ProSimPlus Application Example

Ethanol Plant

Example Purpose
This example illustrates a manufacturing unit of drinks-grade alcohol, (ethanol distillery) with very constraining specifications on purity. The simulation of this process is complex because it involves five distillation columns (two-phase or three-phase) highly inter-connected with many recycles. Moreover the representation of phase equilibria is also particularly complex because of the strong non-ideality of the system: very strict specifications on purity, liquid phase splitting phenomena, multiple azeotropes, etc. The particular point which is detailed in this example is the possibility to define specifications on the output streams of a distillation column or on any multistage separation module in ProSimPlus.

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Corresponding ProSimPlus file	*PSPS_EX_EN-Ethanol-Plant.pmp3*

Energy

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1. PROCESS MODELING

1.1. Process description

The objective of this unit is to produce drinks-grade ethanol, i.e. ethanol with a high purity level.

The process is fed with broth, i.e. an outgoing mixture of a fermentation step, consisting mainly of water, ethanol and small quantities of various impurities which one will seek to eliminate (methanol, 1-Propanol, 2-Methyl-1-Propanol, 1-Butanol, 3-Methyl-1-Butanol, Acetaldehyde or Ethyl Acetate).

This broth is fed at the top of the distillation column with total condenser D530 (streams 1 and 2). The D530 column is an extractive distillation column: it receives in its enrichment section a large amount of water (extracting agent) (stream 34) which sends impurities of the feed that have less affinity for water than alcohol at the top of the column. Alcohol remains in the column bottom and feeds the other diphasic columns D540 and D541 (stream 5 which splits into streams 6 and 7). This step is called purification by hydro-selection.

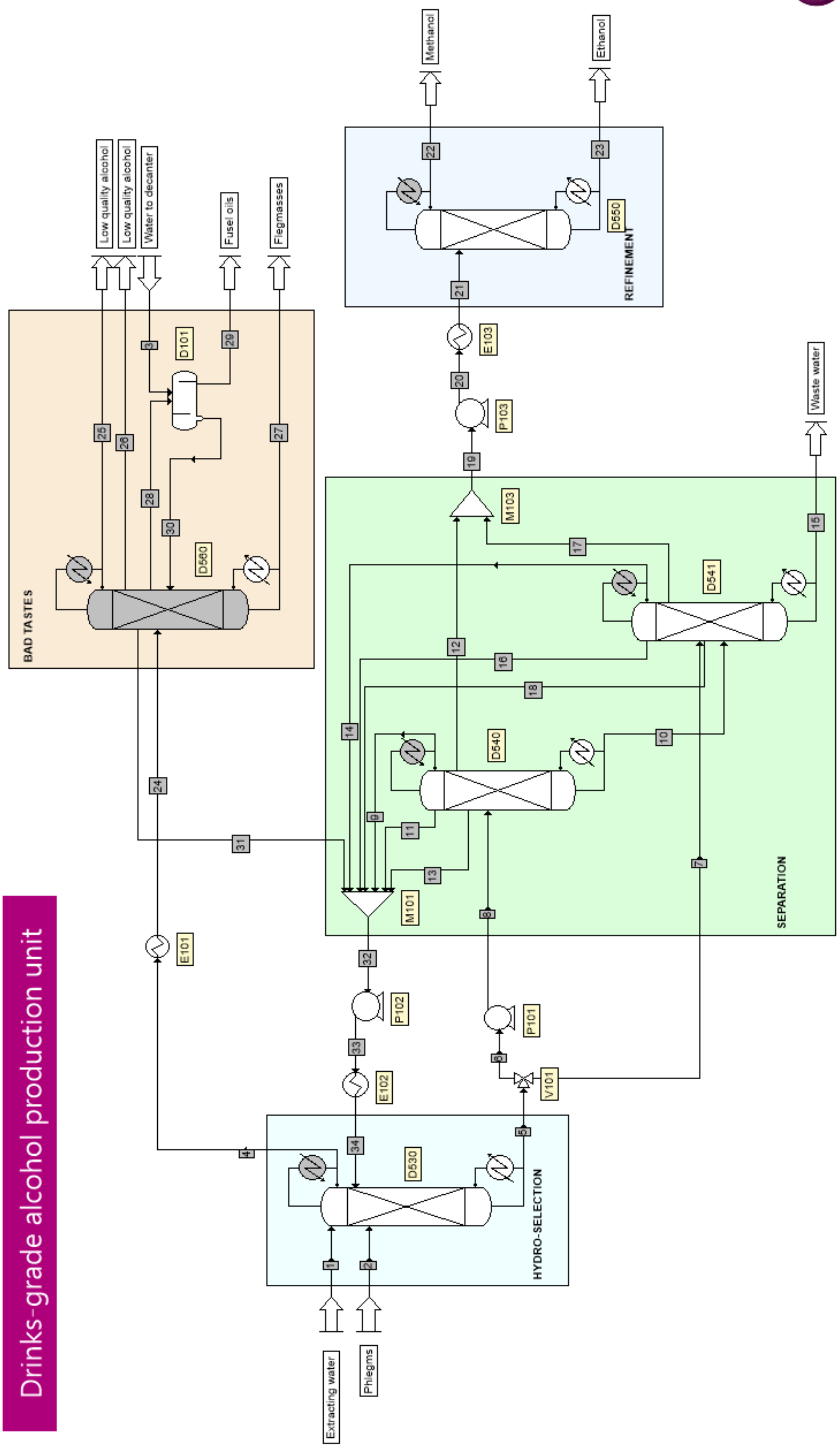
In the D540 and D541 columns, ethanol is extracted in liquid side streams on the upper plates rich in ethanol (streams 12 and 17). The distillate of these columns (streams 9 and 14) and the side streams on lower trays of the columns (streams 11, 13 and 16, 18) are sent back to upstream process, after a remixing (M101) and reheating (E102), at the top of the column D530 (stream 34).

The bottom of the column D540 feeds the D541 column at the lower trays (stream 10). The residue from D541 column primarily consists of water with some impurities (stream 15), with a flowrate similar to that of the one spraying the D530 column.

The ethanol extracted from the columns D540 and D541 is sent in the distillation column D550 (stream 21) to eliminate remaining methanol. Refined alcohol is recovered at the column bottom (stream 23) and the liquid distillate containing a higher concentration of methanol is recovered at the top (stream 22).

The impurities coming from the top of column D530 are sent in the three phase distillation column D560 (also called “column of bad tastes”) (stream 24). Bad quality alcohol is then recovered at the top of this column (streams 25 and 26) whereas the “flegmasses” are found at the bottom (stream 27). Additionally, a side stream is carried out (stream 28) in order to recover oils which are then washed with water in a decanter (D101). The aqueous phase leaving the decanter is returned to the D560 column (stream 30). Extracted oils are known as “fusel” oils (stream 29). Another side stream from the upper plates of the column (stream 31) makes it possible to recycle impurities towards process upstream. The stream is remixed with side streams of the columns D540 and D541 before feeding the top of column D530.

1.2. Process flowsheet



Ethanol plant process flowsheet

1.3. Specification

The main specification imposed on this process is to produce alcohol with 96°GL (equivalent with a mass fraction out of ethanol higher than 94%) and containing only some ppm of the various impurities present in the feed.

1.4. Components

Components taken into account in the simulation are taken from the ProSimPlus standard database:

- Ethanol
- Methanol
- Water
- 1-Propanol
- 2-Methyl-1-Propanol
- Acetaldehyde
- 1-Butanol
- 3-Methyl-1-Butanol
- Ethyl Acetate

1.5. Thermodynamic model

Given the nature of the components involved, the thermodynamic model used for the representation of phase equilibria, as well as other thermodynamic properties required for the simulation is based on the NRTL [1] activity coefficients model.

In order to represent accurately all of the complexity of the system, the binary interaction parameters for this model were obtained by regression of experimental equilibrium values of various concentration ranges. Five sets of binary interaction parameters were regressed:

- The 1st (global, NRTL D530) is used in the column D530 as well as in decanter D101 and modules P101, P102, E101, E102, M101, V101 and the process feeds;
- The 2nd (NRTL D540) is used in column D540;
- The 3rd (NRTL D541) is used in column D541;
- The 4th (NRTL D550) is used in column D550 as well as in modules P103, E103 and M103;
- The 5th (NRTL D560) is used in column D560.

The quality of the calculations carried out with this set of thermodynamic models was evaluated by comparison between the results of simulations and industrial plant data.

1.6. Operating conditions

✓ **Process feeds**

	2	***1***	***3***
Temperature (°C)	74,8	84	20
Pressure (bar)	0,75	0,7	1
Partial mass flowrates (kg/h)			
Ethanol	3490,19	-	-
Acetaldehyde	1,1083	-	-
2-Methyl-1-propanol	3,6958	-	-
1-propanol	1,8369	-	-
1-butanol	0,023	-	-
3-Methyl-1-butanol	8,9073	-	-
Methanol	1,6754	-	-
Ethyl Acetate	0,5624	-	-
Water	382,832	42075,1	199,2

✓ **Column D530**

Column type	Two-phase distillation column
Type of condenser	Total
Number of theoretical stages	51
Extractant feed stage (1)	2
Main feed stage (2)	22
Recycles of froth feed stage (34)	7
Liquid distillate molar flowrate (kmol/h)	100,61
Reflux molar flowrate (kmol/h)	76,27
Top pressure (bar)	0,624
Bottom pressure (bar)	0,865

Additional specifications for column D530:

Specifications		*Product type*	*Components*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Liquid distillate	3-Methyl-1-butanol	0,8315	Liq.	Mass.	Liquid distillate flowrate
2:	Recovery ratio	Liquid distillate	Ethanol	0,0638	Liq.	Mass.	Reflux flowrate

Efficiency of stages (by key words in the "Advanced parameters" tab):

```
EFF=50*1.55
```


✓ **Column D540**

Column type	Two-phase distillation column
Type of condenser	Total
Number of theoretical stages	66
Feed stage (stream 8)	51
Liquid distillate molar flowrate (kmol/h)	1,1611
Reflux molar flowrate (kmol/h)	292,714
Top pressure (bar)	1,888
Bottom pressure (bar)	2,074

Additional specifications for column D540:

Specifications		*Product type*	*Component*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Liquid distillate	Ethanol	0,0194	Liq.	Mass.	Liquid distillate flowrate
2:	Recovery ratio	Side stream 12	Ethanol	0,9307	Liq.	Mass.	Side stream 12 flowrate
3:	Recovery ratio	Side stream 11	Ethanol	0,0333	Liq.	Mass.	Side stream 11 flowrate
4:	Recovery ratio	Bottom liquid product	Water	0,9902	Liq.	Mass.	Reflux flowrate

Side streams:

Streams	*Stage*	*Molar ratio*	*State*
11	43	0,00176	Liquid
12	5	0,03632	Liquid
13	48	0,00425	Liquid

Efficiency of stages:

Stages 1 to 4	1
Stages 5 to 45	0,3
Stages 46 to 65	1

✓ **Column D541**

Column type	Two-phase distillation column
Type of condenser	Total
Number of theoretical stages	66
Feed stage (stream 7)	49
Feed stage (stream 10)	66
Liquid distillate molar flowrate (kmol/h)	1,2221
Reflux molar flowrate (kmol/h)	124,766
Top pressure (bar)	0,3
Bottom pressure (bar)	0,546

Additional specifications for column D541:

Specifications		*Product type*	*Component*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Liquid distillate	Ethanol	0,0414	Liq.	Mass.	Liquid distillate flowrate
2:	Recovery ratio	Side stream 17	Ethanol	0,8887	Liq.	Mass.	Side stream 17 flowrate
3:	Recovery ratio	Side stream 16	Ethanol	0,0393	Liq.	Mass.	Side stream 16 flowrate
4:	Recovery ratio	Bottom liquid product	Water	0,9971	Liq.	Mass.	Reflux flowrate

Side streams:

Streams	*Plate*	*Molar flowrate*	*State*
16	37	0,0007	Liquid
17	5	0,0117	Liquid
18	43	0,0015	Liquid

Efficiency of stages:

Stages 1 to 4	1
Stages 5 to 40	0,4
Stages 41 to 65	1

Initialization value: column top temperature: 46.3 °C

✓ **Column D550**

Column type	Two-phase distillation column
Type of condenser	Total
Number of theoretical stages	51
Feed stage (stream 21)	14
Liquid distillate molar flowrate (kmol/h)	0,85170
Reflux molar flowrate (kmol/h)	138,559
Pressure stage 2 (bar)	0,31
Pressure stage 50 (bar)	0,545

Additional specifications for column D550:

Specifications		*Product type*	*Component*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Liquid distillate	Ethanol	0,0109	Liq.	Mass.	Liquid distillate flowrate
2:	Recovery ratio	Liquid distillate	Methanol	0,3845	Liq.	Mass.	Reflux flowrate

Efficiency of stages: 0,5

✓ **Column D560**

Column type	Three-phase distillation column
Type of condenser	Total
Number of theoretical stages	43
Feed stage (stream 24)	28
Feed stage (stream 30)	34
Liquid distillate molar flowrate (kmol/h)	3,5078
Reflux molar flowrate (kmol/h)	28,443
Top pressure (bar)	0,41
Bottom pressure (bar)	0,55

Additional specifications for column D560 (by key words in the “advanced parameters” tab):

Specifications		*Product type*	*Component*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Liquid distillate	Ethanol	0,467	Liq.	Mass.	Liquid distillate flowrate
2:	Recovery ratio	Side stream 31	Ethanol	0,305	Liq.	Mass.	Side stream 31 flowrate
3:	Recovery ratio	Side stream 26	Ethanol	0,0783	Liq.	Mass.	Side stream 26 flowrate

```
!    1. Ethanol specification (distillate)
SPEC:TAUX=0.4670 CONS=1  SOUT=1  PHASE=L MASS
ACT: DL
!
!    2. Ethanol specification (top side stream)
SPEC:TAUX=0.3050 CONS=1  SOUT=8  PHASE=L MASS
ACT: SOUT=8 PHASE=L
!
!    3. Ethanol specification (second side stream)
SPEC:TAUX=0.0783 CONS=1  SOUT=23 PHASE=L MASS
ACT: SOUT=23 PHASE=L
```

Side streams:

Streams	*Stage*	*Molar flowrate (kmol/h)*	*State*
26	23	0,8459	Liquid
31	8	2,3907	Liquid
28	27	2,8177	Liquid

Efficiency of stages: 0,3

✓ **Heat exchanger E101**

Type of exchanger	Cooler/heater
Temperature (°C)	Bubble temperature
Pressure drop (bar)	0

✓ **Heat exchanger E102**

Type of exchanger	Cooler/heater
Temperature (°C)	88,5
Pressure drop (bar)	0,05

✓ **Heat exchanger E103**

Type of exchanger	Cooler/heater
Temperature (°C)	74,8
Pressure drop (bar)	0,01

✓ **Stream splitter V101**

Splitting ratio (stream 6)	0,664

✓ **Pumps P101**

Exhaust pressure (bar)	2,05
Volumetric efficiency	0,65
Mechanical efficiency	1
Electrical efficiency	1

✓ **Pumps P102**

Exhaust pressure (bar)	0,75
Volumetric efficiency	0,65
Mechanical efficiency	1
Electrical efficiency	1
Fixed liquid physical state	Yes

✓ **Pumps P103**

Exhaust pressure (bar)	0,39
Volumetric efficiency	0,65
Mechanical efficiency	1
Electrical efficiency	1
Fixed liquid physical state	Yes

✓ **Decanter D101**

Temperature	Adiabatic mixing of the feed
Pressure (bar)	Feed pressure.

✓ **Mixer M101**

Type of mixing	Adiabatic

✓ **Mixer M103**

Type of mixing	Adiabatic

1.7. Initialization of tear streams

✓ **34**

Temperature (°C)	88,5
Pressure (bar)	0,7
Total flowrate (kg/h)	600
Mass fraction	
Ethanol	0,66
Water	0,34

✓ **30**

Temperature (°C)	30
Pressure (bar)	0,5
Total flowrate (kg/h)	270
Mass fraction	
Ethanol	0,15
Water	0,85

1.8. "Hints and Tips"

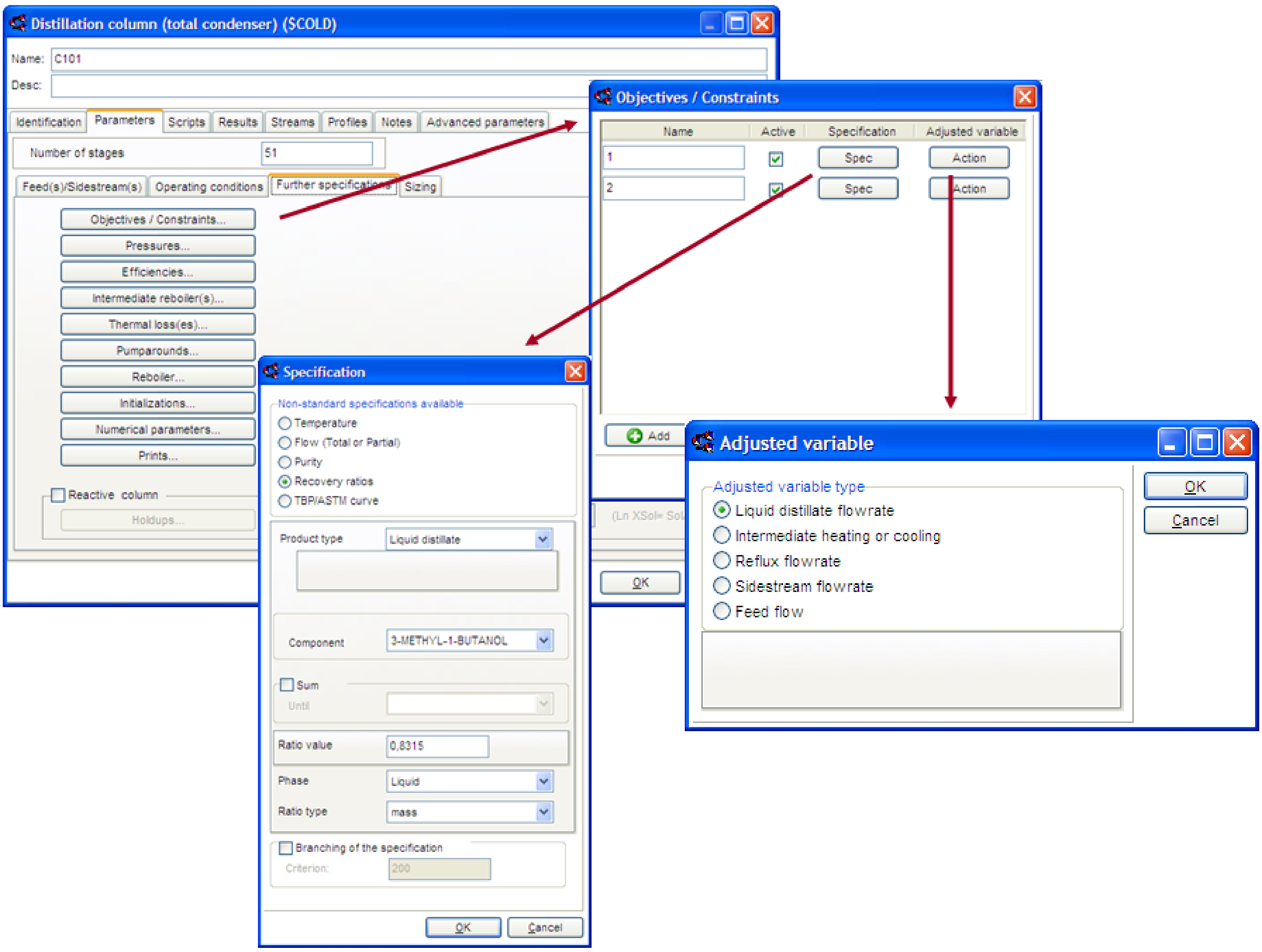
In the modular approach implemented in ProSimPlus, the characteristics (temperature, pressure, composition…) of streams leaving each module are calculated from the knowledge of the parameters of the module and the characteristics of the input streams. In practice, the user often wishes to impose one or more characteristics on the output streams of a module (for example a flowrate a purity level or a recovery ratio). It is frequently the case with the distillation or stripping columns (multistage separators).

The possibility of imposing output parameters (or in other words of setting constraints or "non-standard specification") is available for each column module, under the option "Objectives/Constraints" (module configuration window / Parameters tab / Further Specifications sub-tab). The user chooses the output characteristics to force and the "adjusted variable", i.e. the parameter which will be adjusted to satisfy the constraint. It is possible to impose several constraints and act on several adjusted variables on the same column.

In this example, two non-standard specifications of the D530 column consist in imposing a mass recovery ratio of 3-Methyl-1-Butanol in the distillate of 83,15% and in adjusting the distillate flowrate.

The "Objectives / Constraints" button opens the non-standard specifications definition window. At this level:

- The "Spec" button makes it possible to choose what to impose (here a recovery ratio in the liquid distillate of the component 3-Methyl-1-Butanol, equal to 0,8315 in liquid phase (mass)).
- The "Action" button makes it possible to choose its adjusted variable (Here liquid distillate flowrate).



When using this option, it should be kept in mind that:

- The number of specifications must remain under the degrees of freedom on the operation of a column. For example, on a column of absorption having in entry a vapor stream and a liquid stream and at exit a vapor stream and a liquid stream, it is not possible to impose non-standard specification. On the D530 column there are two degrees of freedom (the liquid distillate flowrate and the reflux flowrate), therefore, one can impose two non-standard specifications.
- The software can satisfy only constraints that are physically possible to reach. For example if one forces to recover all the heavy components in the distillate and the light components in the residue, that will lead to a non-convergence of the column.

It is also to be noted that at the level of the “Objectives / Constraints” window, it is possible to deactivate a predefined non-standard specification. This functionality makes it possible to choose which specification will be taken into account in the calculation. This can be useful when working on the convergence of a particularly complex column.

2. RESULTS

2.1. Comments on results

The calculation sequence (the order of calculation of the modules) is generated automatically.

The convergence of the whole flowsheet is obtained in 9 iterations, leading to 11 passages in the maximum cyclic network.

2.2. Mass and energy balances

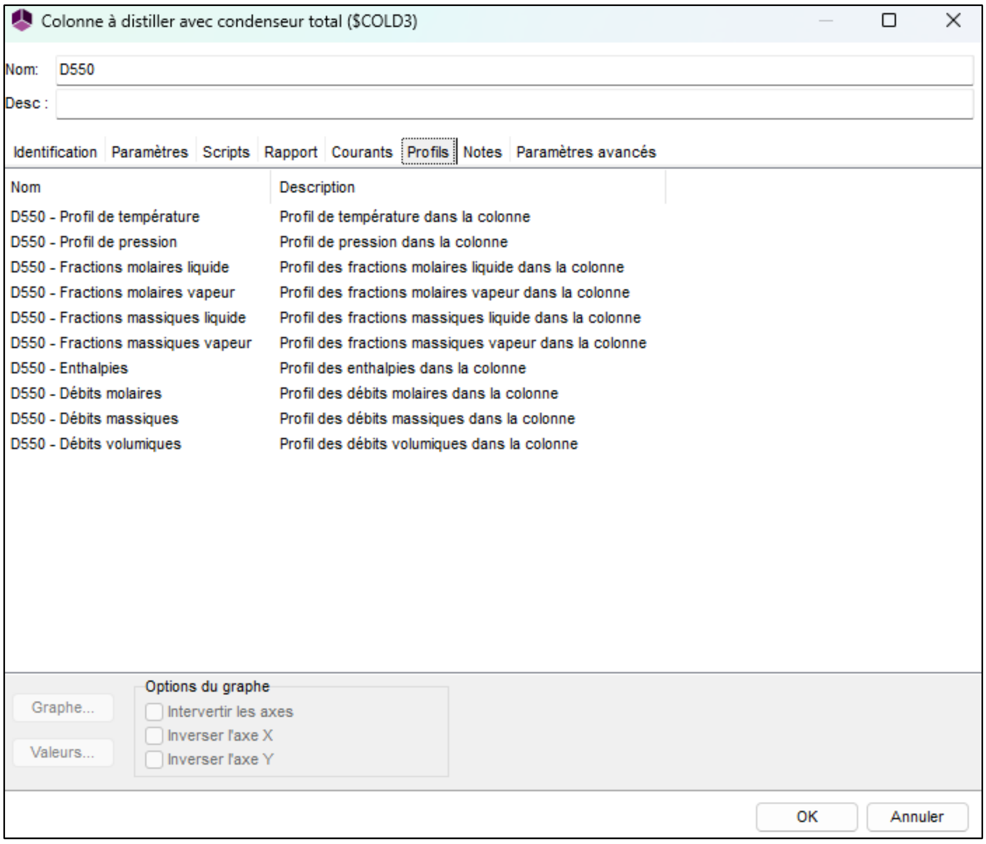
This document presents only the most relevant stream results. In ProSimPlus, mass and energy balances are provided for every stream. Results are also available at the unit operation level (result tab in the configuration window).

Streams		2	1	4	5	10	21
From		Phlegms	Extracting water	D530	D530	D540	E102
To		D530	D530	D560	V101	D541	D550
Partial flows		kg/h	kg/h	kg/h	kg/h	kg/h	kg/h
ETHANOL		3490,19	0	247,267737	3628,40213	0,00729591	3325,7566
ACETALDEHYDE		1,1083	0	1,17693343	0	0	0
2-METHYL-1-PROPANOL		3,6958	0	4,02038814	0,18475065	0	0,00300141
1-PROPANOL		1,8369	0	2,26477859	1,0943653	0	0,01172401
1-BUTANOL		0,023	0	0,00732432	0,01579003	0,01047991	0
3-METHYL-1-BUTANOL		8,9073	0	8,96257799	1,81622897	0	1,1745E-05
METHANOL		1,6754	0	0,02985659	1,92733414	0,00734255	1,6126539
ETHYL ACETATE		0,5624	0	0,58461276	0	0	0
WATER		382,832	42075	1075,02767	41579,9436	27338,5136	204,08179
Total flow	kg/h	3890,8311	42075	1339,34188	45213,3842	27338,5387	3531,46578
Mass fractions							
ETHANOL		0,89702943	0	0,18461884	0,08025062	2,6687E-07	0,94174963
ACETALDEHYDE		0,00028485	0	0,00087874	0	0	0
2-METHYL-1-PROPANOL		0,00094987	0	0,00300176	4,0562E-06	0	8,4990E-07
1-PROPANOL		0,00047211	0	0,00169096	2,4204E-05	0	3,3199E-06
1-BUTANOL		5,9113E-06	0	5,4686E-06	3,4923E-07	3,8334E-07	0
3-METHYL-1-BUTANOL		0,00228931	0	0,00669178	4,0170E-05	0	3,3259E-09
METHANOL		0,0004306	0	2,2292E-05	4,2628E-05	2,6858E-07	0,00045665
ETHYL ACETATE		0,00014454	0	0,00043649	0	0	0
WATER		0,09839337	1	0,80265367	0,91963794	0,99999908	0,05778954
Physical state		Vapor	Liquid	Liquid	Liquid	Liquid	Vapor
Temperature	°C	74,8	84	75,1577507	88,839413	121,425521	74,8
Pressure	bar	0,7499998	0,69999981	0,62399983	0,86499977	2,07399944	0,3851674
Enthalpy	kcal/h	71244,2083	-22037230	-620068,813	-22206316,5	-13285835,5	64026,144
Vapor fraction		1	0	0	0	0	1

Streams		23	22	27	26	25
From		D550	D550	D560	D560	D560
To		Ethanol	Methanol	Flegmasses	Low quality alcohol	Low quality alcohol
Partial flows		kg/h	kg/h	kg/h	kg/h	kg/h
ETHANOL		3289,50585	36,2507457	5,5240365	22,0137558	131,295325
ACETALDEHYDE		0	0	0	0,01364405	1,09220044
2-METHYL-1-PROPANOL		0,00300137	3,8745E-08	0,00606037	1,71204823	0,09512987
1-PROPANOL		0,01172356	4,4485E-06	0,21807512	0,89342595	0,19252216
1-BUTANOL		0	0	0,00109851	0,00205541	2,0885E-05
3-METHYL-1-BUTANOL		1,1745E-05	0	0,21640501	1,81918285	0,00831942
METHANOL		0,99250847	0,62006595	0,00390635	0,00113922	0,02020705
ETHYL ACETATE		0	0	0	0,00546581	0,55436049
WATER		202,723439	1,35835076	1238,10742	10,3852512	11,6855114
Total flow	kg/h	3493,23661	38,2291629	1244,07807	36,8459685	144,943597
Mass fractions						
ETHANOL		0,94167851	0,94824848	0,00444048	0,59745358	0,90583736
ACETALDEHYDE		0	0	0	0,0003703	0,00753535
2-METHYL-1-PROPANOL		8,5919E-07	1,0135E-09	5,5144E-06	0,04646501	0,00065632
1-PROPANOL		3,3561E-06	1,1636E-08	0,00017529	0,02424759	0,00132826
1-BUTANOL		0	0	8,8299E-07	5,5784E-05	1,4409E-07
3-METHYL-1-BUTANOL		3,3623E-09	0	0,00017395	0,04937264	5,7398E-05
METHANOL		0,00028415	0,01621971	3,1400E-06	3,0918E-05	0,00013941
ETHYL ACETATE		0	0	0	0,00014834	0,00382466
WATER		0,05803313	0,03553179	0,99520074	0,28185583	0,08062109
Physical state		Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	°C	63,3009533	55,2321919	83,2207258	63,57261585	56,6963075
Pressure	bar	0,54499985	0,3851674	0,54999985	0,4833332	0,40999989
Enthalpy	kcal/h	-741292,435	-8053,01953	-650479,61	-10481,5494	-32407,9491
Vapor fraction		0	0	0	0	0

2.3. Column profiles

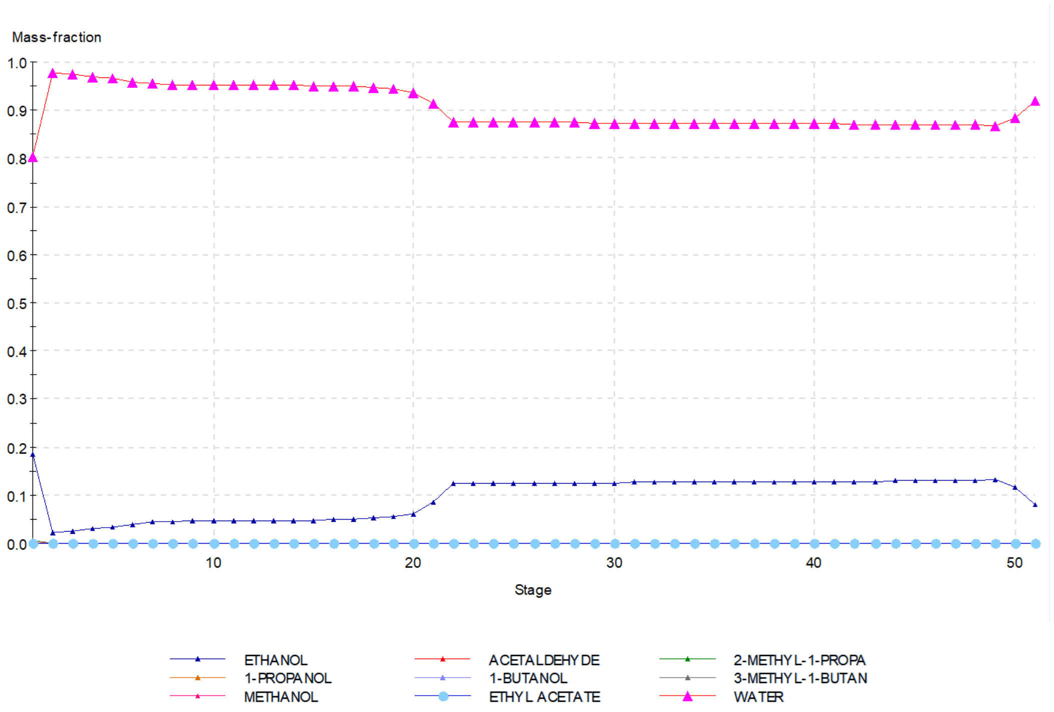
Composition profiles can be accessed after the simulation in each column configuration window, in the "Profiles" tab. Double clicking on the profile will generate the corresponding graph. Here, only the liquid-mole fraction is shown for each column.



Because of the differences in term of order of magnitude, the compositions in liquid phase in columns were represented on two distinct graphs. The first presents the evolution of main components (ethanol and water), the second presents that of impurities.

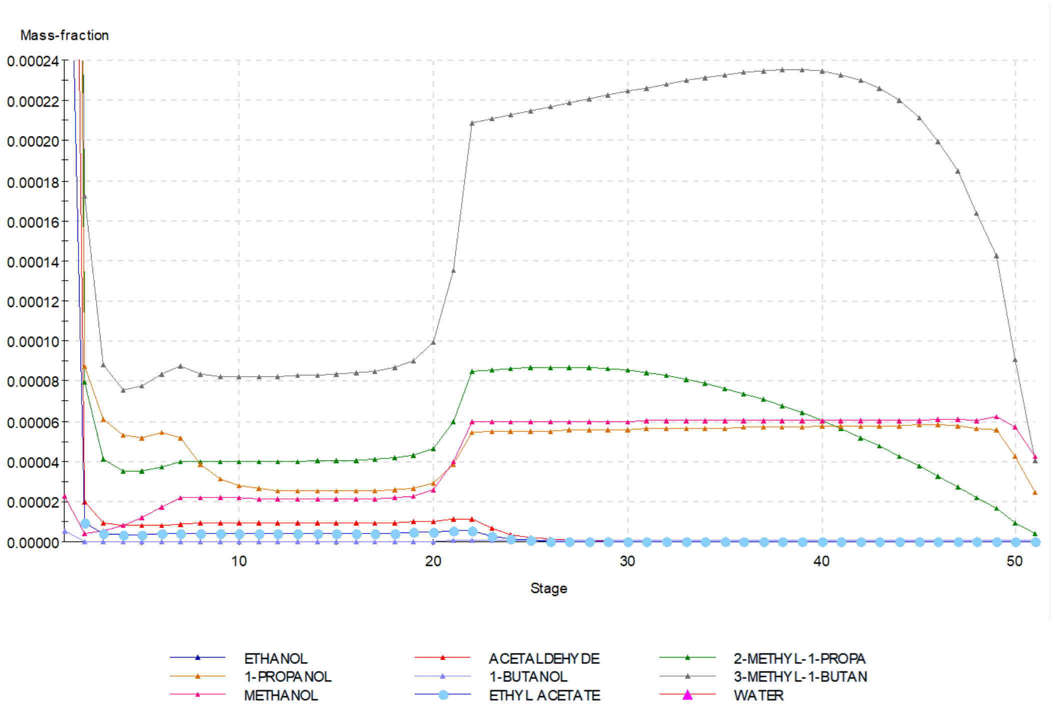
Column D530

D530 - Liquid mass-fractions



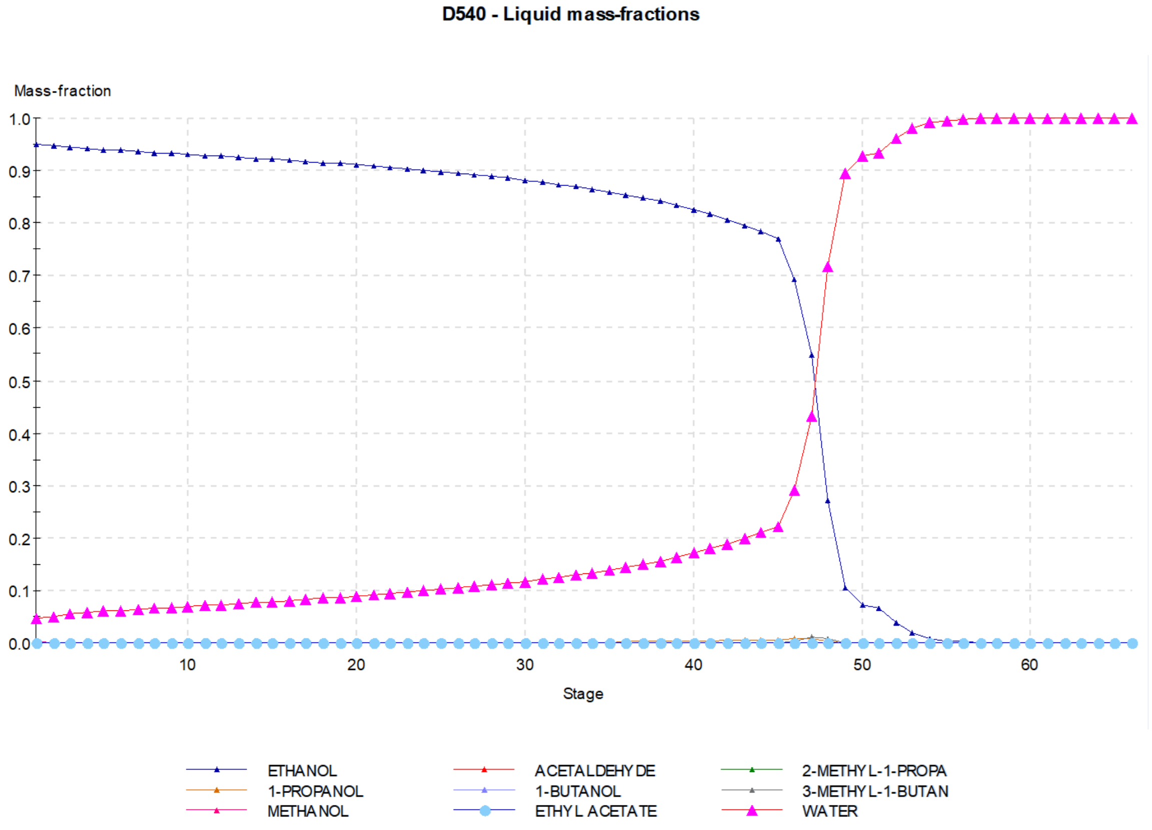
Liquid mass-fractions profile in the column

D530 - Liquid mass-fractions

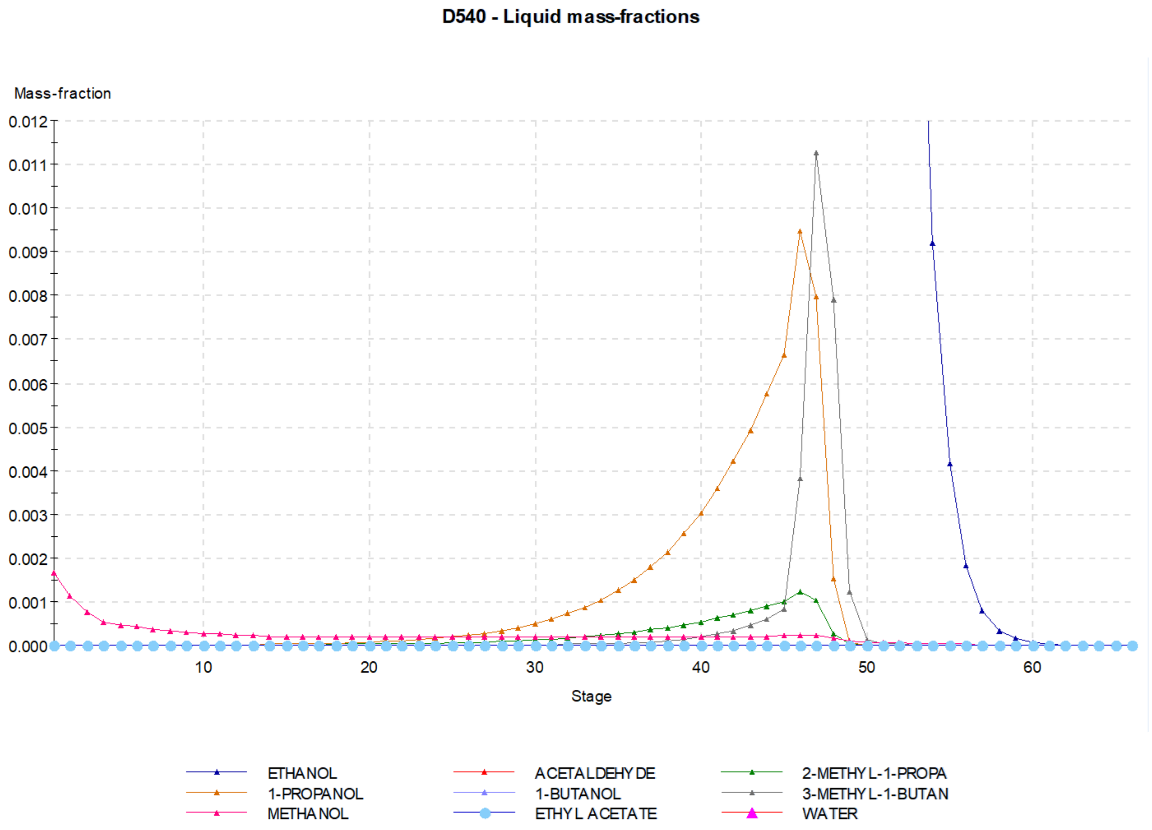


Liquid mass-fractions profile in the column

Column D540

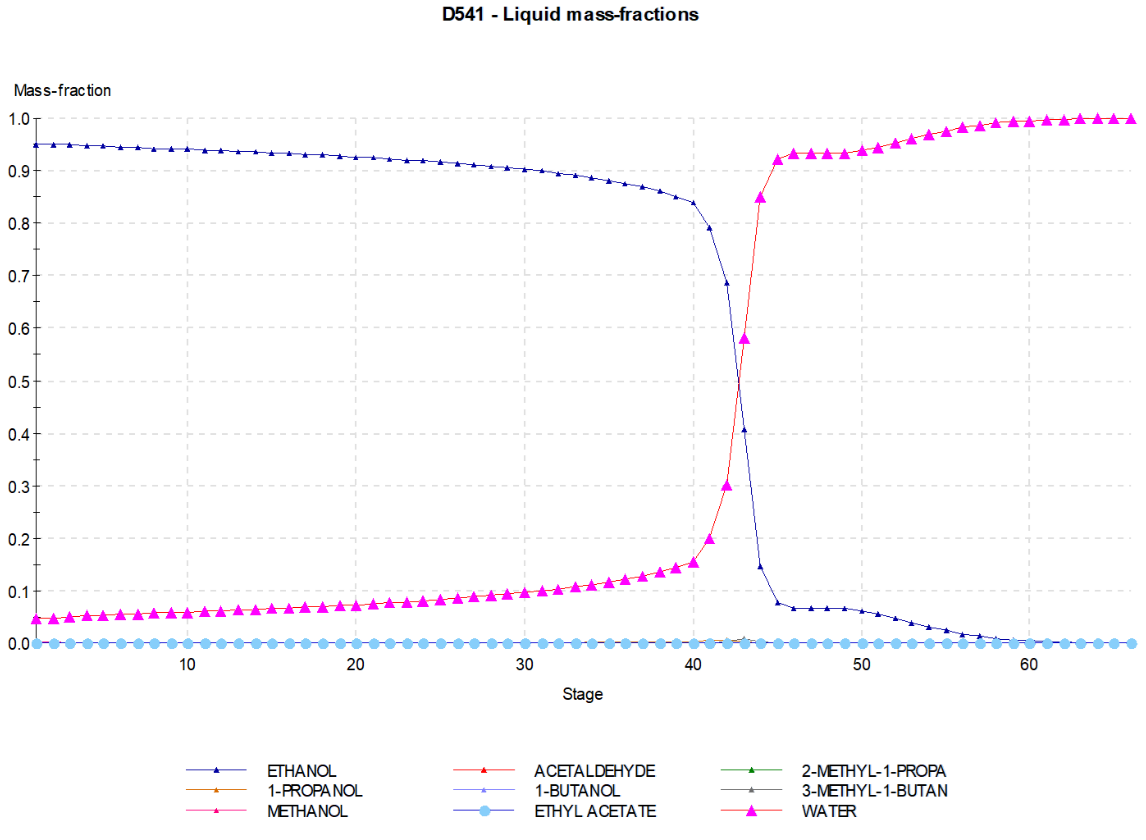


Liquid mass-fractions profile in the column

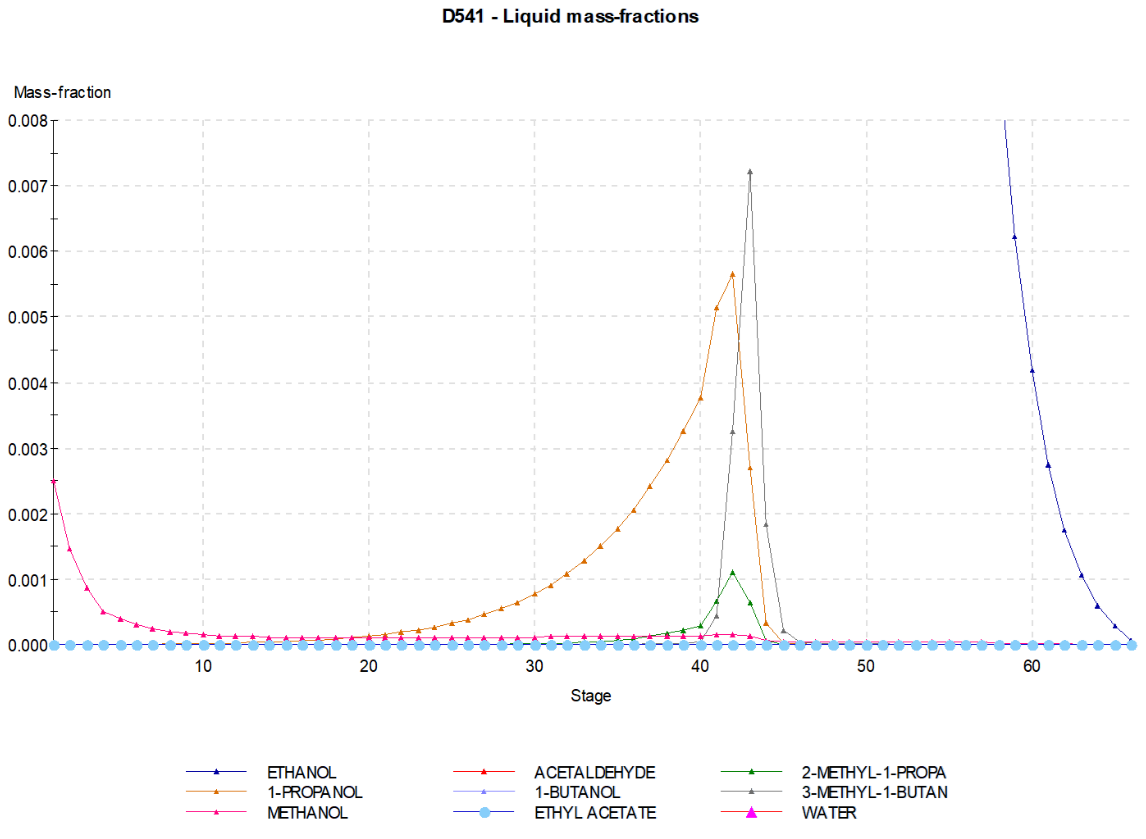


Liquid mass-fractions profile in the column

Column D541

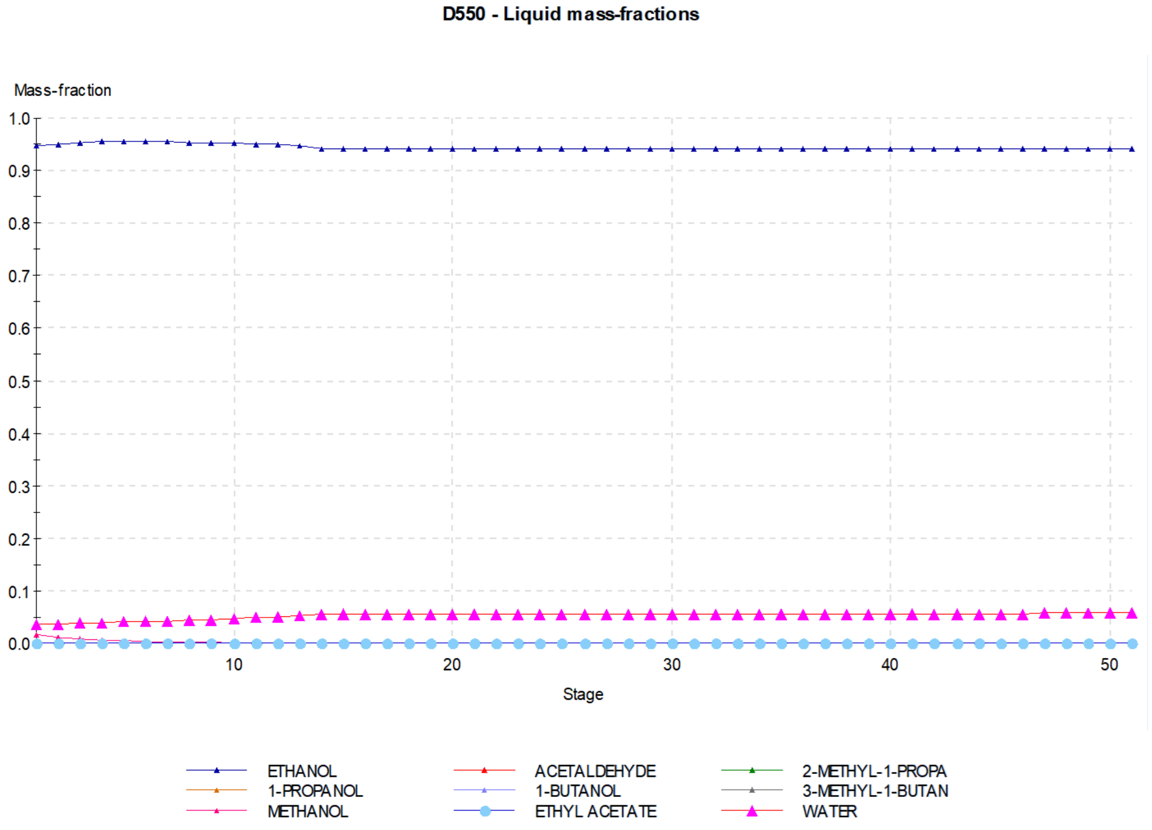


Liquid mass-fractions profile in the column

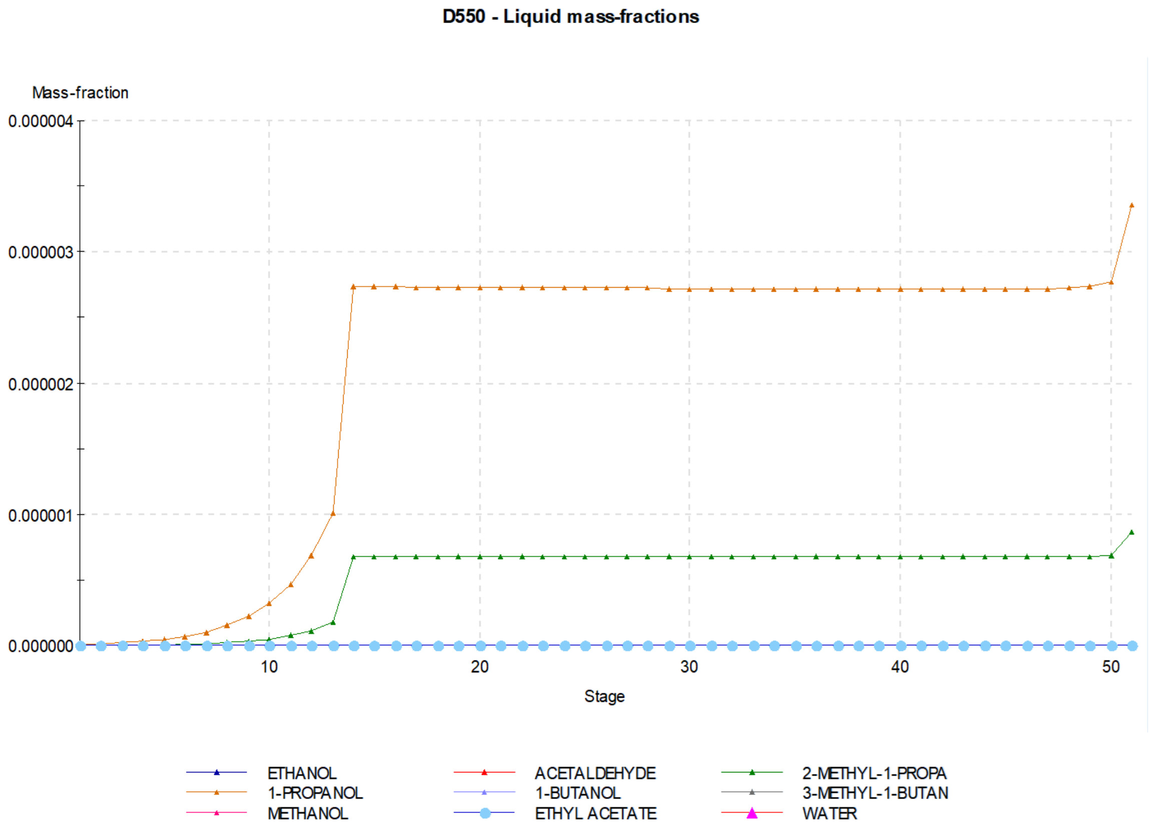


Liquid mass-fractions profile in the column

Column D550

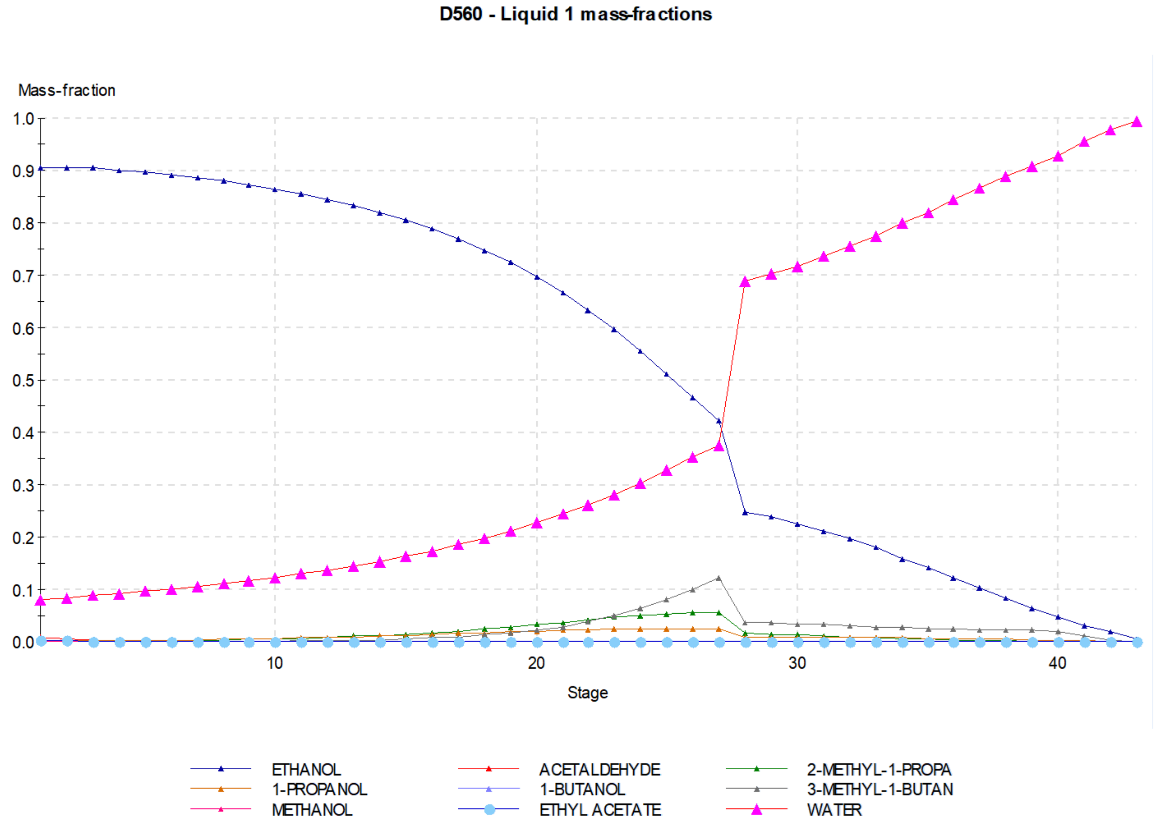


Liquid mass-fractions profile in the column

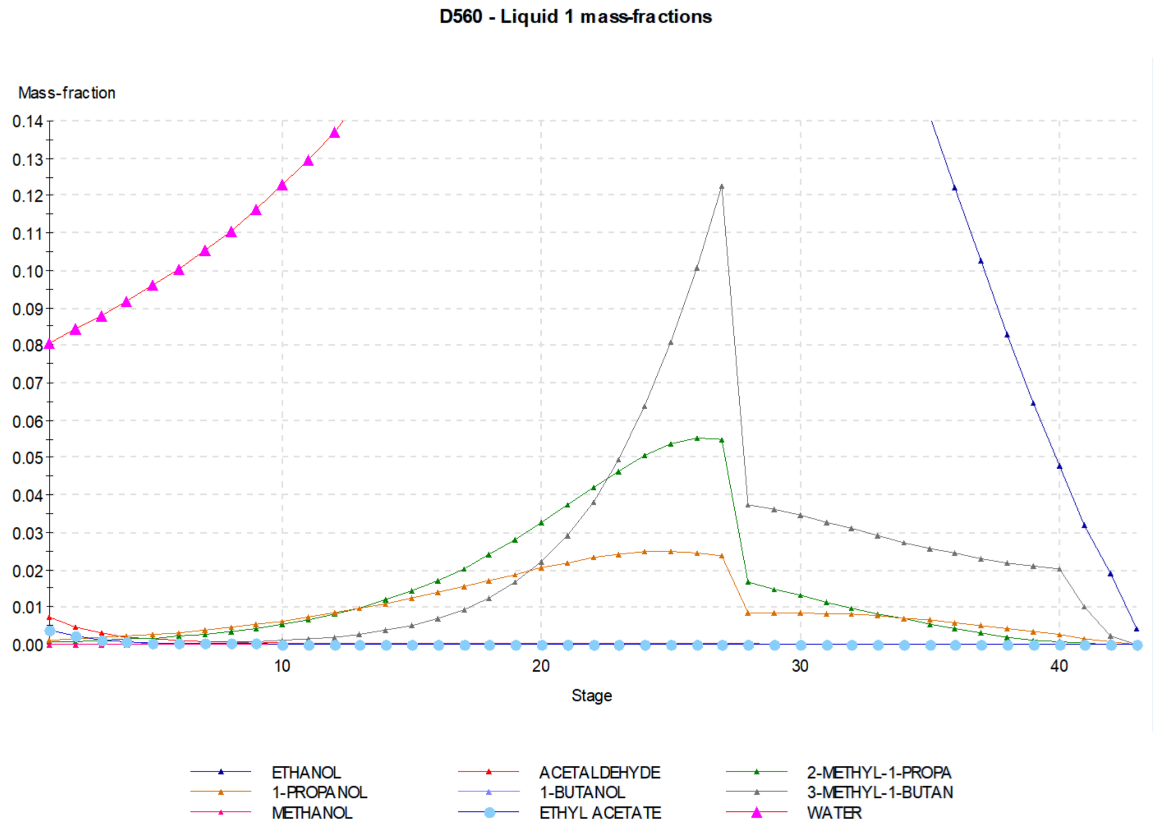


Liquid mass-fractions profile in the column

Column D560



Liquid 1 mass-fractions profile in the column



Liquid 1 mass-fractions profile in the column

3. REFERENCES

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