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ProSimPlus Application Example

Deethanizer with Thermosiphon

Example Purpose
This example deals with the simulation of a deethanizer. The aim of this column is to recover as much as possible of ethane in the overhead product. Thus, the propane and the heavier lie in the bottoms. The particular point which is detailed is the modeling of the thermosiphon reboiler. This equipment is precisely taken into account by the representation of the downcomer and the riser. The pressure drop balance is computed in a Windows Script module.

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Corresponding ProSimPlus files	*PSPS_EX_EN - Deethanizer with thermosiphon - case A.pmp3* *PSPS_EX_EN - Deethanizer with thermosiphon - case B.pmp3*

Energy

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1. MODELING OF THE PROCESS

1.1. Process description

In this example a deethanizer is modeled. The specificity of this column is the use of a thermosiphon as a reboiler.

Vertical thermosiphon reboilers operate by natural circulation of the liquid from the still through the downcomer to the reboiler and of the two-phase mixture from the reboiler through the return piping (the riser). The flow is induced by the hydrostatic pressure imbalance between the liquid in the downcomer and the two-phase mixture in the reboiler tubes. Thermosiphons do not require any pump for recirculation and are generally regarded as less likely to foul in service because of the relatively two-phase high velocities obtained in the tubes. This way of working let them more complicated to model and design than kettle reboilers.

The pressure drop balance is:

$$\Delta P_{static\ head} = \Delta P_{dowmcomer} + \Delta P_{heat\ exchanger} + \Delta P_{riser}$$

The static pressure drop is computed as:

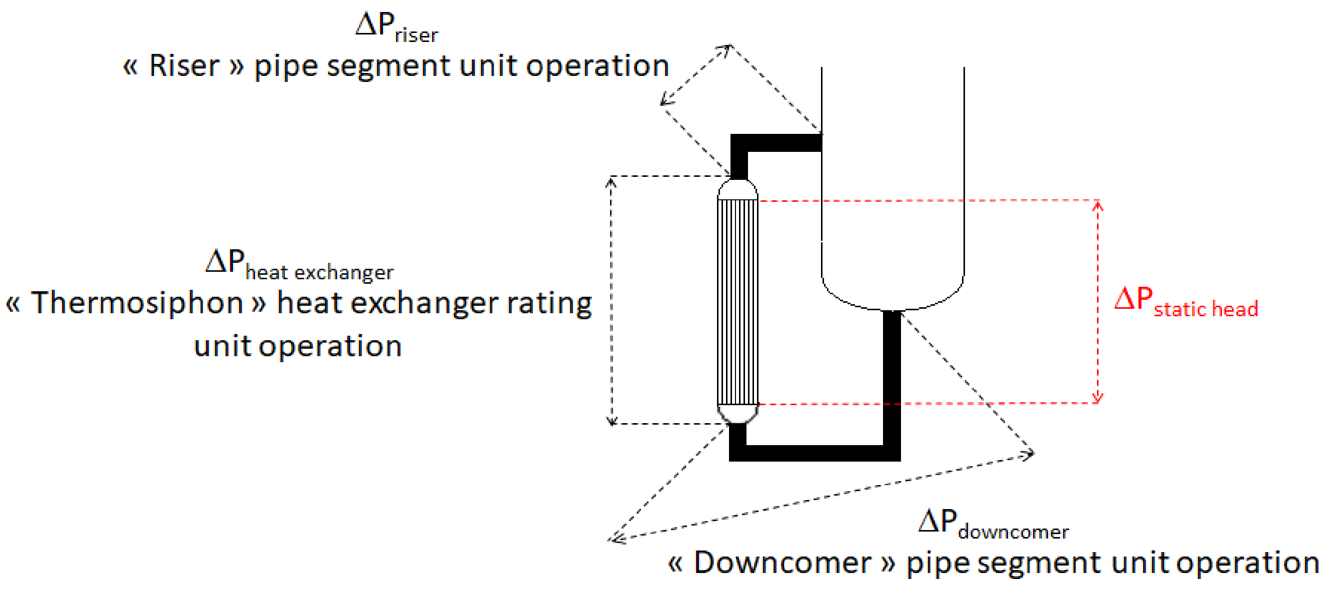
$$\Delta P_{static\ head} = \rho g L_{tubes}$$

The pressure drop between the return of the thermosiphon in the column and the column sump is not taken into account in the pressure drop balance. The static pressure drop due to the possible liquid only phase in the bottom of the thermosiphon is also not taken into account.

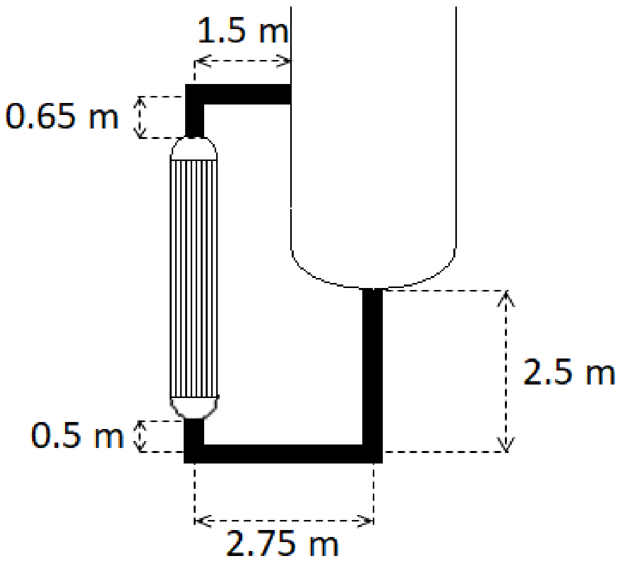
The downcomer, the heat exchanger (including inlet and outlet nozzles) and the riser pressure drops are directly calculated by the corresponding ProSimPlus unit operations. The pressure drop balance is performed in a Windows Script unit operation.

An accurate representation of the thermosiphon is achieved in the simulations by using:

- ✓ Pipe segment unit operations to represent the downcomer and the riser,
- ✓ A heat exchanger rating unit operation to model the thermosiphon itself.



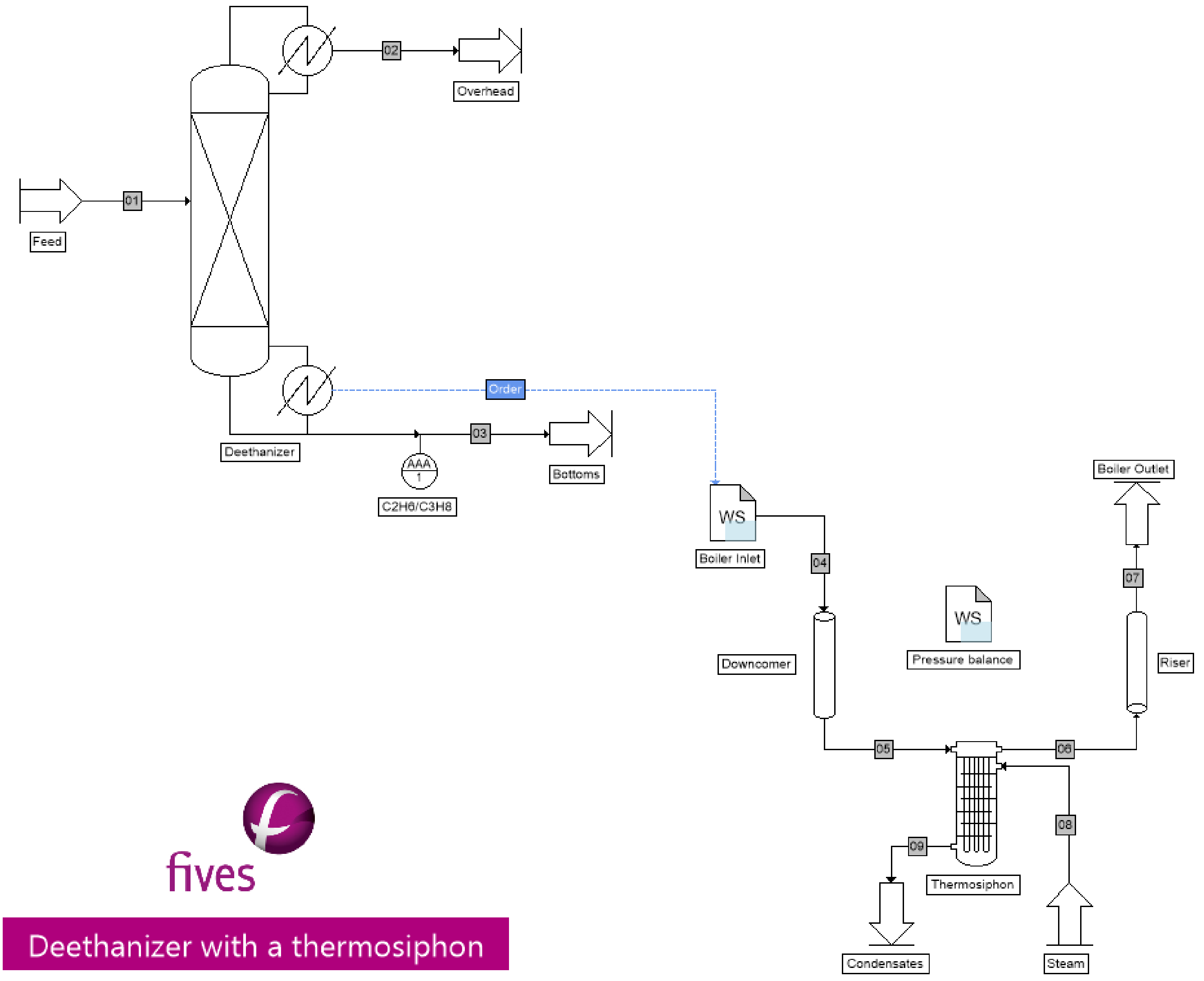
The following installation is modeled in this example:



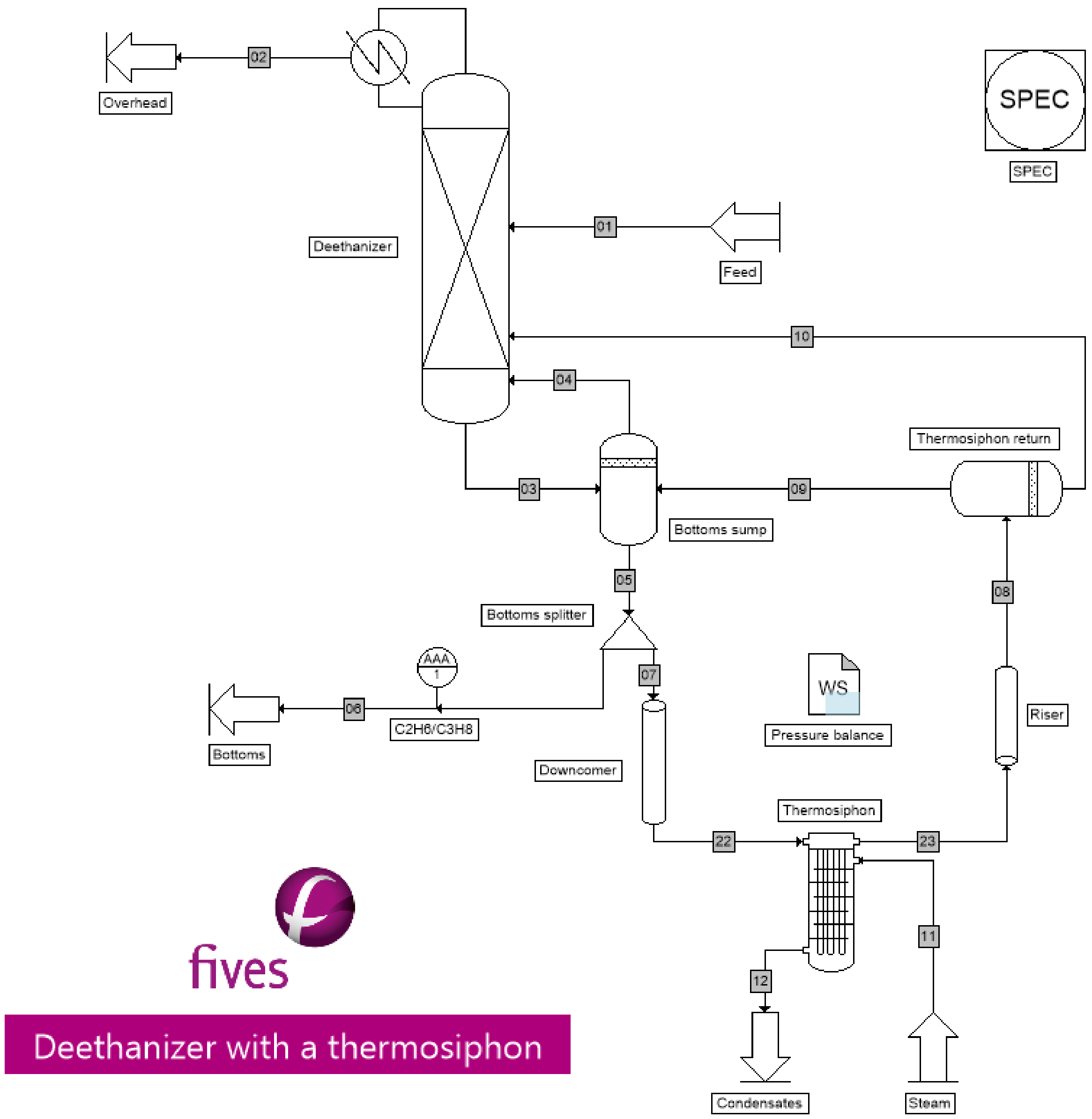
Two simulations are set up. In case A, the thermosiphon is solved after the simulation of the deethanizer. Thus, the deethanizer unit operation model includes the modeling of the thermosiphon. This allows to compute the internal flows characteristics from the specification of the thermosiphon: a vaporization ratio of 0.35. The thermosiphon with the downcomer and the riser can then be calculated. By this way, the design of the thermosiphon can be made. In case B simulation, the thermosiphon is solved in the same time as the deethanizer. In that case, the deethanizer unit operation holds only the condenser. This simulation allows to analyze the interaction between the thermosiphon and the operation of the column.

1.2. Process flowsheet

Case A: Solving of the thermosiphon after the solving of the column.



Case B: Solving of the thermosiphon coupled with the solving of the column.



1.3. Components

The components taken into account in the simulation, their chemical formula and CAS numbers are given in the following table. Pure components physical properties are extracted from the ProSimPlus standard database [ROW17].

Component name	Chemical formula	CAS number
Nitrogen	N_2	7727-37-9
Methane	CH_4	74-82-8
Ethane	C_2H_6	74-84-0
Propane	C_3H_8	74-98-6
Isobutane	C_4H_{10}	75-28-5
n-butane	C_4H_{10}	106-97-8
Isopentane	C_5H_{12}	78-78-4
n-pentane	C_5H_{12}	109-66-0
n-hexane	C_6H_{14}	110-54-3
n-heptane	C_7H_{16}	142-82-5
Water	H_2O	7732-18-5

1.4. Thermodynamic models

The studied process deals with a mixture of hydrocarbons. Thus, the Soave-Redlich-Kwong (SRK) [SOA72] equation of state has been chosen. The binary interaction parameters come from Simulis Thermodynamics database. The liquid molar volume calculation uses the API 6A2.22 model [API82].

For the condensing steam (utility side of the thermosiphon) the specific model for pure water (NBS/NRC steam tables) is used [HAA84].

Each thermodynamic model has its own calculator.

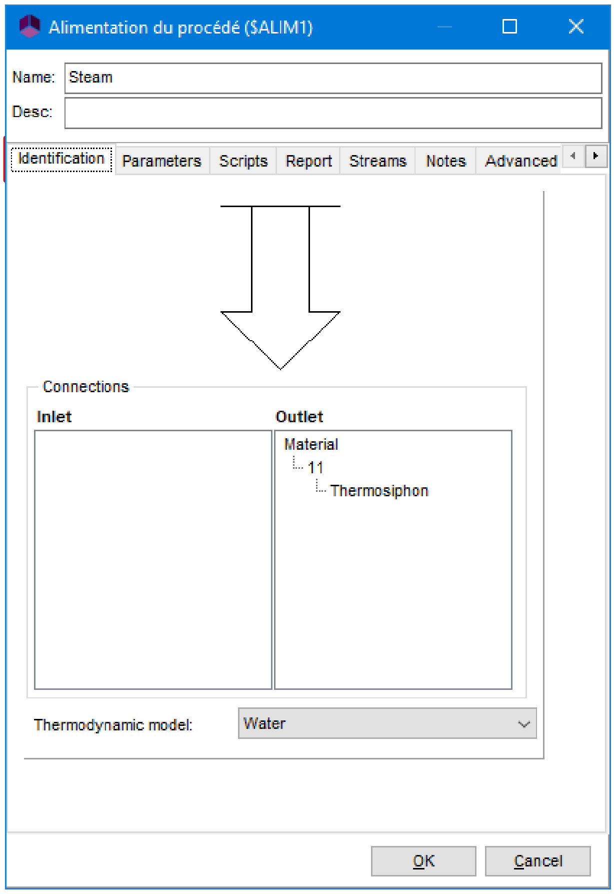
1.5. Operating conditions

1.5.1. Feeds

Process feed	
Mole fraction (-)	
Nitrogen	0.0003
Methane	0.4459
Ethane	0.1983
Propane	0.1909
Isobutane	0.0416
n-butane	0.0460
Isopentane	0.0168
n-pentane	0.0116
n-hexane	0.0296
n-heptane	0.0190
Total flow rate (lbmol/h)	900
Temperature (°C)	-34.45
Pressure (psig)	440

Utility feed	
Mole fraction (-)	
Water	1
Total flow rate (kg/h)	2 714
Temperature (°C)	140
Pressure (psig)	Dew point

Select the calculator with the specific model for pure water for the utility feed.



1.5.2. Deethanizer

For the case A:

Operating parameters	Value
Type	Distillation column with partial condenser
Number of stages (including the condenser and the thermosiphon)	21
Feed stage	10
Vapor distillate flow rate (kmol/h)	261.961285
Molar reflux ratio	0.603738
Pressure profile (psig) Overhead pressure Stage #2 Stage #20	 425 430 440
Reboiler Type Molar vaporization ratio	 Thermosiphon 0.35

ℹ	The thermosiphon reboiler counts as two theoretical stages.

For the case B:

Operating parameters	Value
Type	Stripper with partial condenser
Number of stages (including the condenser)	19
Process feed stage	10
Thermosiphon return stage	19
Molar reflux ratio	0.603738
Pressure profile (psig) Overhead pressure Stage #2 Stage #19	 425 430 439.444444

ℹ	The stages 20 and 21 of the deethanizer of the case A are replaced in the case B by a flash (“Bottoms sumps”) and by the heat exchanger unit operation modeling the thermosiphon (“Thermosiphon”).

1.5.3. Downcomer and riser

Downcomer	
Operating parameters	**Value**
Resolution	
Calculate from	An enthalpy method
Heat transfer	Overall heat exchange
Heat exchanged (kcal/h)	0 (adiabatic)
First segment	
Type	Linear
Objective, calculate	The pressure drop
Diameter (mm)	300
Relative roughness	0
Length (m)	2.5
Angle (°)	-90
Diphasic flow	Estimated
Estimation method	Beggs & Brill
Second segment	
Resistance coefficient (K)	Estimated
Type	Elbow: 90° Std
Diameter (mm)	300
Absolute roughness (m)	0
Third segment	
Type	Linear
Objective, calculate	The pressure drop
Diameter (mm)	300
Relative roughness	0
Length (m)	2.75
Angle (°)	0
Diphasic flow	Estimated
Estimation method	Beggs & Brill
Fourth segment	
Resistance coefficient (K)	Estimated
Type	Elbow: 90° Std
Diameter (mm)	300
Absolute roughness (m)	0
Fifth segment	
Type	Linear
Objective, calculate	The pressure drop
Diameter (mm)	300
Relative roughness	0
Length (m)	0.5
Angle (°)	90
Diphasic flow	Estimated
Estimation method	Beggs & Brill

Riser	
Operating parameters	**Value**
Resolution	
Calculate from	An enthalpy method
Heat transfer	Overall heat exchange
Heat exchanged (kcal/h)	0 (adiabatic)
First segment	
Type	Linear
Objective, calculate	The pressure drop
Diameter (mm)	300
Relative roughness	0
Length (m)	0.65
Angle (°)	90
Diphasic flow	Estimated
Estimation method	Beggs & Brill
Second segment	
Resistance coefficient (K)	Estimated
Type	Elbow: 90° Std
Diameter (mm)	300
Absolute roughness (m)	0
Third segment	
Type	Linear
Objective, calculate	The pressure drop
Diameter (mm)	300
Relative roughness	0
Length (m)	1.5
Angle (°)	0
Diphasic flow	Estimated
Estimation method	Beggs & Brill

1.5.4. Thermosiphon

Operating parameters	Value
Global	
Module type	Heat exchanger rating
Type	TEMA E
Shell	
Diameter (mm)	629
Orientation	Vertical
Number of passes	1
Fouling factor (kcal/h/m²/K)	0
Baffle-shell clearance (mm)	2.5
Tube bank-shell clearance (mm)	7.1
Inlet nozzle diameter (mm)	200
Outlet nozzle diameter (mm)	40
Tubes	
Outlet diameter (in)	1.25
Thickness (in)	0.134
Number	149
Length (ft)	12
Layout pattern	Square
Pitch (in)	1.5625
Type of tubes	Smooth
Fouling factor (kcal/h/m²/K)	0
Material thermal conductivity (W/m/K)	45
Number of passes	1
Tube-baffle clearance (mm)	0.4
Inlet nozzle diameter (mm)	300
Outlet nozzle diameter (mm)	300
Baffles	
Number	11
Inlet spacing (mm)	256
Outlet spacing (mm)	256
Thickness (mm)	7.9
Opening (%)	25
Presence of tubes in the window	Yes
Numerical parameters	
Gravity pressure drop included in the total pressure drop	Yes

1.5.1. Flashs (case B only)

	Bottoms sump	Thermosiphon return
Operating parameters		
Type	Constant pressure and enthalpy	
Pressure (psig)	440	The lowest of the feed streams
Heat duty	Adiabatic	

1.5.2. Stream splitter (case B only)

Operating parameters	Value
Flowrate going to the thermosiphon (kg/h)	72 037.7

> The value of the flowrate going into the thermosiphon is the value calculated by the deethanizer unit operation of case A.

1.5.3. Constraints and recycles module (case B only)

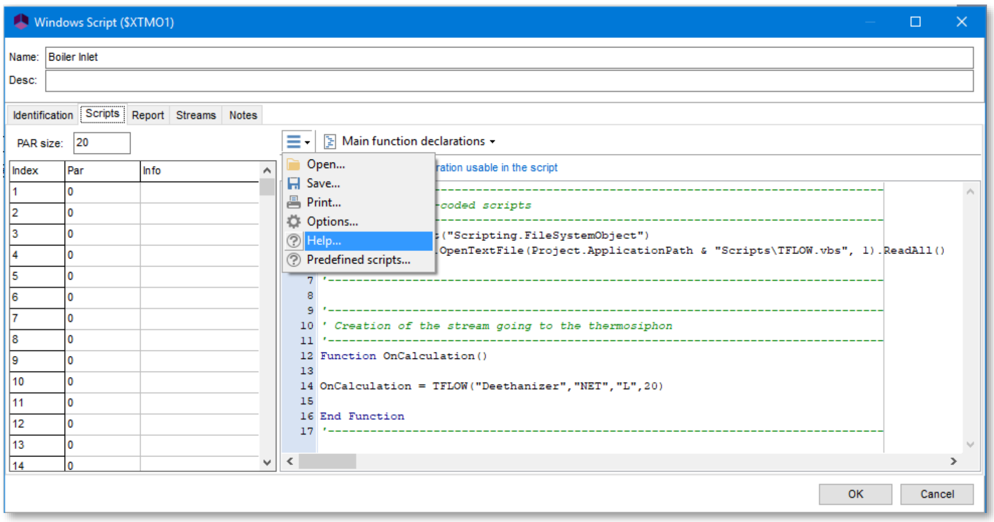
Operating parameters	Value
Tear streams iterative variables	Enthalpies

> The tear stream of case B simulation (stream “04”) is at its dew point. Thus, select enthalpies instead temperatures in order to insure to respect this constraint.

1.6. Windows Script

1.6.1. Case A: Boiler inlet

In the case A, a script is used to create a material stream corresponding to the liquid inside flow of the column going into the thermosiphon. For that, the "TFLOW" pre-coded script is used. The flow incoming in the thermosiphon is the liquid stream of the 20th theoretical stage of the deethanizer column. For more detailed information about scripting, see the on-line help:



```
'-------------------------------------------------------------------------------
' Loading of pre-coded scripts
'-------------------------------------------------------------------------------
With CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\TFLOW.vbs", 1).ReadAll()
End With

'-------------------------------------------------------------------------------
' Creation of the stream going to the thermosiphon
'-------------------------------------------------------------------------------
Function OnCalculation()
 OnCalculation = TFLOW("Déethaniseur","NET","L",20)
End Function
```


1.6.2. Both cases: Pressure drop balance

In both cases, a script is written to perform the pressure drop balance. This scrip uses the “UnitConversion” pre-coded script to obtain the results in the report units selected in ProSimPlus interface.

```
'-------------------------------------------------------------------------------
'Open the script for the units conversions
'-------------------------------------------------------------------------------
With CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\UnitConversion.vbs", 1).ReadAll()
End With

'-------------------------------------------------------------------------------
'Calculation of the pressure drop balance
'-------------------------------------------------------------------------------
Function OnCalculation()
   ' Static head
   ' -----------
  Ltube              = Project.Modules("Thermosiphon").TubesLenght '(m)
  Density            = Project.Modules("Thermosiphon").InputStream(1).Density '(kg/m3)
  DPstatichead       = Density*9.81*Ltube '(Pa)
  DPstatichead       = Convert("Pressure drop", DPstatichead, "Pa", ProSimUnit("Pressure drop"))
  Module.Parameter(1) = ProSimToReport("Pressure drop", DPstatichead)

   ' Pressure drop in the downcomer
   ' ------------------------------
  DPdowncomer = Project.Modules("Downcomer").SegFrictionPressureDrops(1)
  For i = 2 To Project.Modules("Downcomer").NBSEG
    DPdowncomer = DPdowncomer + Project.Modules("Downcomer").SegPressureDrops(i)
  Next
  Module.Parameter(2) = ProSimToReport("Pressure drop", DPdowncomer)

   ' Pressure drop in the heat exchanger
   ' -----------------------------------
  DPecha = Project.Modules("Thermosiphon").TubesPressureDrop +_
           Project.Modules("Thermosiphon").TubesInletNozzlesPressureDrop +_
           Project.Modules("Thermosiphon").TubesOutletNozzlesPressureDrop
  Module.Parameter(3) = ProSimToReport("Pressure drop", DPecha)

   ' Pressure drop in the riser
   ' --------------------------
  DPriser = 0.0
  For i = 1 To Project.Modules("Riser").NBSEG
    DPriser = DPriser + Project.Modules("Riser").SegPressureDrops(i)
  Next
  Module.Parameter(4) = ProSimToReport("Pressure drop", DPriser)
```



```
  ' Total pressure drop
  ' -------------------
  DPtotal             = DPdowncomer + DPecha + DPriser
  Module.Parameter(5) = ProSimToReport("Pressure drop", DPtotal)

  ' Deviation
  ' ---------
  Module.Parameter(6) = abs(DPstatichead - DPtotal)/DPstatichead

  ' Validation of the script
  ' ------------------------
  OnCalculation = True

End Function

'--------------------------------------------------------------------------------
'Printing of the results
'--------------------------------------------------------------------------------
Sub OnPrintResults()
  With Module
    .PrintReport "PRESSURE DROP BALANCE FOR THE THERMOSIPHON"
    .PrintReport "------------------------------------------"
    .PrintReport " "
    .PrintReport " - Static head   : " & FormatNumber(.Parameter(1),0) & " " & ReportUnit("Pressure drop")
    .PrintReport " "
    .PrintReport " - Downcomer     : " & FormatNumber(.Parameter(2),0) & " " & ReportUnit("Pressure drop")
    .PrintReport " - Heat exchanger: " & FormatNumber(.Parameter(3),0) & " " & ReportUnit("Pressure drop")
    .PrintReport " - Riser         : " & FormatNumber(.Parameter(4),0) & " " & ReportUnit("Pressure drop")
    .PrintReport "                  ---------"
    .PrintReport "                   " & FormatNumber(.Parameter(5),0) & " " & ReportUnit("Pressure drop")
    .PrintReport " "
    .PrintReport " - Deviation     : " & FormatNumber(.Parameter(6),2)*100 & "%"
  End With
End Sub
```


1.7. Initializations

The calculation sequence is automatically determined by ProSimPlus. Two tear streams are detected: “04” (gas stream leaving the bottoms sump flash) and “22” (liquid stream incoming the tubes of the thermosiphon). The following initializations are used in the simulation.

Stream	04	22
Mass fraction (-)		
Methane	0.000006	0.000001
Ethane	0.017046	0.007199
Propane	0.610499	0.415365
Isobutane	0.122154	0.120409
n-butane	0.120220	0.133145
Isopentane	0.038025	0.060362
n-pentane	0.024680	0.041679
n-hexane	0.045250	0.127029
n-heptane	0.022122	0.094811
Total flow rate (kg/h)	1 052.7	72 037.7
Temperature (°C)	Dew point	112
Pressure (psig)	440	

The results of case A simulation can also be used to initialize these two tear streams.

1.8. “Hints and tips”

A measurement unit operation is used to compute directly the ethane to propane molar ratio in the bottoms.

2. Results

2.1. Mass and energy balances

This document presents only the most relevant stream results for the case B. The results of the case A are similar. In ProSimPlus, mass and energy balances are provided for all streams. Stream results are also available at the unit operation level ("Stream" tab in the configuration window).

Streams		01	02	03	05
Total flow	kg/h	13528	5330.2	32266	80235
Total flow	kmol/h	408.23	261.86	618.51	1432.7
Mass fractions					
NITROGEN		0.00025361	0.00064365	0	0
METHANE		0.21586	0.54785	1.8074E-006	9.2553E-007
ETHANE		0.17994	0.4456	0.011089	0.0071992
PROPANE		0.25403	0.00591	0.52102	0.41536
ISOBUTANE		0.072966	1.6504E-007	0.1265	0.12041
n-BUTANE		0.080683	2.1369E-008	0.13175	0.13315
ISOPENTANE		0.036578	0	0.049655	0.060362
n-PENTANE		0.025256	0	0.03315	0.041679
n-HEXANE		0.076977	0	0.07861	0.12703
n-HEPTANE		0.057453	0	0.04822	0.094811
WATER		0	0	0	0
Mole fractions					
NITROGEN		0.0003	0.0004677	0	0
METHANE		0.4459	0.69515	5.8776E-006	3.231E-006
ETHANE		0.1983	0.30165	0.019238	0.013408
PROPANE		0.1909	0.0027282	0.6164	0.52753
ISOBUTANE		0.0416	5.7799E-008	0.11354	0.11602
n-BUTANE		0.046	7.484E-009	0.11825	0.12829
ISOPENTANE		0.0168	0	0.035904	0.046854
n-PENTANE		0.0116	0	0.023969	0.032352
n-HEXANE		0.0296	0	0.047587	0.082553
n-HEPTANE		0.019	0	0.025104	0.05299
WATER		0	0	0	0
Physical state		Liq./Vap.	Vapor	Liquid	Liquid
Temperature	°C	-34.45	-37.974	101.72	112.63
Pressure	psig	440	425	439.44	440
Enthalpic flow	kW	-1680.2	-283.18	-1193.2	-2422.5
Vapor molar fraction		0.31124	1	0	0

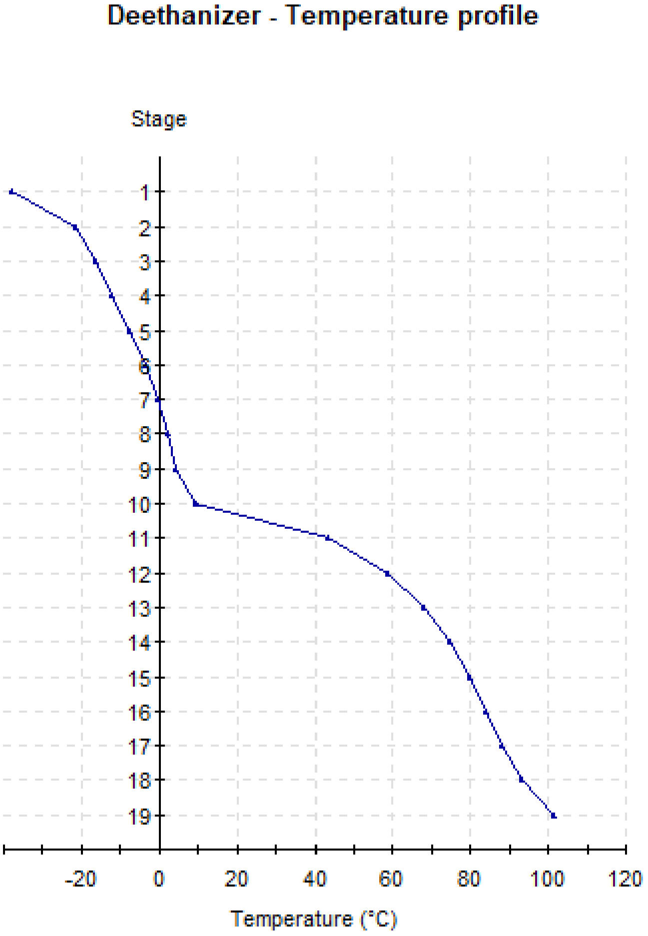
Streams		06	09	10	11
Total flow	kg/h	8197.5	49022	23016	2714
Total flow	kmol/h	146.38	835.44	450.87	150.65
Mass fractions					
NITROGEN		0	0	0	0
METHANE		9.2553E-007	4.1684E-007	2.009E-006	0
ETHANE		0.0071992	0.0048505	0.012202	0
PROPANE		0.41536	0.35001	0.55456	0
ISOBUTANE		0.12041	0.11644	0.12887	0
n-BUTANE		0.13315	0.13379	0.13177	0
ISOPENTANE		0.060362	0.06693	0.046374	0
n-PENTANE		0.041679	0.046928	0.030499	0
n-HEXANE		0.12703	0.15714	0.06289	0
n-HEPTANE		0.094811	0.12392	0.032819	0
WATER		0	0	0	1
Mole fractions					
NITROGEN		0	0	0	0
METHANE		3.2311E-006	1.5247E-006	6.393E-006	0
ETHANE		0.013408	0.0094655	0.020714	0
PROPANE		0.52753	0.46575	0.64199	0
ISOBUTANE		0.11602	0.11755	0.11319	0
n-BUTANE		0.12829	0.13507	0.11573	0
ISOPENTANE		0.046854	0.054433	0.032811	0
n-PENTANE		0.032352	0.038166	0.021579	0
n-HEXANE		0.082553	0.107	0.037254	0
n-HEPTANE		0.05299	0.072565	0.01672	0
WATER		0	0	0	1
Physical state		Liquid	Liquid	Vapor	Vapor
Temperature	°C	112.63	120.84	120.84	140
Pressure	psig	440	439.34	439.34	37.691
Enthalpic flow	kW	-247.51	-1205.2	649	140.53
Vapor molar fraction		0	0	1	1

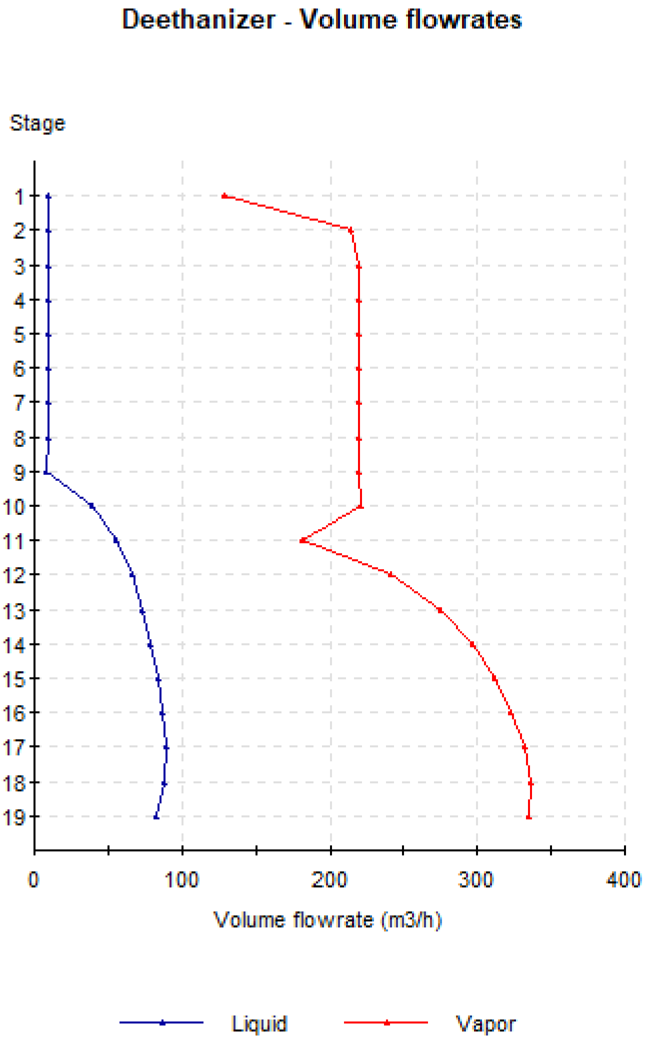
2.2. Process performance

The overhead stream contains the nitrogen and most of the methane and the ethane. This propane loss is less than 1% molar on feed. The ethane to propane molar ratio in the bottoms is close to 0.025.

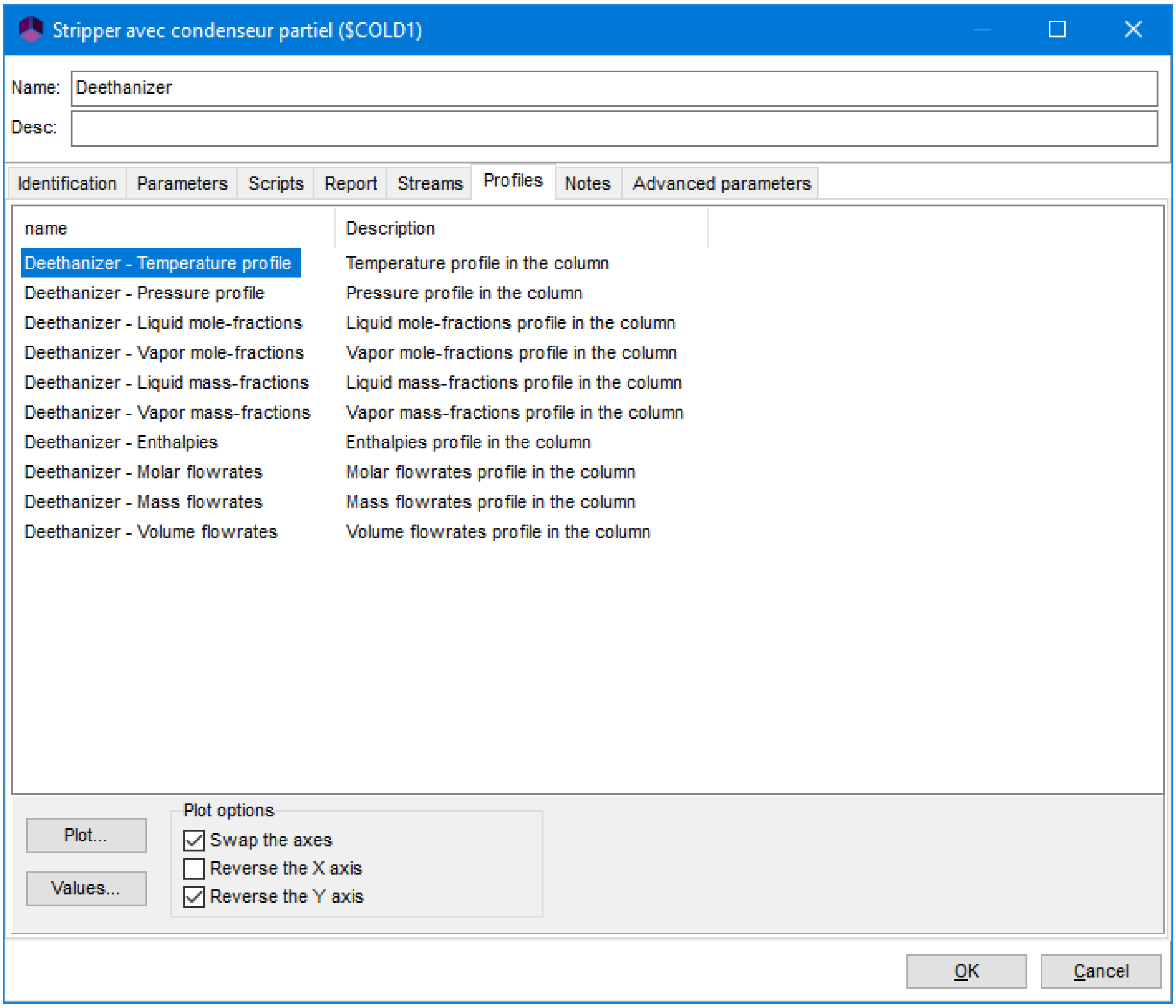
2.3. Deethanizer

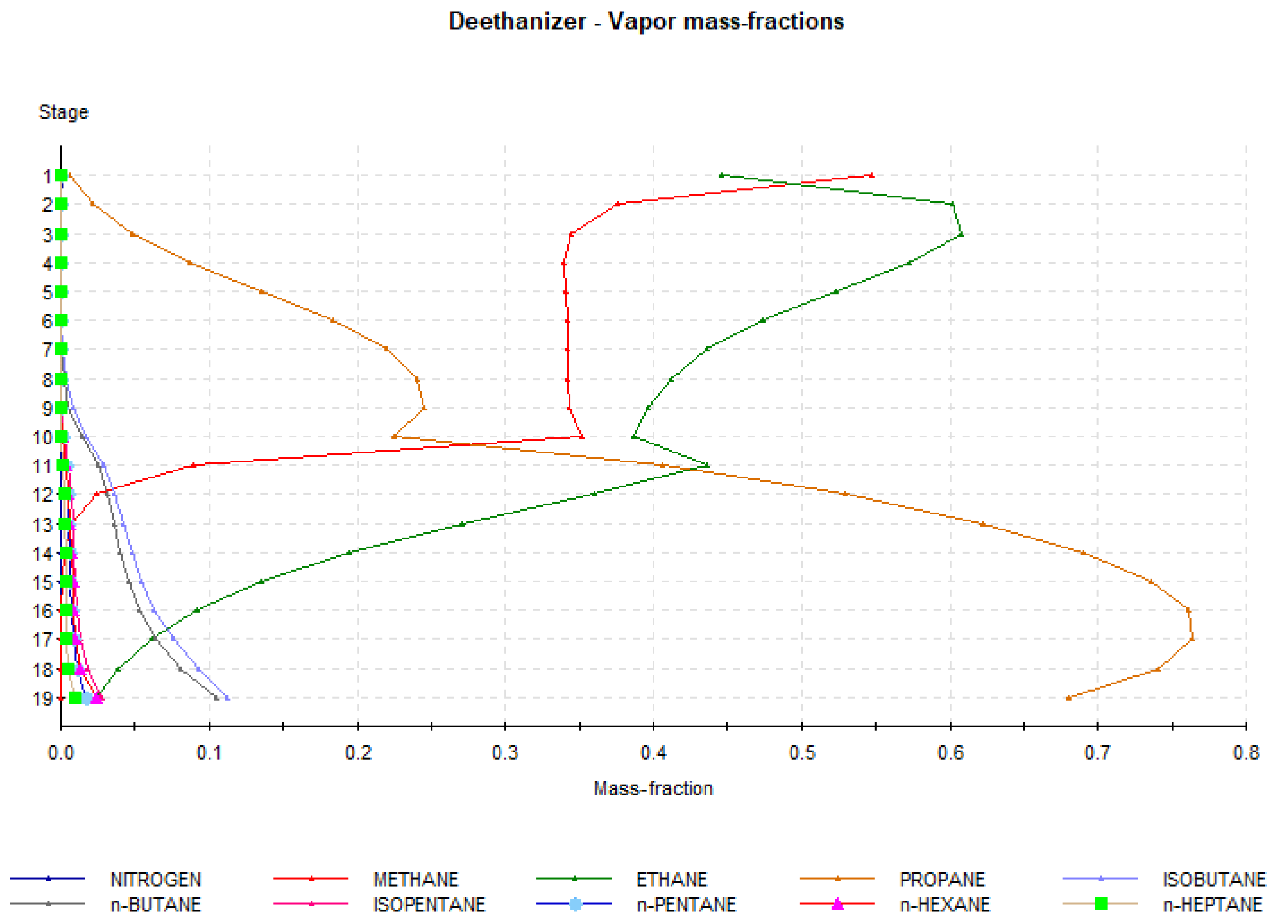
The results are the ones of case B. The results of the case A are similar. The column stages are numbered from top to bottom (plate 1: condenser; plate 2: top plate; plate 19: bottom plate). More profiles are available in the “Profiles” tab of the unit operation.

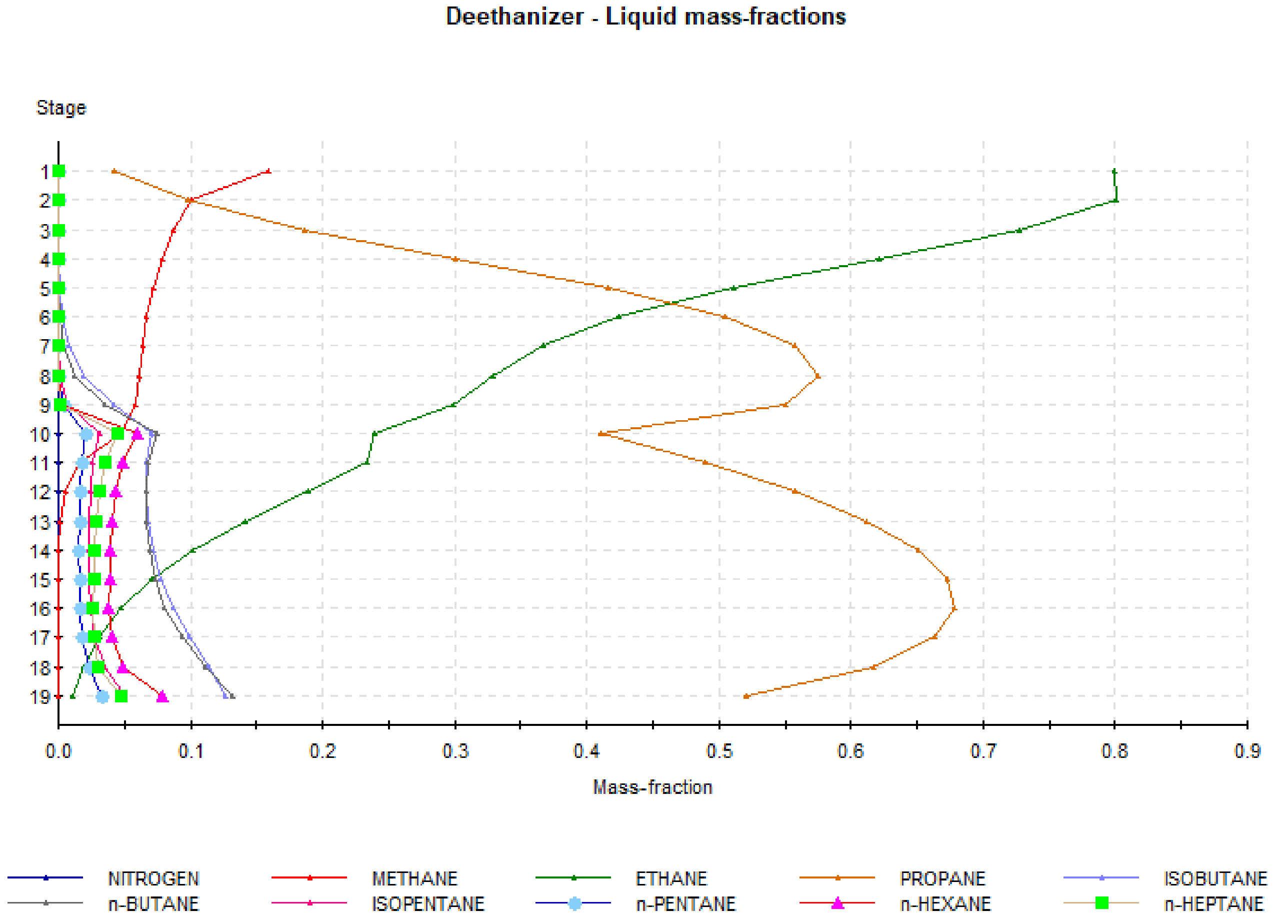




The user can change the graph options to configure them in the way he/she normally does.




Deethanizer - Vapor mass-fractions
Stage
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Mass-fraction
NITROGEN
METHANE
ETHANE
PROPANE
ISOBUTANE
n-BUTANE
ISOPENTANE
n-PENTANE
n-HEXANE
n-HEPTANE



2.4. Thermosiphon

2.4.1. Pressure drop balance

These results are the ones of case B. The results of the case A are similar.

Static head: 142 mbar

Downcomer: 20 mbar

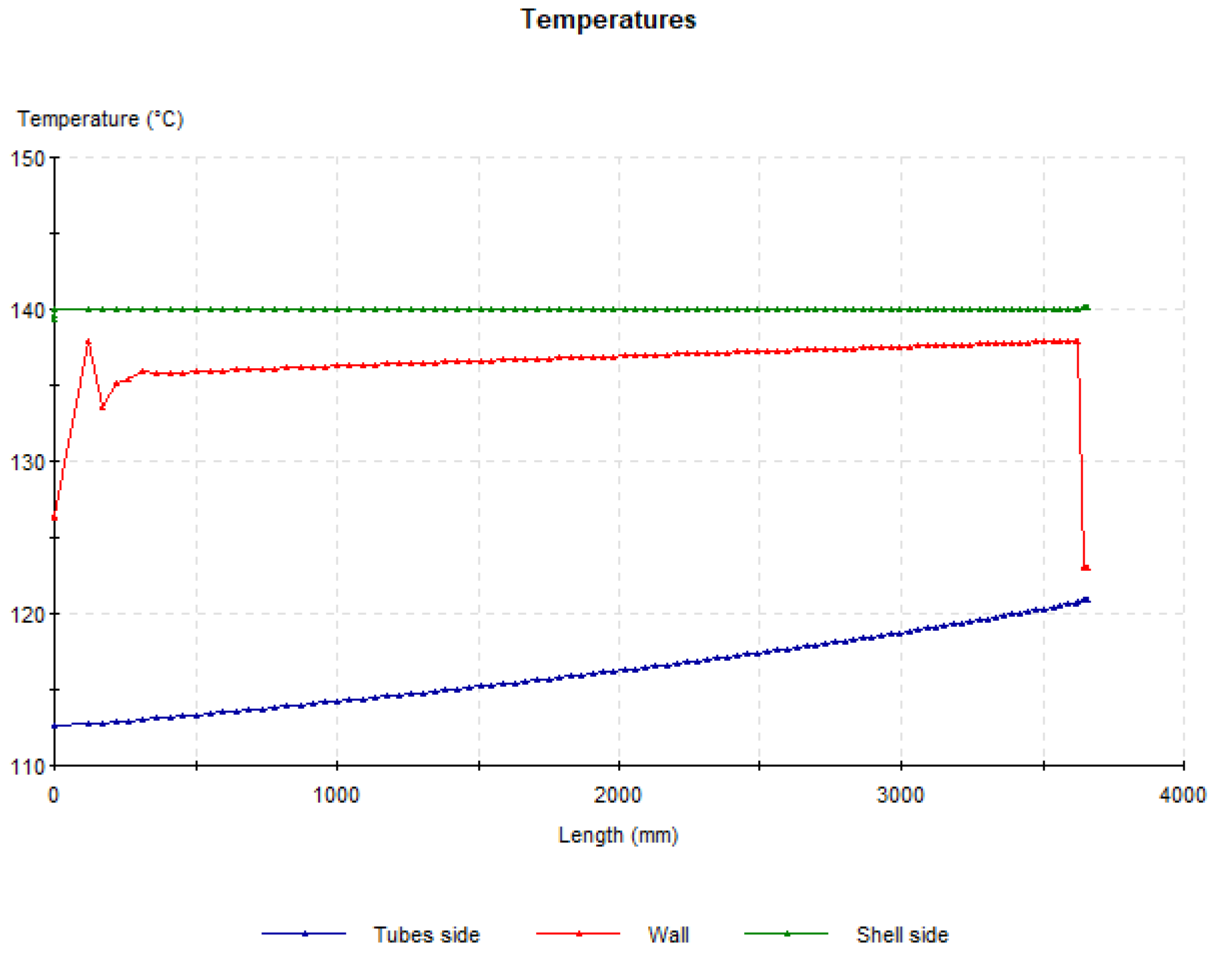
Heat exchanger: 101 mbar

Riser: 21 mbar

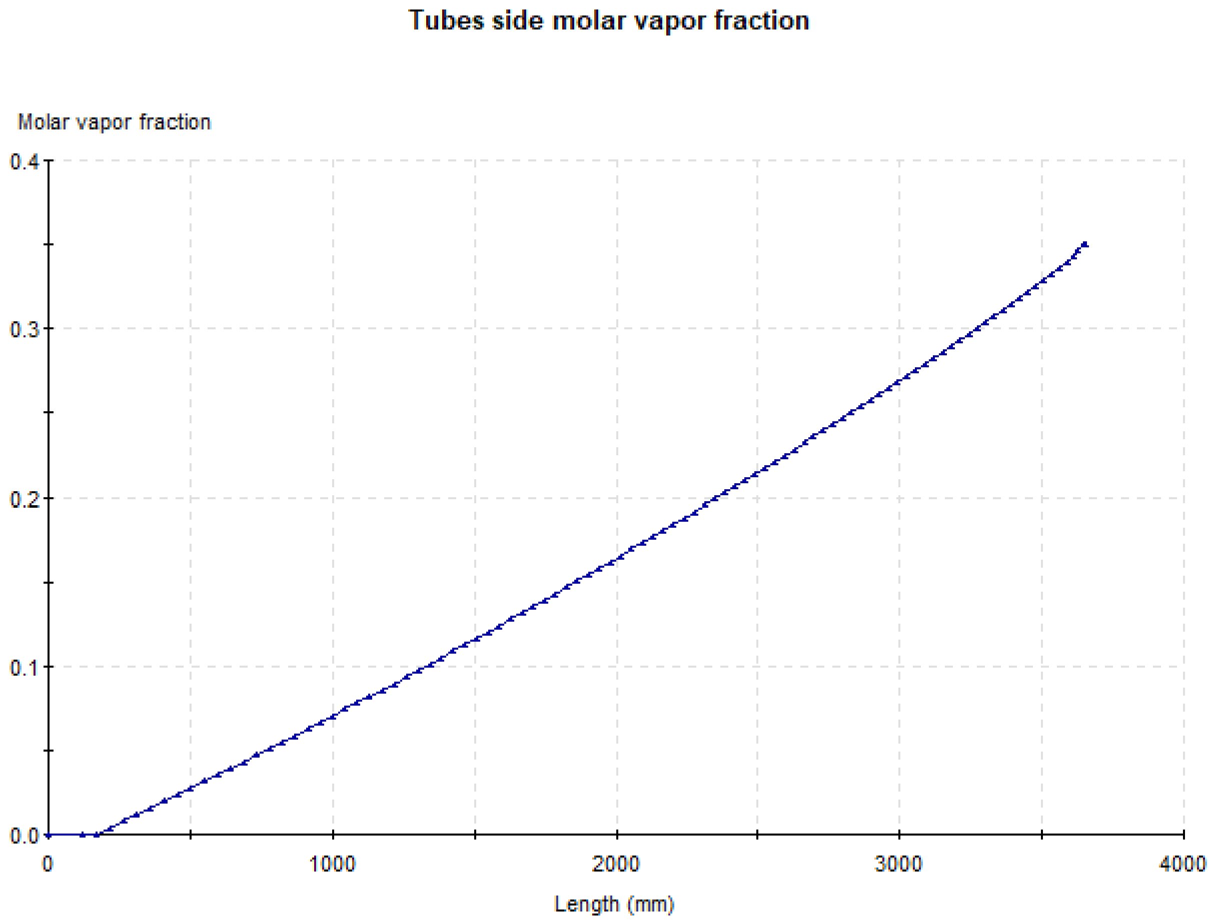
The downcomer + heat exchanger + riser pressure drops (20 mbar + 101 mbar + 21 mbar = 142 mbar) equilibrate the static head (142 mbar). They are calculated and displayed by the windows script module “Pressure drop”.

2.4.2. Profiles

The results are the ones of case B. The results of the case A are similar. More profiles are available in the “Profiles” tab of the unit operation.



Temperatures profile



Tubes side molar vapor fraction profile

3. REFERENCES

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