ProSim

PROSIMPLUS APPLICATION EXAMPLE

NAPHTHALENE SEPARATION

INTEREST OF THIS EXAMPLE
This example illustrates a process to purify naphthalene from a mixture containing 14 components in a three columns distillation train. This example mainly focuses on two-phase (vapor-liquid) distillation columns. For each of the three distillation columns, several specifications are set on the output streams, illustrating the way to set "non-standard" specifications in the multi-stage separation modules of ProSimPlus. This example also demonstrates the way to use modules for measurement of some streams parameters and also how to handle the "information streams" in order to determine the global naphthalene recovery ratio between process input and output.

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

CORRESPONDING PROSIMPLUS FILE	*PSPS_EX_EN-Naphthalene-Separation.pmp3*

.

TABLE OF CONTENTS

1. PROCESS MODELING

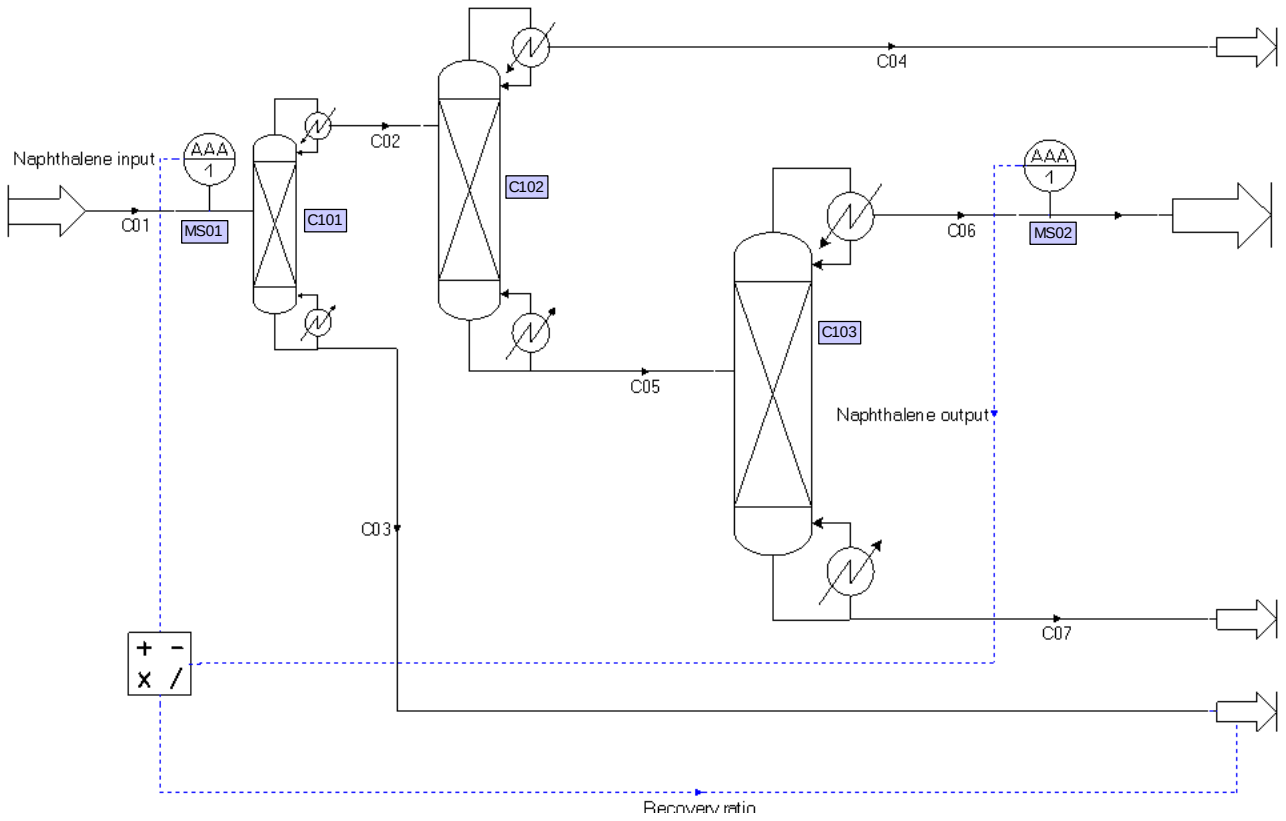
1.1. Process description

The objective of this process is to produce a naphthalene stream with a 97 weight % purity by distillation in a three distillation columns train.

The first column removes Anthracene into the bottom product. The overhead from the first column contains the bulk of the feed and is fed to the second column where the 1,2,4-Trimethylbenzene is removed. A small loss of Naphthalene is allowed in this column. Finally, the last column produces the high purity Naphthalene.

This example is taken from [1].

1.2. Process flowsheet



Naphthalene separation process flowsheet

1.3. Specification

The process specification is to recover a Naphthalene stream with a purity of 97 % wt.

1.4. Components

Components taken into account in the simulation are of two kinds:

- A first set of components are taken from the ProSim standard database, provided with ProSim's software. These components are defined in the table below:

- ❖ Naphthalene
- ❖ 1,2,4-Trimethylbenzene
- ❖ Indene
- ❖ m-Cresol
- ❖ 2,3-Xylenol
- ❖ 2,4-Xylenol
- ❖ n-Dodecane
- ❖ 2-Methylnaphtalene
- ❖ Fluorene
- ❖ Anthracene

- The second set of components for which all the required properties are automatically generated with the pseudo-compound generation service, from the knowledge of the following properties:

Name	*Molecular weight (g/mol)*	*Density*	*NBP (°C)*
Diphenyl	150.425	1.0076	254.6
23 Di Methyl Naph	152.817	1.0407	268.0
Acet. Naph.	152.027	1.0930	279.8
Di BenzoF	164.451	0.9947	274.6

1.5. Thermodynamic model

Given the nature of the compounds involved in the process, the thermodynamic model used to represent phase equilibria and the enthalpy calculations is the Peng-Robinson (PR) [2] cubic equation of state, without binary interaction parameters.

1.6. Operating conditions

✓ Process feed

Temperature (°C)	100
Pressure (mmHg)	780
Mass partial flowrates (kg/h)	
1,2,4-Trimethylbenzene	376.00
Indene	101.00
m-Cresol	5.50
2,4-Xylenol	9.60
n-dodecane	13.20
2,3-Xylenol	5.10
Naphthalene	2266.00
Diphenyl	62.30
23 Di Methyl Naph	78.90
2-Methyl Naphthalene	55.90
Acet. Naph.	72.10
Di Benzof	90.60
Fluorene	110.50
Anthracene	213.00

✓ Column C101

Operating parameters	*Value*
Type of column	Two-phase distillation column
Number of theoretical stages	7
Feed stage	5
Pressure (mmHg) Top	760
Stage 2	780
Reflux molar flowrate (kmol/h)	9 (initialization)
Liquid distillate molar flowrate (kmol/h)	23.9 (initialization)

Additional specifications for column C101:

Specifications		*Product type*	*Component*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Vapor distillate	Naphthalene	0.993	Vap.	Mol.	Vapor distillate flowrate
2:	Recovery ratio	Bottom liquid product	Anthracene	0.995	Liq.	Mol.	Reflux flowrate

✓ Column C102

Operating parameters	*Value*
Type of column	Two-phase distillation column
Number of theoretical stages	14
Feed stage	3
Pressure (mmHg) Top	760
Stage 2	780
Reflux molar flowrate (kmol/h)	43 (initialization)
Liquid distillate molar flowrate (kmol/h)	4.3054 (initialization)

Additional specifications for column C102:

Specifications		*Product type*	*Components*	*Value*	*Phase*	*Type*	*Action*
1:	Purity	Vapor distillate	Naphthalene	0.15	Vap.	Mass.	Vapor distillate flowrate
2:	Recovery ratio	Bottom liquid product	1,2,4-Trimethylbenzene	0.01	Liq.	Mol.	Reflux flowrate

✓ Column C103

Operating parameters		*Value*
Type of column		Two-phase distillation column
Number of theoretical stages		23
Feed stage		14
Pressure (mmHg)	Top	760
	Stage 2	780
Reflux molar flowrate (kmol/h)		17.4014 (initialization)
Liquid distillate molar flowrate (kmol/h)		109.8 (initialization)

Additional specifications for column C103:

Specifications		*Product type*	*Components*	*Value*	*Phase*	*Type*	*Action*
1:	Recovery ratio	Bottom liquid product	Naphthalene	0.0025	Liq.	Mol.	Liquid distillate flowrate
2:	Purity	Vapor distillate	Naphthalene	0.9707	Vap.	Mass	Reflux flowrate

1.7. "Hints and Tips"

✓ Previously to this rigorous simulation, the number of theoretical stages of each column, the feed stage, the reboiler duty and the reflux ratio have been determined thanks to the Short-Cut distillation module available in ProSimPlus.

✓ In order to get the value of the global Naphthalene recovery ratio of this process, the following modules are added to the flowsheet:

- a "Measurement" module on the purified Naphthalene output stream C06. This module measures the partial mass flowrate of Naphthalene in this stream. It generates an information stream "Naphthalene output" which contains in fact the difference between the set-point (0 in the present case) and the partial naphthalene flowrate, i.e. a negative value.
- a "Measurement" module on the process input stream C01. In the same way, this module will generate an information stream "Naphthalene input" containing the opposite of the mass partial flowrate of naphthalene in process feed.
- an "Information stream handler module" which will receive both previously described information streams and calculates the ratio between the mass flowrate of Naphthalene in the process output and in the process feed. Thus, the global Naphthalene recovery ratio is calculated. It must be noted than an information stream must necessarily leave the "Information stream handler module" and it can be sent to any module (here in the process outlet connected to stream C03).

2. RESULTS

2.1. Comments on results

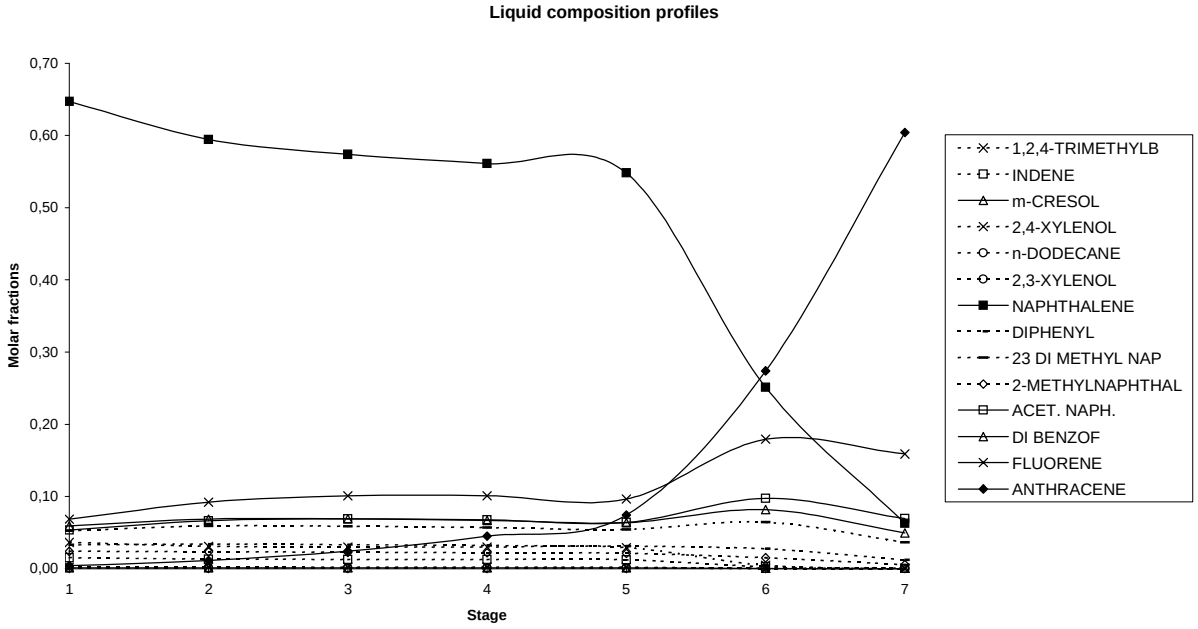
The convergence of the three columns is reached in very few calculations. The output stream C06 effectively contains Naphthalene with a purity of 97% wt. The global recovery ratio of Naphthalene is calculated to be 95.6%.

2.2. Mass and energy balances

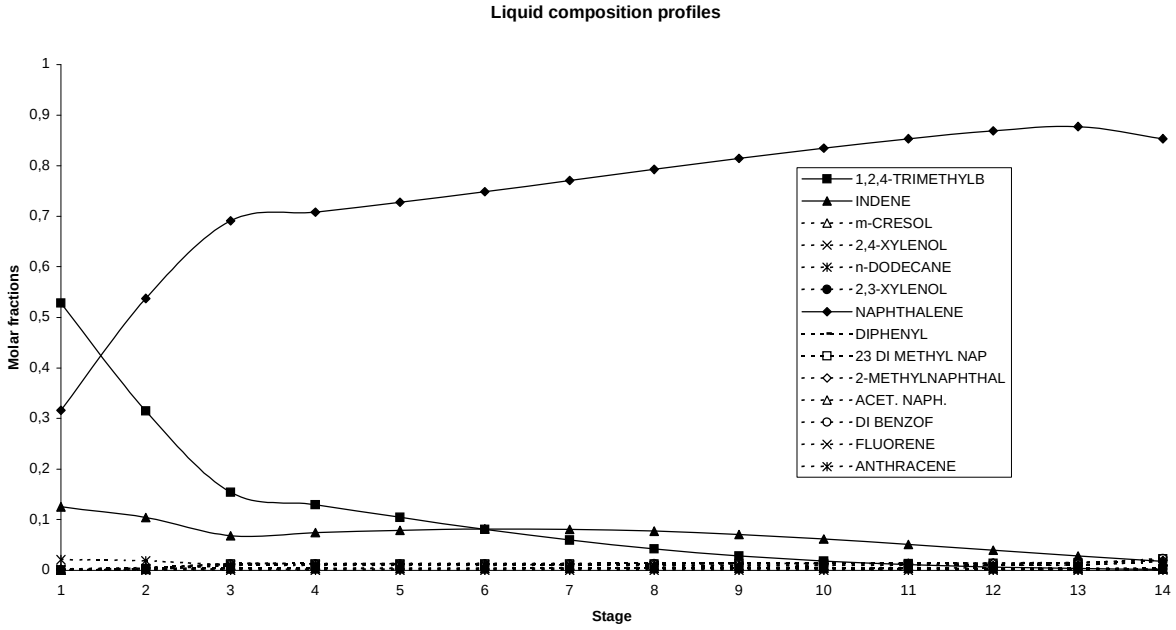
Streams		C01	C02	C03	C04
From		>>>	C101	C101	C102
To		C101	C102	>>>	>>>
Partial flowrates		kg/h	kg/h	kg/h	kg/h
1,2,4-TRIMETHYLBENZENE		376.00	375.89	0.11	372.13
INDENE		101.00	100.91	0.09	60.66
m-CRESOL		5.50	5.49	0.01	0.86
2,4-XYLENOL		9.60	9.57	0.03	0.64
n-DODECANE		13.20	13.20	0.00	11.00
2,3-XYLENOL		5.10	5.08	0.02	0.25
NAPHTHALENE		2266.00	2250.14	15.86	78.70
DIPHENYL		62.30	58.74	3.56	0.08
23 DI METHYL NAPH		78.90	67.94	10.96	0.03
2-METHYLNAPHTHALENE		55.90	54.34	1.56	0.25
ACET. NAPH.		72.10	51.40	20.70	9.85E-03
DI BENZOF		90.60	74.50	16.10	2.04E-02
FLUORENE		110.50	58.58	51.92	8.37E-03
ANTHRACENE		213.00	1.07	211.93	1.31E-06
Total flowrate	kg/h	3459.70	3126.84	332.86	524.64
Mass fractions					
1,2,4-TRIMETHYLBENZENE		0.1087	0.1202	0.0003	0.7093
INDENE		0.0292	0.0323	0.0003	0.1156
m-CRESOL		0.0016	0.0018	3.18E-05	0.0016
2,4-XYLENOL		0.0028	0.0031	0.0001	0.0012
n-DODECANE		0.0038	0.0042	1.31E-05	0.0210
2,3-XYLENOL		0.0015	0.0016	0.0001	0.0005
NAPHTHALENE		0.6550	0.7196	0.0477	0.15
DIPHENYL		0.0180	0.0188	0.0107	0.0002
23 DI METHYL NAPH		0.0228	0.0217	0.0329	6.07E-05
2-METHYLNAPHTHALENE		0.0162	0.0174	0.0047	0.0005
ACET. NAPH.		0.0208	0.0164	0.0622	1.88E-05
DI BENZOF		0.0262	0.0238	0.0484	3.89E-05
FLUORENE		0.0319	0.0187	0.1560	1.60E-05
ANTHRACENE		0.0616	0.0003	0.6367	2.50^{E}-09
Physical state		Liquid	Vapor	Liquid	Vapor
Temperature	°C	100.00	223.34	299.18	181.89
Pressure	mmHg	780.00	760.00	780.00	760.00
Enthalpy	kcal/h	-242963.12	209512.39	6224.06	29454.78
Vapour fraction		0.00	1.00	0.00	1.00

Streams		C05	C06	C07
From		C102	C103	C103
To		C103	>>>	>>
Partial flowrates		kg/h	kg/h	kg/h
1,2,4-TRIMETHYLBENZENE		3.76	3.76	3.89E-08
INDENE		40.26	40.26	2.12E-05
m-CRESOL		4.63	4.63	5.70E-05
2,4-XYLENOL		8.93	8.93	9.32E-04
n-DODECANE		2.20	2.20	1.33E-07
2,3-XYLENOL		4.82	4.82	1.61E-03
NAPHTHALENE		2171.44	2166.01	5.43
DIPHENYL		58.66	1.94E-03	58.65
23 DI METHYL NAPH		67.91	7.30E-06	67.91
2-METHYLNAPHTHALENE		54.09	7.82E-01	53.31
ACET. NAPH.		51.39	0	51.39
DI BENZOF		74.48	1.69E-06	74.48
FLUORENE		58.57	0	58.57
ANTHRACENE		1.06	0	1.07
Total flowrate	kg/h	2602.20	2231.39	370.81
Mass fractions				
1,2,4-TRIMETHYLBENZENE		0.0014	0.0017	1.05E-10
INDENE		0.0155	0.0180	5.72E-08
m-CRESOL		0.0018	0.0021	1.54E-07
2,4-XYLENOL		0.0034	0.0040	2.51E-06
n-DODECANE		0.0008	0.0010	3.58E-10
2,3-XYLENOL		0.0019	0.0022	4.35E-06
NAPHTHALENE		0.8345	0.9707	0.0146
DIPHENYL		0.0225	8.70E-07	0.1582
23 DI METHYL NAPH		0.0261	3.27E-09	0.1831
2-METHYLNAPHTHALENE		0.0208	3.51E-04	0.1438
ACET. NAPH.		0.0197	0	0.1386
DI BENZOF		0.0286	7.58E-10	0.2009
FLUORENE		0.0225	0	0.1580
ANTHRACENE		0.0004	0	0.0029
Physical state		Liquid	Vapor	Liquid
Temperature	°C	221.62	218.46	265.16
Pressure	mmHg	780.00	780.00	780.00
Enthalpy	kcal/h	-42553.90	141503.76	1940.57
Vapour fraction		0.00	1.00	0.00

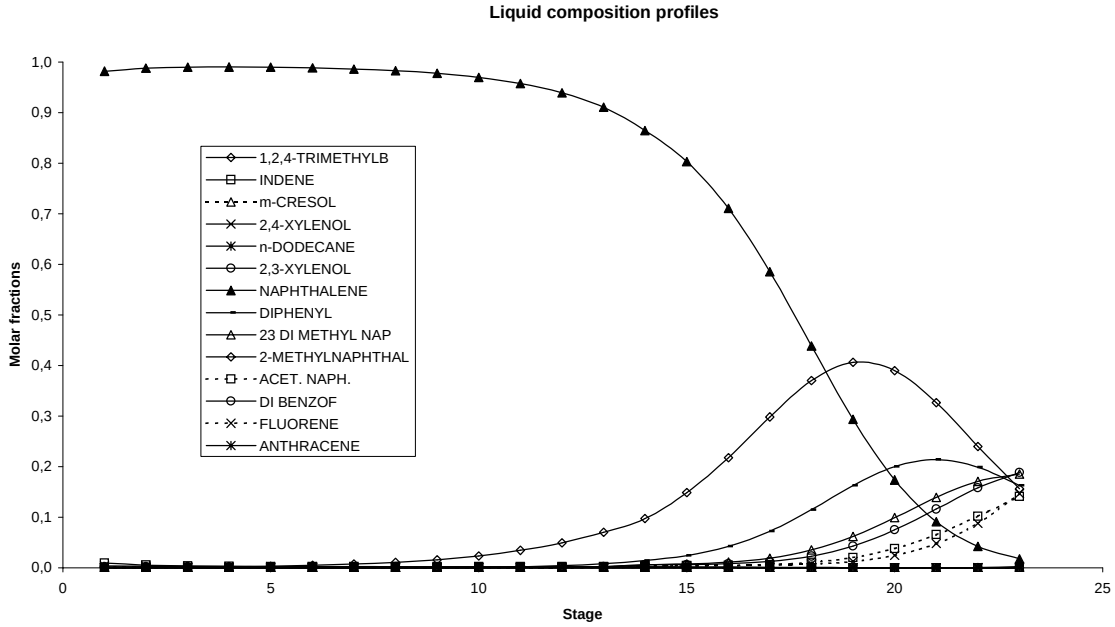
2.3. Column C101 composition profiles



2.4. Column C102 composition profiles



2.5. Column C103 composition profiles



3. REFERENCES

[1] Application Briefs
Process Simulation Program
Simulation Sciences Inc.
Revision 1, Jan 1983

[2] Peng Y.D., Robinson D.B.
"A new two constant equation of state"
I.E.C. Fundam., 15, 1, 59-64 (1976)

