

PROSIMPLUS HNO₃ APPLICATION EXAMPLE

MONO-PRESSURE PROCESS

EXAMPLE PURPOSE

This document presents a mono-pressure nitric acid production process. It is a rather usual process of industrial production of nitric acid. The main equipment specific to ProSimPlus HNO₃ simulator are used in this simulation: absorption column of nitrous vapors, nitrous vapors condenser, oxidation reactors, heat exchangers with oxidation volumes, etc.

It's an example of pure simulation, without any specification on the outlet streams.

The particular points which are detailed in this example are the simulation of a DeNO_x reactor on the tail gas and the use of an external stream to take into account the cooling water of the nitrous vapors' condenser.

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| CORRESPONDING PROSIMPLUS FILES | <i>PSPH_EX_EN-Mono-pressure-process.pmp3</i> |
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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. Fives 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.

Energy

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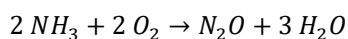
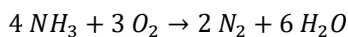
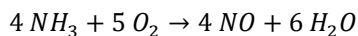
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1. PROCESS MODELING

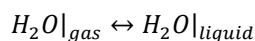
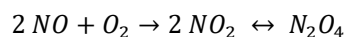
1.1. Process description

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

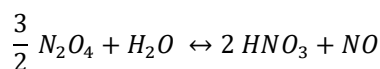
- ✓ Ammonia oxidation



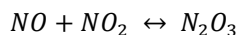
- ✓ Oxidation of the nitric oxide and condensation of the combustion water



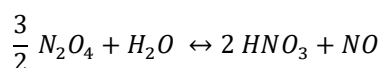
- ✓ Fixing of the nitrogen tetroxide



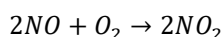
The mathematical representations of the equilibria and kinetics of the reactions described here above are complex. Side reactions occur, in particular the formation of nitrogen trioxide:



The mono-pressure process (catalytic oxidation and absorption at the same pressure) relies on the reaction:



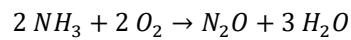
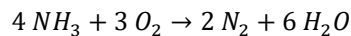
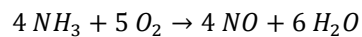
The main characteristic of this reaction is that each time two molecules of nitric acid are formed there is also production of one molecule of nitric oxide (NO). This molecule of NO has to be oxidized in NO₂, and then absorbed and so on. These successive oxidations are mainly done in gas phase in oxido-absorption tower where the reactions of nitric acid production and NO oxidation are performed in parallel:



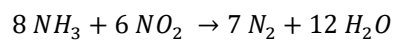
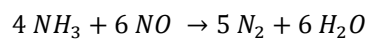
In this process, condensation and absorption are done at the same pressure as the oxidation, between approximately 5 and 10 bars. Thus, only one compressor is used. The absorption tower has a bleaching stage in its lower part.

The process flowsheet is given in paragraph 1.2. The liquid ammonia is vaporized by cooling water (E101), filtered before overheating (E102) and sent in an air – ammonia mixer (M101). The filtered atmospheric air is compressed (K101) and then splitted in two streams by the valve V103: the primary air (Air S06) goes to the air – ammonia mixer (M101) and the secondary air goes to the bleaching column (C102). Before, a part of the air is withdrawn for the instrumentation in the valve V102. The air – ammonia mixture is sent to the reactor (R101).

For the reactor modelling, three main reactions are taken into account:



The gas after combustion is composed of nitrogen oxides, nitrogen and oxygen. Its sensible heat is recovered in a series of heat exchangers (E103, E104, E105 and E106). After condensation (E107), a huge quantity of weak nitric acid is formed and sent to the absorption tower (C101). The gas mixed with the air leaving the bleaching tower C102 in the mixer M103 is sent to the sieve trays of the absorption tower (C101). This column has cooling coils on its trays. Process water is introduced at the top of this column and nitric acid at the desired concentration is withdrawn at its bottom. Then, this acid goes to the bleaching column (C102). A stripping by the secondary air (Air S08) is done in this equipment. The gas leaving the main absorber C101 is sent in a series of gas-gas heat exchangers (E108, E109 and E105). Then the gas is mixed with a low quantity of ammonia to react in a catalytic reactor to reduce the amount of NO_x in the tail gas. This reactor (R102) is operated around 270°C; the conversion in this reactor can be modelled by the two following reactions:

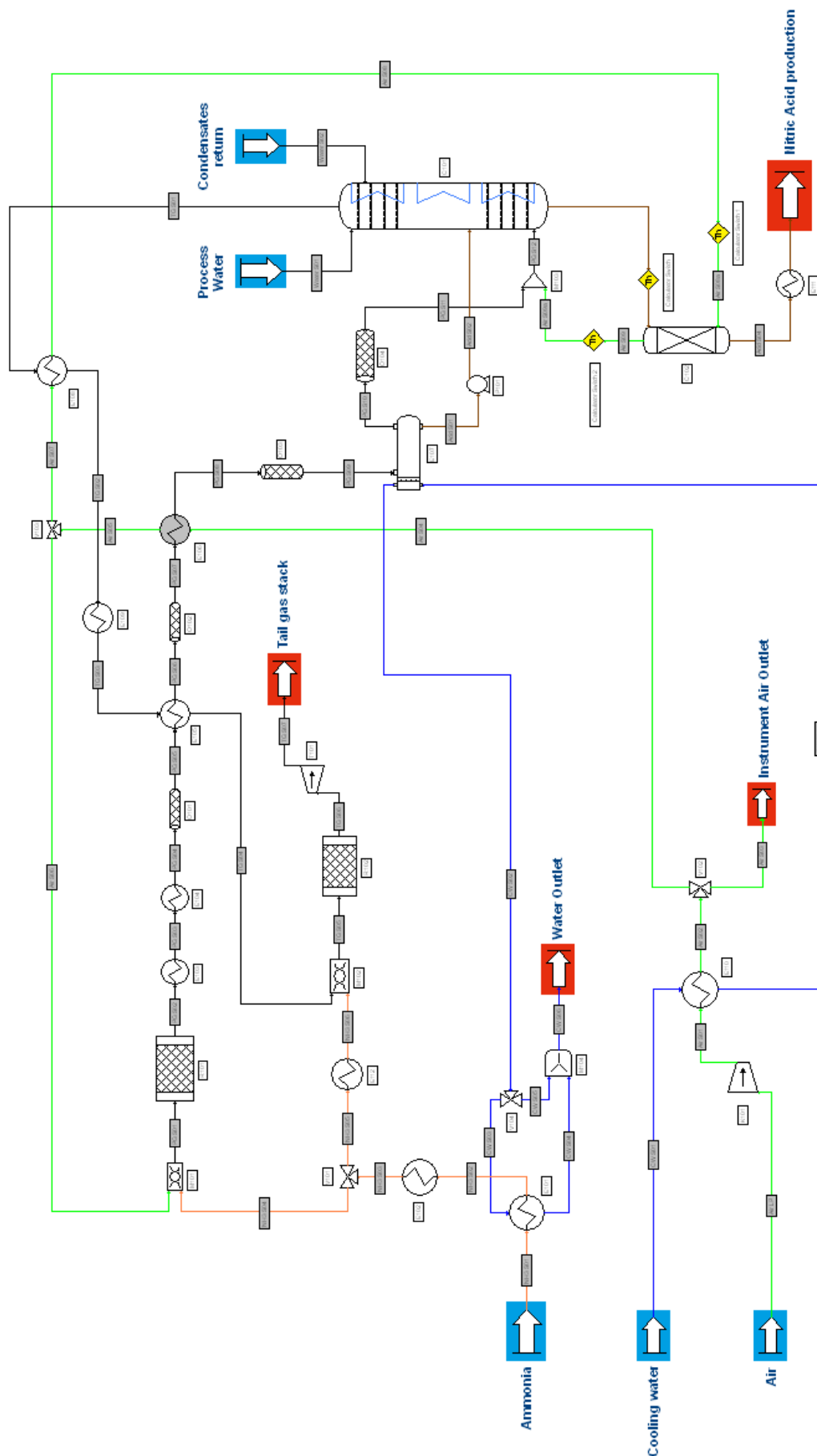


The NO_x-depleted tail gas is sent in an expander (T101) and then to the stack.

In parallel, steam is produced by heat integration (not modelled in this example). In addition, cooling water goes successively in the condenser E107 and in the heat exchanger E101.

The objective of this process is to produce 1 000 t/d of nitric acid (eq. 100%) at a concentration of 58% wt.

1.2. Process flowsheet



1.3. Components

The components involved in the simulation, their chemical formula and CAS Registry Numbers^{® 1} 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 [®] |
|--------------------|-------------------------------|-------------------------|
| Ammonia | NH ₃ | 7664-41-7 |
| Oxygen | O ₂ | 7782-44-7 |
| Nitrogen | N ₂ | 7727-37-9 |
| Nitric oxide | NO | 10102-43-9 |
| Nitrogen dioxide | NO ₂ | 10102-44-0 |
| Nitrogen tetroxide | N ₂ O ₄ | 10544-72-6 |
| Nitrous oxide | N ₂ O | 10024-97-2 |
| Nitric acid | HNO ₃ | 7697-37-2 |

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 NO_x solubility and the complexity of the H₂O – HNO₃ 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. This model is also used in the E111 product acid cooler.

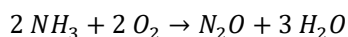
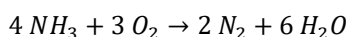
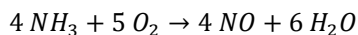
For the cooling water circuit, the “Specific thermodynamic model for water” is used [HAA84]. To be able to select this model, only water must be present in the calculator’s list of compounds. This model is used in the cooling water process feed, V104 three-way valve and the M104 mixer.

¹ CAS Registry Numbers[®] are the intellectual property of the American Chemical Society and are used by Fives ProSim SAS with the express permission of ACS. CAS Registry Numbers[®] have not been verified by ACS and may be inaccurate.

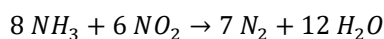
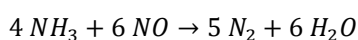
1.5. Chemical reactions

NO oxidation, NO₂ 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 only reactions to be described are following ones. These reactions have to be described for the calculator using "HNO₃ specific" thermodynamic model.

- ✓ Ammonia combustion



- ✓ NO_x reduction



These different reactions are defined as:

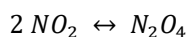
- ✓ Reaction type: Controlled
- ✓ Kinetic model: Instantaneous
- ✓ Heat of reaction: Computed from the standard enthalpies of formation at 25°C.

The instantaneous kinetic model is chosen because conversion ratios are specified for each reaction in the reactors R101 and R102 (§ 1.6.2).

Two reaction sets must be created:

- ✓ One with the ammonia combustion reactions only,
- ✓ One with the NO_x reduction reactions only.

The NO₂ dimerization equilibrium in the gas phase is taken into account in the bleaching column. Indeed, this column is modelled by a non-specific module of ProSimPlus HNO₃ (§ 1.6.8). This reaction must be described for the calculator using the "Engels (strong acids)" thermodynamic model.



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 NO₂ and 1 for the N₂O₄.

The heat of reaction is computed from the standard enthalpies of formation at 25°C.

1.6. **Operating conditions**

1.6.1. **Process feeds**

| | Ammonia | Process water | Condensates return | Cooling water |
|-------------------------------|---------|---------------|--------------------|---------------|
| Partial mass flow rate (kg/h) | | | | |
| Ammonia | 11 874 | 0 | 0 | 0 |
| Water | 24 | 3 555 | 12 520 | 2 000 000 |
| Temperature (°C) | 10 | 25 | 25 | 22 |
| Pressure (bar) | 14 | 6.5 | 6.6 | 4.2 |

| | Air |
|--------------------------------------|---------|
| Mole fraction (-) | |
| Oxygen | 0.29 |
| Nitrogen | 0.71 |
| Total flow rate (Nm ³ /h) | 165 178 |
| Relative humidity (%) | 46 |
| Temperature (°C) | 25 |
| Pressure (bar) | 1 |

1.6.2. **Reactors**

✓ R101 ammonia burner

| Operating parameters | Value |
|---|-------------------------|
| Reactor type | Simple |
| Reaction set | Ammonia combustion |
| Ammonia conversion ratio (%) | |
| $4 \text{ NH}_3 + 5 \text{ O}_2 \rightarrow 4 \text{ NO} + 6 \text{ H}_2\text{O}$ | 96.2 of NH ₃ |
| $4 \text{ NH}_3 + 3 \text{ O}_2 \rightarrow 2 \text{ N}_2 + 6 \text{ H}_2\text{O}$ | 3.7 of NH ₃ |
| $2 \text{ NH}_3 + 2 \text{ O}_2 \rightarrow \text{N}_2\text{O} + 3 \text{ H}_2\text{O}$ | 0.1 of NH ₃ |
| Thermal behavior | Adiabatic |
| Pressure drop (bar) | 0.05 |

✓ R102 NOx reduction catalytic reactor

| Operating parameters | Value |
|---|--------------------------|
| Reactor type | Simple |
| Reaction set | NOx reduction |
| Conversion ratio | |
| $4 NH_3 + 6 NO \rightarrow 5 N_2 + 6 H_2O$ | 90.0% of NO |
| $8 NH_3 + 6 NO_2 \rightarrow 7 N_2 + 12 H_2O$ | 28.5% of NO ₂ |
| Thermal behavior | Adiabatic |
| Pressure drop (bar) | 0.1 |

✓ Oxidation reactors

These modules model the oxidation of the NO and the dimerization of the NO₂ in the gas volumes of pipes.

| | O101 | O102 | O103 | O104 |
|--|----------------------|------|------|------|
| Operating parameters | Value | | | |
| Reactor type | Simplified plug flow | | | |
| Oxidation volume (m ³) | 9 | 28 | 6 | 2 |
| Calculation of the exchanged heat duty | Adiabatic | | | |
| Oxidation efficiency | 1 | | | |
| Reactions | | | | |
| Oxidation reaction rate constant | Koukolik | | | |
| Dimerization equilibrium constant | Koukolik | | | |
| Pressure drop (bar) | 0.01 | | | |

1.6.3. Heat exchangers

✓ Generalized heat exchangers.

| | E101 | E105 | E108 | E110 |
|-------------------------|-------|------|------|------|
| Operating parameters | Value | | | |
| Hot stream | | | | |
| Outlet temperature (°C) | - | 250 | 100 | 102 |
| Pressure drop (bar) | 0.05 | | | |
| Cold stream | | | | |
| Outlet temperature (°C) | 34 | - | | |
| Pressure drop (bar) | 4.80 | 0.05 | 0.02 | 0.05 |

✓ Generalized heat exchanger HNO₃

| | E106 |
|------------------------------------|--------|
| Operating parameter | Value |
| Hot stream | |
| Outlet temperature (°C) | 175 |
| Pressure drop (bar) | 0.05 |
| Oxidation volume (m ³) | 7.4873 |
| Cold stream | |
| Outlet temperature (°C) | - |
| Pressure drop (bar) | 0.05 |
| Oxidation volume (m ³) | 0 |

The following parameters are used for the heat exchanger for accounting of the chemical reactions:

- 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

✓ Cooler/Heater

| | E102 | E103 | E104 | E109 | E111 | E112 |
|------------------------------------|-------|------|--------|------|------|------|
| Operating parameters | Value | | | | | |
| Outlet temperature (°C) | 120 | 450 | 350 | 100 | 45 | 180 |
| Pressure drop (bar) | 1.50 | 0.05 | | 0.01 | 0.05 | 1.15 |
| Oxidation volume (m ³) | 0 | | 1.9514 | 0 | | |

The following parameters are used for the heat exchanger in which the chemical reactions are taken into account (E104, 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
- Taking into account a maximum temperature for the oxidation: Yes

✓ E107 nitrous vapors condenser

| Operating parameters | Value |
|--|----------------------|
| Tubes length (m) | 9 |
| Number of tubes | 2 100 |
| Circulation of the vapors | Inside the tubes |
| Inner diameter of the tubes (mm) | 25.40 |
| Equivalent diameter (mm) | 25.47 |
| Cooling water | |
| Flow direction | Counter-current |
| Heat transfer coefficients (kcal/h/m ² /K) | |
| Oxido-absorption | 290 |
| Oxidation | 215 |
| Pressure drop (bar) | 0.07 |
| Reactions | |
| Calculation of the oxidation rate constant | Koukolik |
| Calculation of the dimerization equilibrium constant | Koukolik |
| Calculation of the absorption constant of N ₂ O ₄ in water | Miller (bubble caps) |
| Number of intermediate points for print | 21 |

1.6.4. Three-way valves

| | Operating parameters | Value |
|------|---|--------------|
| V101 | Mass flow rate of the stream "NH3 S05" | 87.4 kg/h |
| V102 | Mass flow rate of the stream "Air S03" | 1 006.8 kg/h |
| V103 | Splitting ratio of the stream "Air S06" | 79.931111% |
| V104 | Splitting ratio of the stream "CW S03" | 80% |

1.6.5. Mixers

| | M101 | M102 | M103 | M104 |
|-----------------------|--------------|------|----------------------------------|-------|
| Operating parameters | Value | | | |
| Type | Static mixer | | Other mixer | Mixer |
| Outlet pressure (bar) | 7.60 | 6.35 | Equal to the lowest of the feeds | |

1.6.6. Compressor, turbine and pump

✓ K101 air compressor

| Operating parameters | Value |
|---------------------------|------------------------|
| Type | Compressor |
| Discharge pressure (bar) | 7.8 |
| Isentropic efficiency (-) | 0.845 |
| Mechanical efficiency (-) | 1 |
| Chemical reactions | Not taken into account |

✓ T101 tail gas expander

| Operating parameters | Value |
|---------------------------|---------|
| Type | Turbine |
| Discharge pressure (bar) | 1.03 |
| Isentropic efficiency (-) | 0.83 |
| Mechanical efficiency (-) | 1 |
| Electrical efficiency (-) | 1 |



It's possible to model a turbo-expander by sending the power available at the turbine to the compressor using an information stream. This is detailed in the example "PSPH_EX_EN – dual-pressure process".

✓ P101 centrifugal pump

| Operating parameters | Value |
|---------------------------|------------------|
| Type | Centrifugal pump |
| Discharge pressure (bar) | 7.5 |
| Volumetric efficiency (-) | 0.65 |
| Mechanical efficiency (-) | 1 |
| Electrical efficiency (-) | 1 |

1.6.7. Oxido-absorption column

✓ C101 oxido-absorption column

| Operating parameters | Value |
|--|------------------------------------|
| Type | Plate oxido-absorption column |
| Number of plates | 35 |
| Column diameter (m) | 6.1 |
| Holes diameter (mm) | 2 |
| Fraction free area (%) | 2.60 |
| Column temperature profile | Calculated from the temperatures |
| Intermediate feeds | |
| Return condensates | Plate 2 |
| Weak acid from the nitrous vapors condenser | Plate 32 |
| 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) | 0.77 |
| 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 35: bottom plate).

The following table presents the parameters of the plates.

| Plate | Oxidation efficiency | Oxidation volume (m ³) | Hydrodynamic model | Absorption efficiency | Tray spacing (m) | Temperature (°C) |
|-------|----------------------|------------------------------------|--------------------|-----------------------|------------------|------------------|
| 1 | 1 | 65.8 | Plug flow reactor | Atroschenko 2 | 2.25 | 29.4 |
| 2 | 1 | 65.8 | Plug flow reactor | Atroschenko 2 | 2.25 | 29.6 |
| 3 | 1 | 65.8 | Plug flow reactor | Atroschenko 2 | 2.25 | 30.0 |
| 4 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.25 | 30.6 |
| 5 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.00 | 31.4 |
| 6 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.00 | - |
| 7 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.00 | - |
| 8 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.00 | - |
| 9 | 1 | 51.1 | Plug flow reactor | Atroschenko 2 | 2.00 | - |
| 10 | 1 | 51.1 | Plug flow reactor | Atroschenko 2 | 1.75 | - |
| 11 | 1 | 51.1 | Plug flow reactor | Atroschenko 2 | 1.75 | - |
| 12 | 1 | 51.1 | Plug flow reactor | Atroschenko 2 | 1.75 | - |
| 13 | 1 | 51.1 | Plug flow reactor | Atroschenko 2 | 1.75 | - |
| 14 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.75 | - |
| 15 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 16 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 17 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 18 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 19 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 20 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 21 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 22 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 23 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 24 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 25 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 26 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 27 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 28 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 29 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 30 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 31 | 1 | 35.4 | Plug flow reactor | Atroschenko 2 | 1.21 | - |
| 32 | 1 | 78.9 | Plug flow reactor | Atroschenko 2 | 1.21 | 52.0 |
| 33 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.70 | 52.9 |
| 34 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.00 | 54.5 |
| 35 | 1 | 58.4 | Plug flow reactor | Atroschenko 2 | 2.00 | 57.0 |

1.6.8. Bleaching column

- ✓ Calculator switch

These modules are used to change the thermodynamic model between the section of the process which uses the “HNO3 specific” model and the section which uses the “Engels (strong acids)” model. The calculation of the liquid enthalpies being not rigorously the same between these two models, the use of a “Calculator switch” unit is necessary in order not to distort the enthalpy balance. The “Engels (strong acids)” model is used in the C102 bleaching column and the E111 product acid cooler. The “HNO3 specific” model is used in the rest of the process.

| Unit operation | Thermodynamic model | Outlet physical stage |
|---------------------|-----------------------|-----------------------|
| Calculator Switch | Engels (strong acids) | Calculated |
| Calculator Switch 1 | | |
| Calculator Switch 2 | HNO3 specific | |

- ✓ C102 Bleaching column

| Operating parameters | Value |
|------------------------------|---|
| Column type | Absorber |
| Thermodynamic model | Engels |
| Number of theoretical stages | 8 |
| Pressure drop (bar) | 0.41 |
| Stage efficiency | 1 for each stage |
| Reactive column | NO ₂ /N ₂ O ₄ equilibrium in gas phase |
| Print profiles | Complete |

1.7. Initializations

The calculation sequence is automatically determined by ProSimPlus HNO3. Two tear streams are identified: “Air S09” (outlet gas stream of the bleaching column) and “PG S07” (stream between the modules “O102” and “E106”). The following initializations of these streams are used in the simulation.

| Stream | Air S09 | PG S07 |
|-----------------------|-----------|---------|
| Mass fraction (-) | | |
| Oxygen | 0.22 | 0.03 |
| Nitrogen | 0.74 | 0.71 |
| Nitric oxide | 0 | 0.04 |
| Nitrogen dioxide | 0 | 0.10 |
| Nitric acid | 0.03 | 0 |
| Water | 0.01 | 0.12 |
| Mass flow rate (kg/h) | 44 000 | 180 000 |
| Temperature (°C) | Dew point | 300 |
| Pressure (bar) | 7.24 | 7.38 |

2. RESULTS

2.1. Mass and Energy Balance

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 produc... | Acid S01 | Acid S03 | Air LP | Air S04 | Air S06 | Air S08 |
|----------------------|--------------------|----------------|----------|-------------|------------|------------|-----------|-----------|
| From | | E111 | E107 | C101 | Air feed | V102 | V103 | E108 |
| Total flow (mass) | t/d | 1725.6 | 792.28 | 1731.5 | 5074.8 | 5050.6 | 4037 | 1013.6 |
| Total flow (molar) | Nm ³ /h | 52321 | 27132 | 52212 | 1.6518E005 | 1.6439E005 | 1.314E005 | 32992 |
| Mass fractions | | | | | | | | |
| AMMONIA | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| OXY GEN | | 0.00019363 | 0 | 0 | 0.23078 | 0.23078 | 0.23078 | 0.23078 |
| NITROGEN | | 0.00010932 | 0 | 0 | 0.76006 | 0.76006 | 0.76006 | 0.76006 |
| NITRIC OXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| NITROGEN DIOXIDE | | 3.2354E-010 | 0 | 0.00010018 | 0 | 0 | 0 | 0 |
| NITROGEN TETROXIDE | | 0 | 0 | 0.0041807 | 0 | 0 | 0 | 0 |
| NITROUS OXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| NITRIC ACID | | 0.58112 | 0.47529 | 0.58102 | 0 | 0 | 0 | 0 |
| WATER | | 0.41857 | 0.52471 | 0.4147 | 0.0091548 | 0.0091548 | 0.0091548 | 0.0091548 |
| Mole fractions | | | | | | | | |
| AMMONIA | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| OXY GEN | | 0.00018638 | 0 | 0 | 0.20694 | 0.20694 | 0.20694 | 0.20694 |
| NITROGEN | | 0.0001202 | 0 | 0 | 0.77848 | 0.77848 | 0.77848 | 0.77848 |
| NITRIC OXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| NITROGEN DIOXIDE | | 2.1661E-010 | 0 | 6.7444E-005 | 0 | 0 | 0 | 0 |
| NITROGEN TETROXIDE | | 0 | 0 | 0.0014073 | 0 | 0 | 0 | 0 |
| NITROUS OXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| NITRIC ACID | | 0.28406 | 0.2057 | 0.28558 | 0 | 0 | 0 | 0 |
| WATER | | 0.71564 | 0.7943 | 0.71295 | 0.014581 | 0.014581 | 0.014581 | 0.014581 |
| Physical state | | Liquid | Liquid | Liquid | Vapor | Vapor | Vapor | Vapor |
| Temperature | °C | 45 | 49.426 | 57 | 25 | 102 | 236.18 | 100 |
| Pressure | bar | 7.6 | 7.25 | 7.24 | 1 | 7.75 | 7.7 | 7.65 |
| Enthalpic flow | kW | -1.6669E005 | -89450 | -1.6632E005 | -7217.6 | -2584.8 | 4421 | -542.8 |
| Molar vapor fraction | | 0 | 0 | 0 | 1 | 1 | 1 | 1 |

| Streams | | CW S01 | CW S02 | CW S06 | NH3 S01 | NH3 S04 | PG S02 | PG S09 |
|----------------------|-------|----------------|-------------|-------------|-----------|-----------|-------------|-------------|
| From | | Cooling w ater | E107 | M104 | NH3 feed | V101 | R101 | O103 |
| Total flow (mass) | t/d | 48000 | 48000 | 48000 | 285.55 | 283.45 | 4320.4 | 4320.4 |
| Total flow (molar) | Nm3/h | 2.4883E006 | 2.4883E006 | 2.4883E006 | 15657 | 15542 | 1.5082E005 | 1.4557E005 |
| Mass fractions | | | | | | | | |
| AMMONIA | | 0 | 0 | 0 | 0.99798 | 0.99798 | 0 | 0 |
| OXY GEN | | 0 | 0 | 0 | 0 | 0 | 0.064173 | 0.02267 |
| NITROGEN | | 0 | 0 | 0 | 0 | 0 | 0.71219 | 0.71219 |
| NITRIC OXIDE | | 0 | 0 | 0 | 0 | 0 | 0.11098 | 0.03314 |
| NITROGEN DIOXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0.11907 |
| NITROGEN TETROXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0.00027466 |
| NITROUS OXIDE | | 0 | 0 | 0 | 0 | 0 | 8.4605E-005 | 8.4605E-005 |
| NITRIC ACID | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| WATER | | 1 | 1 | 1 | 0.0020171 | 0.0020171 | 0.11258 | 0.11258 |
| Mole fractions | | | | | | | | |
| AMMONIA | | 0 | 0 | 0 | 0.99809 | 0.99809 | 0 | 0 |
| OXY GEN | | 0 | 0 | 0 | 0 | 0 | 0.053654 | 0.019637 |
| NITROGEN | | 0 | 0 | 0 | 0 | 0 | 0.68016 | 0.70467 |
| NITRIC OXIDE | | 0 | 0 | 0 | 0 | 0 | 0.098948 | 0.030613 |
| NITROGEN DIOXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 0.071735 |
| NITROGEN TETROXIDE | | 0 | 0 | 0 | 0 | 0 | 0 | 8.274E-005 |
| NITROUS OXIDE | | 0 | 0 | 0 | 0 | 0 | 5.1428E-005 | 5.3282E-005 |
| NITRIC ACID | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| WATER | | 1 | 1 | 1 | 0.0019071 | 0.0019071 | 0.16719 | 0.17321 |
| Physical state | | Liquid | Liquid | Liquid | Liquid | Vapor | Vapor | Vapor |
| Temperature | °C | 22 | 38.857 | 37.071 | 10 | 120 | 929.25 | 182.21 |
| Pressure | bar | 4.2 | 4.15 | 4.1 | 14 | 7.7 | 7.55 | 7.32 |
| Enthalpic flow | kW | -1.3638E006 | -1.3246E006 | -1.3288E006 | -13071 | -8235.2 | -3814.2 | -57528 |
| Molar vapor fraction | | 0 | 0 | 0 | 0 | 1 | 1 | 1 |

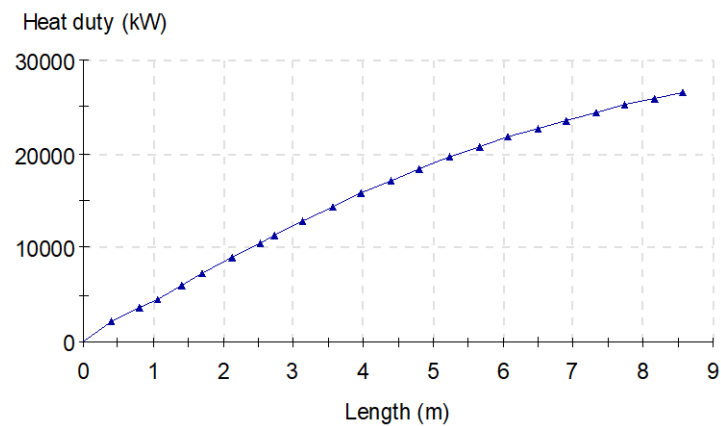
| Streams | | PG S12 | TG S05 | TG S07 | Water S01 | Water S02 |
|----------------------|-------|-------------|-------------|-------------|----------------|---------------|
| From | | M103 | M102 | T101 | Process w a... | Condensate... |
| Total flow (mass) | t/d | 4547.7 | 3996.4 | 3996.4 | 85.32 | 300.48 |
| Total flow (molar) | Nm3/h | 1.463E005 | 1.3302E005 | 1.3303E005 | 4423 | 15577 |
| Mass fractions | | | | | | |
| AMMONIA | | 0 | 0.00052382 | 0.0003661 | 0 | 0 |
| OXY GEN | | 0.060346 | 0.032221 | 0.032221 | 0 | 0 |
| NITROGEN | | 0.84595 | 0.96267 | 0.96298 | 0 | 0 |
| NITRIC OXIDE | | 0.027653 | 0.00041465 | 4.1465E-005 | 0 | 0 |
| NITROGEN DIOXIDE | | 0.046412 | 0.00011735 | 8.3908E-005 | 0 | 0 |
| NITROGEN TETROXIDE | | 0.014013 | 1.9983E-011 | 7.5964E-010 | 0 | 0 |
| NITROUS OXIDE | | 8.0377E-005 | 9.1466E-005 | 9.1466E-005 | 0 | 0 |
| NITRIC ACID | | 0.00072183 | 3.8672E-007 | 3.8672E-007 | 0 | 0 |
| WA TER | | 0.0048189 | 0.0039655 | 0.0042158 | 1 | 1 |
| Mole fractions | | | | | | |
| AMMONIA | | 0 | 0.00086299 | 0.00060311 | 0 | 0 |
| OXY GEN | | 0.054747 | 0.028253 | 0.028251 | 0 | 0 |
| NITROGEN | | 0.87664 | 0.96419 | 0.96443 | 0 | 0 |
| NITRIC OXIDE | | 0.026753 | 0.00038773 | 3.877E-005 | 0 | 0 |
| NITROGEN DIOXIDE | | 0.029286 | 7.1572E-005 | 5.117E-005 | 0 | 0 |
| NITROGEN TETROXIDE | | 0.0044212 | 6.0937E-012 | 2.3163E-010 | 0 | 0 |
| NITROUS OXIDE | | 5.3014E-005 | 5.8309E-005 | 5.8305E-005 | 0 | 0 |
| NITRIC ACID | | 0.00033254 | 1.7219E-007 | 1.7218E-007 | 0 | 0 |
| WA TER | | 0.0077652 | 0.0061761 | 0.0065653 | 1 | 1 |
| Physical state | | Vapor | Vapor | Vapor | Liquid | Liquid |
| Temperature | °C | 56.324 | 270.6 | 93.386 | 25 | 25 |
| Pressure | bar | 7.24 | 6.35 | 1.03 | 6.5 | 6.6 |
| Enthalpic flow | kW | 4421.4 | 9456.6 | 645.53 | -15660 | -55150 |
| Molar vapor fraction | | 1 | 1 | 1 | 0 | 0 |

2.2. Process Performance

This process produces 1 003 t/d of nitric acid (eq. 100%) at a purity of 58.1% wt. The NO_x content at the outlet of the oxido-absorption column is 460 ppmv eq. NO. After the NO_x abbatment reactor, the NO_x content is 90 ppmv eq. NO.

2.3. Nitrous vapors condenser profiles

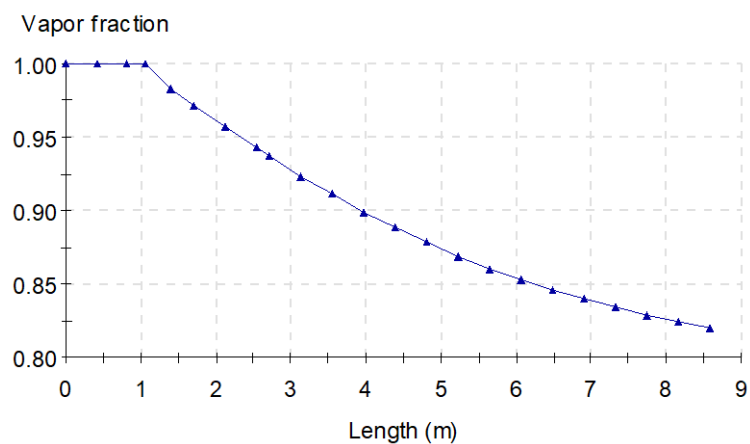
E107 - Heat duty



Heat duty

The following curve shows that 8% of the length of the heat exchanger is used to cool the inlet process gas down to its dew point, only gas phase reactions are occurring in this section while the oxido-absorption phenomena is occurring in the remaining part of the condenser.

E107 - Mass vapor fraction

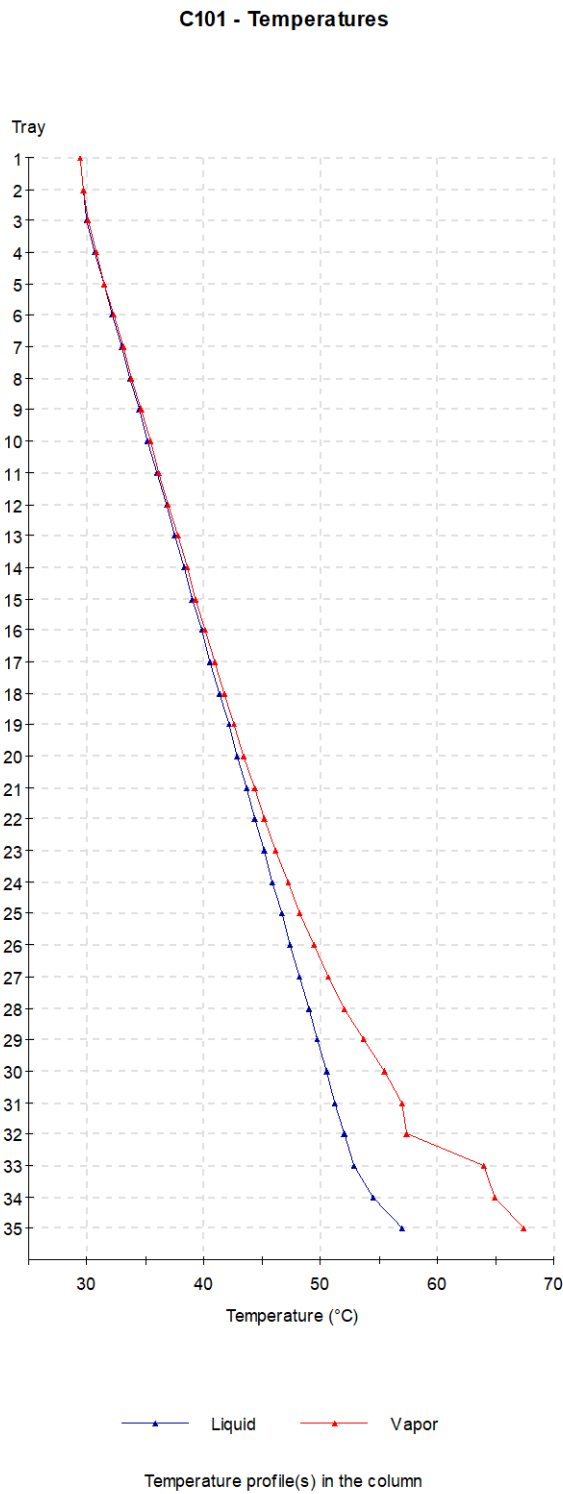


Mass vapor fraction profiles along the condenser

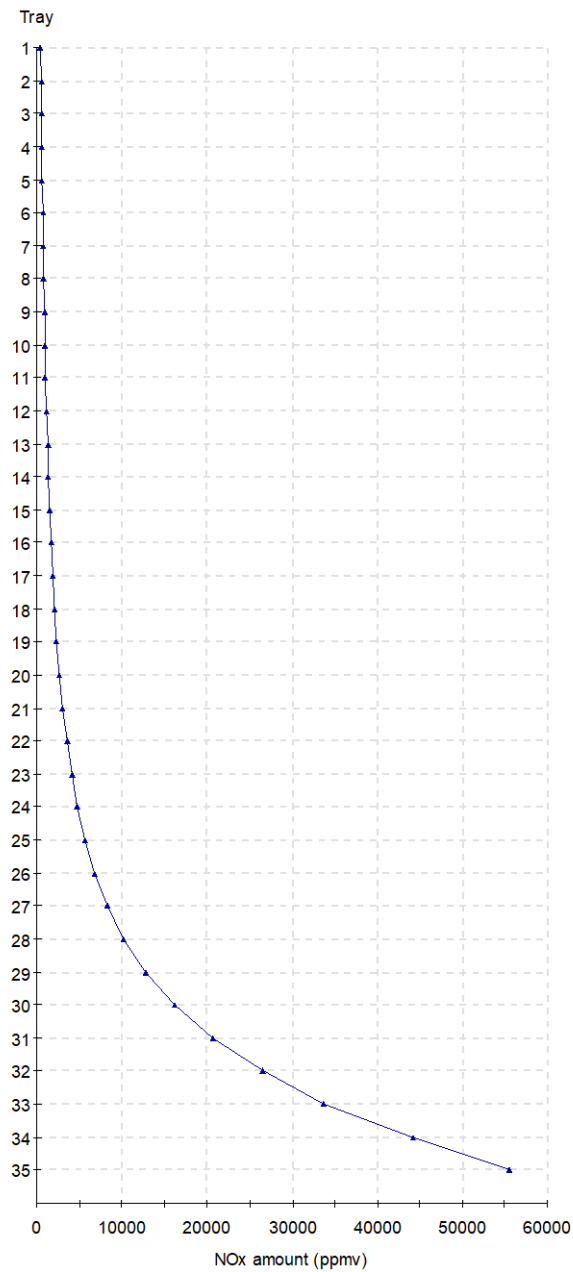
2.4. Columns profiles

2.4.1. C101 oxido-absorption column

The column stages are numbered from top to bottom (plate 1: top plate; plate 35: bottom plate).

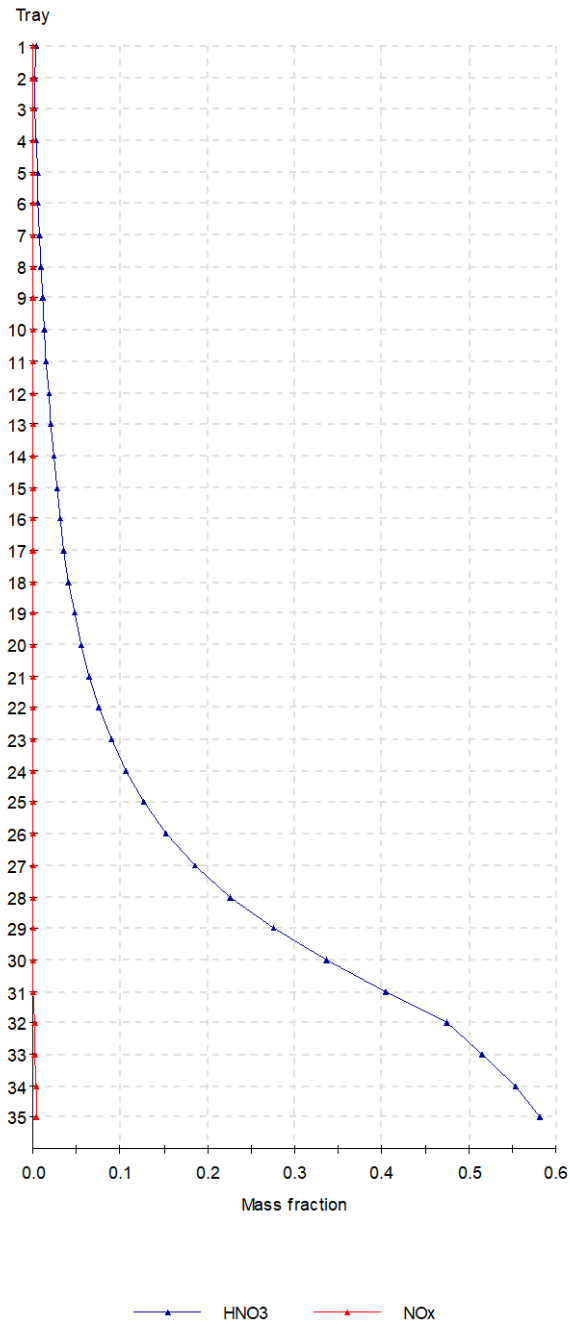


C101 - Amount of NOx (ppmv)



Amount of NOx profile in the column

C101 - Liquid mass fractions

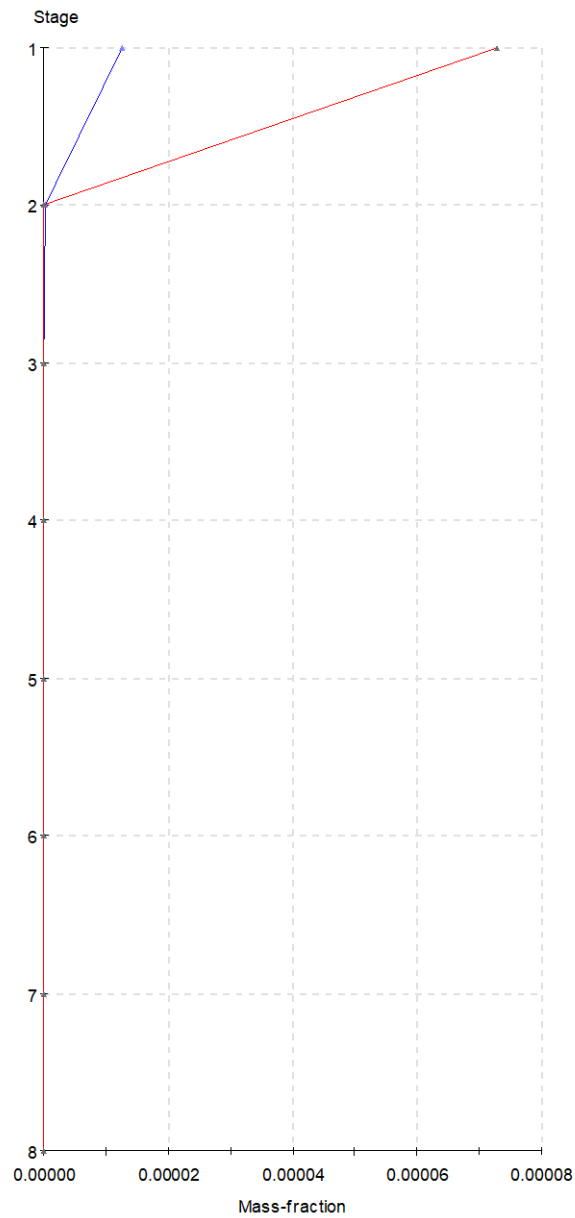


Liquid mass fractions profiles in the column

2.4.2. C102 bleaching column

The column stages are numbered from top to bottom (plate 1: top plate; plate 8: bottom plate).

C102 - Liquid mass-fractions



— NITROGEN DIOXIDE — NITROGEN TETROXI

Liquid mass-fractions profile in the column

3. REFERENCES

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