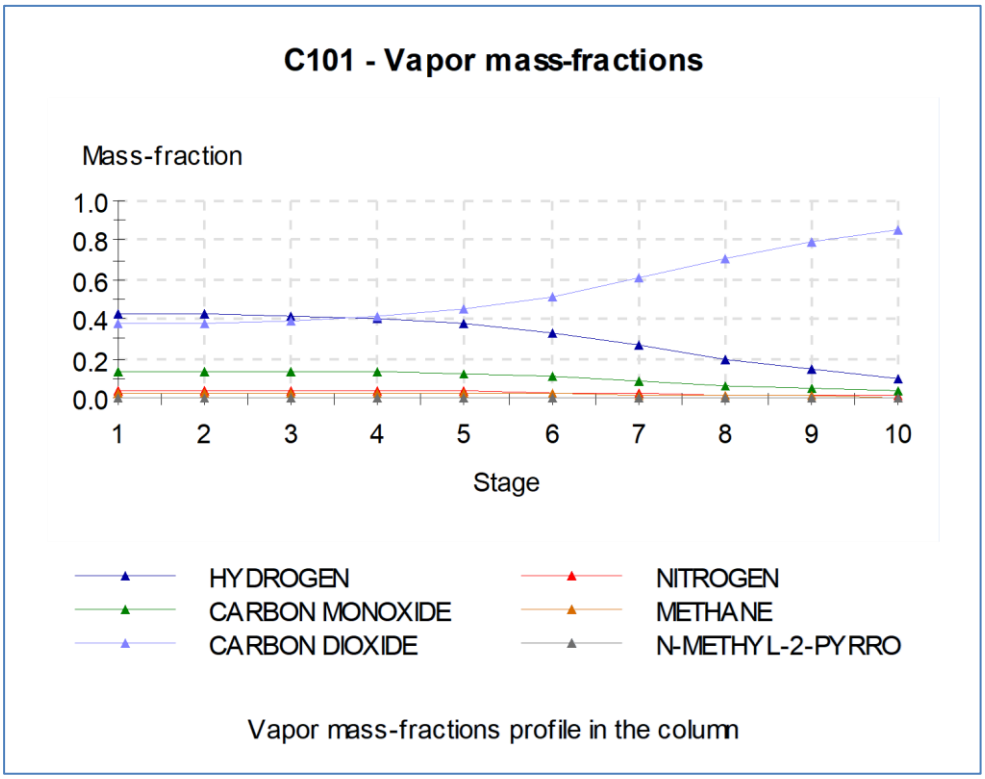
Temperature profile in the column



Volume flow rates profile in the column



Liquid mass-fractions profile in the column



Vapor mass-fractions profile in the column

3. REFERENCES

[CHE02] CHEN J., FISCHER K., GMEHLING J., “Modification of PSRK Mixing Rules and Results for Vapor – Liquid Equilibria, Enthalpy of Mixing and Activity Coefficients at Infinite Dilution”, Fluid Phase Equilib., 200, 411-429 (2002)

[GME95] GMEHLING J., “From UNIFAC to Modified UNIFAC to PSRK with the Help of DDB”, Fluid Phase Equilib., 107, 1-29 (1995)

[HOL91] HOLDERBAUM T., GMEHLING J., “PSRK: A Group Contribution Equation of State Based on UNIFAC”, Fluid Phase Equilib., 70, 251-265 (1991)

[KOH97] KOHL A., NIELSEN R., “Gas Purification”, Gulf Publishing, 5th edition (1997)

[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)

