# PROSIMPLUS HNO3 APPLICATION EXAMPLE

# PACKED COLUMN FOR NOX ABSORPTION

| EXAMPLE PURPOSE |
|---|
| This example uses a column with two packing beds to absorb the NOx of a gas stream with a weak solution of nitric acid. The flow rate of this solution is determined to respect the NOx content of the gas stream leaving the column. |

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

| CORRESPONDING PROSIMPLUS HNO3 FILE | *PSPH_EX_EN-Packed-column.pmp3* |
|---|---|

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# 1. Modelling of the process

## 1.1. Process description

In this example the absorption of the NOx present in a gas stream is realized in a column with two packing beds with a weak solution of nitric acid. The flow in the column is counter-current. Each section has a recirculation stream to allow a sufficient wetting of the packing. The description of the physico-chemical phenomena involved is based on a rate-based approach. This approach assumes that the production of nitric acid is done by the reaction scheme described hereafter. The two-layer theory is used to evaluate the different transfer flux. It's assumed that the gas and liquid flows are of plug flow types.

- ✓ Gas phase reactions
  - o NO oxidation

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

  - o $NO_2$ dimerization

$$2\,NO_2 \leftrightarrow N_2O_4$$

  - o $N_2O_3$ formation

$$NO + NO_2 \leftrightarrow N_2O_3$$

- ✓ Reaction at the gas-liquid interface
  - o $N_2O_4$ absorption with chemical reactions
    a. Transfer by diffusion of $NO_2$ and $N_2O_4$ (at equilibrium) from the gas phase to the interface.
    b. Dissolution of $N_2O_4$ in water.
    c. Hydrolysis of $N_2O_4$ and fast decomposition of $HNO_2$:

$$N_2O_4 + H_2O \leftrightarrow HNO_2 + HNO_3$$

$$3\,HNO_2 \leftrightarrow HNO_3 + H_2O + 2\,NO$$

These two reactions are combined to calculate the equilibrium constant:

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

  - o Absorption of $N_2O_3$ with chemical reactions
    a. Transfer by diffusion of $N_2O_3$ (at equilibrium) from the gas phase to the interface.
    b. Dissolution of $N_2O_3$ in water.
    c. Hydrolysis of $N_2O_3$:

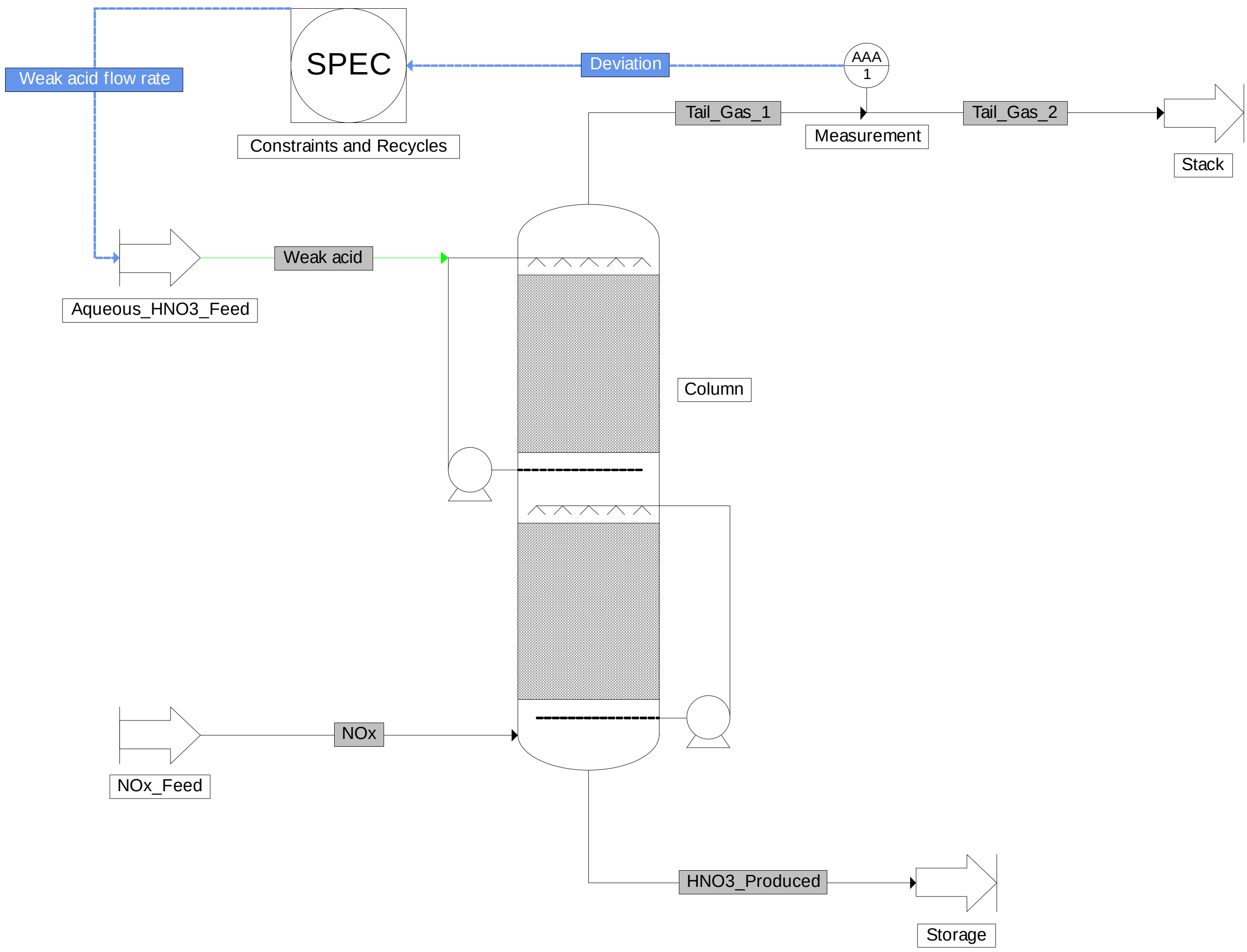
$$N_2O_3 + H_2O \leftrightarrow 2\,HNO_2$$

- ✓ Reaction in liquid phase
  - o Decomposition of $HNO_2$

$$3\,HNO_2 \leftrightarrow HNO_3 + H_2O + 2\,NO$$

## 1.2. Process flowsheet

The gas flux containing the NOx enters in the column by the stream "NOx". The weak nitric acid solution used to absorb the NOx is fed by the stream "Weak acid". The "Measurement" module is used to compute the deviation between the NOx content of the gas stream leaving the column and the specified value: 6 000 ppmv. The "Constraints and Recycles" module minimizes this deviation by acting on the weak acid flow rate.



## 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.

| Components | 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 |
| Nitrous oxide | $N_2O$ | 10024-97-2 |
| Nitrous acid | $HNO_2$ | 7782-77-6 |
| Nitrogen trioxide | $N_2O_3$ | 10544-73-7 |

## 1.4. Thermodynamic model

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.

## 1.5. Chemical reactions

The reactions involved in the oxido-absorption column are pre-coded inside the module. Thus, they don’t have to be described by the user.

## 1.6. Operating parameters

✓ Process feeds

| **Feed** | NOx | Weak acid |
|---|---|---|
| **Mass fraction** | | |
| **Water** | 0.0018 | 0.8351 |
| **Nitric oxide** | 0.0304 | 0 |
| **Nitrogen dioxide** | 0.0340 | 0 |
| **Nitrogen tetroxide** | 0.0369 | 0 |
| **Nitrogen** | 0.3532 | 0 |
| **Oxygen** | 0.1030 | 0 |
| **Nitric acid** | 0 | 0.1649 |
| **Nitrous oxide** | 0.4407 | 0 |
| **Flow rate (kg/h)** | 5 775 | 3 360 |
| **Temperature (°C)** | 21.5 | 22.1 |
| **Pressure (bar)** | 2.45 | 2.45 |

✓ Absorption column with two beds of packing

| | Top section | Bottom section |
|---|---|---|
| **Packing** | | |
| **Type** | Raschig rings | |
| **Material** | Ceramic | |
| **Specific area ($m^2/m^3$)** | 120 | 92 |
| **Nominal size (mm)** | 38 | 50 |
| **Equivalent diameter (mm)** | 35.8 | 64.55 |
| **Void fraction (-)** | 0.68 | 0.74 |
| **Height (m)** | 4 | |
| **Column diameter (m)** | 1.98 | |
| **Flow direction** | Counter-current | |
| **Recirculation stream** | | |
| **Mass flow rate (t/d)** | 30 | 60 |
| **Temperature (°C)** | 20 | 25 |
| **Oxidation volume** | | |
| **Bottom ($m^3$)** | 4.3 | |
| **Middle ($m^3$)** | 6.0 | |
| **Top ($m^3$)** | 6.7 | |
| **Temperature profile inside the column** | | |
| **Temperature (°C)** | 29 | |
| **Pressure profile inside the column** | | |
| **Pressure drop (bar)** | 0.2 | |
| **Parameters** | | |
| **Print profiles** | Mass | |
| **Intermediate points** | 10 | |

✓ Specifications

| Specifications | Value |
|---|---|
| Amount of NOx (ppmv) | 6 000 |

✓ Acting variables

| Acting variables |
|---|
| Feed flow rate of weak acid |

✓ "Constraints and recycles" module

The default parameters are used for this module.

# 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 | | HNO3_Prod... | NOx | Tail_Gas_1 | Tail_Gas_2 | Weak acid |
|---|---|---|---|---|---|---|
| Total flow | kg/h | 9948.1 | 5575 | 4895.9 | 4895.9 | 9269 |
| Total flow | Nm3/h | 10285 | 3510.2 | 3173.6 | 3173.6 | 10174 |
| Mass fractions | | | | | | |
| WATER | | 0.7628 | 0.0017316 | 0.0083989 | 0.0083989 | 0.8351 |
| NITRIC OXIDE | | 0 | 0.03039 | 0.0022362 | 0.0022362 | 0 |
| NITROGEN DIOXIDE | | 0 | 0.03398 | 0.0043027 | 0.0043027 | 0 |
| NITROGEN TETROXIDE | | 0 | 0.036929 | 0.00023612 | 0.00023612 | 0 |
| NITROGEN | | 0 | 0.35325 | 0.40225 | 0.40225 | 0 |
| OXYGEN | | 0 | 0.10303 | 0.080733 | 0.080733 | 0 |
| NITRIC ACID | | 0.23352 | 0 | 8.8888E-006 | 8.8888E-006 | 0.1649 |
| NITROUS OXIDE | | 0 | 0.44069 | 0.50182 | 0.50182 | 0 |
| NITROUS ACID | | 0.0036802 | 0 | 0 | 0 | 0 |
| NITROGEN TRIOXIDE | | 0 | 0 | 1.297E-005 | 1.297E-005 | 0 |
| Mole fractions | | | | | | |
| WATER | | 0.91796 | 0.0034216 | 0.01612 | 0.01612 | 0.94656 |
| NITRIC OXIDE | | 0 | 0.036053 | 0.0025769 | 0.0025769 | 0 |
| NITROGEN DIOXIDE | | 0 | 0.026293 | 0.0032338 | 0.0032338 | 0 |
| NITROGEN TETROXIDE | | 0 | 0.014287 | 8.8734E-005 | 8.8734E-005 | 0 |
| NITROGEN | | 0 | 0.44889 | 0.49649 | 0.49649 | 0 |
| OXYGEN | | 0 | 0.11462 | 0.087237 | 0.087237 | 0 |
| NITRIC ACID | | 0.080342 | 0 | 4.8775E-006 | 4.8775E-006 | 0.053437 |
| NITROUS OXIDE | | 0 | 0.35644 | 0.39424 | 0.39424 | 0 |
| NITROUS ACID | | 0.0016971 | 0 | 0 | 0 | 0 |
| NITROGEN TRIOXIDE | | 0 | 0 | 5.9E-006 | 5.9E-006 | 0 |
| Physical state | | Liquid | Vapor | Vapor | Vapor | Liquid |
| Temperature | °C | 29 | 21.5 | 30.751 | 30.751 | 22.1 |
| Pressure | bar | 2.45 | 2.45 | 2.05 | 2.05 | 2.45 |
| Enthalpic flow | kW | -35537 | 1416.3 | 1139.8 | 1139.8 | -35519 |
| Vapor molar fraction | | 0 | 1 | 1 | 1 | 0 |

## 2.2. Process performance

The gas entering the column has a NOx content of 90 920 ppmv eq. NO. To decrease this value to 6 000 ppmv eq. NO in the outlet gas, a flow rate of weak nitric acid of 9 267 kg/h is needed.

## 2.3. Profiles in the column

The position 0 m corresponds to the bottom of the bottom packing section (column bottom). The position 4 m corresponds to the top of the bottom packing section and to the bottom of the top packing section (column middle). The position 8 m corresponds to the top of the top packing section (column top). The heights corresponding to the oxidation volumes (bottom, middle, top) are not taken into account on these graphs. This explains the jump in the nitric acid mass fraction curve.