ProSim

PROSIMPLUS APPLICATION EXAMPLE

ECONOMIC EVALUATION OF A TOLUENE HYDRODEALKYLATION PROCESS

EXAMPLE PURPOSE
This example presents the economic evaluation of a toluene hydrodealkylation process with ProSimPlus. The hydrodealkylation reactor is fed with pre-heated hydrogen and toluene. The products of the reaction (benzene, biphenyl and methane) and the residual reactants are separated by a flash and three separation units. The recycling allows to reinject a part of the residual reactants into the hydrodealkylation reactor. This example especially illustrates the use of the ProSimPlus "Economic evaluation" module on a process including different types of unit operations (reactors, columns, pumps, heat exchangers…).

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CORRESPONDING PROSIMPLUS FILES	*PSPS_E18_EN – HDA Toluene Process Cost FMM.pmp3* *PSPS_E18_EN – HDA Toluene Process Cost PEM.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. 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.

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1. INTRODUCTION

This example is carried out on benzene production process by toluene hydrodealkylation. This process was especially used after the Second World War to convert a toluene excess (produced as a consequence of the stop of its use in the TNT production) into benzene. This benzene is mainly used to produce cyclohexane that is a nylon precursor.

The diversity of equipment of this process allows to illustrate the use of the “Economic evaluation” unit operation in ProSimPlus. This unit operation aims to evaluate the investment and operating costs of a process. The economic evaluation is a step to determine the viability of a process.

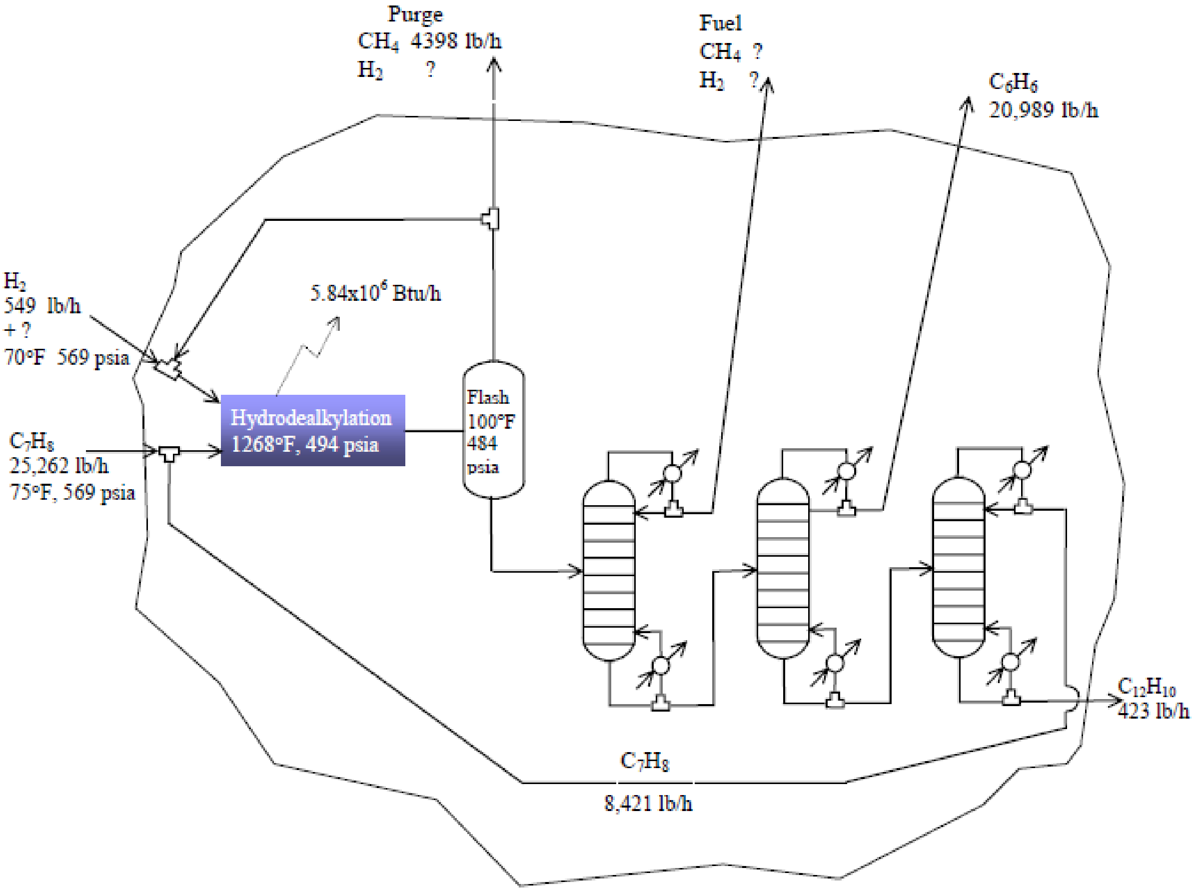
Two economic evaluation methods are available in this module: the Functional Modules Method (FMM) and the Pré-Estime Method (PEM) developed by CHAUVEL *et al.* [CHA03]. The FMM that is essentially based on process parameters (flowrate, pressure, temperature…) gives a quick economic evaluation and a good order of magnitude for the investment costs. Whereas the PEM provides a more precise evaluation by taking into account the sizing characteristics of equipment. Moreover the “Economic evaluation” unit operation allows the user to easily implement his own cost evaluation methods.

These two methods are used and compared in this example.

2. PROCESS MODELING

2.1. Process presentation

The principle diagram of the studied process is the following [SEI04]:



A part of the data necessary to build this example comes from the DOUGLAS book [DOU88].

The hydrodealkylation reactor is fed with hydrogen, benzene and the recycling streams at 650 °C and 36 bar.

The protocol to separate the reaction products is the following:

- A flash at the outlet of the reaction section allows to recycle the hydrogen that did not react
- A first distillation column allows the recuperation of the light gas (CH_4 and H_2)
- A second column is used to purify the benzene
- A third column aims to collect the non-converted toluene at the head (recycled stream) and the biphenyl at the bottom

Two main specifications have been imposed in the process:

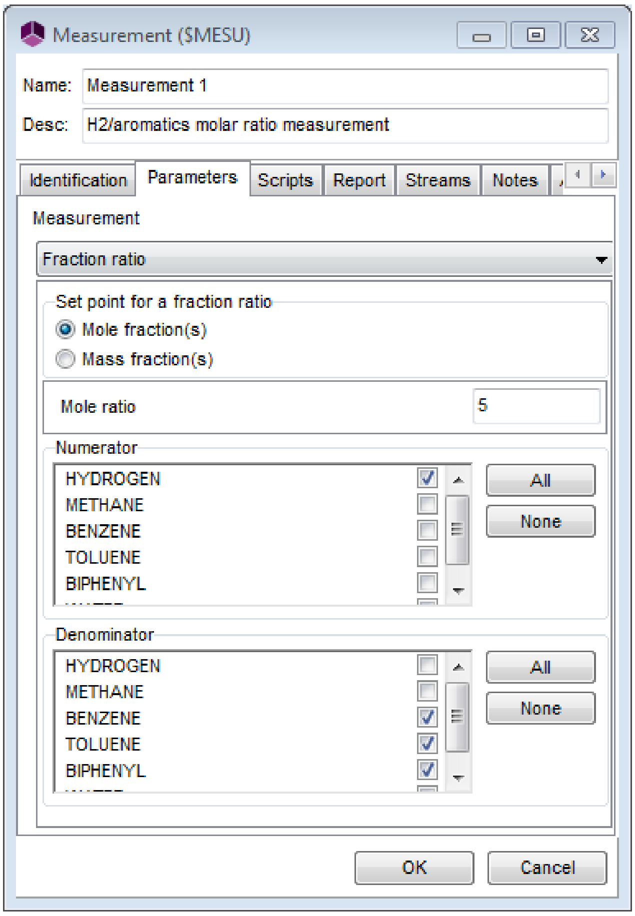
- A hydrogen/aromatics (benzene, toluene, biphenyl) molar ratio of 5% at the inlet of the R1 reactor to avoid cokefaction
  (Measurement between streams 4 and 5)
- A benzene production of 120 kmol/h
  (Measurement between streams 21 and 22)

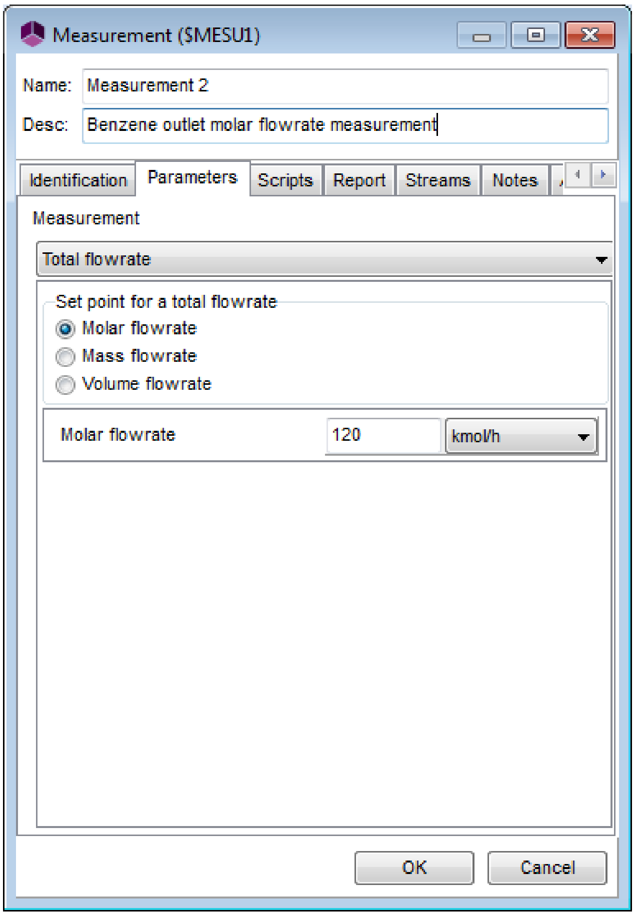
The two action variables are:

- The hydrogen feed total flowrate
- The toluene feed total flowrate

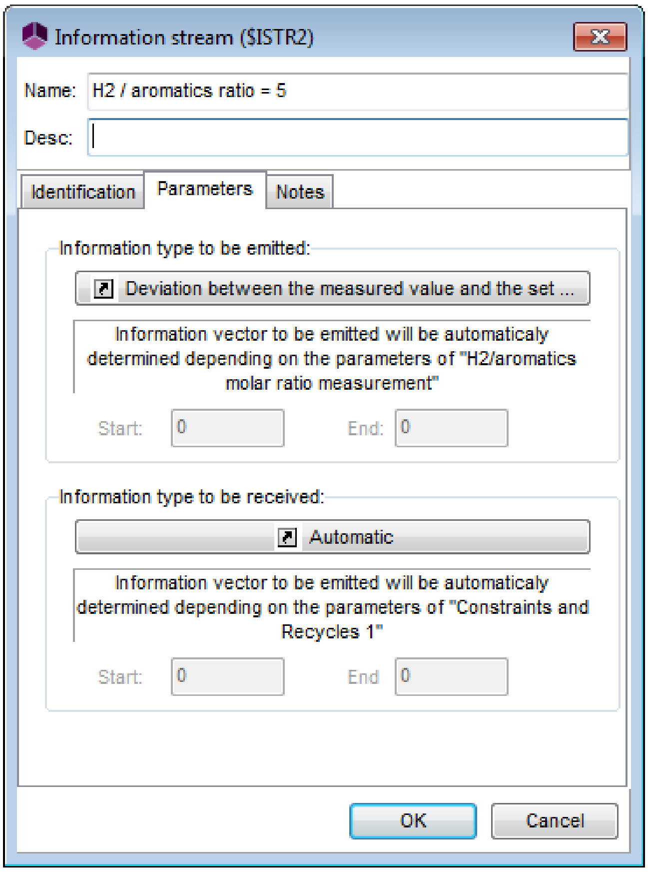
To take these specifications into account with ProSimPlus, a "Constraints and Recycles" block unit has been added to the flowsheet. This block unit is connected with two information streams to the measurements and feed unit operations as presented in the part **2.2 Process flowsheet**.

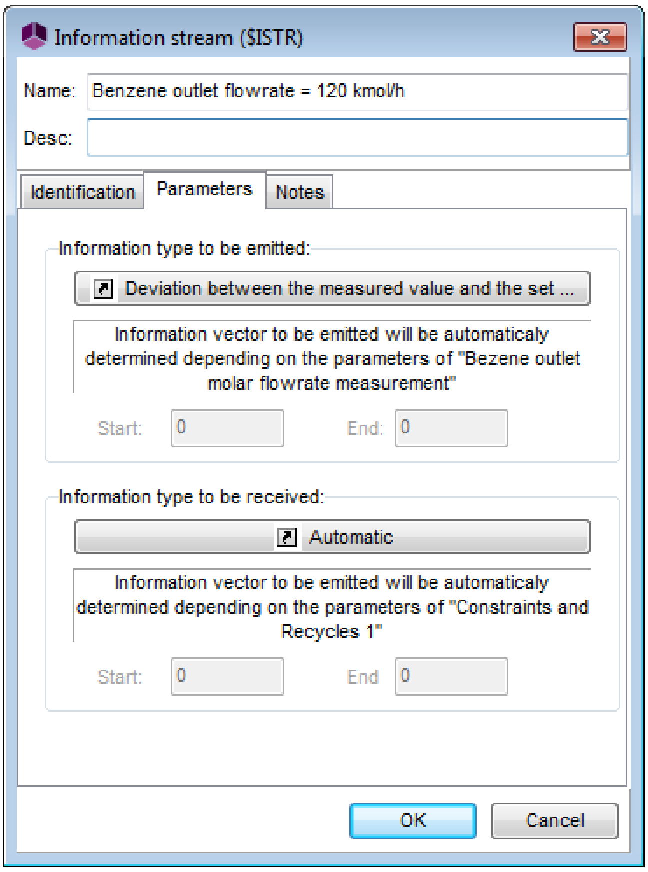
The data entered in the measurements are presented in the screenshots below:

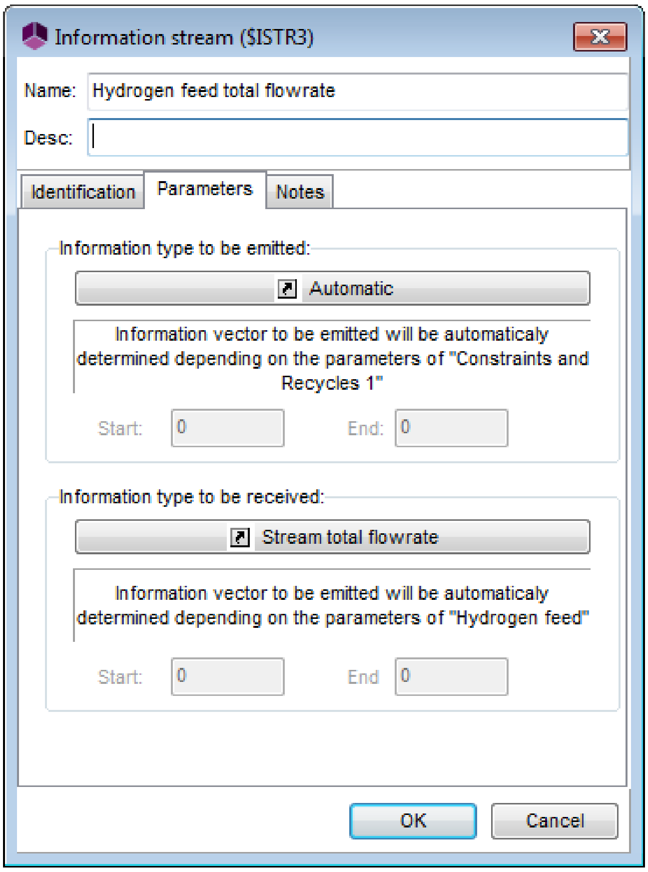


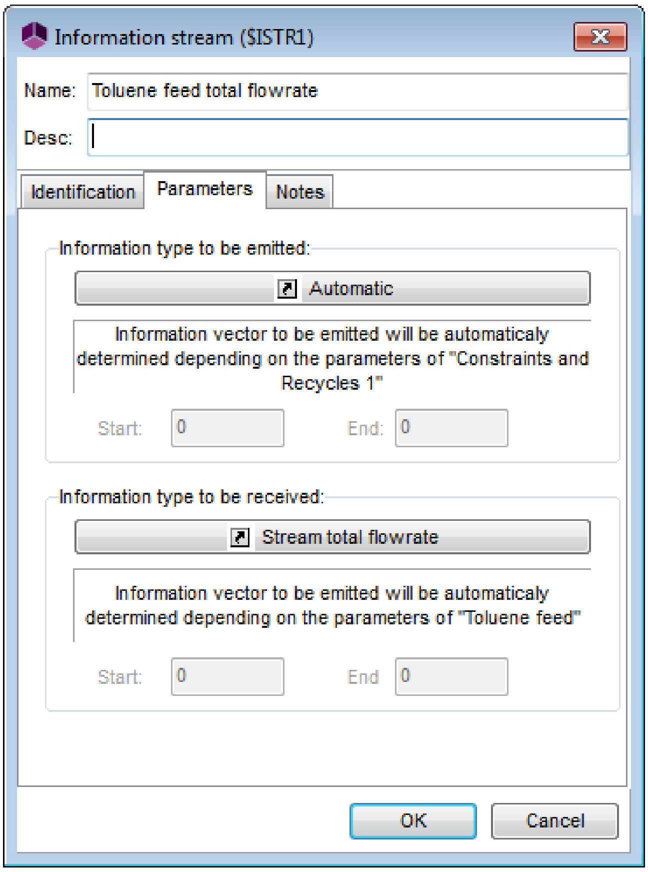


The data entered in the information streams are gathered in the screenshots below:

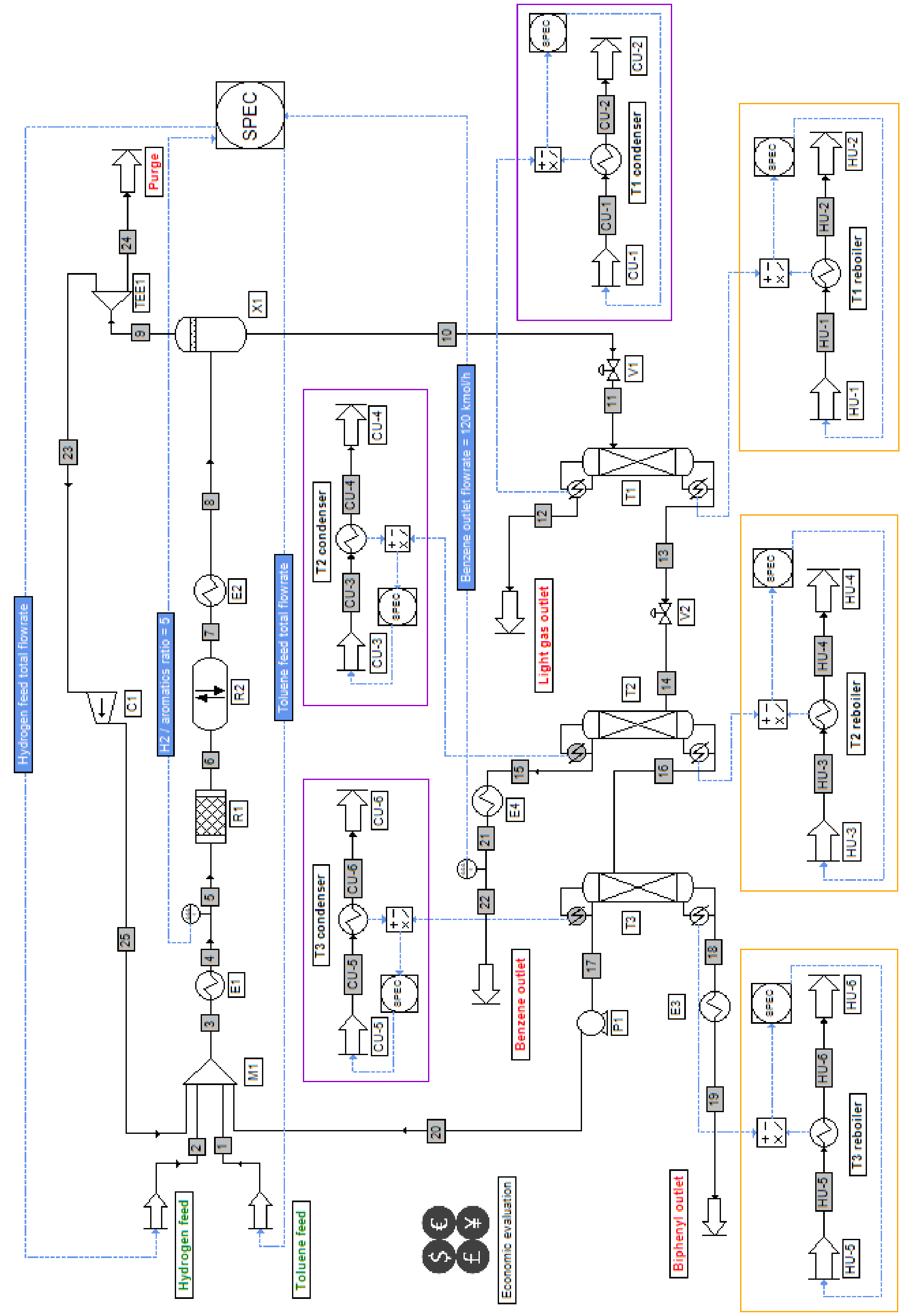








2.2. Process flowsheet



Flowsheet of the toluene hydrodealkylation unit

In order to improve the readability of the process flowsheet, the inlets and outlets (except the utilities) are respectively in green and red characters and the part of the process representing the column condensers and reboilers are respectively framed in purple and orange.

2.3. Compounds

The compounds taken into consideration in this example are listed in the table below:

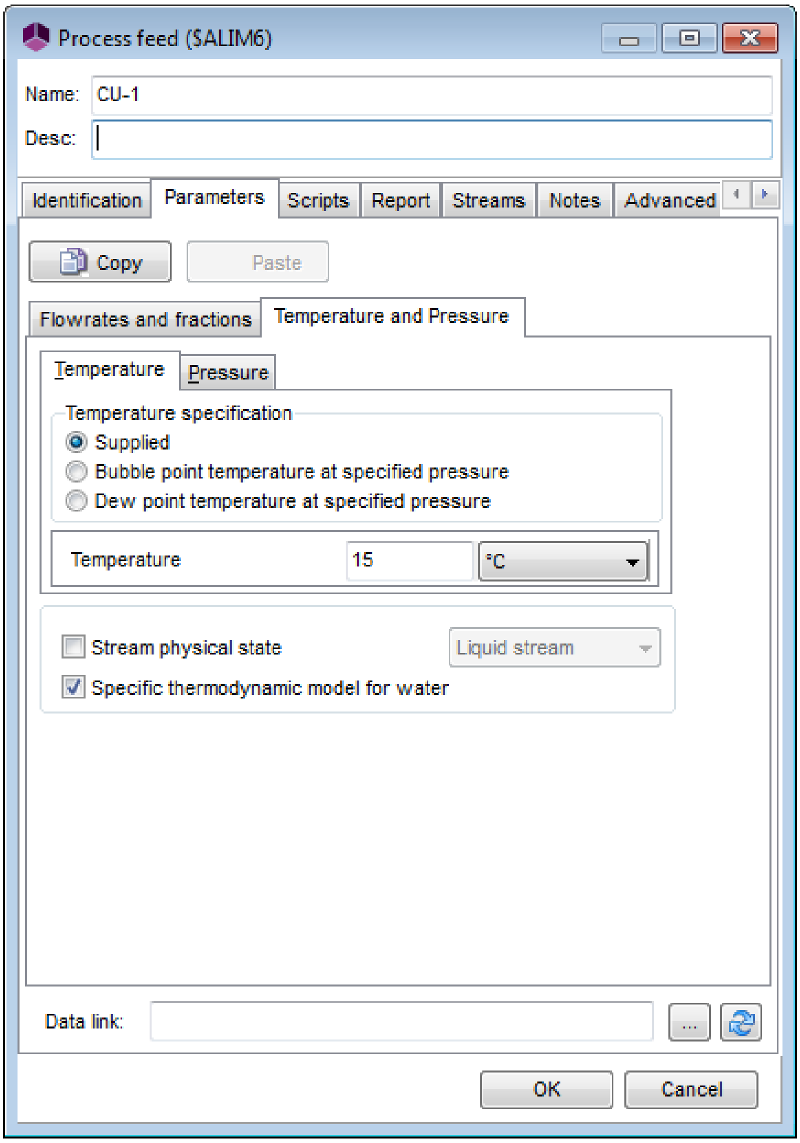
Name	Chemical formulae	CAS number
Hydrogen	H_2	1333-74-0
Methane	CH_4	74-82-8
Benzene	C_6H_6	71-43-2
Toluene	C_7H_8	108-88-3
Biphenyl	$C_{12}H_{10}$	92-52-4
Water	H_2O	7732-18-5

Water is only considered as a utility and is not in contact with the other compounds.

2.4. Thermodynamic model

The system considered contains hydrocarbons and derived hydrocarbons and hydrogen. The working pressure never exceeds 100 bars. As a consequence, the SRK model [SOA72] has been chosen. The binary interaction coefficients from the ProSim database are used.

The specific thermodynamic model for water is used for the hot and cold utilities calculation (HU and CU). To use this model, the "Specific thermodynamic model for water" box has been ticked in the utility streams (HU-1, 3 and 5 and CU-1, 3 and 5) as shown below:



2.5. Chemical reactions

In the hydrodealkylation reactor, the following reaction takes place:

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4 \quad (\Delta H_R = -50 \text{ kJ/mol})$$

The toluene conversion ratio in this reaction is 0.75.

In ProSimPlus, the reaction is simulated in the “Simple reactor” unit operation (R1) and has been defined as follow:

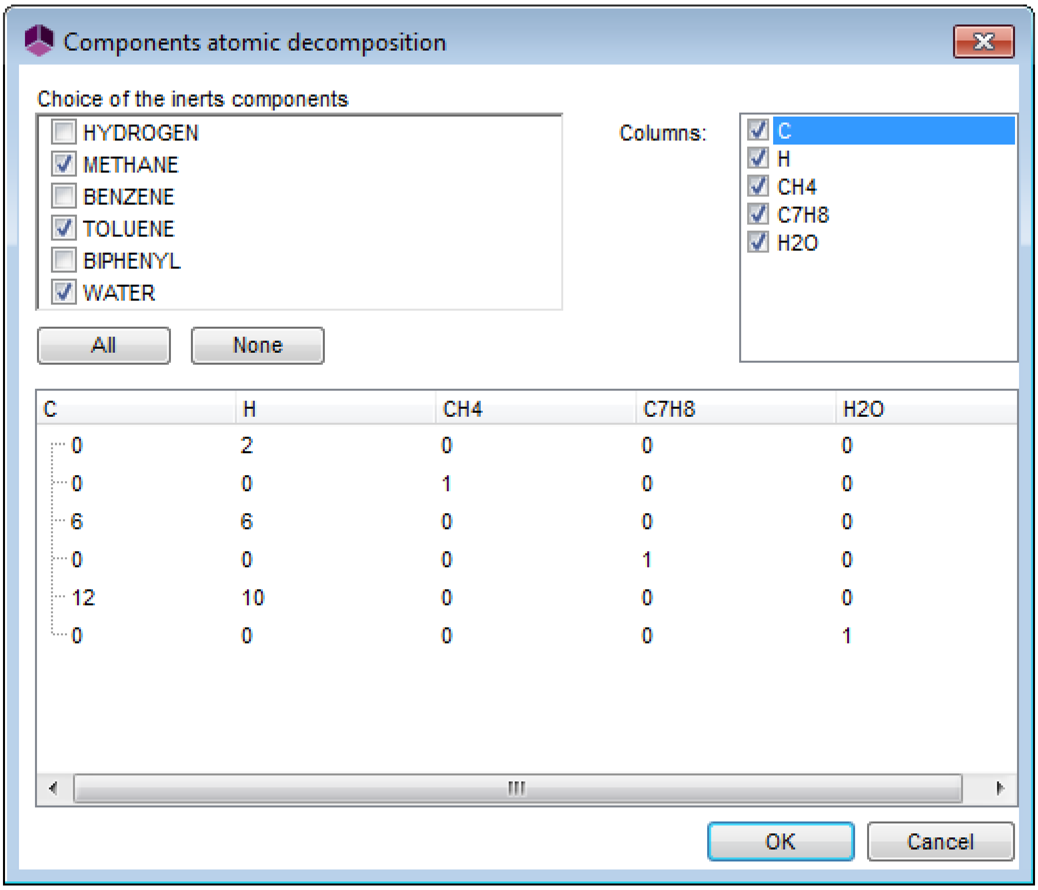
Reaction	$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$
Reaction type	Controlled
Kinetic model	Instantaneous
Heat of reaction (kJ/mol)	-50

Furthermore, a secondary reaction occurs producing biphenyl from benzene:

$$2\ C_6H_6 \leftrightarrow C_{12}H_{10} + H_2$$

To model this reaction, the « Equilibrium reactor » has been used (R2). The selected method is the minimization of Gibbs free energy. The physical state of the compounds is vapor.

The components atomic decomposition entered in the R2 reactor is the following one:



2.6. Operating conditions

All the operating conditions required to define the process are summarized in this part. The data in green are initial values:

- ✓ Hydrogen feed

	Hydrogen feed
H_2 molar fraction	0.95
CH_4 molar fraction	0.05
Total molar flowrate (kmol/h)	200
Temperature (°C)	37.85
Pressure (bar)	37

- ✓ Toluene feed

	Toluene feed
C_7H_8 molar fraction	1
Total molar flowrate (kmol/h)	150
Temperature (°C)	37.85
Pressure (bar)	37

- ✓ Cold utilities (CU) and hot utilities (HU)

	T1 condenser CU-1	***T2 condenser CU-3***	***T3 condenser CU-5***	***T1 reboiler HU-1***	***T2 reboiler HU-3***	***T3 reboiler HU-5***
Mass fraction H_2O	1	1	1	1	1	1
Total mass flowrate (t/h)	1	100	100	10	10	10
Pressure (bar)	1	1	1	15	5	60
Temperature (°C)	15	15	15	Dew temperature	Dew temperature	Dew temperature

✓ Reactors

Operating parameters	*Reactor 1 R1*	*Reactor 2 R2*
Reactor type	Simple	Equilibrium
Reaction set	Hydrodealkylation	-
Outlet temperature (°C)	684	Inlet temperature
Outlet pressure (bar)	34.5	Inlet pressure

✓ Separators

Operating parameters	*Flash X1*
Separator type	Liquid-vapor separator
Temperature (°C)	38
Pressure (bar)	32

✓ Columns

Operating parameters	*Distillation column T1*	*Distillation column T2*	*Distillation column T3*
Column type	2-phase distillation column with partial condenser	2-phase distillation column with total condenser	2-phase distillation column with total condenser
Number of theoretical stages	10	40	7
Feed stage	2	20	2
Distillate flowrate (kmol/h): vapor (partial condenser) liquid (total condenser)	0.05*	120	Calculated
Molar reflux ratio	0.05	1.3	0.06
Reboiler heat duty (kcal/h)	Calculated	Calculated	353 943
Column head pressure (bar)	10.2	1.5	2
Column bottom pressure (bar)	10.2	2	2
Stages efficiency	1	1	1

*: Related to 1 kmol/h feeds flowrate

T1 column further specifications:

Specification		***Product type***	***Compound***	***Value***	***Type***	***Action***
1:	Purity	Vapor distillate	BENZENE	0.01	Molar	Vapor distillate flowrate

T2 column further specifications:

Specification		***Product type***	***Compound***	***Value***	***Type***	***Action***
1:	Purity	Liquid distillate	BENZENE	0.995	Molar	Liquid distillate flowrate

✓ Heat exchangers

Name	***Type***	***Outlet temperature (°C)***	***Pressure drop (bar)***
E1	Cooler/Heater	650	1
E2	Cooler/Heater	38	0.5
E3	Cooler/Heater	38	0.2
E4	Cooler/Heater	30	0.5
T1 condenser	Cooler/Heater	25	0
T2 condenser	Cooler/Heater	25	0
T3 condenser	Cooler/Heater	25	0
T1 reboiler	Cooler/Heater	Bubble temperature	0
T2 reboiler	Cooler/Heater	Bubble temperature	0
T3 reboiler	Cooler/Heater	Bubble temperature	0

- ✓ *Compressors*

Operating parameters	*Compressor C1*
Exhaust pressure (bar)	37
Isentropic efficiency	0.65
Mechanical efficiency	1

- ✓ *Pumps*

Operating parameters	*Pump P1*
Exhaust pressure (bar)	37
Volumetric efficiency	0.65
Mechanical efficiency	1

- ✓ *Mixers*

Operating parameter	*Mixer M1*
Outlet pressure (bar)	Equal to the lowest of the feed

- ✓ *Valves*

Operating parameter	*Expansion valve V1*	*Expansion valve V2*
Outlet pressure (bar)	10.2	1.8

- ✓ *Stream splitters*

Operating parameters	*Stream splitter TEE1*
Splitting ratio stream 23	0.92
Outlet pressure (bar)	Equal to the feed pressure

2.7. Drum and distillation columns sizing

ProSimPlus allows to size equipment like drums or distillation columns. This sizing is particularly useful for an economic evaluation with the PEM.

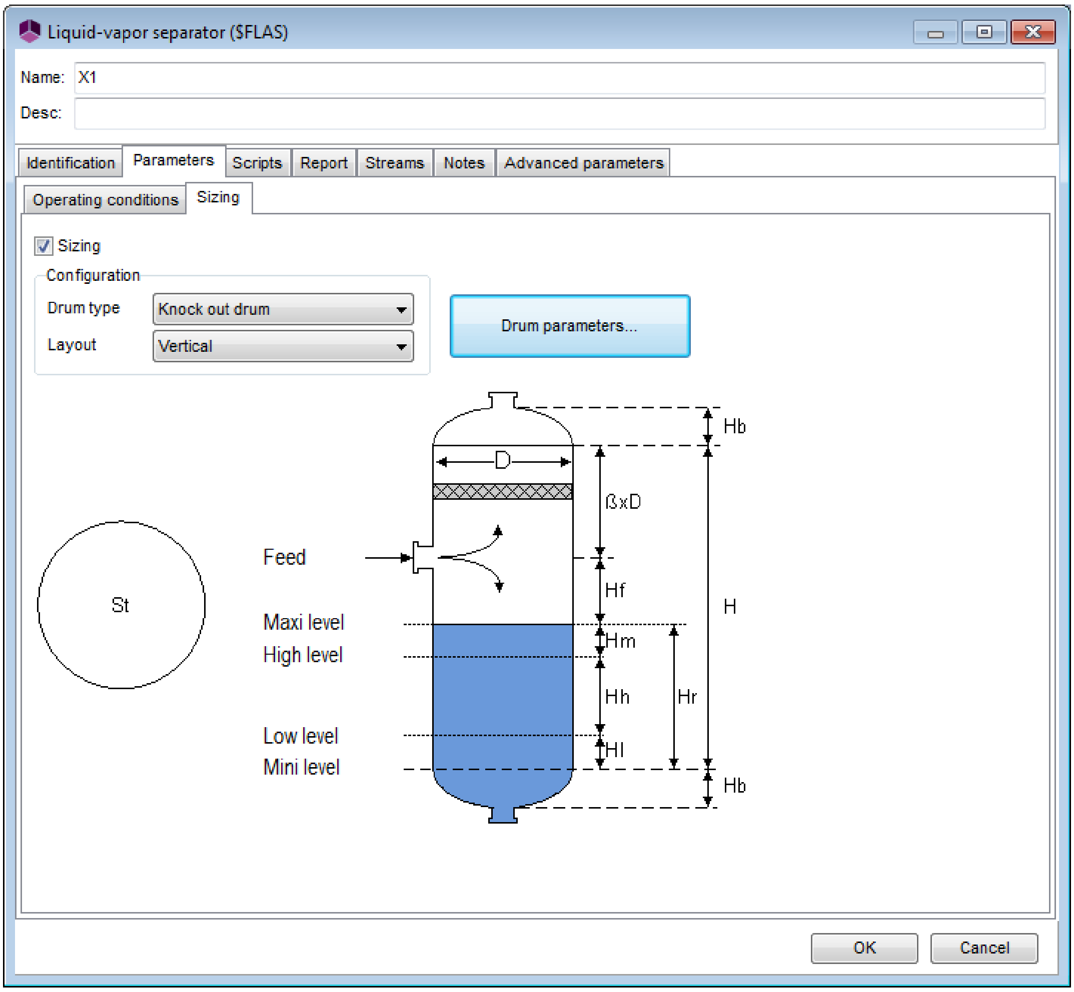
2.7.1. X1 drum sizing

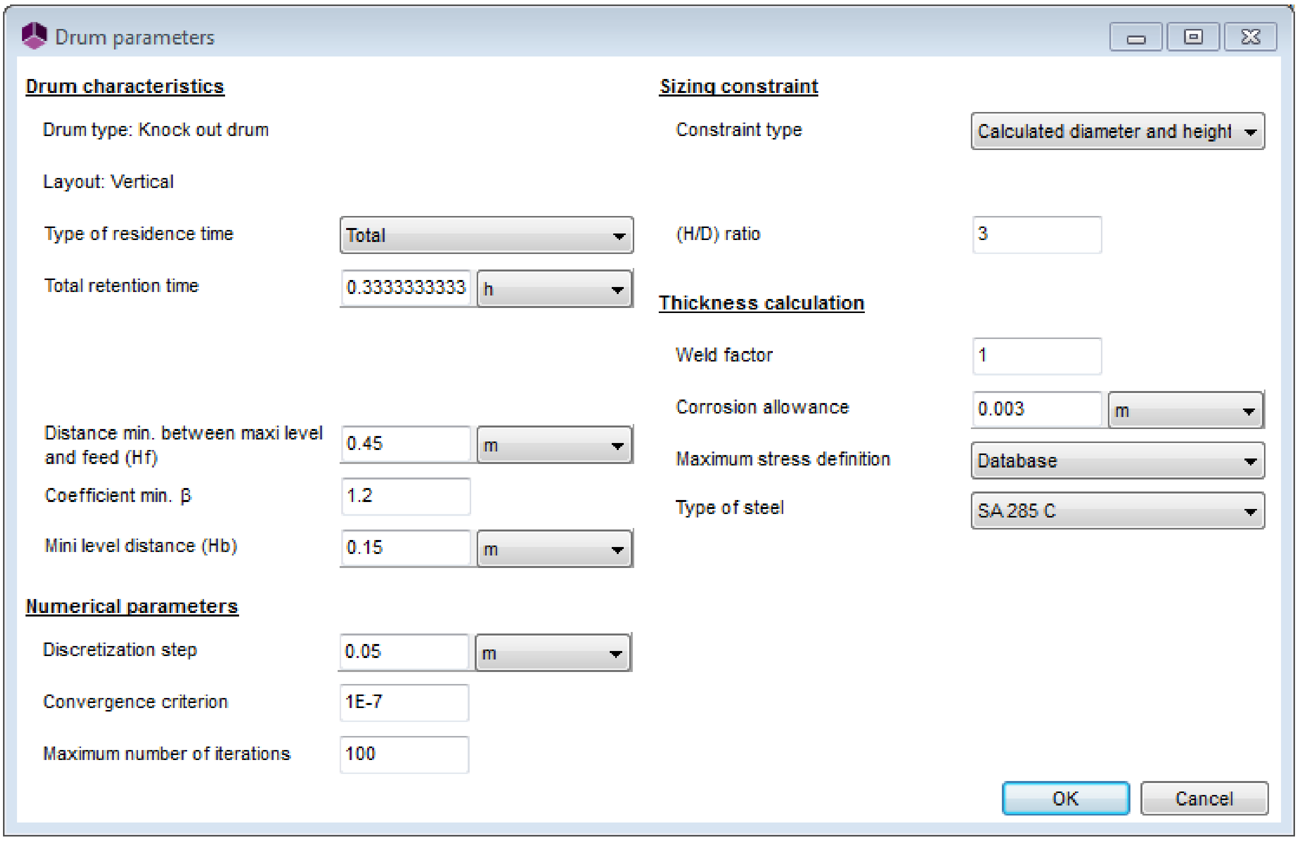
To size the X1 drum, the edition window of the X1 unit operation has to be opened, and the subtab "Sizing" located in the tab "Parameters" has to be selected. The "Sizing" box has to be ticked and the configuration of the drum has to be defined. As shown next page, the vertical knock out drum has been chosen.

Click on the "Drum parameters" button and enter the required parameter as presented next page.

Each parameter has been set by default excepted:

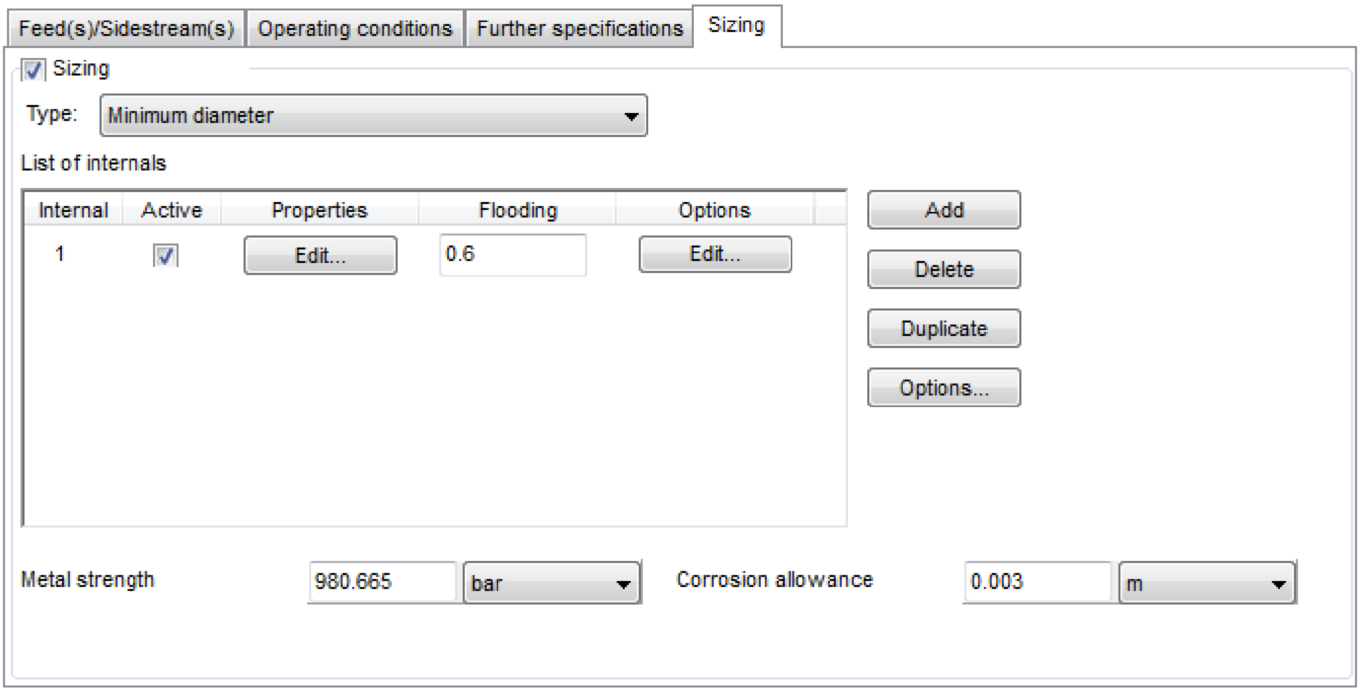
- Type of residence time: Total
- (H/D) ratio: 3
- Type of steel: SA 285 C




Drum parameters
Drum characteristics
Drum type: Knock out drum
Layout: Vertical
Type of residence time
Total
Total retention time
0.3333333333
h
Distance min. between maxi level and feed (Hf)
0.45
m
Coefficient min. β
1.2
Mini level distance (Hb)
0.15
m
Numerical parameters
Discretization step
0.05
m
Convergence criterion
1E-7
Maximum number of iterations
100
Sizing constraint
Constraint type
Calculated diameter and height
(H/D) ratio
3
Thickness calculation
Weld factor
1
Corrosion allowance
0.003
m
Maximum stress definition
Database
Type of steel
SA 285 C
OK
Cancel

2.7.2. T1, T2 and T3 columns sizing

As for drums, to size the columns, proceed as follows: open the edition window and the subtab “Sizing” located in the tab “Parameters”. Then choose the sizing type “Minimum diameter” and the following configuration for the three columns:



The metal strength and the corrosion allowance are parameters used in the calculation of the column shell and the bottoms thickness.

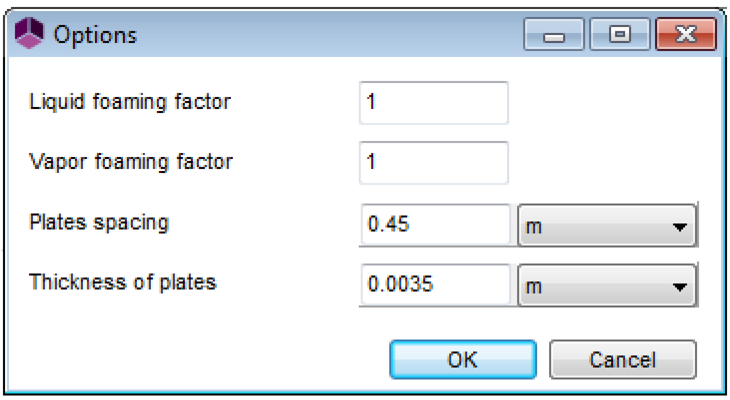
To add an internal in the list of internals, click on “Add”. The data to be entered in the section “Properties” and “Options” (accessible by clicking on the respective “Edit…” buttons) are gathered below:

T1 column:

“Properties” section:

Internal type: select “Nutter valve trays” and let the parameter by default.

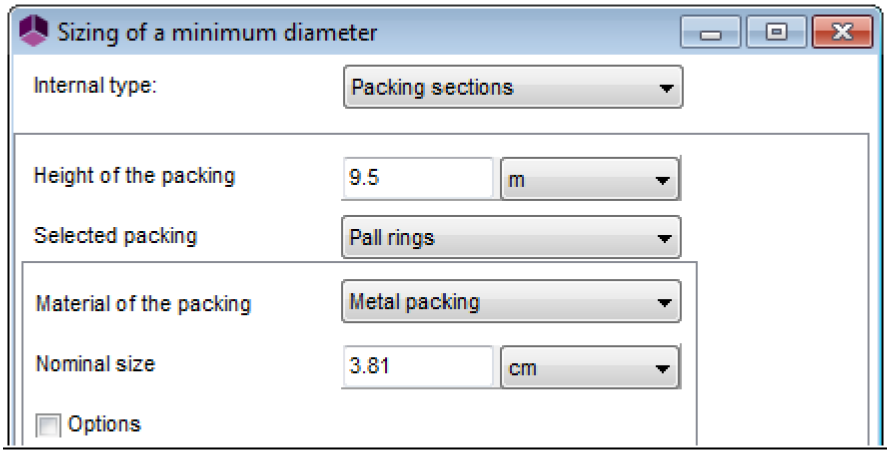
“Options” section: enter the following configuration:



T2 column:

“Properties” section:

Internal type: select “Packing sections” and the following configuration:



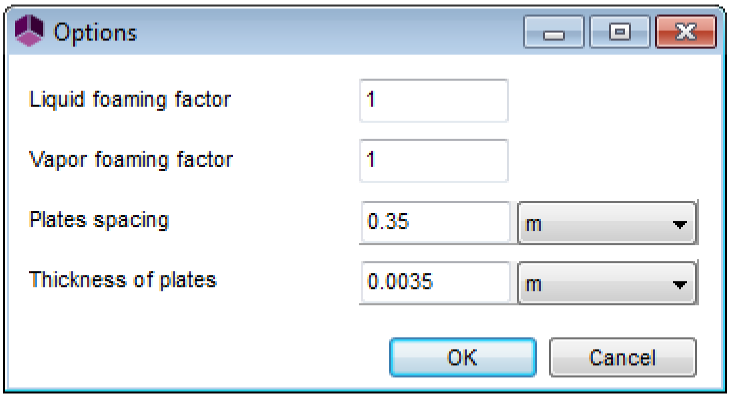
“Options” section: let the options by default.

T3 column:

“Properties” section:

Internal type: select “Nutter valve trays” and let the parameter by default.

“Options” section: enter the following configuration:

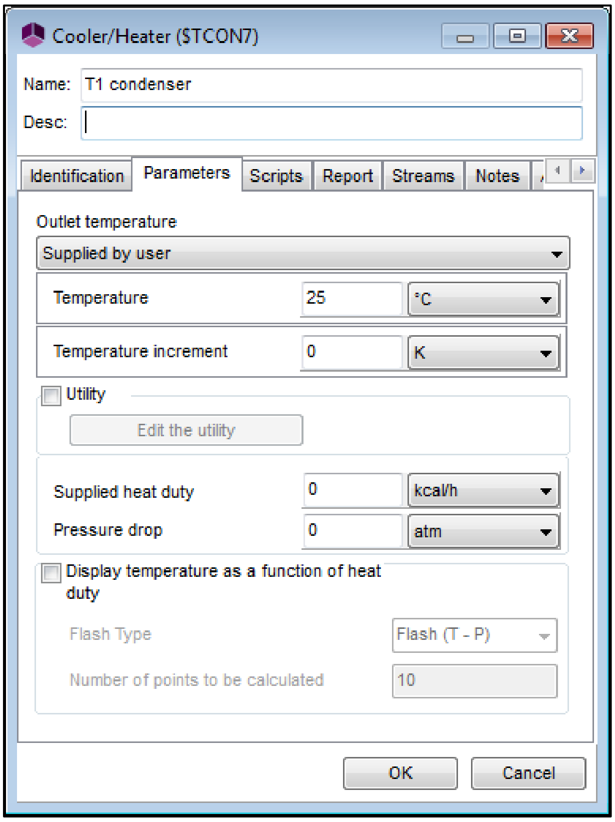


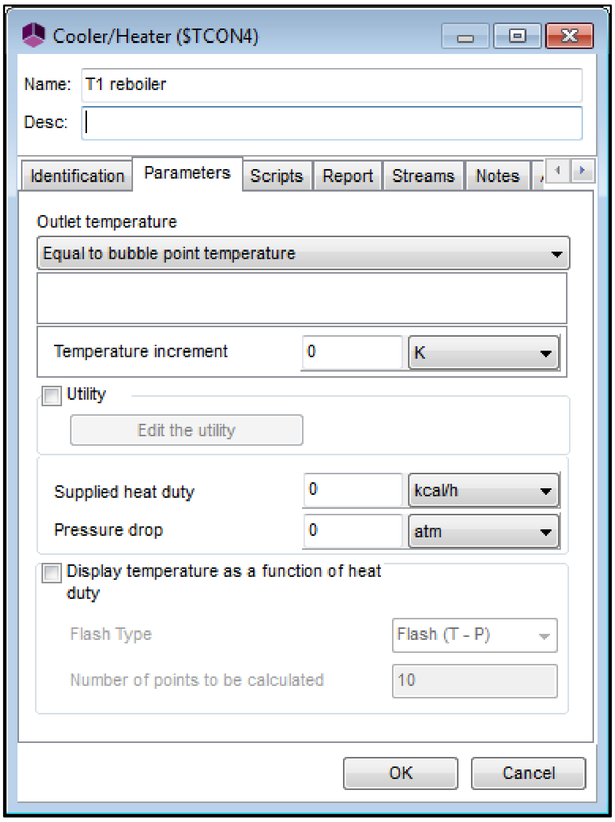
2.7.3. Utilities consumption in the condensers and reboilers of the T1, T2 and T3 columns

The condensers and reboilers have been simulated with "Cooler/Heater" unit operations. The physical characteristics of the utility employed are gathered in the table of the part **2.6 Operating conditions.**

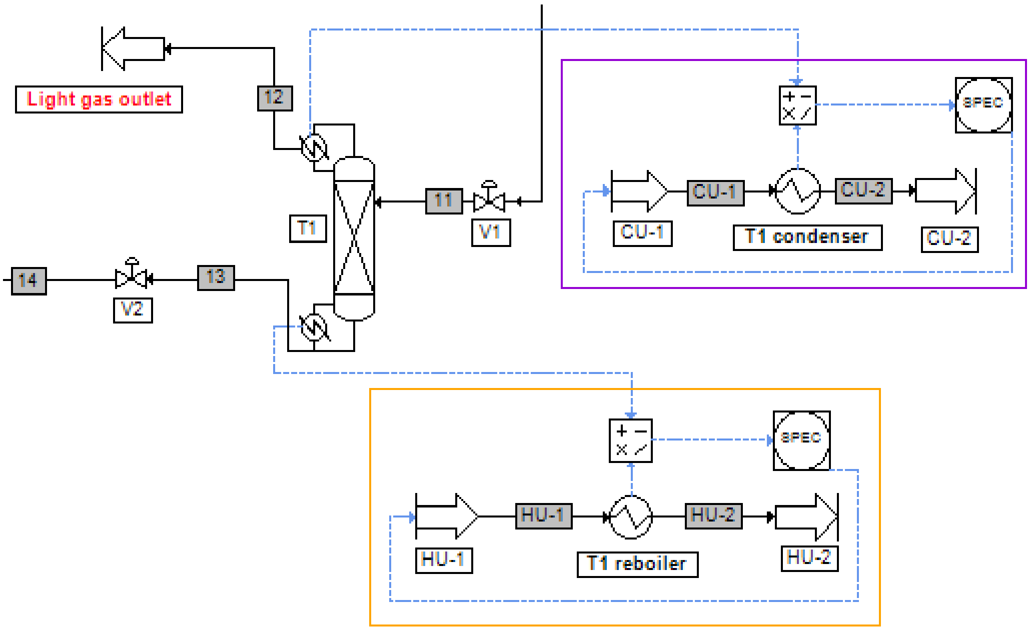
We use 15°C and 1 atm liquid water in the condensers and saturated vapor with different pressure levels in the reboilers.

We impose the water temperature at the condensers outlet to be 25°C. In the reboilers, we want to use completely and only the vaporization heat duty. To do so, we impose the outlet temperature to the bubble temperature. The following windows contain the configuration entered in the condenser and the reboiler of the T1 column:

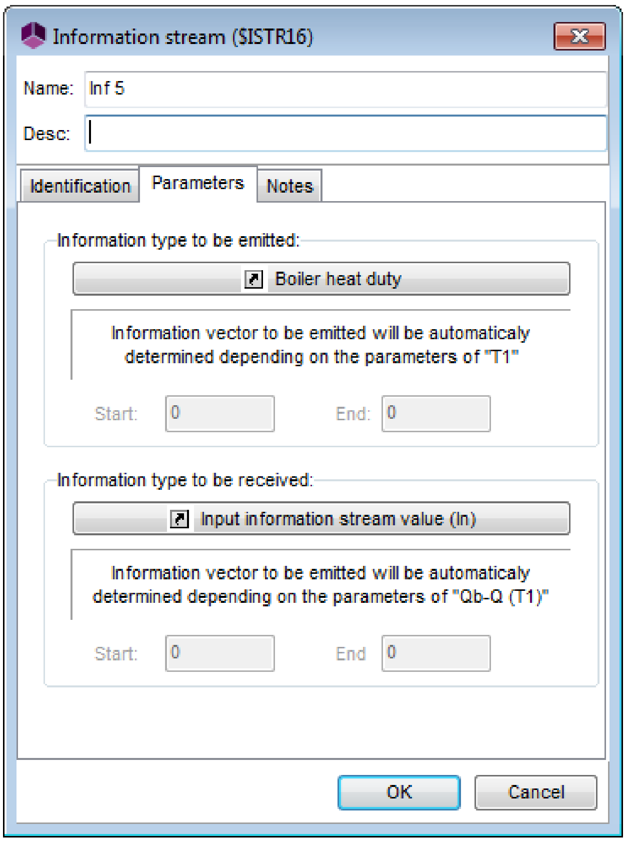


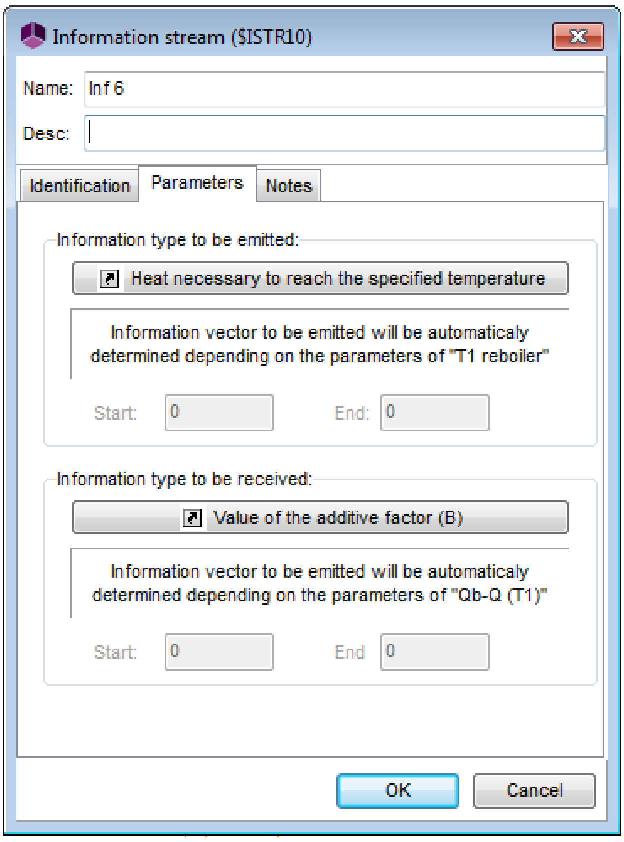


To determine the necessary utility flowrates needed, we use a SPEC block unit as presented below in the case of the T1 column:



The approach is the same for the reboilers and condensers of the different columns: we take the heat duty values of the reboiler (or the condenser) of the column and “Cooler/Heater” unit operation using information streams. We link these streams to an information stream handler as presented hereafter in the case of the T1 column reboiler:

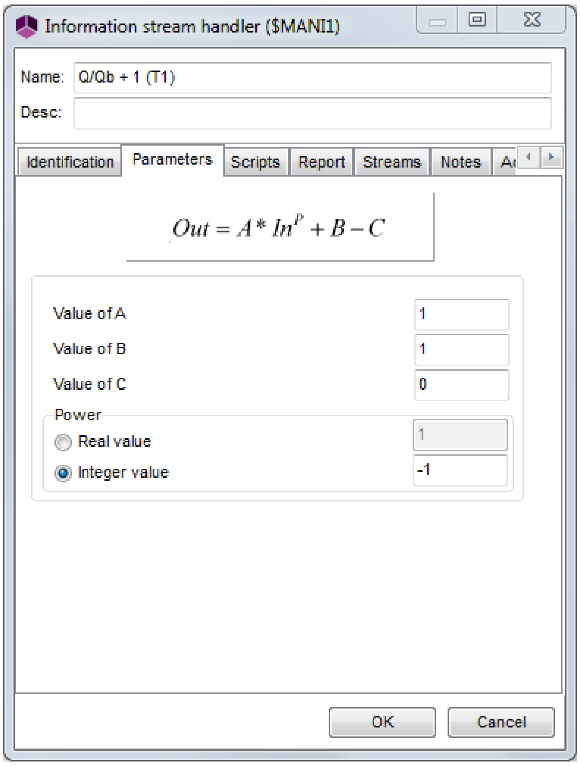




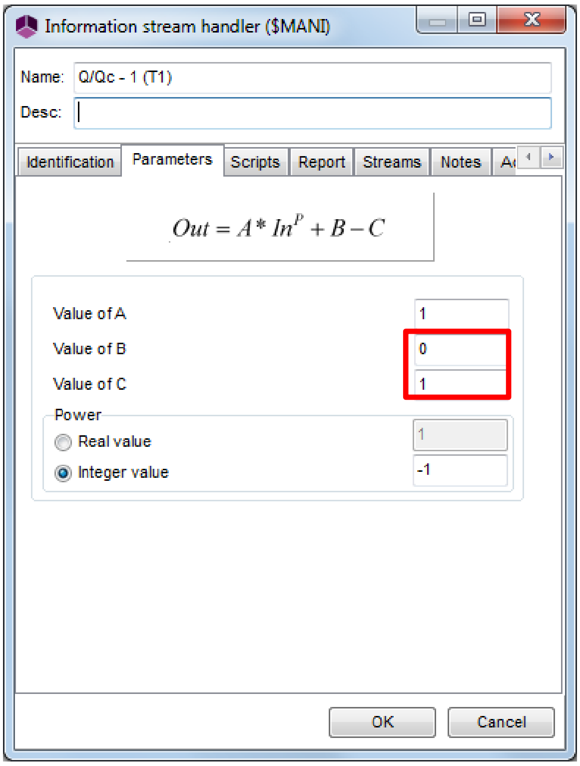
In the information stream handler we want to calculate the difference between the boiler (or condenser) heat duty to heat duty calculated in the related “Cooler/Heater” unit operation ratio and 1.

The reboiler and condenser heat duties are positive and the related "Cooler/Heater" heat duties are respectively negative and positive. A particular attention to the signs while configuring information stream handlers has then to be paid. The correct configurations in the cases of the boiler and the condenser are given hereafter:

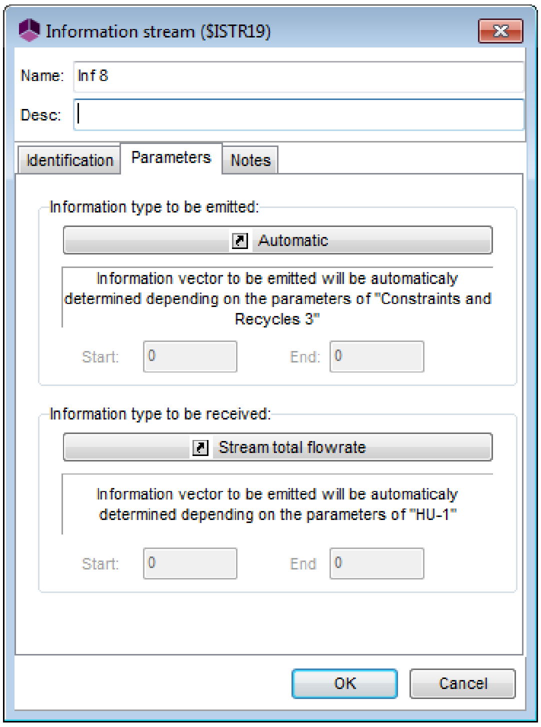
Reboiler



Condenser



The difference between the reboiler (or condenser) heat duty of the column to the one calculated in the related "Cooler/Heater" unit operation ratio and 1 is then sent to the SPEC block unit. This SPEC block unit is linked to the utility feed unit operation by an information stream configured as follow:



So the SPEC block unit will adjust the utility flowrate in order to cancel the difference between the heat duties ratio and 1. This way, the "Cooler/Heater" unit operation will represent the boiler (or the condenser) and the calculated utility flowrate will correspond to the utility flowrate circulating in the reboiler (or the condenser). The obtained mass flowrates are summarized in the following table:

	T1 condenser ***CU-1***	***T2 condenser*** ***CU-3***	***T3 condenser*** ***CU-5***	***T1 reboiler*** ***HU-1***	***T2 reboiler*** ***HU-3***	***T3 reboiler*** ***HU-6***
Mass flowrate (kg/h)	774	199 611	32 881	2 095	2 840	943

3. SIMULATION RESULTS

3.1. Comments on results

The calculation sequence (order of calculation of the unit operations) is automatically generated. The tear stream "5" is initialized with the following characteristics:

	Tear stream "5"
H_2 molar fraction	0.36
CH_4 molar fraction	0.57
C_6H_6 molar fraction	0.005
C_7H_8 molar fraction	0.065
Total molar flowrate (kmol/h)	2600
Temperature (°C)	650
Pressure (bar)	36

Two input flowrates are adjusted in order to reach the right operating conditions for the hydrodealkylation reaction (H_2/aromatics molar ratio of 5%) and the 120 kmol/h benzene production with a molar purity of 99.5%.
The required feed flowrates are 199.6 kmol/h hydrogen and 127.9 kmol/h toluene.

3.2. Mass and energy balances

This document only presents 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).

Inlet/outlet streams (except utilities):

Streams		1	2	12	19	22	24
From		Toluene feed	Hydrogen feed	T1	E3	Measurement 2	TEE1
To		M1	M1	Light gas outlet	Biphenyl outlet	Benzene outlet	Purge
Partial flows		kmol/h	kmol/h	kmol/h	kmol/h	kmol/h	kmol/h
HYDROGEN		0	189.6	0.8	0	0	64.8
METHANE		0	10.0	8.4	0	0	128.7
BENZENE		0	0	0.09	3.3E-07	119.4	1.5
TOLUENE		127.9	0	3.6E-03	1.3E-01	0.6	0.2
BIPHENYL		0	0	1E-09	3.0	0	3E-05
WATER		0	0	0	0	0	0
Total flow	kmol/h	127.9	199.6	9.2	3.1	120.0	195.1
Mole fractions							
HYDROGEN		0	0.950	0.082	0	0	0.332
METHANE		0	0.050	0.908	0	0	0.659
BENZENE		0	0	1.0E-02	1E-07	0.995	8E-03
TOLUENE		1	0	4E-04	0.041	0.005	9E-04
BIPHENYL		0	0	1E-10	0.959	0	2E-07
WATER		0	0	0	0	0	0
Physical state		Liquid	Vapor	Vapor	Liquid	Liquid	Vapor
Temperature	°C	37.85	37.85	18.75	38	30	38
Pressure	bar	37.0	37.0	10.2	1.8	1.0	32.0
Enthalpic flow	kcal/h	-1 095 998	18 343	-849	-44 548	-940 762	8 135
Vapor molar fraction		0	1	1	0	0	1

Inlet/outlet streams (hot utilities):

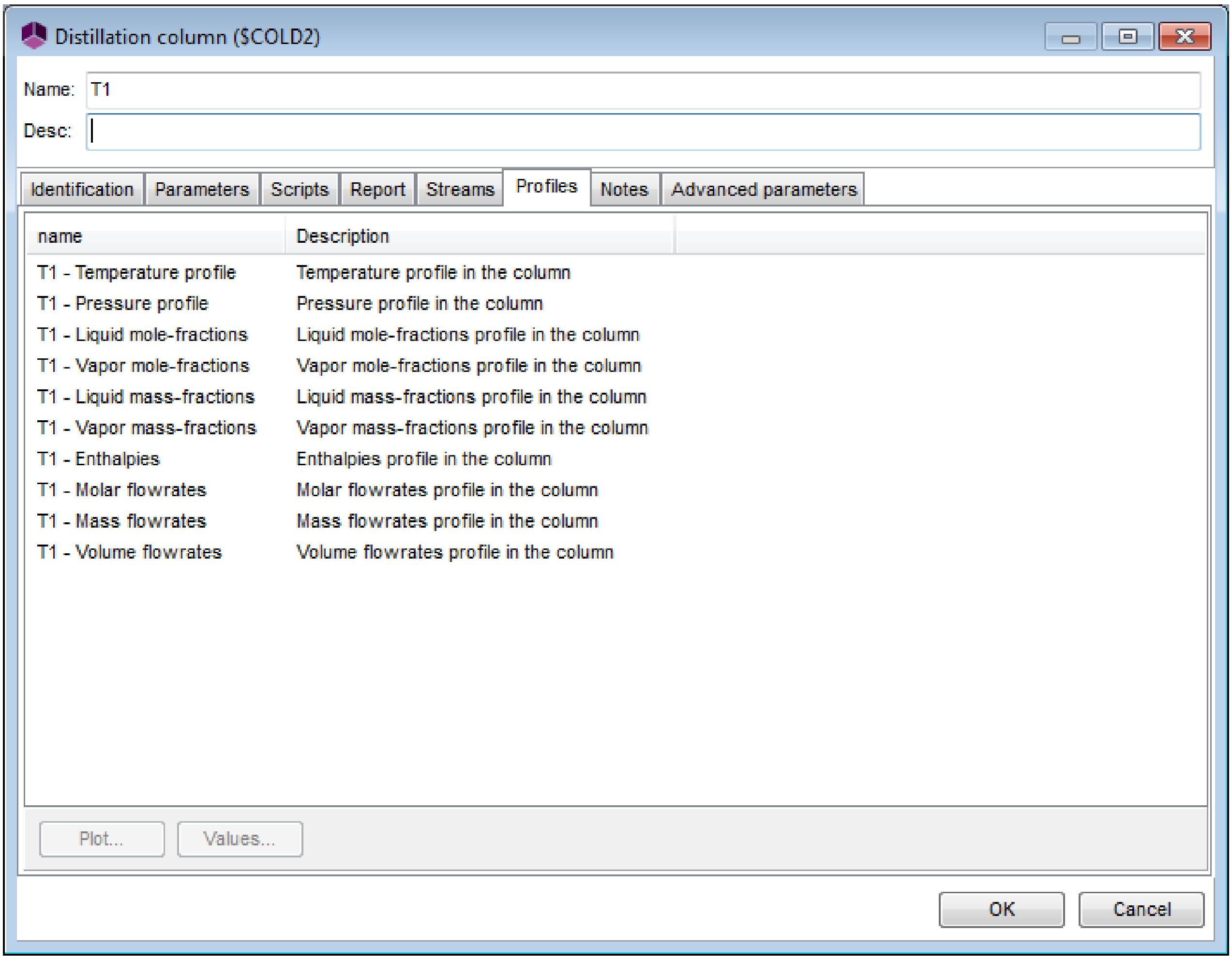
Streams		HU-1	HU-2	HU-3	HU-4	HU-5	HU-6
From		HU-1	T1 reboiler	HU-3	T2 reboiler	HU-5	T3 reboiler
To		T1 reboiler	HU-2	T2 reboiler	HU-4	T3 reboiler	HU-6
Partial flows		kmol/h	kmol/h	kmol/h	kmol/h	kmol/h	kmol/h
WATER		116.3	116.3	157.6	157.6	52.3	52.3
Total flow	kmol/h	116.3	116.3	157.6	157.6	52.3	52.3
Mole fractions							
WATER		1	1	1	1	1	1
Physical state		Vapor	Liquid	Vapor	Liquid	Vapor	Liquid
Temperature	°C	198.3	198.3	151.9	151.9	275.6	275.6
Pressure	bar	15.0	15.0	5.0	5.0	60.0	60.0
Enthalpic flow	kcal/h	122 186	-852 310	136 547	-1 294 340	53 300	-300 643
Vapor molar fraction		1	0	1	0	1	0

Inlet/outlet streams (cold utilities):

Streams		CU-1	CU-2	CU-3	CU-4	CU-5	CU-6
From		CU-1	T1 condenser	CU-3	T2 condenser	CU-5	T3 condenser
To		T1 condenser	CU-2	T2 condenser	CU-4	T3 condenser	CU-6
Partial flows		kmol/h	kmol/h	kmol/h	kmol/h	kmol/h	kmol/h
WATER		42.9	42.9	11 080.1	11 080.1	1 825.2	1 825.2
Total flow	kmol/h	42.9	42.9	11080.1	11080.1	1825.2	1825.2
Mole fractions							
WATER		1	1	1	1	1	1
Physical state		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	°C	15.0	25.0	15.0	25.0	15.0	25.0
Pressure	bar	1.0	1.0	1.0	1.0	1.0	1.0
Enthalpic flow	kcal/h	-459 378	-451 643	-118 526 712	-116 531 022	-19 524 602	-19 195 857
Vapor molar fraction		0	0	0	0	0	0

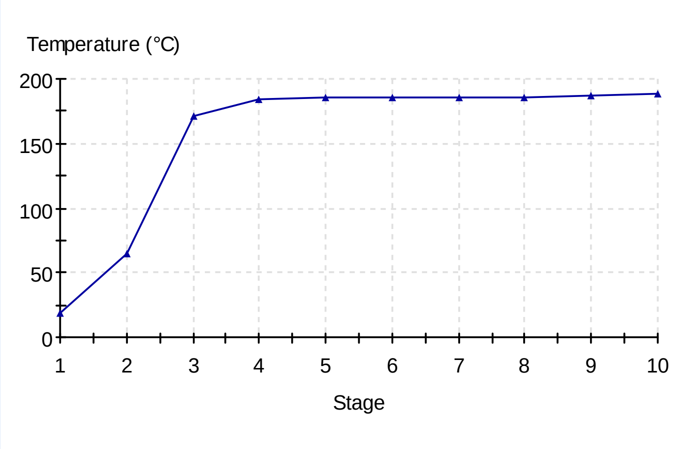
3.3. Column profiles

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. It is important to note that, in ProSimPlus, the first stage correspond to the condenser and the last stage to the reboiler (numbering from top to bottom).



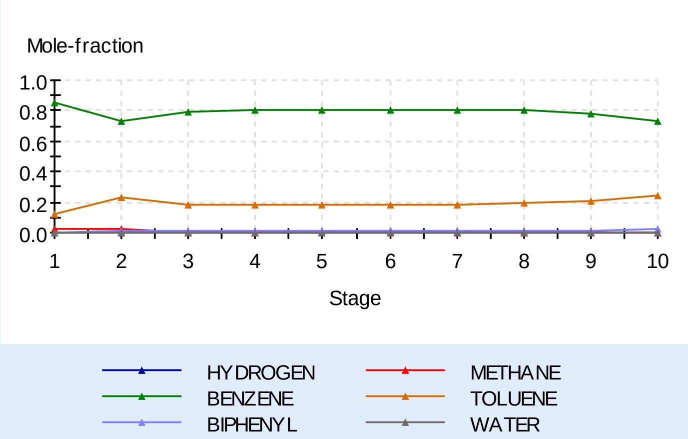
T1 column

T1 - Temperature profile



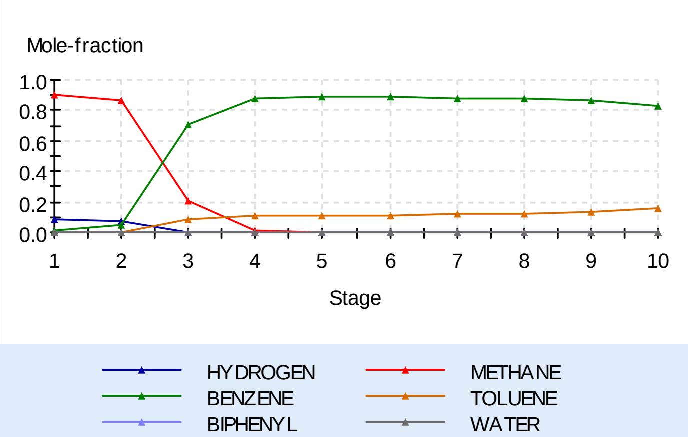
Temperature profile in the column

T1 - Liquid mole-fractions



Liquid mole-fractions profile in the column

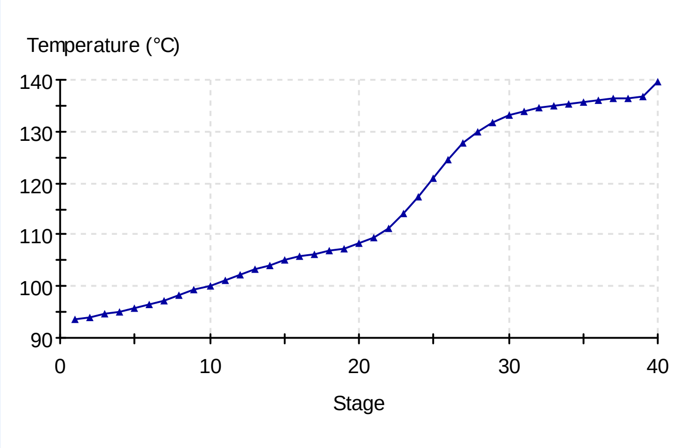
T1 - Vapor mole-fractions



Vapor mole-fractions profile in the column

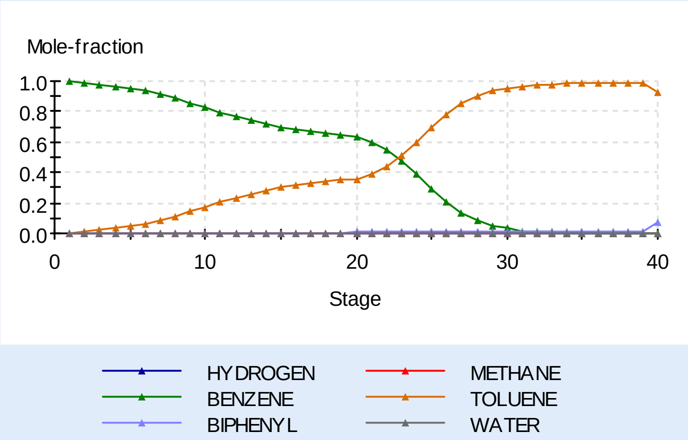
T2 column

T2 - Temperature profile



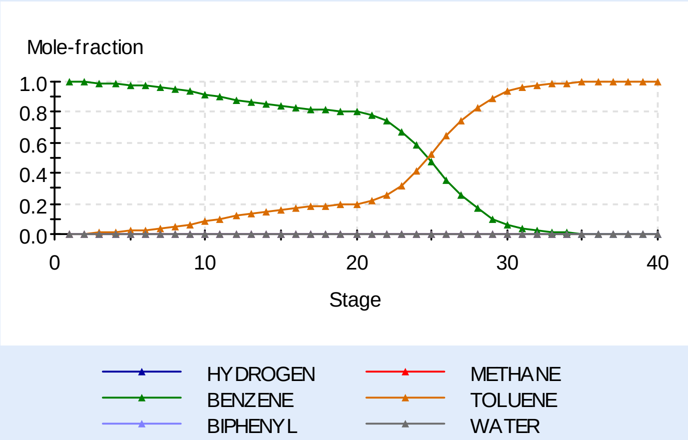
Temperature profile in the column

T2 - Liquid mole-fractions



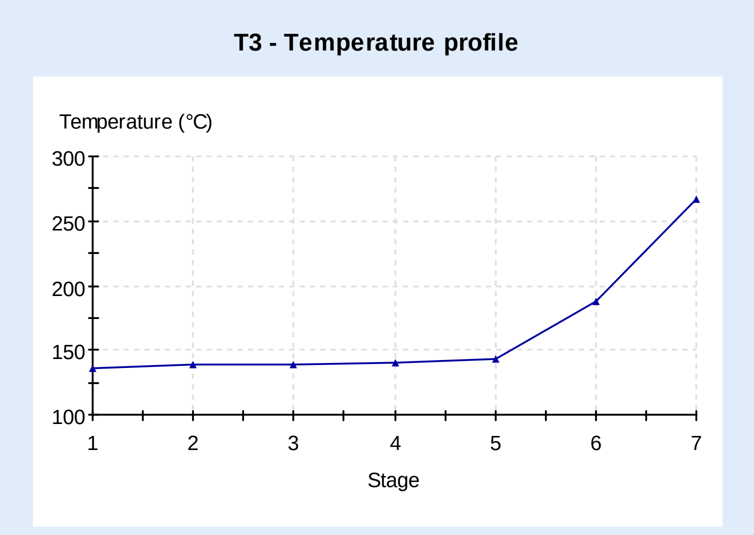
Liquid mole-fractions profile in the column

T2 - Vapor mole-fractions

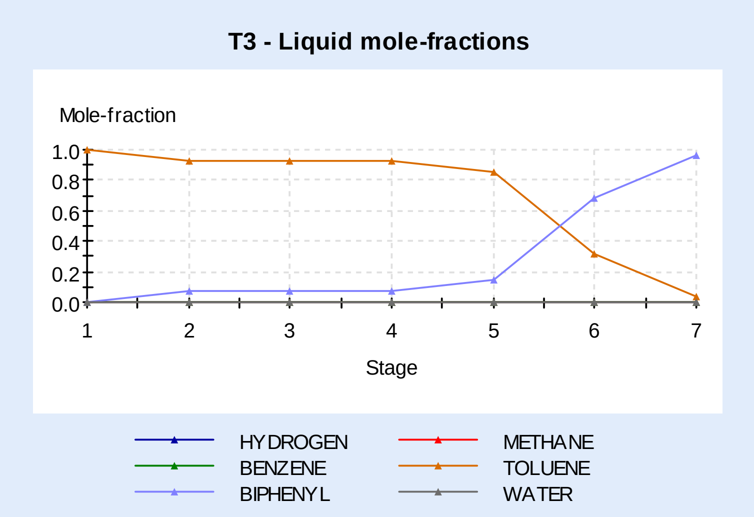


Vapor mole-fractions profile in the column

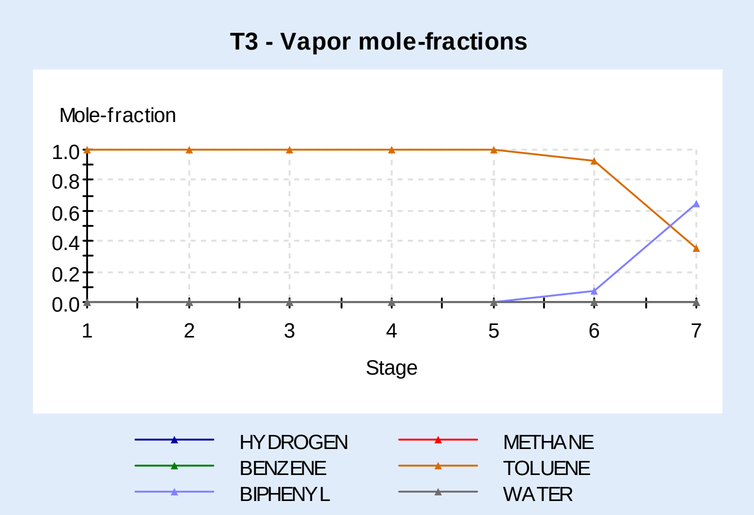
T3 column



Temperature profile in the column



Liquid mole-fractions profile in the column



Vapor mole-fractions profile in the column

3.4. Sizing results

The sizing results of the concerned unit operations are accessible in the simulation report. The sizing results that will be used for the economic evaluation are presented hereafter:

X1 drum:

Height (m)	5.1
Diameter (m)	1.7
Thickness (mm)	30.8

T1 column:

Internal diameter (m)	1.022
External diameter (m)	1.050
Shell thickness (mm)	14

The tray diameter is considered equal to the internal diameter. To determine the T1 column height, we consider that it contains 8 real trays. The space between two trays is 0.45 m and we consider that there is the same space between the top tray and the column top, and the bottom tray and the column bottom.

So the column height is:

$$H_1 = 0.45 \times (8 - 1 + 2) = 4.05\ m$$

T2 column:

Internal diameter (m)	1.288
External diameter (m)	1.300
Shell thickness (mm)	6

The column height is evaluated considering that one theoretical stage (except boiler and condenser) is equivalent to 0.50 m packing height. The column height is then:

$$H_2 = 0.50 \times (40 - 2) = 19\ m$$

The packing volume V is estimated with the following formulae:

$$V = \pi \times \frac{Internal\ diameter^2}{4} \times H_2 = 25\ m^3\ (rounded\ up)$$

T3 column:

Internal diameter (m)	0.69
External diameter (m)	0.70
Shell thickness (mm)	5

The tray thickness is considered equal to the internal diameter. To determine the T1 column height, we consider that it contains 5 real trays. The space between two trays is 0.35 m and we consider that there is the same space between the top tray and the column top, and the bottom tray and the column bottom.

The column height is then:

$$H_3 = 0.35 \times (5 - 1 + 2) = 2.10\ m$$

4. ECONOMIC EVALUATION

The ProSimPlus economic evaluation deals with the following points:

- equipment **initial** and **secondary investment** cost calculation
- equipment **residual value** calculation at the end of the time horizon
- equipment **maintenance** cost calculation
- **operating gains** and **costs** calculation
- **economic indicators** calculation
- **schedule**
- **economic indicators** profiles

The economic indicators are:

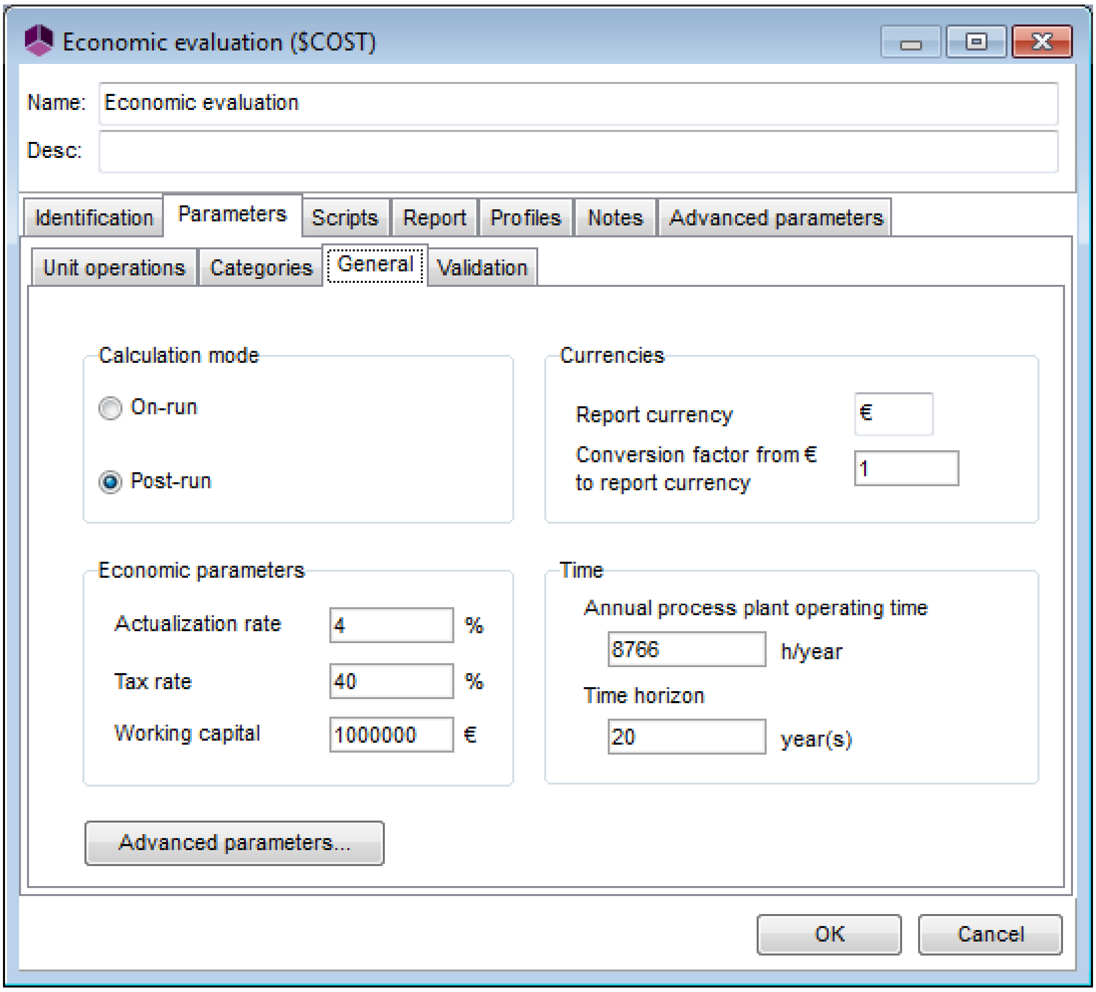
- **pay out time**
- **rate of return**
- equipment **residual values**
- **cumulative discounted cash flow** of the process
- **net discounted value** of the process

This economic evaluation is carried out by putting the "Economic evaluation" unit operation on the flowsheet as shown hereafter:

This part describes the parameters used for the economic evaluation and the corresponding results.

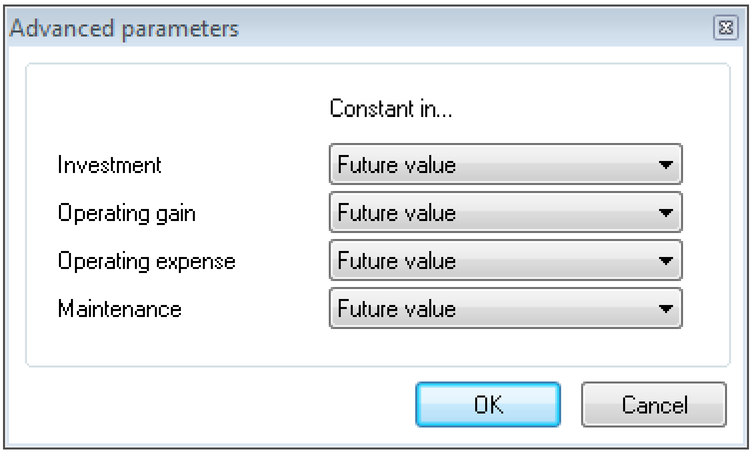
4.1. Economic evaluation general parameters

The general parameters entered in this example are shown below:



Since no parameter of the economic evaluation unit operation is used for optimization, the “Post-run” calculation mode has been chosen. The default currency (€) has been kept. The annual process plant operating time corresponds to the maximum (a continuous functioning of the plant 24/24 for 365.25 days a year). For more information about the general parameters, please refer to the Online Help.

The advanced parameters chosen for this example are the following ones:



4.2. Initial investment cost

In ProSimPlus, two methods are available to carry out the initial investment cost calculation of the equipment. These methods (the Functional Modules Method (FMM) and the Pré-Estime Method (PEM)) are described in the "Manual fo Process Economic Evaluation – New, revised and expanded edition" from CHAUVEL *et al.* [CHA03].

They allow to calculate:

- the equipment **base prices** (prices **before** the application of correction factors related for instance to the type, the material and the operating conditions of the equipment)
- the equipment **unassembled real prices** (prices **after** the application of correction factors previously mentioned and **before** the additional cost for **assembly**)
- the equipment **assembled real prices** (real prices **after** the application of the additional cost for **assembly** and of a size correction factor in the case of the PEM)
- the **equipment categories prices** (sum of the assembled real prices of the equipment belonging to a category).

In this example, the economic evaluation was carried out using each of the two methods.

Most of the data required to use these two methods are already pre-filled with default values when placing the "Economic evaluation module" on the flowsheet. A part of the data has to be supplied by the user as it is the case for equipment sizing data when using the PEM or for equipment material choice.

In this example, all the unit operations of the flowsheet except the feeds, the measurements, the valves, the mixer and the stream splitter are taken into account for the initial investment calculation. The considered unit operations are gathered in the following table:

Considered unit operations
C1
E1
E2
E3
E4
P1
R1 + R2
T1
T1 condenser
T1 reboiler
T2
T2 condenser
T2 reboiler
T3
T3 condenser
T3 reboiler
X1

Remark: the reactor of the process is simulated using two unit operations (a simple reactor unit operation and an equilibrium reactor unit operation). These two unit operations represent in reality one reactor. So for this economic evaluation, the reactor price is evaluated considering only one unit operation noted R1+R2 in this document.

4.2.1. Functional Modules Method (FMM)

The FMM has the advantage of not requiring equipment sizing data. It uses the operating parameters that are mostly pre-filled by recuperation of the simulation results to calculate the base prices. Carbon steel is the default value for the material correction factors but other choices are available in the ProSimPlus database. For some unit operations, the assembly correction factors depend on technological or operating aspects. In this case, the default values can also be modified by the user.

The first step of the FMM is to choose the functional module used to calculate the cost of each operation. A default value is assigned to each ProSimPlus unit operation but this value can be modified.

For this example, the functional modules chosen for each unit operation are:

Unit operation	Module type (FMM)
C1	Compression
E1	Heating furnace
E2	Heat exchanger
E3	Heat exchanger
E4	Heat exchanger
R1 + R2	Homogeneous fixed bed reactor with external pump system
T1	Distillation
T2	Distillation
T3	Distillation
X1	Drum

Remark: the FMM calculates the price of an unit operation (distillation, compression, reaction…). The “Distillation” functional module of the FMM includes especially the condenser and the reboiler. The “Ti condenser” and “Ti reboiler” (i = 1 to 3) unit operations prices must not be calculated otherwise their price will be considered twice.

For each functional module, parameters are required to calculate the operation base price. Parameters are pre-filled and related to the simulation results, others have to be manually entered. The following table gathers the parameters needed by the FMM in this example:

Unit operation	Parameters							
C1	DEB (kmol/h)	2244					COMP (-)	1.1563
E1	Q (Mkcal/h)	21.96						
E2	Q (Mkcal/h)	7.85	U (kcal/h/m²/°C)	500	TML (°C)	59		
E3	Q (Mkcal/h)	0.10	U (kcal/h/m²/°C)	600	TML (°C)	93		
E4	Q (Mkcal/h)	0.25	U (kcal/h/m²/°C)	500	TML (°C)	35		
R1 + R2	DEB (kmol/h)	2611	TS (s)	10	PRES (bar)	36.0		
T1	DEDIST (kmol/h)	9	XLEC (mole%)	5	PTE (bar)	10.2	VORM (-)	50
T2	DEDIST (kmol/h)	120	XLEC (mole%)	73.74	PTE (bar)	1.5	VORM (-)	2.23
T3	DEDIST (kmol/h)	40	XLEC (mole%)	92.64	PTE (bar)	2.0	VORM (-)	33.73
X1	DEB (kmol/h)	2611	TS (s)	1200	PRES (bar)	32.0		

Abbreviations: DEB: flowrate, Q: heat duty, DEDIST: distillate output, U: heat overall transfer coefficient, TS: residence time, XLEC: light ends in the feed molar ratio, TML: log mean temperature, PRES: pressure, PTE: column top pressure, COMP: compression factor, VORM: average relative volatility

Key: Black numeral value: pre-filled by ProSimPlus and related to a simulation result, red numeral value: to be supplied by the user (can be a simulation result), purple numeral value: see below

In the case of the E2 heat exchanger, the heat duty (23.5 Mkcal/h) and the log mean temperature (177 °C) are out of their respective variation intervals defined by CHAUVEL *et al.* [CHA03]. Nevertheless, to determine the base price of this exchanger, we have to assimilate it to 3 heat exchangers with a quantity of heat exchanged and a log mean temperature divided by 3 so they will belong to their respective variation interval. The base price of the E2 heat exchanger is then the sum of the base prices of this 3 exchangers.

For the heat exchanger E3, the heat duty is below the variation interval defined by CHAUVEL *et al.* [CHA03]. The heat duty has then been considered equal to the lower bound of the correlation variation interval (0.10 Mkcal/h).

The following table gathers the base prices obtained using the FMM:

			Variation interval	
Unit operation	**Module type (FMM)**	**Base price (€)**	**Min bound (€)**	**Max bound (€)**
C1	Compression	393 288	78 980	2 632 651
E1	Heating furnace	698 381	155 326	1 184 693
E2	Heat exchanger	95 226	2 633	526 530
E3	Heat exchanger	1 674	2 633	526 530
E4	Heat exchanger	5 503	2 633	526 530
R1 + R2	Homogeneous fixed bed reactor with external pump system	232 746	5 265	3 948 976
T1	Distillation	11 546	26 327	13 163 255
T2	Distillation	85 527	26 327	13 163 255
T3	Distillation	13 109	26 327	13 163 255
X1	Drum	719 492	5 265	3 948 976

After analyzing the results, we remark that three unit operations (in red) have a base price inferior to the variation domain defined by CHAUVEL *et al.* [CHA03]. The authors recommend in this case to take the minimum value of the variation interval. We have done that here by simply adding the following instruction in the calculation function:

If Base price < Min bound then Base price = Min bound. This instruction is written as follow:

```
if BasePrice < MinBasePrice * 210.365074668267 * 1.25146771037182 then
    BasePrice = MinBasePrice * 210.365074668267 * 1.25146771037182
end if
```

Where: BasePrice: base price (1985kFF)

210.365074668267: conversion factor from 1985kFF to mid-2000€

1.25146771037182: conversion factor from mid-2000€ to 2015€

The new base price table obtained is as follows:

Unit operation	**Module type (FMM)**	**Base price (€)**
C1	Compression	393 288
E1	Heating furnace	698 381
E2	Heat exchanger	95 226
E3	Heat exchanger	2 633
E4	Heat exchanger	5 503
R1 + R2	Homogeneous fixed bed reactor with external pump system	232 746
T1	Distillation	26 327
T2	Distillation	85 527
T3	Distillation	26 327
X1	Drum	719 492

Correction factors have to be applied to determine the unassembled and assembled real prices of equipment. The following table gathers this correction factors from the ProSimPlus database:

	Correction factor					
	Materials		Other		Erection	
Unit operation	**Description**	**Value**	**Description**	**Value**	**Description**	**Value**
C1	Carbon steel	0	Pressure < 75 bar	0	Centrifugal	2.91
E1	Carbon steel	0	Pressure 30 -70 bar	0.1		1.31
E2	CS/CS	0	Pressure 30 -40 bar	0.35		2.84
E3	CS/CS	0	Pressure < 10 bar	0		2.84
E4	CS/CS	0	Pressure < 10 bar	0		2.84
R1 + R2	Carbon steel	0			With shell and without quench	8.2
T1	Carbon steel	0			Detente/separation	3.39
T2	Carbon steel	0				3.39
T3	Carbon steel	0				3.39
X1	Carbon steel	0			Detente/separation	2.72

The unassembled and assembled real prices obtained are gathered in the following table:

Unit operation	Module type (FMM)	Unassembled real price (€)	Assembled real price (€)
C1	Compression	393 288	1 144 467
E1	Heating furnace	768 220	984 718
E2	Heat exchanger	128 555	303 771
E3	Heat exchanger	2 633	7 477
E4	Heat exchanger	5 503	15 629
R1	Homogeneous fixed bed reactor with external pump system	232 746	1 908 519
T1	Distillation	26 327	89 247
T2	Distillation	85 527	289 938
T3	Distillation	26 327	89 247
X1	Drum	719 492	1 957 017

The category total price is simply the sum of the assembled real prices of the equipment belonging to the category. The following table gathers the obtained results:

Category (FMM)	Equipment in the category	Category price (€)
Drums	X1	1 957 017
Compression	C1	1 144 467
Distillation	T1, T2, T3	468 431
Heat exchangers	E2, E3, E4	326 877
Heating furnaces	E1	984 718
Homogeneous fixed bed reactors with external pump system with shell and without quench	R1 + R2	1 908 519
Total	**(Process)**	**6 790 029**

4.2.2. Pré-Estime Method (PEM)

In the PEM, the evaluation of the initial investment cost is based on sizing aspects. In some complex cases (reactors and columns for example), the equipment can be divided into sub-equipment whose prices are separately evaluated. The following table gathers the equipment type (for the PEM) used for the prices calculation of each ProSimPlus unit operation:

Unit operation	Equipment type (PEM)
C1	**Centrifugal compressor**
E1	**Heating furnace**
E2	**Air-cooler**
E3	**Tube-type heat exchanger**
E4	**Tube-type heat exchanger**
P1	**Centrifugal pump (driver included)**
R1 + R2	**Pressure vessel (Reactor)**
	Shell
	Bottoms
	Accessories
T1	**Pressure vessel (Column)**
	Shell
	Bottoms
	Skirt
	Accessories
	Trays (8) (Valve, Carbon steel, 3.5 mm)
T1 condenser	**Tube-type heat exchanger**
T1 reboiler	**Tube-type heat exchanger**
T2	**Pressure vessel (Column)**
	Shell
	Bottoms
	Skirt
	Accessories
	Packing (Pall rings, Carbon steel, 1.5 in)
T2 condenser	**Tube-type heat exchanger**
T2 reboiler	**Tube-type heat exchanger**
T3	**Pressure vessel (Column)**
	Shell
	Bottoms
	Skirt
	Accessories
	Trays (5) (Valve, Carbon steel, 3.5 mm)
T3 condenser	**Tube-type heat exchanger**
T3 reboiler	**Tube-type heat exchanger**
X1	**Pressure vessel (Drum)**
	Shell
	Bottoms
	Accessories

Key: In bold letters: full equipment, in thin letters: sub-equipment

One or more parameters are required to determine the base price of equipment or sub-equipment. The following table shows the required parameters to use the PEM in this method. Attention has been paid to have the PEM parameters coherent with the FMM parameters.

Unit operation	Equipment type (PEM)	Parameter	Value
C1	**Centrifugal compressor**	Power (kW)	361.3
E1	**Heating furnace**	Calorific power (Gcal/h)	21.96
E2	**Air-cooler**	Fluid to be cooled inlet temperature (°C)	684
		Fluid to be cooled outlet temperature (°C)	38
		Air inlet temperature (°C)	20
		Fluid designation	Cooling: light hydrocarbons
		Heat duty to be removed (kcal/h)	2.35E+07
E3	**Tube-type heat exchanger**	Exchanger surface (m²)	1.8
E4	**Tube-type heat exchanger**	Exchanger surface (m²)	14.1
P1	**Centrifugal pump (driver included)**	Pression d'entrée (bar)	2
		Pression de sortie (bar)	37
		Flowrate (m3/h)	5.04
R1 + R2	**Pressure vessel (Reactor)**		
	Shell	Diameter (mm)	2000
		Weight (kg)	10374
	Bottoms	Diameter (mm)	2000
		Weight (kg)	2961
	Accessories	Weight (Shell + Bottoms) (kg)	13335
T1	**Pressure vessel (Column)**		
	Shell	Diameter (mm)	1050
		Weight (kg)	1471
	Bottoms	Diameter (mm)	1050
		Weight (kg)	264
	Skirt	Diameter (mm)	1050
		Weight (kg)	622
	Accessories	Weight (Shell + Bottoms + Skirt) (kg)	2357
	Trays (8) (Valve, Carbon steel, 3.5 mm)	Material and thickness	AO 3.5 mm
		Trays diameter (m)	1.022
		Trays number	8
T1 condenser	**Tube-type heat exchanger**	Exchanger surface (m²)	128.6
T1 reboiler	**Tube-type heat exchanger**	Exchanger surface (m²)	176.3
T2	**Pressure vessel (Column)**		
	Shell	Diameter (mm)	1300
		Weight (kg)	3661
	Bottoms	Diameter (mm)	1300
		Weight (kg)	178
	Skirt	Diameter (mm)	1300
		Weight (kg)	1156
	Accessories	Weight (Shell + Bottoms + Skirt) (kg)	4995
	Packing (Pall rings, Carbon steel, 1.5 in)	Dimension (mm)	38.1
		Packing type	Carbon steel Pall rings
		Volume (m3)	25
T2 condenser	**Tube-type heat exchanger**	Exchanger surface (m²)	26.4
T2 reboiler	**Tube-type heat exchanger**	Exchanger surface (m²)	138.5
T3	**Pressure vessel (Column)**		
	Shell	Diameter (mm)	700
		Weight (kg)	182
	Bottoms	Diameter (mm)	700
		Weight (kg)	178
	Skirt	Diameter (mm)	700
		Weight (kg)	415
	Accessories	Weight (Shell + Bottoms + Skirt) (kg)	633
	Trays (5) (Valve, Carbon steel, 3.5 mm)	Material and thickness	AO 3.5 mm
		Trays diameter (m)	0.69
		Trays number	5
T3 condenser	**Tube-type heat exchanger**	Exchanger surface (m²)	16.5
T3 reboiler	**Tube-type heat exchanger**	Exchanger surface (m²)	64.8
X1	**Pressure vessel (Drum)**		
	Shell	Diameter (mm)	1700
		Weight (kg)	6596
	Bottoms	Diameter (mm)	1700
		Weight (kg)	1583
	Accessories	Weight (Shell + Bottoms) (kg)	8180

Key: black numerical value: pre-filled by ProSimPlus and related to a simulation result, red numerical value: to be supplied by the user, purple numerical value: calculated during the simulation if the simulation has been done otherwise has to be entered by the user, blue numerical value: weight calculation formulae (to be entered by the user) from [CHA03] and using sizing variables calculated during simulation.

The drum, reactors and columns weight have been calculated with the method presented in CHAUVEL *et al.* [CHA03]:

The shell weight is determined as follows:

$$shell\ weight\ (kg) = 24.7\ .\ D'.\ H.\ e$$

Where D': shell diameter (m)

H: shell height or length (m)

e: shell thickness (mm)

The bottoms weight is calculated as follows:

$$bottoms\ weight\ (kg) = unit\ weight.\ e$$

Where e: bottoms thickness (here considered equal to the shell thickness) (mm)

unit weight: bottoms weight (kg) for a unit thickness (1 mm)

The curve giving the unit weight as a function of the shell diameter is available in [CHA03]. By regressing this curve, we obtain the following equation:

$$unit\ weight\ (kg) = \exp(2.83 + 2.23 \ln(\mathrm{D}') - 0.32 \ln(\mathrm{D}')^2 +\ 0.13 \ln(\mathrm{D}')^3)$$

To calculate the skirt weight we use the same equation as for the shell weight but using the skirt height and thickness.

The column diameters were calculated using the sizing method of the ProSimPlus "Distillation column" unit operations. The other entered values (in red) are orders of magnitude that are coherent with the FMM.

For heat exchangers, the exchanger surface is coherent with the FMM values and estimated as follows:

$$A = \frac{Q}{U\ .\ TML}$$

Where A: exchanger surface (m²)

Q: heat duty (kcal/h)

U: overall transfer coefficient (kcal/h/m²/°C)

TML: log mean temperature (°C)

The following table gathers the base prices calculated using the PEM:

Unit operation	Equipment type (PEM)	Base price (€)
C1	**Centrifugal compressor**	**630 416**
E1	**Heating furnace**	**1 132 299**
E2	**Air-cooler**	**87 565**
E3	**Tube-type heat exchanger**	**4 417**
E4	**Tube-type heat exchanger**	**10 225**
P1	**Centrifugal pump (driver included)**	**54 492**
R1 + R2	Shell	43 294
	Bottoms	12 357
	Accessories	41 475
	Pressure vessel (Reactor)	**97 126**
T1	Shell	7 303
	Bottoms	1 311
	Skirt	3 088
	Accessories	16 952
	Trays (8) (Valve, Carbon steel, 3.5 mm)	1 777
	Pressure vessel (Column)	**30 431**
T1 condenser	**Tube-type heat exchanger**	**35 248**
T1 reboiler	**Tube-type heat exchanger**	**44 265**
T2	Shell	17 201
	Bottoms	836
	Skirt	5 431
	Accessories	22 274
	Packing (Pall rings, Carbon steel, 1.5 in)	34 572
	Pressure vessel (Column)	**80 314**
T2 condenser	**Tube-type heat exchanger**	**13 790**
T2 reboiler	**Tube-type heat exchanger**	**37 135**
T3	Shell	989
	Bottoms	196
	Skirt	2 255
	Accessories	10 512
	Trays (5) (Valve, Carbon steel, 3.5 mm)	802
	Pressure vessel (Column)	**14 754**
T3 condenser	**Tube-type heat exchanger**	**10 989**
T3 reboiler	**Tube-type heat exchanger**	**22 603**
X1	Shell	28 790
	Bottoms	6 909
	Accessories	17 821
	Pressure vessel (Drum)	**53 520**

Key: In bold letters: full equipment, in thin letters: sub-equipment

To determine the unassembled real prices, correction factors have to be applied. The table hereafter gathers the correction factors used with the notation employed by CHAUVEL *et al.* [CHA03] (for example: fp: pressure correction factor). All this factors are included in the ProSimPlus database.

Unit operation	Equipment type (PEM)	Correction factors											
C1	**Centrifugal compressor**	ft (Electric motor)	1	fpmax (<75 bar)	1	fm (Cast steel)	1						
E1	**Heating furnace**	fd (Furnaces for heating the heat transfer fluid)	0.15	fm (Carbon steel)	0	fp (30-70 bar)	0.1						
E2	**Air-cooler**	fe (e = 2,77 mm)	1	fp (P = 30 to 50 bar)	1.1	fl (l = 10 m)	1	fN (N = 6 rows)	1	fm (Carbon steel)	1		
E3	**Tube-type heat exchanger**	fd (AES)	1	fl (16 ft ; 4,9 m)	1	fnp (2 passes)	1	fp (P < 10 bar, Tubes and shells)	1	ft (T < 350 °C)	1	fm (CS/CS)	1
E4	**Tube-type heat exchanger**	fd (AES)	1	fl (16 ft ; 4,9 m)	1	fnp (2 passes)	1	fp (P < 10 bar, Tubes and shells)	1	ft (T < 350 °C)	1	fm (CS/CS)	1
P1	**Centrifugal pump (driver included)**	fd ("Process" horizontal with vertical seal)	1	fe (Electric motor)	1	fm (Cast steel)	1	ft (<150°C)	1	fp (< 20 bar suction)	1		
R1 + R2	Shell	fe (e = 42 mm)	0.84	fm (SA 240 304)	2.3			fpf (Columns and reactors)	1.15				
	Bottoms	fe (e = 42 mm)	0.84	fm (SA 240 304)	2.3	ff (1,5 m < D' <= 2 m)	2	fpf (Columns and reactors)	1.15				
	Accessories	fam (SA 240 304)	2.5					fpf (Columns and reactors)	1.15				
	Pressure vessel (Reactor)												
T1	Shell	fe (e = 14 mm)	0.88	fm (SA 285 C)	1			fpf (Columns and reactors)	1.15				
	Bottoms	fe (e = 14 mm)	0.88	fm (SA 285 C)	1	ff (1 m < D' <= 1,5 m)	2.5	fpf (Columns and reactors)	1.15				
	Skirt	fe (e = 8 mm)	1.02					fpf (Columns and reactors)	1.15				
	Accessories	fam (SA 285 C)	1.00					fpf (Columns and reactors)	1.15				
	Trays (8) (Valve, Carbon steel, 3.5 mm)	fpl (Valve)	1	fe (e = 3,5 mm)	1.25	fpa (1 passe)	1	fam (Carbon steel)	1	fpn (0-15)	1	Trays number	8
	Pressure vessel (Column)												
T1 condenser	**Tube-type heat exchanger**	fd (AES)	1	fl (16 ft ; 4,9 m)	1	fnp (2 passes)	1	fp (P 10 to 20 bar, Tubes)	1.07	ft (T < 350 °C)	1	fm (CS/CS)	1
T1 reboiler	**Tube-type heat exchanger**	fd (BKT)	1.25	fl (16 ft ; 4,9 m)	1.00	fnp (2 passes)	1.00	fp (P 10 to 20 bar, Tubes and shells)	1.12	ft (T < 350 °C)	1.00	fm (CS/CS)	1.00
T2	Shell	fe (e = 6 mm)	1.20	fm (SA 285 C)	1			fpf (Columns and reactors)	1.15				
	Bottoms	fe (e = 6 mm)	1.20	fm (SA 285 C)	1	ff (1 m <= D' <= 1,5 m)	2.5	fpf (Columns and reactors)	1.15				
	Skirt	fe (e = 12 mm)	0.91					fpf (Columns and reactors)	1.15				
	Accessories	fam (SA 285 C)	1					fpf (Columns and reactors)	1.15				
	Packing (Pall rings, Carbon steel, 1.5 in)	fv (V < 50 m3)	1					fpf (Columns and reactors)	1.15				
	Pressure vessel (Column)												
T2 condenser	**Tube-type heat exchanger**	fd (AES)	1	fl (16 ft ; 4,9 m)	1	fnp (2 passes)	1	fp (P < 10 bar, Tubes)	1	ft (T < 350 °C)	1	fm (CS/CS)	1
T2 reboiler	**Tube-type heat exchanger**	fd (BKT)	1.25	fl (16 ft ; 4,9 m)	1.00	fnp (2 passes)	1.00	fp (P < 10 bar, Tubes and shells)	1.00	ft (T < 350 °C)	1.00	fm (CS/CS)	1.00
T3	Shell	fe (e = 5 mm)	1.44	fm (SA 285 C)	1			fpf (Columns and reactors)	1.15				
	Bottoms	fe (e = 5 mm)	1.44	fm (SA 285 C)	1	ff (D' < 1 m)	2.8	fpf (Columns and reactors)	1.15				
	Skirt	fe (e = 8 mm)	1.02					fpf (Columns and reactors)	1.15				
	Accessories	fam (SA 285 C)	1					fpf (Columns and reactors)	1.15				
	Trays (5) (Valve, Carbon steel, 3.5 mm)	fpl (Valve)	1	fe (e = 3,5 mm)	1.25	fpa (1 passe)	1	fam (Carbon steel)	1	fpn (0-15)	1	Trays number	5
	Pressure vessel (Column)												
T3 condenser	**Tube-type heat exchanger**	fd (AES)	1	fl (16 ft ; 4,9 m)	1	fnp (2 passes)	1	fp (P < 10 bar, Tubes)	1	ft (T < 350 °C)	1	fm (CS/CS)	1
T3 reboiler	**Tube-type heat exchanger**	fd (BKT)	1.25	fl (16 ft ; 4,9 m)	1.00	fnp (2 passes)	1.00	fp (P 40 to 65 bar, Tubes and shells)	1.81	ft (T < 350 °C)	1.00	fm (CS/CS)	1.00
X1	Shell	fe (e = 30,8 mm)	0.80	fm (SA 285 C)	1			fpf (Drums)	1.1				
	Bottoms	fe (e = 30,8 mm)	0.80	fm (SA 285 C)	1	ff (1,5 m < D' <= 2 m)	2	fpf (Drums)	1.1				
	Accessories	fam (SA 285 C)	1					fpf (Drums)	1.1				
	Pressure vessel (Drum)												

Key: refer to [CHA03], fpf: final price correction factor (see [CHA03] p. 333) and fv: packing volume correction factor (see [CHA03] p. 359)

The unassembled real prices are gathered in the table below:

Unit operation	Equipment type (PEM)	Unassembled real price (€)
C1	**Centrifugal compressor**	**630 416**
E1	**Heating furnace**	**1 415 374**
E2	**Air-cooler**	**96 321**
E3	**Tube-type heat exchanger**	**4 609**
E4	**Tube-type heat exchanger**	**10 670**
P1	**Centrifugal pump (driver included)**	**54 492**
R1 + R2	Shell	95 892
	Bottoms	54 740
	Accessories	119 241
	Pressure vessel (Reactor)	**269 872**
T1	Shell	7 426
	Bottoms	3 332
	Skirt	3 606
	Accessories	19 495
	Trays (8) (Valve, Carbon steel, 3.5 mm)	2 554
	Pressure vessel (Column)	**36 413**
T1 condenser	**Tube-type heat exchanger**	**39 354**
T1 reboiler	**Tube-type heat exchanger**	**64 664**
T2	Shell	23 830
	Bottoms	2 897
	Skirt	5 680
	Accessories	25 615
	Packing (Pall rings, Carbon steel, 1.5 in)	39 758
	Pressure vessel (Column)	**97 779**
T2 condenser	**Tube-type heat exchanger**	**14 390**
T2 reboiler	**Tube-type heat exchanger**	**48 436**
T3	Shell	1 635
	Bottoms	906
	Skirt	2 634
	Accessories	12 089
	Trays (5) (Valve, Carbon steel, 3.5 mm)	1 153
	Pressure vessel (Column)	**18 417**
T3 condenser	**Tube-type heat exchanger**	**11 467**
T3 reboiler	**Tube-type heat exchanger**	**53 363**
X1	Shell	25 429
	Bottoms	12 206
	Accessories	19 603
	Pressure vessel (Drum)	**57 238**

Key: In bold letters: full equipment, in thin letters: sub-equipment

The calculation of the assembled real price from the unassembled real price is more complex in the case of the PEM than in the case of the FMM. Indeed an assembly factor is taken into account but also a size factor. This size factor represents a decrease or an increase of the equipment depending on the "size" of the ordered batch: for instance ordering a batch of 10 heat exchangers allows to save money on the total assembled real price instead of ordering the 10 heat exchangers separately.

This size factor is defined for each equipment category (in the PEM sense) and depends on the sum of the unassembled real prices of the equipment belonging to the category.

The following table shows the assembled real price of each piece of equipment and its respective category (in the PEM sense):

Unit operation	Equipment type (PEM)	Category (PEM)	Assembled real price (€)
C1	Centrifugal compressor	Centrifugal compressors and drivings	1 929 869
E1	Heating furnace	Heating furnaces	3 170 112
E2	Air-cooler	Air-coolers	260 887
E3	Tube-type heat exchanger	Tubular heat exchangers	16 514
E4	Tube-type heat exchanger	Tubular heat exchangers	38 230
P1	Centrifugal pump (driver included)	Pumps and drivings	187 652
R1 + R2	Pressure vessel (Reactor)	Columns and reactors	606 524
T1	Pressure vessel (Column)	Columns and reactors	141 892
T1 condenser	Tube-type heat exchanger	Tubular heat exchangers	134 358
T1 reboiler	Tube-type heat exchanger	Tubular heat exchangers	183 971
T2	Pressure vessel (Column)	Columns and reactors	376 158
T2 condenser	Tube-type heat exchanger	Tubular heat exchangers	51 559
T2 reboiler	Tube-type heat exchanger	Tubular heat exchangers	148 525
T3	Pressure vessel (Column)	Columns and reactors	69 556
T3 condenser	Tube-type heat exchanger	Tubular heat exchangers	41 085
T3 reboiler	Tube-type heat exchanger	Tubular heat exchangers	114 285
X1	Pressure vessel (Drum)	Drums	191 689
Total	**(Process)**	**(Process)**	**7 662 867**

To calculate the total price of an equipment category, the sum of the assembled real prices of the equipment belonging to the category is done. The results are gathered in the table below:

Category (PEM)	Category price (€)
Air-coolers	260 887
Drums	191 689
Columns and reactors	1 194 131
Centrifugal compressors and drivings	1 929 869
Tubular heat exchangers	728 527
Heating furnaces	3 170 112
Pumps and drivings	187 652
Total (Process)	**7 662 867**

4.2.3. Results comparison (FMM and PEM)

The following table contains the initial investment costs of the operations evaluated by the FMM and the PEM (that is why the P1 pump is not present):

		Unassembled real price (€)		Assembled real price (€)	
Unit operation	**Equipment type**	**FMM**	**PEM**	**FMM**	**PEM**
C1	Compressor	393 288	630 416	1 144 467	1 929 869
E1	Heating furnace	768 220	1 415 374	984 718	3 170 112
E2	Heat exchanger	128 555	96 321	303 771	260 887
E3	Heat exchanger	2 633	4 609	7 477	16 514
E4	Heat exchanger	5 503	10 670	15 629	38 230
R1 + R2	Reactor	232 746	269 872	1 908 519	606 524
T1*	Distillation column (partial condenser)	26 327	140 432	89 247	460 222
T2*	Distillation column (total condenser)	85 527	160 604	289 938	576 243
T3*	Distillation column (total condenser)	26 327	83 246	89 247	224 927
X1	Separation drum	719 492	57 238	1 957 017	191 689
Total		**2 388 616**	**2 868 782**	**6 790 029**	**7 475 215**

*: in this table, the prices of the columns take into account the prices of the reboilers and of the condensers for the PEM

We remark that the prices of some operations are noticeably different for the two methods. The FMM and the PEM are indeed two distinct cost evaluation methods: the first one is mainly based on operating parameters and estimates the price of a functional unit (distillation, reaction…) whereas the second one takes equipment sizing aspects into account.

Considering the total initial investment costs the results are nevertheless of the same order of magnitude with a deviation of around 18% on the total unassembled real price and 10% on the total assembled real price.

4.3. Secondary investment cost and residual value

For each unit operation for which the initial investment cost was defined, it is necessary to specify a life time. As soon as the life time of a piece of equipment has been reached, this piece needs to be rebought. The secondary investment cost of a piece of equipment is then defined as the sum of the rebuy costs of this piece on the time horizon.

The life time also allows to determine the residual value of a piece of equipment that is to say the resale price of this piece every year. In the economic evaluation unit operation, we consider that the decreasing of the residual value of a piece of equipment is linear with time.

If the rebuy year of a piece of equipment occurs the last year of the time horizon, then the piece is not rebought this year and its residual value is null.

The equipment life times considered in this example are gathered in the table hereafter:

Unit operation	Life time (an)
C1	10
E1	10
E2	10
E3	10
E4	10
P1	10
R1 + R2	15
T1	15
T1 condenser	15
T1 reboiler	15
T2	15
T2 condenser	15
T2 reboiler	15
T3	15
T3 condenser	15
T3 reboiler	15
X1	15

*: only defined for the PEM

The following tables indicate for each unit operation the number of equipment changes, the total secondary investment cost and the residual value at the end of the time horizon:

Functional Modules Method:

Unit operation	Number of equipment changes	Total secondary investment (€)	Residual value (€)
C1	1	772 254	0
E1	1	664 460	0
E2	1	204 976	0
E3	1	5 045	0
E4	1	10 546	0
R1 + R2	1	1 058 490	580 682
T1	1	49 498	27 155
T2	1	160 803	88 216
T3	1	49 498	27 154
X1	1	1 085 388	595 438

Pré-Estime method:

Unit operation	Number of equipment changes	Total secondary investment (€)	Residual value (€)
C1	1	1 303 750	0
E1	1	2 141 614	0
E2	1	176 246	0
E3	1	11 156	0
E4	1	25 827	0
P1	1	126 771	0
R1 + R2	1	336 781	184 540
T1	1	78 788	43 172
T1 condenser	1	74 604	40 880
T1 reboiler	1	102 153	55 975
T2	1	208 868	114 449
T2 condenser	1	28 629	15 687
T2 reboiler	1	82 471	45 190
T3	1	38 622	21 163
T3 condenser	1	22 813	12 501
T3 reboiler	1	63 459	34 772
X1	1	106 438	58 323

4.4. Maintenance cost

The annual maintenance cost of each piece of equipment (in €/year) can be either defined as a constant, be calculated as a percentage of the investment cost (unassembled or assembled real price) or be calculated by a user formulae.

In this example we have considered that the annual maintenance cost of the equipment corresponds to 5% percent of their assembled real price.

The annual maintenance cost of each piece of equipment is indicated in the following tables.

Functional Modules Method:

Unit operation	Module type (FMM)	Maintenance (€/year)
C1	Compressor	57 223
E1	Heating furnace	49 236
E2	Heat exchanger	15 189
E3	Heat exchanger	374
E4	Heat exchanger	781
R1 + R2	Reactor	95 426
T1	Distillation column (partial condenser)	4 462
T2	Distillation column (total condenser)	14 497
T3	Distillation column (total condenser)	4 462
X1	Separation drum	97 851
Total	**Process**	**339 501**

Pré-Estime Method:

Unit operation	Equipment type (PEM)	Maintenance (€/year)
C1	Compressor	96 493
E1	Heating furnace	158 506
E2	Air-cooler	13 044
E3	Tube-type heat exchanger	826
E4	Tube-type heat exchanger	1 911
P1	Centrifugal pump	9 383
R1 + R2	Reactor	30 326
T1	Column	7 095
T1 condenser	Tube-type heat exchanger	6 718
T1 reboiler	Tube-type heat exchanger	9 199
T2	Column	18 808
T2 condenser	Tube-type heat exchanger	2 578
T2 reboiler	Tube-type heat exchanger	7 426
T3	Column	3 478
T3 condenser	Tube-type heat exchanger	2 054
T3 reboiler	Tube-type heat exchanger	5 714
X1	Drum	9 584
Total	**Process**	**383 143**

4.5. Operating gains and costs

The operating gains and costs include the following points:

- gains and costs of the process inlets and outlets
- costs of the utilities defined in the unit operations
- production gains and consumption costs of electricity

The following gathers the data used to calculate the operating gains and costs of the example.

Gains and costs of the process inlets and outlets:

Unit operation	Consumption / production type	Price (€/t)
Hydrogen feed	Raw material	34
Toluene feed	Raw material	291
Benzene outlet	Product	383
Biphenyl outlet	Product	250
Light gas outlet	Product	308
Purge	Product	308
CU-1	Utility	0
CU-3	Utility	0
CU-5	Utility	0
HU-1	Utility	20
HU-3	Utility	15
HU-5	Utility	25

Costs of the utilities defined in the unit operations:

Unit operation	Utility type of use	Utility description	Price (€/MWh)
E1	Heat duty	Natural gas	20
E2	Heat duty	Air (20°C)	0
E3	Heat duty	Cold water (15°C)	0
E4	Heat duty	Cold water (15°C)	0
R1	Heat duty	Cold water (15°C)	0
R2	Heat duty	Cold water (15°C)	0
X1	Heat duty	Natural gas	20

Remarks:

- Cold water and air costs are neglected
- Natural gas has been chosen to feed the E1 furnace and to heat the heat transfer fluid in the X1 drum (the heat transfer losses have been neglected)
- The utility consumption in the reactor is the sum of the consumptions in the R1 and R2 unit operations
- The row "Utility description" does not appear in the economic evaluation unit operation but is present in this document to precise the hypothesis of the example

Production gains and consumption costs of electricity:

Unit operation	Electricity	Price (€/MWh)
C1	Consumption	40
P1	Consumption	40

Results:

Operating gains:

	Operating gains (€/year)
Unit operation	**Product**
Benzene outlet	31 499 069
Biphenyl outlet	1 043 463
Light gas outlet	386 546
Purge	6 288 027
Total	**39 217 104**

Operating expenses:

	Operating cost (€/year)			
Unit operation	**Raw material**	**Utility**	**Consumed electricity**	**Total**
C1	0	0	126 684	126 684
E1	0	4 475 279	0	4 475 279
HU-1		367 210	0	367 210
HU-3		373 398	0	373 398
HU-5		206 633	0	206 633
Hydrogen feed	161 613	0	0	161 613
P1	0	0	2 643	2 643
Toluene feed	30 070 261	0	0	30 070 261
X1	0	2 932	0	2 932
Total	**30 231 8744**	**5 425452**	**129 327**	**35 786 654**

The **operating balance** (difference between operating gains and cost) is equal to **3 430 450 €/year**.

4.6. Schedule

The economic evaluation unit operation supplies a schedule on the time horizon specified by user. The actualization is taken into account. The definitions of the results given in the schedule are available in the ProSimPlus Online Help. For instance we can have access to the depreciation, the cumulative discounted cash flow or the net discounted value.

The following pages contain the schedules obtained for this example with the FMM and the PEM.

Year	Investment cost	Maintenance cost	Operating gain	Operating expense	Depreciation	Operating cost	Net income	Cash flow	Discount factor	Discounted cash flow	Cumulative discounted cash flow	Residual value	Discounted residual value	Net discounted value
	(€)	(€)	(€)	(€)	(€)	(€)	(€)	(€)		(€)	(€)	(€)	(€)	(€)
0	7 790 029	0	0	0	0	0	0	-7 790 029	1,000	-7 790 029	-7 790 029	6 790 029	6 790 029	0
1	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,962	1 858 255	-5 931 774	6 255 492	6 014 896	1 044 660
2	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,925	1 786 783	-4 144 991	5 720 954	5 289 344	2 068 909
3	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,889	1 718 061	-2 426 930	5 186 417	4 610 706	3 072 772
4	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,855	1 651 982	-774 949	4 651 880	3 976 446	4 056 302
5	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,822	1 588 444	813 495	4 117 342	3 384 155	5 019 578
6	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,790	1 527 350	2 340 845	3 582 805	2 831 543	5 962 703
7	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,760	1 468 606	3 809 451	3 048 268	2 316 433	6 885 802
8	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,731	1 412 121	5 221 572	2 513 730	1 836 758	7 789 020
9	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,703	1 357 808	6 579 380	1 979 193	1 390 555	8 672 522
10	2 456 061	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	-523 477	0,676	-353 642	6 225 738	3 900 717	2 635 185	9 536 487
11	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,650	1 255 370	7 481 108	3 366 180	2 186 606	10 317 295
12	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,625	1 207 087	8 688 195	2 831 643	1 768 636	11 081 428
13	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,601	1 160 660	9 848 855	2 297 105	1 379 582	11 829 011
14	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,577	1 116 020	10 964 875	1 762 568	1 017 839	12 560 189
15	4 333 968	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	-2 401 383	0,555	-1 333 403	9 631 472	5 561 998	3 088 380	13 275 117
16	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,534	1 031 823	10 663 295	5 027 461	2 684 202	13 881 406
17	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,513	992 137	11 655 432	4 492 924	2 306 547	14 475 353
18	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,494	953 978	12 609 411	3 958 386	1 953 971	15 057 010
19	0	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	1 932 585	0,475	917 287	13 526 697	3 423 849	1 625 104	15 626 444
20	-3 889 312	339 501	39 217 104	35 786 652	534 537	36 321 189	1 737 549	5 821 897	0,456	2 657 038	16 183 735	2 889 312	1 318 644	16 183 735

Schedule (FMM)

Year	Investment cost	Maintenance cost	Operating gain	Operating expense	Depreciation	Operating cost	Net income	Cash flow	Discount factor	Discounted cash flow	Cumulative discounted cash flow	Residual value	Discounted residual value	Net discounted value
	(€)	(€)	(€)	(€)	(€)	(€)	(€)	(€)		(€)	(€)	(€)	(€)	(€)
0	8 662 867	0	0	0	0	0	0	-8 662 867	1,000	-8 662 867	-8 662 867	7 662 867	7 662 867	0
1	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,962	1 879 020	-6 783 846	6 965 234	6 697 340	875 032
2	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,925	1 806 750	-4 977 096	6 267 600	5 794 749	1 742 209
3	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,889	1 737 260	-3 239 836	5 569 967	4 951 681	2 600 841
4	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,855	1 670 442	-1 569 394	4 872 334	4 164 892	3 450 302
5	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,822	1 606 195	36 801	4 174 701	3 431 300	4 290 028
6	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,790	1 544 418	1 581 219	3 477 068	2 747 977	5 119 510
7	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,760	1 485 017	3 066 236	2 779 434	2 112 142	5 938 295
8	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,731	1 427 901	4 494 137	2 081 801	1 521 152	6 745 979
9	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,703	1 372 982	5 867 119	1 384 168	972 498	7 542 204
10	5 603 263	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	-3 649 081	0,676	-2 465 189	3 401 930	6 289 797	4 249 162	8 326 656
11	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,650	1 269 399	4 671 329	5 592 164	3 632 563	8 953 473
12	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,625	1 220 576	5 891 905	4 894 531	3 057 110	9 573 612
13	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,601	1 173 631	7 065 536	4 196 898	2 520 548	10 186 658
14	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,577	1 128 491	8 194 027	3 499 265	2 020 738	10 792 240
15	2 059 604	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	-105 423	0,555	-58 538	8 135 489	4 861 236	2 699 272	11 390 025
16	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,534	1 043 353	9 178 842	4 163 602	2 222 981	11 935 732
17	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,513	1 003 224	10 182 067	3 465 969	1 779 336	12 474 776
18	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,494	964 639	11 146 706	2 768 336	1 366 528	13 006 862
19	0	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	1 954 181	0,475	927 537	12 074 243	2 070 703	982 843	13 531 729
20	-2 373 069	383 143	39 217 104	35 786 652	697 633	36 484 285	1 639 691	4 327 251	0,456	1 974 901	14 049 144	1 373 069	626 651	14 049 144

Schedule (PEM)

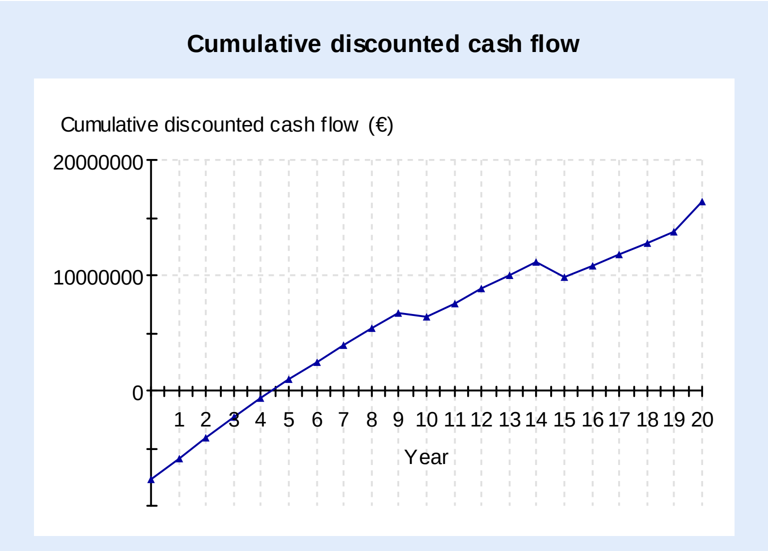
4.7. Profiles supplied by the economic evaluation unit operation

The economic evaluation unit operation supplies the following profiles:

- cumulative discounted cash flow function of time
- net discounted cash flow function of time
- discounted residual value of the process function of time
- cumulative discounted cash flow function of discount rate

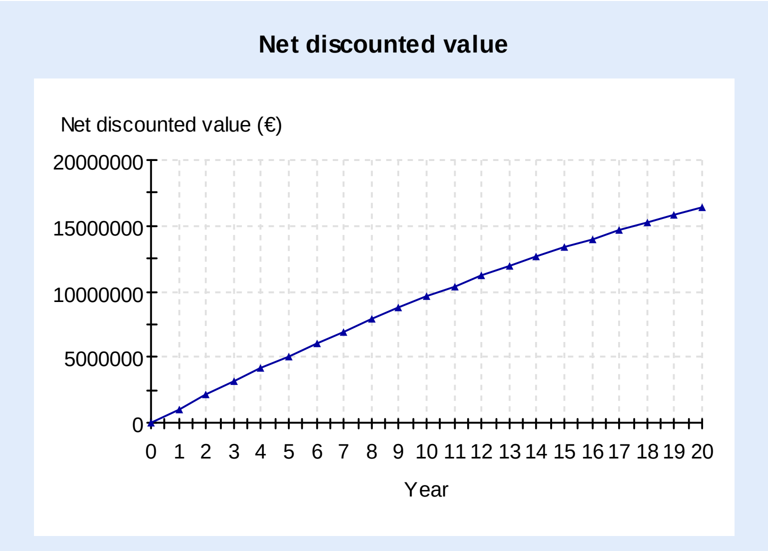
The following shows the profiles obtained in the example with the FMM and the PEM.

Profiles obtained with the FMM:



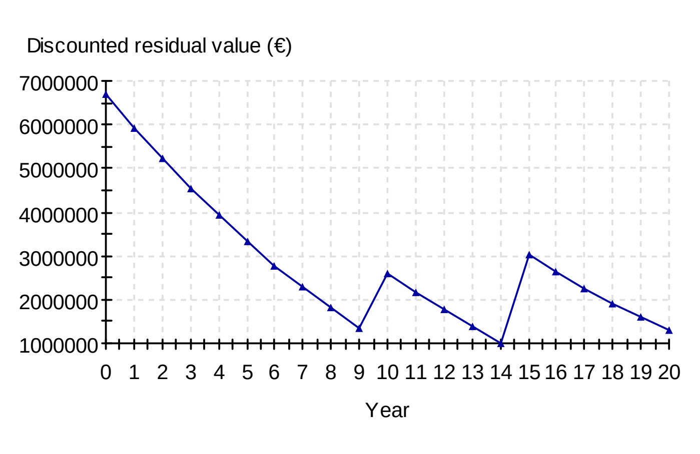
Cumulative discounted cash flow vs. Time

On this curve, we can remark that the pay out time (time when the cumulative discounted cash flow becomes positive) is around 4.5 years.



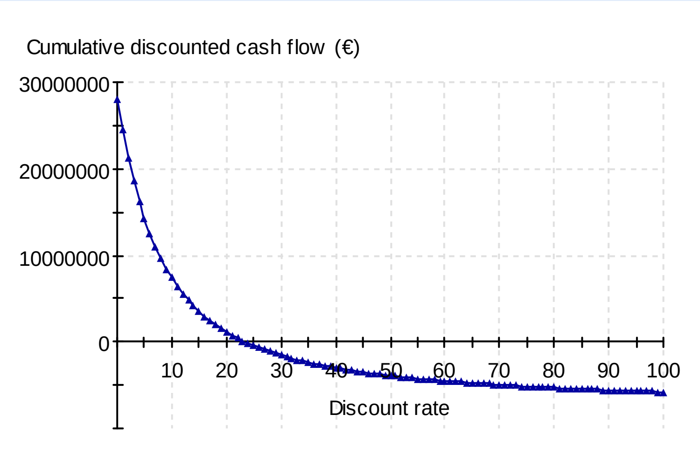
Net discounted value vs. Time

Discounted residual value



Discounted residual value vs.Time

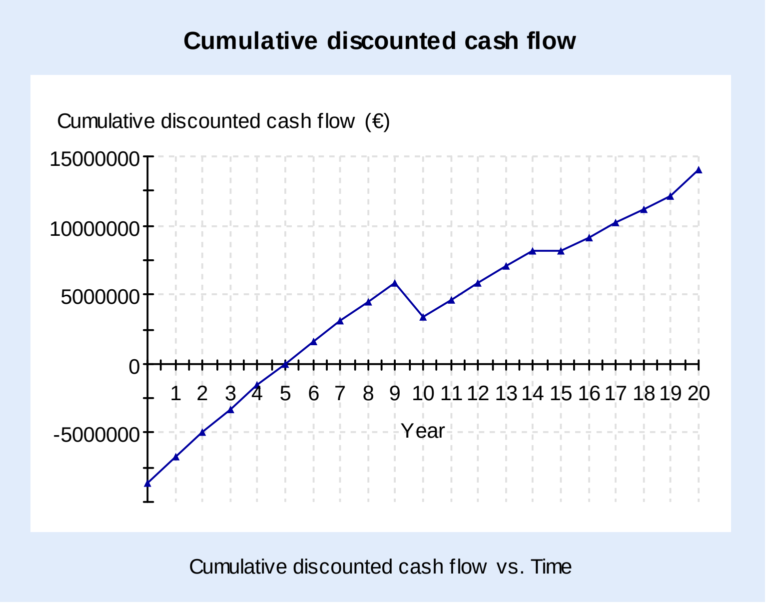
Rate of return



Cumulative discounted cash flow vs. Discount rate

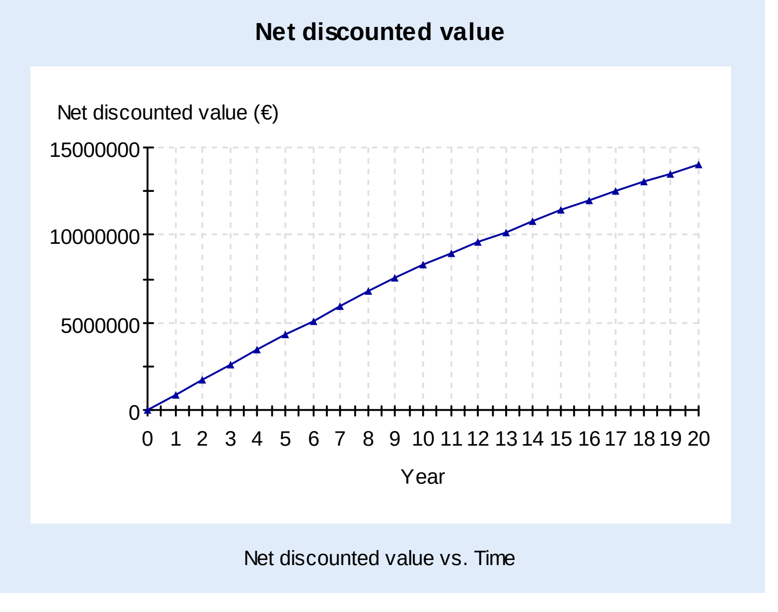
On this last curve, we can remark that the rate of return (discount rate for which the cumulative discounted cash flow at the end of the time horizon is null) is around 23%.

Profiles obtained with the PEM:



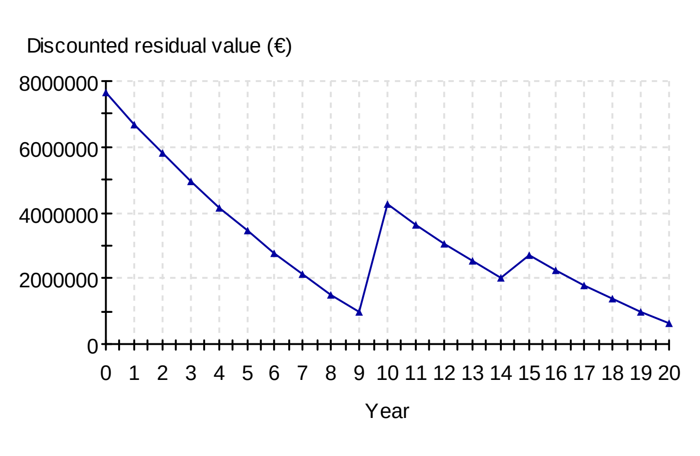
Cumulative discounted cash flow vs. Time

On this curve, we can remark that the pay out time is around 5 years.



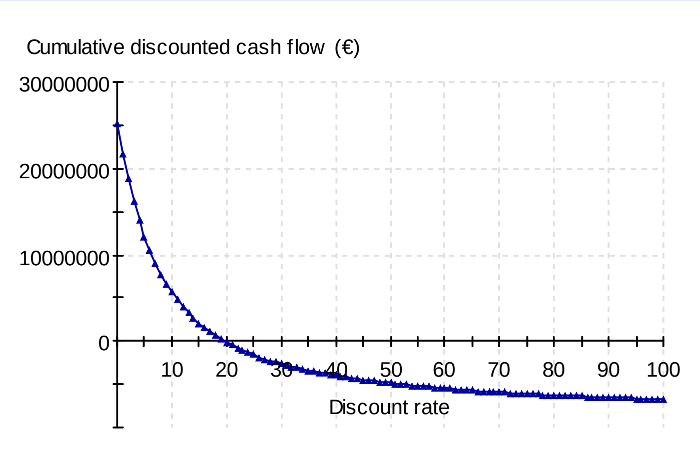
Net discounted value vs. Time

Discounted residual value



Discounted residual value vs.Time

Rate of return



Cumulative discounted cash flow vs. Discount rate

On this last curve, we can remark that the rate of return is around 20%.

4.8. Summary of the economic evaluation results

The economic evaluation unit operation supplies a global economic balance of the process that summarizes the different results previously described.

The results obtained using the FMM are:

OVERALL RESULTS (discounted values)

☐ Define global currency

Initial investment cost	=	7 790 028.74	(€)
Total secondary investment cost	=	4 065 725.28	(€)
Residual value at the time horizon	=	1 318 644.12	(€)
Maintenance cost	=	339 501.44	(€/AN)
Operating balance	=	3 430 446.46	(€/AN)
Operating gain	=	39 217 100.39	(€/AN)
Products	=	39 217 100.39	(€/AN)
Remunerative inputs	=	0.00	(€/AN)
Produced electricity	=	0.00	(€/AN)
Operating expense	=	35 786 653.93	(€/AN)
Raw materials	=	30 231 874.17	(€/AN)
Utilities	=	5 425 452.29	(€/AN)
Consumed electricity	=	129 327.46	(€/AN)
Waste (reprocessing)	=	0.00	(€/AN)
Pay out time	=	4.49	(AN)
Rate of return	=	23.12	(%)

The results obtained using the PEM are:

OVERALL RESULTS (discounted values)

☐ Define global currency

Initial investment cost	=	8 662 866.78	(€)
Total secondary investment cost	=	4 928 988.53	(€)
Residual value at the time horizon	=	626 650.98	(€)
Maintenance cost	=	383 143.34	(€/AN)
Operating balance	=	3 430 446.49	(€/AN)
Operating gain	=	39 217 100.72	(€/AN)
Products	=	39 217 100.72	(€/AN)
Remunerative inputs	=	0.00	(€/AN)
Produced electricity	=	0.00	(€/AN)
Operating expense	=	35 786 654.23	(€/AN)
Raw materials	=	30 231 874.43	(€/AN)
Utilities	=	5 425 452.33	(€/AN)
Consumed electricity	=	129 327.47	(€/AN)
Waste (reprocessing)	=	0.00	(€/AN)
Pay out time	=	4.98	(AN)
Rate of return	=	19.65	(%)

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