

PROSIMPLUS APPLICATION EXAMPLE

PACKED COLUMN FOR NO_x ABSORPTION

EXAMPLE PURPOSE

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

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CORRESPONDING PROSIMPLUS FILES

PSPH_EX_EN-Packed-column.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. 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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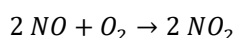
1. PROCESS MODELING

1.1. Process description

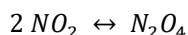
In this example the absorption of the NOx present in a gas stream is realized in a column with two packing beds with a weak solution of nitric acid. The flow in the column is counter-current. Each section has a recirculation stream to allow a sufficient wetting of the packing. The description of the 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

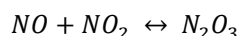
- NO oxidation



- NO₂ dimerization



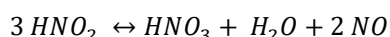
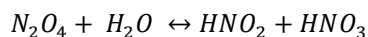
- N₂O₃ formation



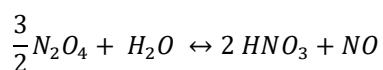
✓ Reaction at the gas-liquid interface

- N₂O₄ absorption with chemical reactions

- Transfer by diffusion of NO₂ and N₂O₄ (at equilibrium) from the gas phase to the interface.
- Dissolution of N₂O₄ in water.
- Hydrolysis of N₂O₄ and fast decomposition of HNO₂:

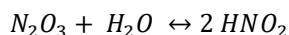


These two reactions are combined to calculate the equilibrium constant:



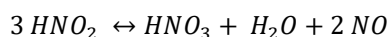
- Absorption of N₂O₃ with chemical reactions

- Transfer by diffusion of N₂O₃ (at equilibrium) from the gas phase to the interface.
- Dissolution of N₂O₃ in water.
- Hydrolysis of N₂O₃:



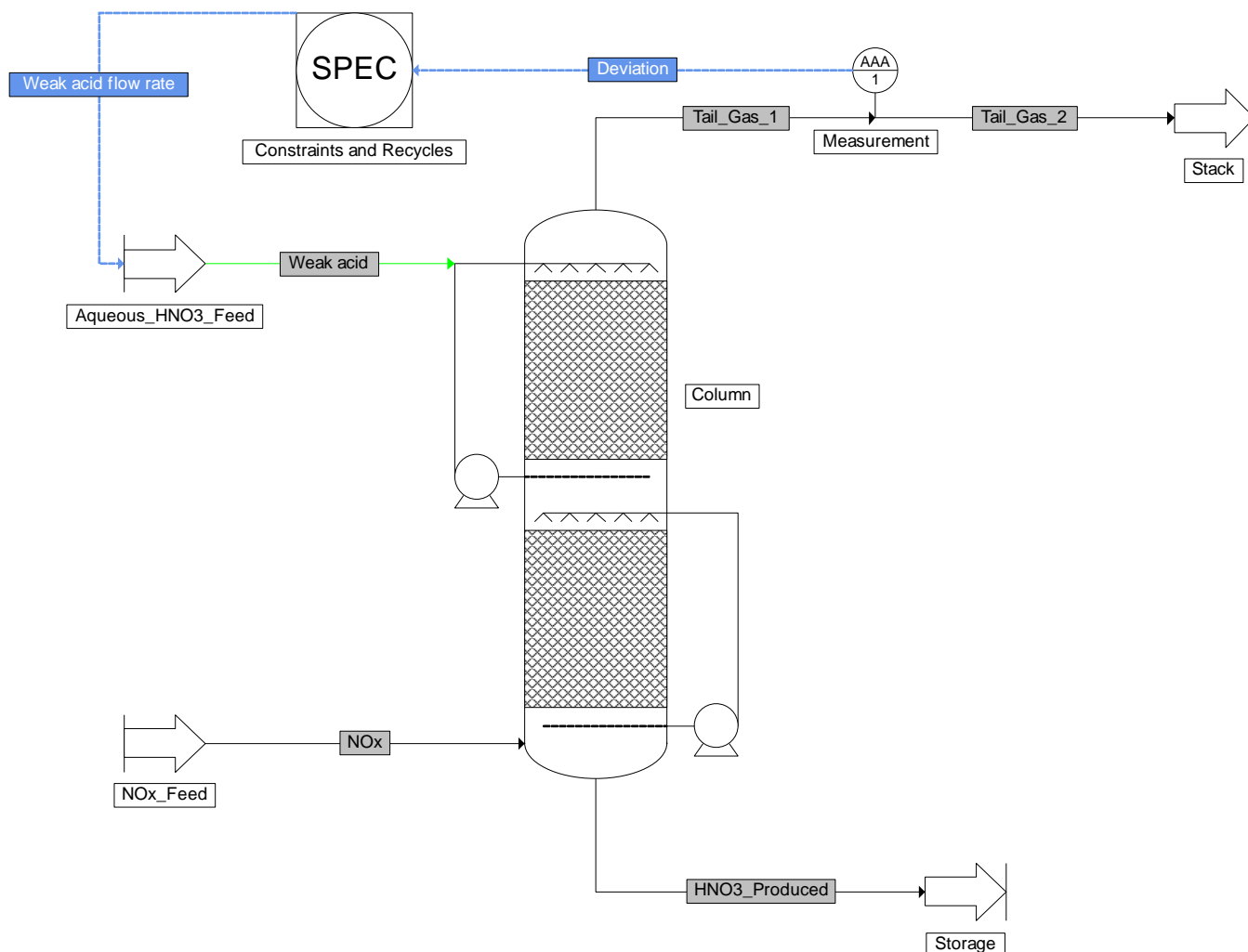
✓ Reaction in liquid phase

- Decomposition of HNO₂



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 registry numbers¹ 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 ₂ O	7732-18-5
Nitric oxide	NO	10102-43-9
Nitrogen dioxide	NO ₂	10102-44-0
Nitrogen tetroxide	N ₂ O 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 ₂ O	10024-97-2
Nitrous acid	HNO ₂	7782-77-6
Nitrogen trioxide	N ₂ O 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 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.

1.6. 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 (m²/m³)	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 (m³)	4.3	
Middle (m³)	6.0	
Top (m³)	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 NO _x (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 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		HNO ₃ _Prod...	NO _x	Tail_Gas_1	Tail_Gas_2	Weak acid
Total flow	kg/h	9948.1	5575	4895.9	4895.9	9269
Total flow	Nm ³ /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

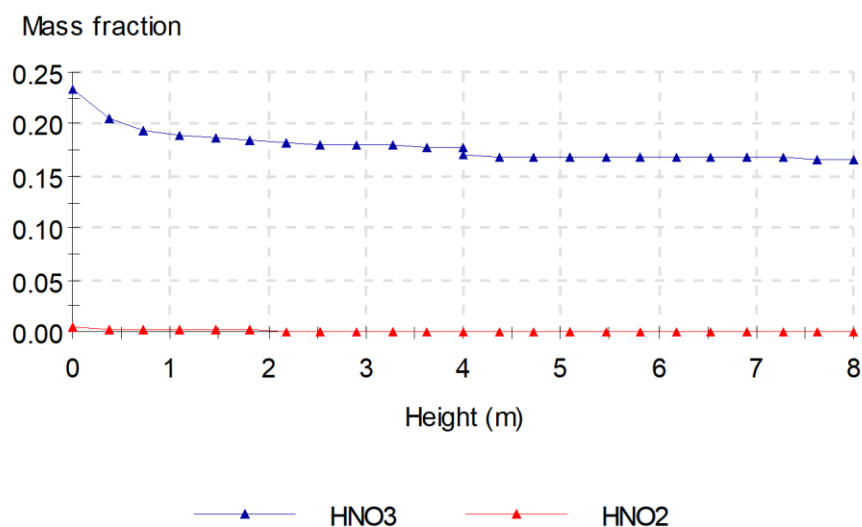
2.2. Process Performance

The gas entering the column has a NO_x 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.

Column - Liquid mass fractions



Column - Amount of NOx

