PROSIMPLUS HNO3 APPLICATION EXAMPLE

DUAL-PRESSURE PROCESS

EXAMPLE PURPOSE
This example corresponds to a dual-pressure nitric acid production process. It is a rather usual process of industrial production of nitric acid. The main modules specific to the simulator ProSimPlus HNO3 are used in this simulation: absorption column of nitrous vapors, nitrous vapors condenser, oxidation reactors, heat exchangers with oxidation volumes, nitrous vapor compressors, etc. The particular points which are detailed in this example are: ✓ Use of a constraints and recycles module to reach a set of specifications, ✓ Compressors – expanders coupling using information streams to model the turbo-expander and use of a constraints and recycles module to balance the powers. ✓ The separation of a heat exchanger between a cooler/heater and a simple heat exchanger to avoid a recycle stream by using an information stream.

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CORRESPONDING PROSIMPLUS HNO3 FILE	*PSPH_E02_EN – Dual-pressure process.pmp3*

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1. MODELING OF THE PROCESS

1.1. Process description

This example is extracted from [BAD96] and [CLA96], which describe summarily the process. The production of nitric acid includes three main steps:

- ✓ Ammonia oxidation

$$4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$$

$$4\,NH_3 + 3\,O_2 \rightarrow 2\,N_2 + 6\,H_2O$$

$$2\,NH_3 + 2\,O_2 \rightarrow N_2O + 3\,H_2O$$

- ✓ Oxidation of the nitric oxide and condensation of the combustion water

$$2\,NO + O_2 \rightarrow 2\,NO_2 \leftrightarrow N_2O_4$$

$$H_2O|_{gaz} \leftrightarrow H_2O|_{liquide}$$

- ✓ Fixing of the nitrogen tetroxide

$$\frac{3}{2}\,N_2O_4 + H_2O \leftrightarrow 2\,HNO_3 + NO$$

The mathematical representations of the equilibria and kinetics of the reactions described here above is complex. Side reactions occur, in particular the formation of nitrogen trioxide:

$$NO + NO_2 \leftrightarrow N_2O_3$$

The dual-pressure process (pressure of the absorption sensibly higher than the one of the catalytic oxidation) lies on the reaction:

$$\frac{3}{2}\,N_2O_4 + H_2O \leftrightarrow 2\,HNO_3 + NO$$

The main characteristic of this reaction is that each time two molecules of nitric acid are formed there is also production of one molecule of nitric oxide (NO). This molecule of NO has to be oxidized in NO_2, and then absorbed and so on. These successive oxidations are mainly done in gas phase in oxido-absorption tower where the reactions of nitric acid production and NO oxidation are performed in parallel:

$$2NO + O_2 \rightarrow 2NO_2$$

This process is mainly characterized by the use of two different pressures for the ammonia oxidation and the absorption of the nitrogen oxides. This ensures a high yield in nitrogen and decreases the consumption of platinum.

The process flowsheet is given in paragraph 1.2. The liquid ammonia is vaporized (E101), then after overheating (E102), is sent in an air – ammonia mixer (AIR NH3 MIXER). The atmospheric air is compressed (AIR COMPRESSOR), then divided in two streams: the primary air (HP AIR 2) sent to the air – ammonia mixer (AIR NH3 MIXER) and the secondary air sent to the bleaching column (BLEACHING COLUMN). The air – ammonia mixture is sent to the burner (BURNER).

For the reactor modelling, three global reactions are taken onto account:

$$4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$$

$$4\,NH_3 + 3\,O_2 \rightarrow 2\,N_2 + 6\,H_2O$$

$$2\,NH_3 + 2\,O_2 \rightarrow N_2O + 3\,H_2O$$

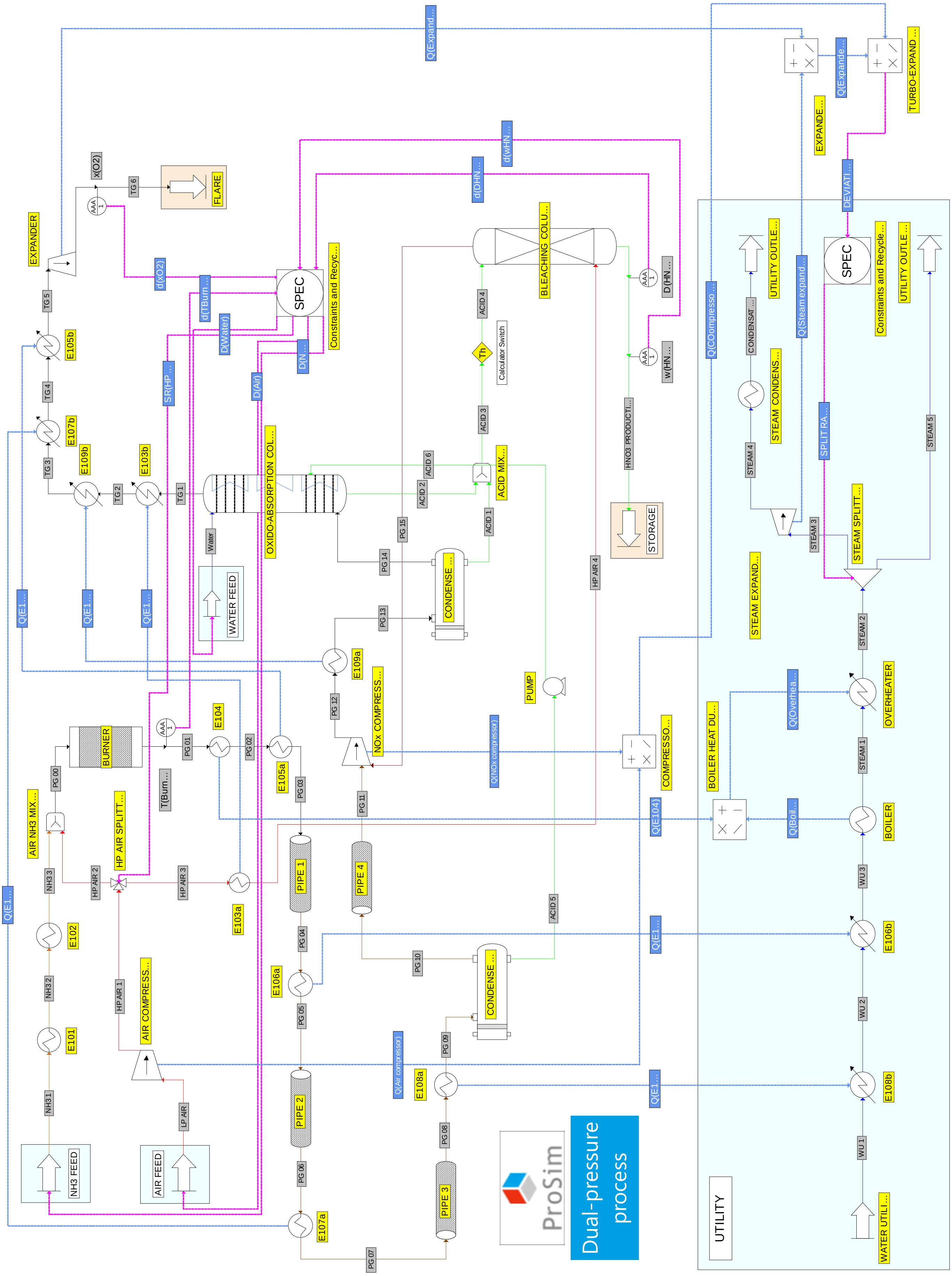
The gas after combustion is composed of nitrogen oxides, nitrogen and oxygen. Its sensible heat is recovered in a series of heat exchangers (E104, E105, E106, E107 and E108). After condensation (CONDENSER 1), a huge quantity of weak nitric acid is formed and sent to the absorption tower (OXIDO-ABSORPTION COLUMN). The second compressor (NOx COMPRESSOR) received the gas coming from the first condenser and from the bleaching column. After cooling in the heat exchanger (E109), these gases enter in the sieve trays oxido-absorption column (OXIDO-ABSORPTION COLUMN). Process water is introduced at the top of this column and nitric acid at the whished concentration is withdrawn at its bottom. Then, this acid goes to the bleaching column (BLEACHING COLUMN). A stripping by the secondary air (HP AIR 4) is done in this equipment. The gas leaving the absorber C101 is sent to a serie of gas-gas heat exchangers (E103, E105, E107 and E109) and then in an expander (EXPANDER). The gas leaves the process via a stack. The possible reactor for NOx reduction is not modeled in this example. This aspect is detailed in the example “PSPH_E01_EN - Mono-pressure process”.

In parallel, steam is produced by energy integration. For that, the water is preheated (E106 and E108), then the steam is produced in the boiler (BOILER) and overheated (OVERHEATER). A part of this steam is expanded (STEAM EXPANDER) to bring the mechanical energy needed by the process. This steam is then condensed (STEAM CONDENSER). From a practical point of view, the two compressors (AIR COMPRESSOR and NOx COMPRESSOR) are on the same shaft than the two expanders (EXPANDER and STEAM EXPANDER). Information streams and information stream handler modules are used to model this coupling.

The objective of this process is to produce 1 000 t/d of nitric acid (eq. 100%) at a concentration of 58% mass. At the steam production level, this plant produces 15 bars steam by energy integration.

The oxygen amount in the tail gas is fixed at 2.5% volume (mol.). The temperature at the outlet of the burner is fixed to 890°C. The water flow rate for absorption, the ammonia feed flow rate, the air feed flow rate and the ratio between the primary and the secondary air are automatically adjusted to ensure this production. The amount of steam expanded is adjusted to balance the power available at the turbines and those necessary for the compressors.

1.2. Process flowsheet



1.3. Components

Components taken into account in the simulation, their chemical formula and CAS numbers are presented in the following table. Pure components physical properties are extracted from the ProSimPlus HNO3 specific database ("HNO3").

Component name	Chemical formula	CAS number
Water	H_2O	7732-18-5
Nitric oxide	NO	10102-43-9
Nitrogen dioxide	NO_2	10102-44-0
Nitrogen tetroxide	N_2O_4	10544-72-6
Nitrogen	N_2	7727-37-9
Oxygen	O_2	7782-44-7
Nitric acid	HNO_3	7697-37-2
Ammonia	NH_3	7664-41-7
Nitrous oxide	N_2O	10024-97-2

1.4. Thermodynamic models

For the main part of the process, the "HNO3 specific" thermodynamic model is selected. This model takes into account the non-ideality of the liquid phase through correlations based on experimental data of partial pressures of water and nitric acid over aqueous solutions of nitric acid. The perfect gas model is used for the gas phase. A correlation based on experimental data is used to take into account the excess enthalpies of the water – nitric acid binary.

For the bleaching column the "Engels (strong acids)" thermodynamic model is used. This model well represents the NOx solubility and the complexity of the H_2O – HNO_3 equilibria. The "H*=DH0f, ideal gas, 25°C, 1 atm" enthalpy basis is selected instead of the default one of this model, to ensure the coherence with the "HNO3 specific" model.

For the cooling water circuit, the "Specific thermodynamic model for water" is used [HAA84].

1.5. Chemical reactions

NO oxidation, NO_2 dimerization and nitric acid oxido-absorption reactions are pre-coded. Thus, they don't have to be described by the user for modules specific to ProSimPlus HNO3. The reactions to be described are the ones for the combustion of the ammonia:

$$4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$$

$$4\,NH_3 + 3\,O_2 \rightarrow 2\,N_2 + 6\,H_2O$$

$$2\,NH_3 + 2\,O_2 \rightarrow N_2O + 3\,H_2O$$

These different reactions are defined as:

- ✓ Reaction type: Controlled
- ✓ Kinetic model: Instantaneous

The instantaneous kinetic model is chosen because conversion ratios are specified for each reaction in the reactors "BURNER" (§ 1.6.1).

The NO_2 dimerization equilibrium in gas phase is taken into account in the bleaching column. Indeed this column is modelled by a non-specific module of ProSimPlus HNO3 (§ 1.6.1).

$$2\,NO_2 \;\leftrightarrow\; N_2O_4$$

The equilibrium constant used is the one proposed by [KOU68]:

$$Ln(K_3) = -21.24366 + \frac{6891.64}{T}$$

⚠	The partial orders are 2 for the NO_2 and 1 for the N_2O_4.

The heats of reaction of these different reactions are computed from the standard enthalpies of formation at 25°C.

Two reaction sets have to be created:

- ✓ One with only the ammonia combustion reactions,
- ✓ One with only the NO_2 dimerization reaction.

1.6. Operating conditions

1.6.1. Nitric acid production process

- ✓ Process feeds

Feed	NH3 FEED	AIR FEED	WATER FEED
Molar fraction			
Nitrogen	0	0.776	0
Oxygen	0	0.206	0
Ammonia	1	0	0
Water	0	0.018	1
Total flow rate (t/d)	280	5000	365
Temperature (°C)	10	25	20
Pressure (bar)	14	1	10

- ✓ “BURNER” ammonia combustion burner

Operating parameters	**Value**
Reactor type	Simple
Reaction set	Ammonia combustion
Ammonia conversion ratio (%)	
$4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O$	96.2
$4\ NH_3 + 3\ O_2 \rightarrow 2\ N_2 + 6\ H_2O$	3.7
$2\ NH_3 + 2\ O_2 \rightarrow N_2O + 3\ H_2O$	0.1
Thermal behavior	Adiabatic
Pressure drop (bar)	0.05

- ✓ Oxidation reactors

These modules model the oxidation of the NO and the dimerization of the NO_2 in the gas volumes of pipes.

	PIPE 1	PIPE 2	PIPE 3	PIPE 4
Reactor type	Simplified plug flow			
Oxidation volume (m^3)	20	25	20	20
Calculation of the exchanged heat duty	Adiabatic			T = 85°C
Oxidation efficiency	1			
Reactions				
Calculation of the oxidation reaction rate constant	Koukolik			
Calculation of the dimerization equilibrium constant	Koukolik			
Pressure drop (bar)	0.0125			

- ✓ Cooler/Heater modules

Name	Outlet temperature (°C)	Pressure drop (bar)	Oxidation volume (m^3)
E101	Dew temperature	8	0
E102	80	0.05	0
E103a	70	0.05	0
E104	440	0.05	0
E105a	290	0.05	1.8
E106a	220	0.05	1.8
E107a	180	0.05	1.8
E108a	110	0.05	1.8
E109a	125	0.05	1.8

The following parameters are used for the heat exchangers in which the chemical reactions are taken into account (the ones with an oxidation volume different from 0):

- Hydrodynamic model: Plug flow
- Oxidation efficiency: 1
- Calculation of the oxidation rate constant: Koukolik
- Calculation of the dimerization equilibrium constant: Koukolik
- Take into account of a maximum temperature for the oxidation: Yes

- ✓ Simple heat exchangers

Name	Heat duty (kW)	Pressure drop (bar)	Oxidation volume (m^3)
E103b	0	0.05	0
E105b	0	0.05	0
E107b	0	0.05	0
E109b	0	0.05	0

The heat duties are sent by information streams from the corresponding cooler/heater modules (E103a, E105a, E107a and E109a).

- ✓ Nitrous vapors condensers

	CONDENSER 1	CONDENSER 2
Tubes length (m)	6	
Number of tubes	840	250
Circulation of the vapors	Inside the tubes	
Inner diameter of the tubes (mm)	25.4	
Equivalent diameter (mm)	0	
Cooling water		
Temperature (°C)	20	15
Flow rate (kg/h)	375 000	271 000
Flow direction	Counter-current	
Heat transfer coefficients (kcal/h/m^2/K)		
Oxido-absorption	300	600
Oxidation	0	
Pressure drop (bar)	0.05	
Reactions		
Calculation of the oxidation rate constant	Koukolik	
Calculation of the dimerization equilibrium constant	Koukolik	
Calculation of the absorption constant of N_2O_4 in water	Miller (bubble caps)	
Number of intermediate points for print	10	

- ✓ Compressors

	AIR COMPRESSOR	NOx COMPRESSOR
Discharge pressure (bar)	4.6	10
Efficiency		
Isentropic	0.845	0.795
Mechanical	1	
Reactions		
Taken into account	No	Yes
Dimerization equilibrium constant	-	Koukolik
Equilibrium of N_2O_3 formation	-	Miller

- ✓ “EXPANDER” tail gas expander

Operating parameters	Value
Type	Expander
Discharge pressure (bar)	1
Isentropic efficiency (-)	0.83
Mechanical efficiency (-)	1
Electrical efficiency (-)	1

- ✓ “PUMP” centrifugal pump

Operating parameters	Value
Type	centrifugal pump
Discharge pressure (bar)	11
Volumetric efficiency (-)	0.65
Mechanical efficiency (-)	1
Electrical efficiency (-)	1

- ✓ “HP AIR SPLITTER” splitter

Operating parameters	Value
Type	Three way valve
Splitting ratio of the stream HP AIR 2 (primary air)	0.80
Automatically calculated stream	HP AIR 3 (secondary air)
Outlet pressure	Equal to the feed pressure

- ✓ Mixers

The default parameters are used for the two mixers “AIR NH3 MIXER” and “ACID MIXER3.

✓ “OXIDO-ABSORPTION COLUMN”

Operating parameters	**Value**
Type	Plate oxido-absorption column
Number of plates	30
Column diameter (m)	5
Holes diameter (mm)	5
Fraction free area (%)	4.82
Column temperature profile	Calculated from the temperatures
Outlet acid stream temperature (°C)	25
Weak acid intermediate feed “ACID 6”	Tray 25
NOx in the liquid phase	
NO oxidized (%)	0
NOx solubility in the liquid phase	Taken into account
Henry constant	Calculated from the internal model
Total pressure drop (bar)	0.8
Correlations	
Calculation of the oxidation rate constant	Koukolik
Calculation of the dimerization equilibrium constant	Koukolik
Equilibrium of the NOx – water – nitric acid system	Zhidkov
Print profiles	Complete

⚠	The column stages are numbered from top to bottom (plate 1: top plate; plate 30: bottom plate).

The following table presents the parameters of the plates.

Plate	Oxidation efficiency	Oxidation volume (m^3)	Hydrodynamic model	Absorption efficiency	Liquid height (m)	Temperature (°C)
1	1	23.2	Plug flow reactor	Atroschenko 3	0.1	22
2	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
3	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
4	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
5	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
6	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
7	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
8	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
9	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
10	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
11	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
12	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
13	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
14	1	23.2	Plug flow reactor	Atroschenko 3	0.1	-
15	1	23.2	Plug flow reactor	Atroschenko 3	0.1	31
16	1	11.6	Plug flow reactor	Atroschenko 3	0.1	33
17	1	11.6	Plug flow reactor	Atroschenko 3	0.1	35
18	1	11.6	Plug flow reactor	Atroschenko 3	0.1	37
19	1	11.6	Plug flow reactor	Atroschenko 3	0.1	38
20	1	11.6	Plug flow reactor	Atroschenko 3	0.1	38
21	1	11.6	Plug flow reactor	Atroschenko 3	0.1	39
22	1	11.6	Plug flow reactor	Atroschenko 3	0.1	40
23	1	11.6	Plug flow reactor	Atroschenko 3	0.1	40
24	1	11.6	Plug flow reactor	Atroschenko 3	0.1	40
25	1	11.6	Plug flow reactor	Atroschenko 3	0.1	40
26	1	11.6	Plug flow reactor	Atroschenko 3	0.1	41
27	1	11.6	Plug flow reactor	Atroschenko 3	0.1	42
28	1	11.6	Plug flow reactor	Atroschenko 3	0.1	43
29	1	11.6	Plug flow reactor	Atroschenko 3	0.1	44
30	1	11.6	Plug flow reactor	Atroschenko 3	0.1	45

- ✓ Calculator switch

This module is used to change the thermodynamic model from the “HNO3 specific” one used in the previous modules to the “Engels (strong acids)” used in the bleaching column. The calculation of the liquid enthalpies being not the same between these two models, the use of a “Calculator switch” module is necessary in order to not distort the enthalpy balance on the bleaching column. In the case of the switch from the “HNO3 specific” model to the “Engels (strong acids)” model, and inversely, the “Calculator switch” module is necessary only on liquid streams (except if they leave the process).

Operating parameters	**Value**
Thermodynamic model	Engels
Outlet physical state	Calculated

- ✓ “BLEACHING COLUMN”

Operating parameters	**Value**
Column type	Absorber
Thermodynamic model	Engels
Number of theoretical stages	5
Overhead pressure (bar)	4.2
Pressure drop (bar)	0.2
Stage efficiency	1 for each stage
Reactive column	NO_2/N_2O_4 equilibrium in gas phase
Print profiles	Complete

1.6.2. Specifications of the nitric acid production process

✓ Specifications

Specifications	Value
Outlet temperature of the ammonia combustion burner (°C)	890
Oxygen amount in the tail gas (% molar)	2.5
Concentration of the produced nitric acid (% mass)	58
Mass flow rate (eq. 100%) of the produced nitric acid (t/j)	1 000

✓ Acting variables

Acting variables
Ammonia feed flow rate
Air feed flow rate
Water feed flow rate of the oxido-absorption column
Splitting ratio between the primary air and the secondary air

✓ “Constraints and Recycles”

Operating parameters	Value
Numerical method	Broyden with Jacobian matrix by finite differences
Step size of the recycle streams variables proportional to	The variable
Step size of the adjusted variables proportional to	The variable
Tear streams	“PG 15” (top stream of the bleaching column)
Other parameters	Default values

ProSimPlus HNO3 determines automatically the calculation sequence and the tear streams. The tear stream selected by default (“PG 12” outlet stream of the NOx compressor) needs an initialization to reach the convergence of the simulation. To avoid this, another stream, “PG 15”, is selected directly in the module “Constraints and Recycles”. Thus, this choice avoids the need to specify an initialization of the tear stream.

1.6.3. Utility production

- ✓ Process feed

Feed	WATER UTILITY
Molar fraction	
Water	1
Total flow rate (t/d)	1 130
Temperature (°C)	20
Pressure (bar)	15

- ✓ “STEAM EXPANDER”

Operating parameters	Value
Type	Expander
Discharge pressure (bar)	1.05
Isentropic efficiency (-)	0.85
Mechanical efficiency (-)	1
Electrical efficiency (-)	1

- ✓ “STEAM SPLITTER” splitter

Operating parameters	Value
Type	Stream splitter
Splitting ratio of the stream STEAM 3 (steam expanded)	0.90
Automatically calculated stream	“STEAM 5” (steam not expanded)
Outlet pressure	Equal to the feed pressure

- ✓ Cooler/Heater modules

Name	Outlet temperature (°C)	Pressure drop (bar)	Oxidation volume (m^3)
BOILER	Dew temperature	0.05	0
STEAM CONDENSER	Bubble temperature	0.05	0

- ✓ Simple heat exchangers

Name	Heat duty (kW)	Pressure drop(bar)	Oxidation volume (m^3)
E106b	0	0.5	0
E108b	0	0.05	0
OVERHEATER	0	0.05	0

The heat duties of the simple heat exchangers E106b and E108b are transmitted by information streams from the corresponding cooler/heater modules (E106a and E108a).

The heat duty of the simple heat exchanger "OVERHEATER" is the sum of the heat duties calculated by the cooler/heater modules "E104" and "BOILER". The information is transmitted by information stream and the sum is computed by an "Information stream handler" module (§ 1.7). The parameters of these different items are the following:

- Information stream from the cooler/heater "E104" to the information stream handler "BOILER HEAT DUTY"

Parameters	Value
Information type to be emitted	Heat necessary to reach the specified temperature
Information type to be received	Input information stream value (In)

- Information stream from the cooler/heater "BOILER" to the information stream handler "BOILER HEAT DUTY"

Parameters	Value
Information type to be emitted	Heat necessary to reach the specified temperature
Information type to be received	Value of the additive factor (B)

- Information stream from the information stream handler "BOILER HEAT DUTY" to the simple heat exchanger "OVERHEATER"

Parameters	Value
Information type to be emitted	Output information stream value (Out)
Information type to be received	Heat duty

- Information stream handler "BOILER HEAT DUTY"

Parameters	Value
A	1
B	0
C	0
Power	1 (Integer value)

1.6.4. Coupling of the compressors and the expanders

In this process, the compressors "AIR COMPRESSOR" and "NOx COMPRESSOR" and the expanders "EXPANDER" and "STEAM EXPANDER" compose a turbo-expander. The objective is to adjust the steam flow rate expanded by action on the splitting ratio of the "STEAM SPLITTER" in order to balance the power consumption of the compressors ("AIR COMPRESSOR" and "NOx COMPRESSOR") and the power available at the expanders ("EXPANDER" and "STEAM EXPANDER"). For that, several information stream handlers (§ 1.7) as well as a constraints and recycles module are used. Several information streams link these different items.

- ✓ Sum of the power of the compressors "AIR COMPRESSOR" and "NOx COMPRESSOR"
  - o Information stream from the compressor "NOx COMPRESSOR" to the information stream handler "COMPRESSORS"

Parameters	Value
Information type to be emitted	Mechanical power
Information type to be received	Input information stream value (In)

  - o Information stream from the compressor "AIR COMPRESSOR" to the information stream handler "COMPRESSORS"

Parameters	Value
Information type to be emitted	Mechanical power
Information type to be received	Value of the additive factor (B)

  - o Information stream handler "COMPRESSORS"

Parameters	Value
A	1
B	0
C	0
Power	1 (Integer value)

- ✓ Sum of the power of the expanders "EXPANDER" and "STEAM EXPANDER"
  - o Information stream from the expander "EXPANDER" to the information stream handler "EXPANDERS"

Parameters	Value
Information type to be emitted	Mechanical power
Information type to be received	Input information stream value (In)

  - o Information stream from the expander "STEAM EXPANDER" to the information stream handler "EXPANDERS"

Parameters	Value
Information type to be emitted	Mechanical power
Information type to be received	Value of the additive factor (B)

- Information stream handler “EXPANDERS”

Parameters	Value
A	1
B	0
C	0
Power	1 (Integer value)

- ✓ Calculation of the deviation between the power needed for the compressors and the power available at the turbines and action on the splitting ratio of the “STEAM SPLITTER” splitter
    - Information stream from the information stream handler “COMPRESSORS” to the information stream handler “TURBO-EXPANDER”

Parameters	Value
Information type to be emitted	Output information stream value (Out)
Information type to be received	Input information stream value (In)

- Information stream from the information stream handler “EXPANDERS” to the information stream handler “TURBO-EXPANDER”

Parameters	Value
Information type to be emitted	Mechanical power
Information type to be received	Value of the additive factor (B)

> The two values are summed although we wish to compute the deviation between the power needed for the compressors and the power available at the turbines. In fact, the power needed for a compressor are negative values, whereas the power available for a turbine are positive values.

- Information stream handler “TURBO-EXPANDER”

Parameters	Value
A	1
B	0
C	0
Power	1 (Integer value)

- Information stream from the information stream handler “TURBO-EXPANDER” to the “Constraints and Recycles 1” constraints and recycles module

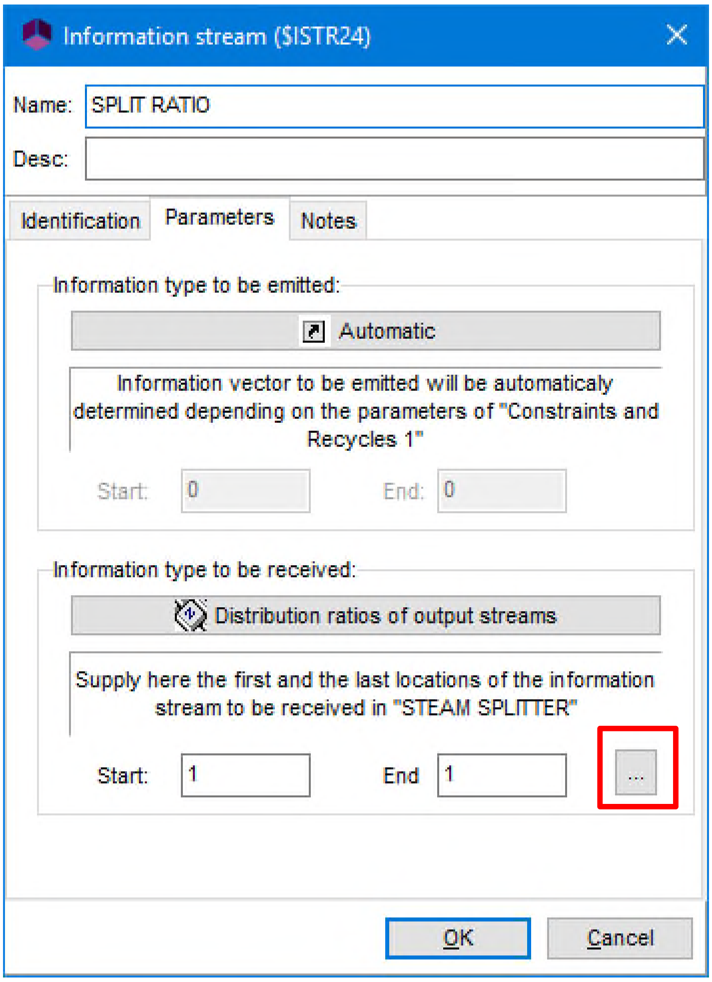
Parameters	Value
Information type to be emitted	Output information stream value (Out)
Information type to be received	Automatic

- The default values are kept for the module “Constraints and Recycles 1”

- Information stream from the module “Constraints and Recycles 1” to the splitter “STEAM SPLITTER”

Parameters	Value
Information type to be emitted	Automatic
Information type to be received	Distribution ratios of output streams

Regarding the information type to be received, well select the stream for which the splitting ratio is specified and not the stream automatically calculated. The choice is done from the bottom red framed of the following figure.



Name: SPLIT RATIO

Desc:

Information type to be emitted: Automatic

Information vector to be emitted will be automaticaly determined depending on the parameters of "Constraints and Recycles 1"

Start: 0 End: 0

Information type to be received: Distribution ratios of output streams

Supply here the first and the last locations of the information stream to be received in "STEAM SPLITTER"

Start: 1 End: 1

1.7. “Tips and tricks”

To minimize the risk of errors and to correct more easily those eventually committed, it’s advisable to proceed in four steps to build this example:

1. Simulation of the nitric acid production part without the specifications, the utility production and the coupling between the compressors and the turbines.
2. Add of the specifications to the previous simulation.
3. Add of the utility production part to the previous simulation.
4. Add of the coupling between the compressors and the turbines to the previous simulation.

In this simulation example, most of the heat exchangers are simulated by decoupling the hot stream and the cold stream. This way of modeling a two-stream heat exchanger avoids a recycle stream that would penalize the calculations by decoupling the heat exchanger into two parts.

Several “Information stream handler” modules are used. In ProSimPlus HNO3 this module performs simple operation on information streams: add a constant (B), subtract a constant (C), multiply its contents (A and P = 1), divide its contents (A and P = -1) or raised its contents to an entire or real power (P). The result of this operation is available in the outlet information stream of the “Information stream handler” module:

$$Inlet = A * (Outlet)^P + B - C$$

In this formula, A, B, C, and P are constants specified by the user. By putting several information streams in an "Information stream handler" module and playing on their position in the module parameter zone, it’s possible to use their information to specify the values of the constants A, B, C and P. Thus, operations between several information streams can be performed. Using several modules of this type, it’s possible to perform more complex operations. For more complex operation on information streams it’s advised to use a “Windows Script” module.

It’s possible in ProSimPlus HNO3 to use several constraints and recycles modules in one simulation. In this example for a better readability of the simulation, two constraints and recycles modules are used:

- ✓ One for the process itself: “Constraints and Recycles”
- ✓ The other for the steam production “Constraints and Recycles 1”

Using several constraints and recycles modules has an effect on the calculation sequence of the module (the list of the calculations automatically determined by ProSimPlus HNO3) and on the convergence of each cycle. But this has no effect on the results obtained at convergence.

This possibility could be used in some case for ease of the convergence of complex flowsheet, or, like here, to not unnecessarily complicate the representation of the process.

2. RESULTS

2.1. Mass and energy balances

This document presents only the most relevant stream results. In ProSimPlus HNO3, mass and energy balances are provided for all streams. Results are also available at the unit operation level ("Report" tab in the configuration window).

Streams		ACID 1	ACID 2	ACID 5	CONDENSA...	HNO3 PROD...	HP AIR 4	LP AIR
From		CONDENSE...	OXIDO-ABS...	CONDENSE...	STEAM CO...	w (HNO3)	E103a	AIR FEED
Total flow	t/d	161.3	1596.2	258.96	965.58	1724.1	814.68	4999.7
Total flow	Nm3/h	6457.1	46030	11629	50055	52352	26552	1.6295E005
Mass fractions								
WATER		0.68103	0.38143	0.81268	1	0.41976	0.011317	0.011317
NITRIC OXIDE		0	0	0	0	0	0	0
NITROGEN DIOXIDE		0	0.00014369	0	0	0	0	0
NITROGEN TETROXIDE		0	0.022554	0	0	0	0	0
NITROGEN		0	0	0	0	9.197E-005	0.75864	0.75864
OXYGEN		0	0	0	0	0.00014285	0.23004	0.23004
NITRIC ACID		0.31897	0.59587	0.18732	0	0.58	0	0
AMMONIA		0	0	0	0	0	0	0
NITROUS OXIDE		0	0	0	0	0	0	0
Mole fractions								
WATER		0.88191	0.6857	0.93818	1	0.71666	0.018	0.018
NITRIC OXIDE		0	0	0	0	0	0	0
NITROGEN DIOXIDE		0	0.00010115	0	0	0	0	0
NITROGEN TETROXIDE		0	0.0079388	0	0	0	0	0
NITROGEN		0	0	0	0	0.00010098	0.776	0.776
OXYGEN		0	0	0	0	0.00013731	0.206	0.206
NITRIC ACID		0.11809	0.30626	0.061824	0	0.28311	0	0
AMMONIA		0	0	0	0	0	0	0
NITROUS OXIDE		0	0	0	0	0	0	0
Physical state		Liquid	Liquid	Liquid	Liquid	Liquid	Vapor	Vapor
Temperature	°C	92.009	45	81.628	99.632	51.109	70	25
Pressure	bar	9.9	9.9	4.2125	1	4.4	4.55	1
Enthalpic flow	kW	-21663	-1.4501E005	-39835	-23803	-1.6633E005	-998.56	-8790
Vapor molar fraction		0	0	0	0	0	1	1

Streams		NH3 1	PG 01	PG 09	PG 10	PG 13	PG 14	STEAM 2
From		NH3 FEED	T(Burner)	E108a	CONDENSE...	E109a	CONDENSE...	OVERHEAT...
Total flow	t/d	283.6	4468.6	4468.6	4209.6	5057.7	4896.4	1130
Total flow	Nm3/h	15552	1.5583E005	1.5177E005	1.3942E005	1.6503E005	1.5755E005	58579
Mass fractions								
WATER		0	0.1113	0.1113	0.066506	0.056185	0.034099	1
NITRIC OXIDE		0	0.10757	0.050098	0.052814	0.02445	0.024414	0
NITROGEN DIOXIDE		0	0	0.086644	0.08031	0.10571	0.095129	0
NITROGEN TETROXIDE		0	0	0.0014708	0.0053727	0.0026833	0.010449	0
NITROGEN		0	0.71243	0.71243	0.75625	0.75161	0.77637	0
OXYGEN		0	0.068624	0.03798	0.038659	0.05878	0.058934	0
NITRIC ACID		0	0	0	0	0.00051388	0.00053081	0
AMMONIA		1	0	0	0	0	0	0
NITROUS OXIDE		0	8.2007E-005	8.2007E-005	8.7052E-005	7.2455E-005	7.4842E-005	0
Mole fractions								
WATER		0	0.16545	0.16988	0.1041	0.089267	0.054937	1
NITRIC OXIDE		0	0.096005	0.045909	0.049634	0.023323	0.023616	0
NITROGEN DIOXIDE		0	0	0.051787	0.049226	0.065765	0.060016	0
NITROGEN TETROXIDE		0	0	0.00043955	0.0016466	0.00083472	0.003296	0
NITROGEN		0	0.68106	0.6993	0.76127	0.76795	0.80439	0
OXYGEN		0	0.057432	0.032637	0.034068	0.052578	0.053456	0
NITRIC ACID		0	0	0	0	0.00023342	0.0002445	0
AMMONIA		1	0	0	0	0	0	0
NITROUS OXIDE		0	4.9899E-005	5.1234E-005	5.5775E-005	4.7119E-005	4.9355E-005	0
Physical state		Liquid	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	°C	10	890	110	81.628	125	92.009	391.36
Pressure	bar	14	4.55	4.2625	4.2125	9.95	9.9	14.8
Enthalpic flow	kW	-12902	-6352.1	-61350	-29945	-29222	-13940	9022.6
Vapor molar fraction		0	1	1	1	1	1	1

Streams		STEAM 5	TG 6	Water	WU 1
From		STEAM SPLI...	x(O2)	WATER FEED	WATER UTI...
Total flow	t/d	164.42	3926.4	367.26	1130
Total flow	Nm3/h	8523.5	1.3051E005	19039	58579
Mass fractions					
WATER		1	0.0018222	1	1
NITRIC OXIDE		0	0.00059144	0	0
NITROGEN DIOXIDE		0	0.00084391	0	0
NITROGEN TETROXIDE		0	2.7866E-009	0	0
NITROGEN		0	0.96818	0	0
OXYGEN		0	0.028473	0	0
NITRIC ACID		0	1.3384E-007	0	0
AMMONIA		0	0	0	0
NITROUS OXIDE		0	9.3332E-005	0	0
Mole fractions					
WATER		1	0.0028418	1	1
NITRIC OXIDE		0	0.00055379	0	0
NITROGEN DIOXIDE		0	0.00051539	0	0
NITROGEN TETROXIDE		0	8.5091E-010	0	0
NITROGEN		0	0.97103	0	0
OXYGEN		0	0.025	0	0
NITRIC ACID		0	5.9677E-008	0	0
AMMONIA		0	0	0	0
NITROUS OXIDE		0	5.9579E-005	0	0
Physical state		Vapor	Vapor	Liquid	Liquid
Temperature	°C	391.36	171.47	20	20
Pressure	bar	14.8	1.0132	10	15
Enthalpic flow	kW	1312.8	5934.9	-67495	-32202
Vapor molar fraction		1	1	0	0

2.2. Process performance

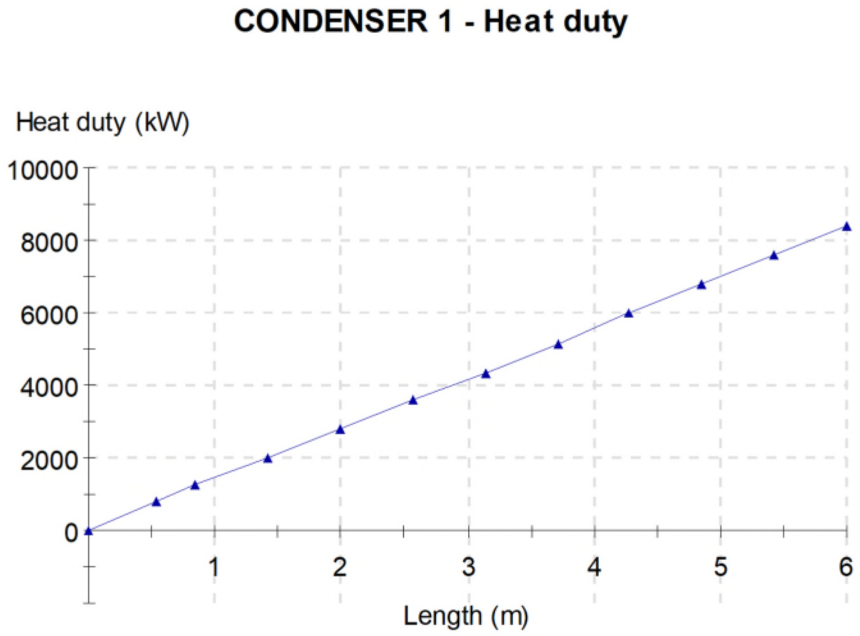
The production of 1 000 t/d of nitric acid eq. 100% at a concentration of 58% mass with this process while having a temperature of 890°C at the outlet of the ammonia burner and 2.5% molar of oxygen in the tail gas needs:

- ✓ 284 t/d of ammonia
- ✓ 5 000 t/d of air with 84% for the primary air (NH_3 combustion) and the remainder (16%) for the secondary air (bleaching of the produced nitric acid)
- ✓ 367 t/d of process water for the oxido-absorption

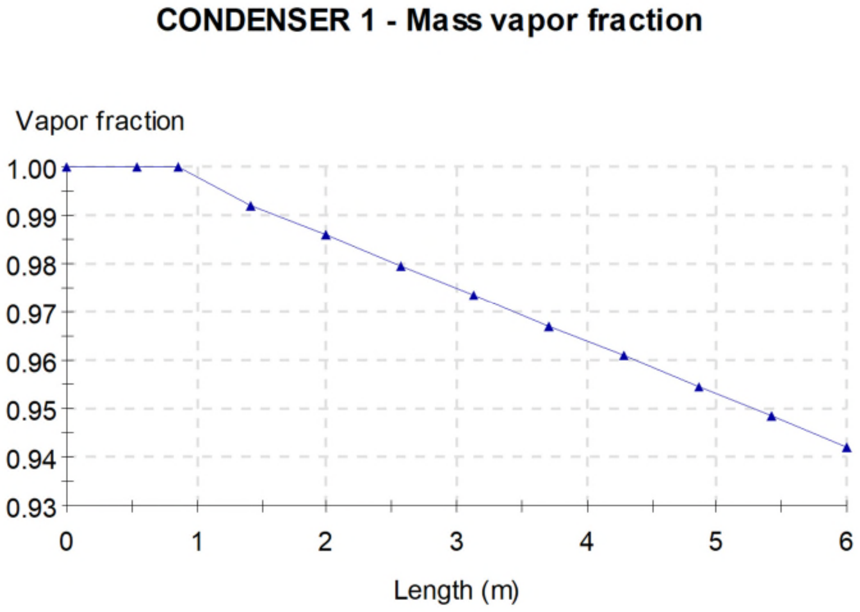
The NOx amount at the outlet of the oxido-absorption column is 1 070 ppmv eq. NO.

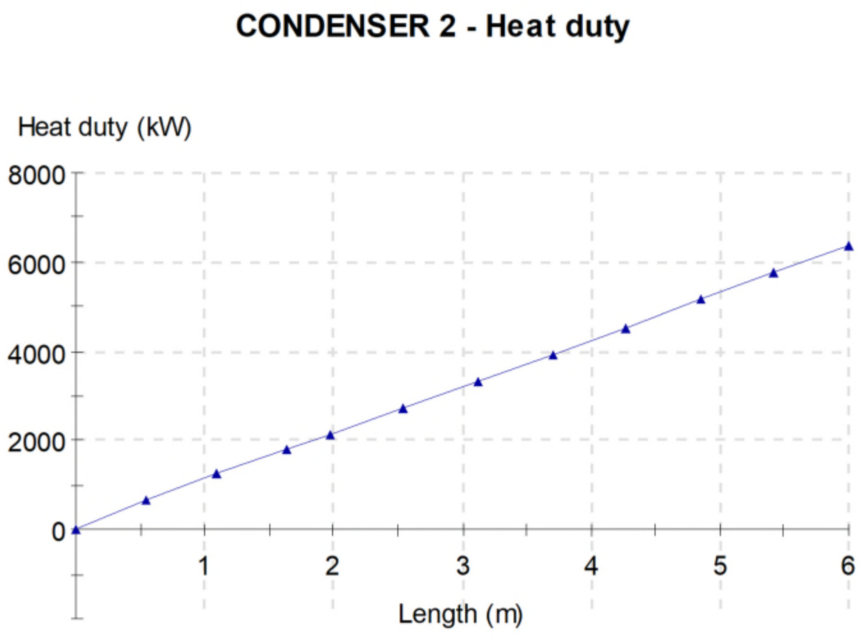
The balance between the consumption of compressors and the power available at the turbines needs to expand 86% of the 15 bar steam produced (966 t/d).

2.3. Nitrous vapors condensers profiles

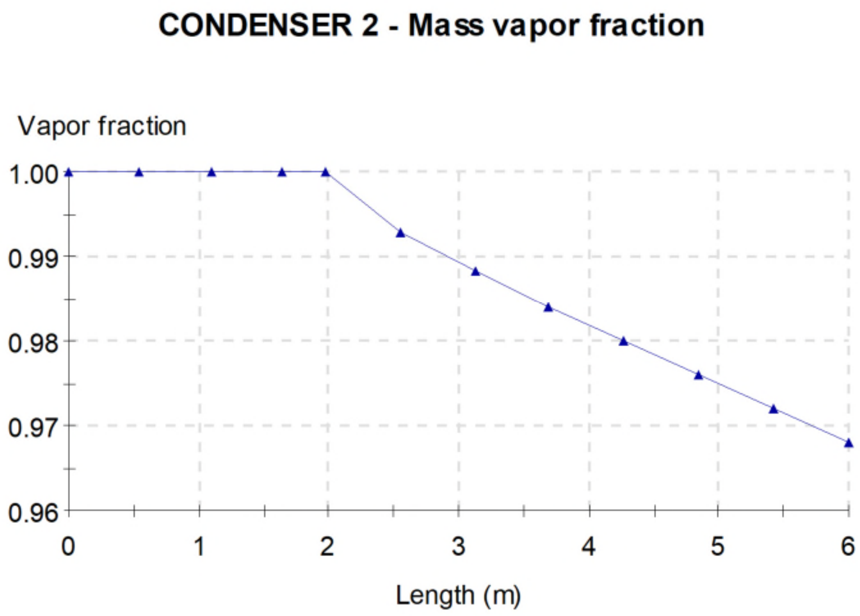


The following curve shows that 15% of the length of the "CONDENSER 1" are not used for the oxido-absorption.





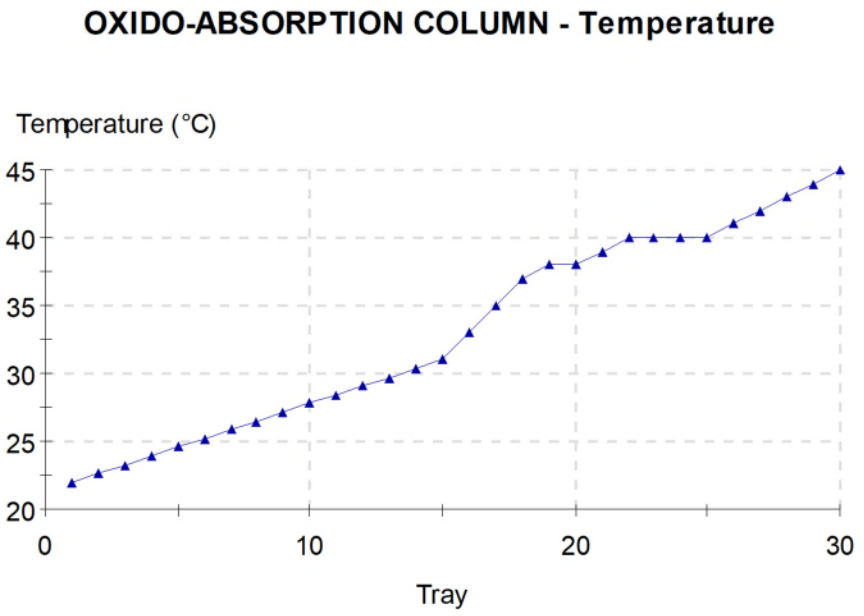
The following curve shows that 33% of the length of the "CONDENSER 2" are not used for the oxido-absorption.

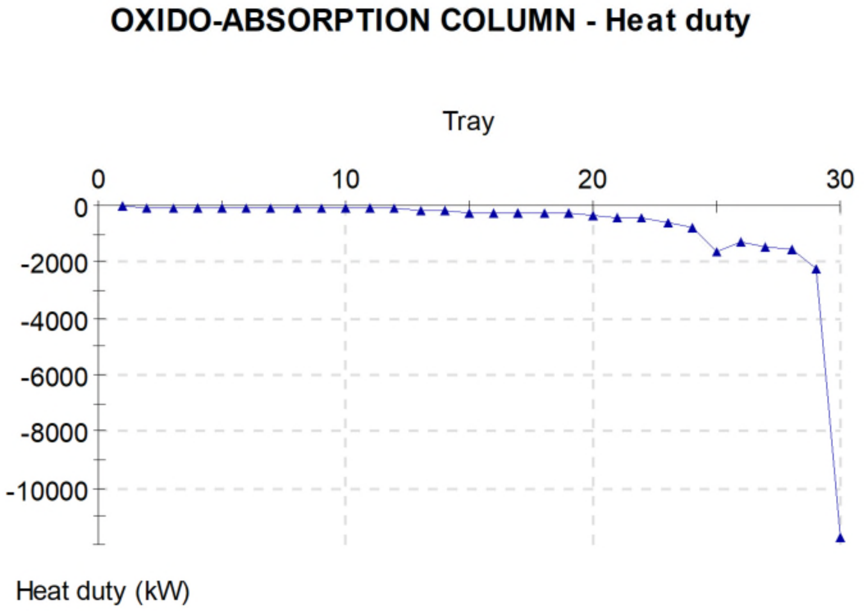


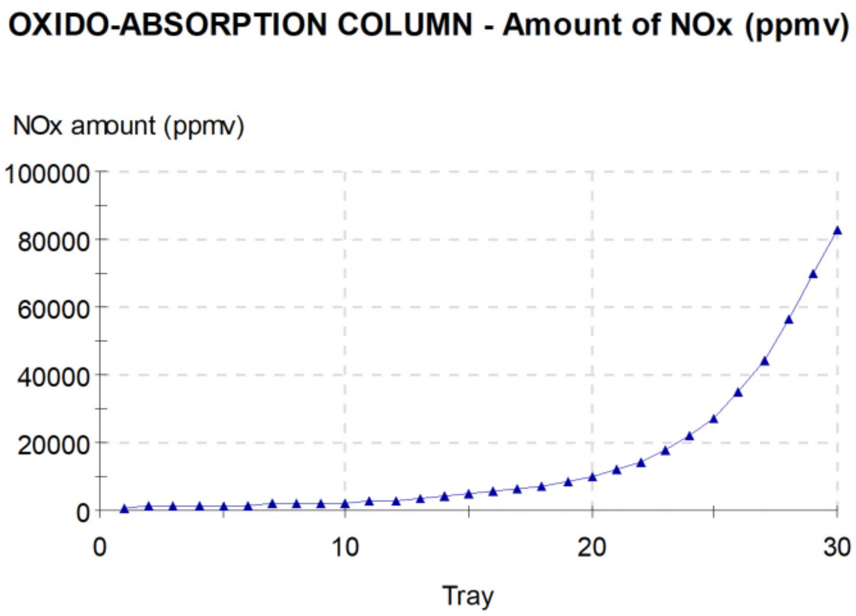
2.4. Columns profiles

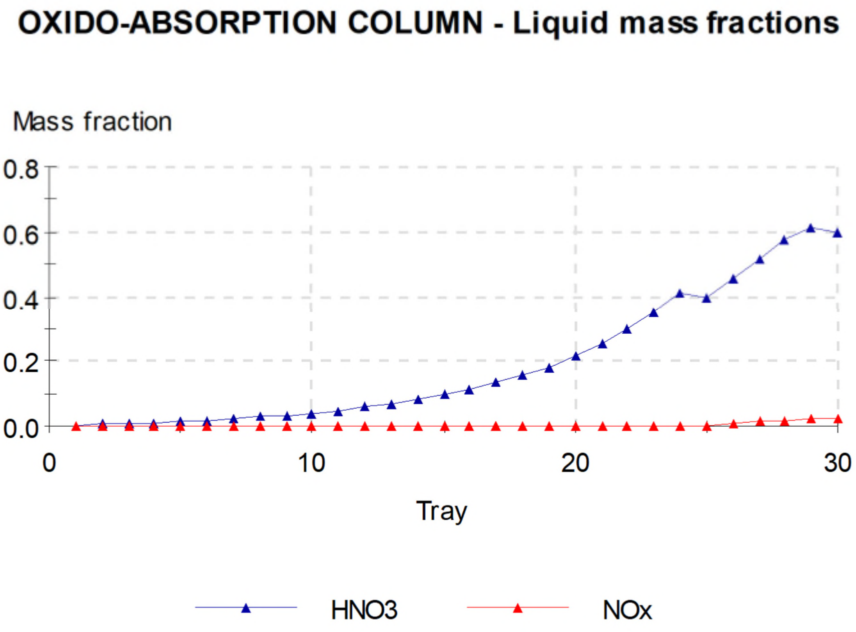
2.4.1. Oxido-absorption column

The column stages are numbered from top to bottom (plate 1: top plate; plate 30: bottom plate).



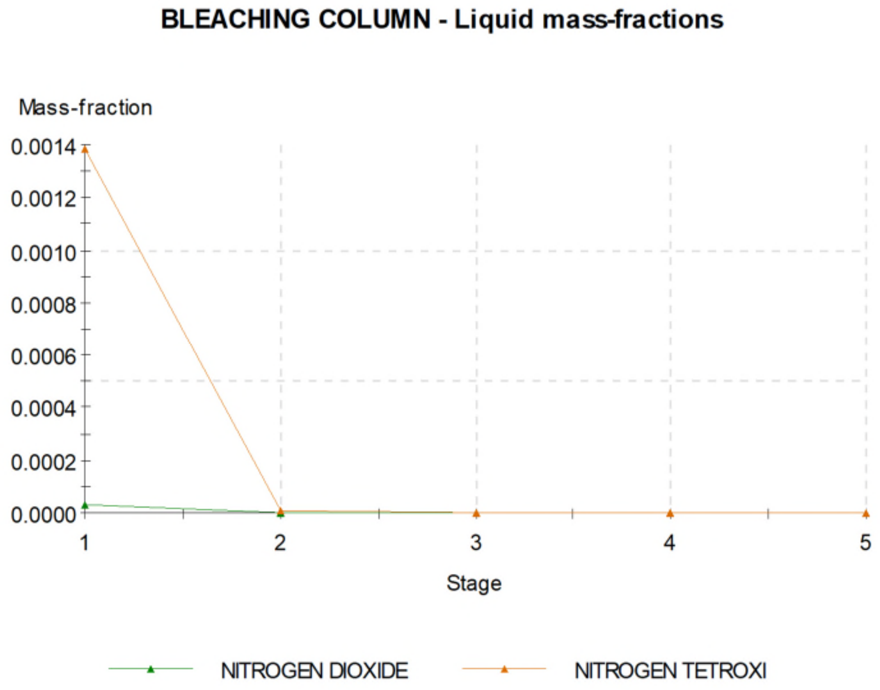



OXIDO-ABSORPTION COLUMN - Amount of NOx (ppmv)
NOx amount (ppmv)
100000
80000
60000
40000
20000
0
0
10
20
30
Tray


OXIDO-ABSORPTION COLUMN - Liquid mass fractions
Mass fraction
0.8
0.6
0.4
0.2
0.0
0
10
20
30
Tray
HNO3
NOx

2.4.2. Bleaching column

The column stages are numbered from top to bottom (plate 1: top plate; plate 5: bottom plate).



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