



ProSimPlus HNO₃

Simulation of Nitric Acid Plants And Nitrous Vapors Absorption

The only software fully dedicated to nitric acid production processes.

To face economic, environmental or safety challenges inherent to their activity, actors of the fertilizer industry, and nitric acid producers in particular, cannot be satisfied anymore with general simulation software. They need a reliable and efficient tool, capable of representing the full complexity of their production process.

ProSimPlus HNO₃ is a process engineering tool specifically designed to model nitric acid production plants and nitrous vapors absorption units.

It is used in design phases as well as in plant operations for process optimization, unit debottlenecking or plant revamping. Thanks to a reliable modeling of the steady-state behavior of the installation, it helps to generate significant improvements in efficiency and profitability as well as to increase reactivity when facing new regulations.

- ▶ **Industry specific equipment:** absorption columns, nitrous vapors condensers, etc.
- ▶ **Many years of experience** in properties calculations and in chemical reactions readily available.
- ▶ **Complete mass and energy balances** on the installation without time-consuming convergence tests.
- ▶ **An easy-to-use graphical user interface** for instant usability and fast learning.
- ▶ **A reference software** selected by leading actors in the field.



Why a specific software?

The complexity of the physical and chemical phenomena involved in nitric acid processes (chemical reactions in gas phase in nearly all the equipment pieces, thermodynamic properties not easy to model...) and the specificity of the equipment used in these units make the simulation of these processes nearly impossible with a general purpose simulation software. Typically, sizing parameters (pipes volume, absorption column trays spacing...) must be taken into account at early stages of process design as, when adding oxidation volumes, they affect the mass and energy balances. This is generally not the case in other processes and these parameters are therefore not taken into account in standard simulation software. Some operating or engineering companies have developed specific in-house programs for the main unit operations but, beside usual maintenance and permanence issues, they often lack in flexibility and efficiency when looking at a complete process.

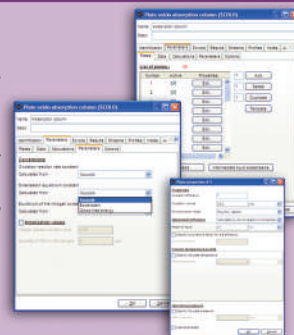
ProSimPlus HNO₃ is built on over 30 years of experience in the modeling of nitric acid plants and nitrous vapors absorption units (thesis of Prof. Xavier Joulia – 1981 "Contribution au développement d'un programme général de simulation – Application à l'analyse du fonctionnement d'un atelier de production d'acide nitrique"). Since then, this know-how has constantly been enriched, updated and validated.

Represent your processes accurately

In addition to the unit operation library usually available in general simulation packages, ProSimPlus HNO₃ offers a full set of specific equipment used in nitric acid production processes, in particular:

- **Absorption columns** for nitrous vapors by aqueous nitric acid solutions: chemical reactions in gas phase, mass transfer with chemical reaction in liquid phase, plate or packing towers, spray columns, plate coolers, etc.
- **Nitrous vapors condensers** using rate-based approach or simplified model.
- **Chemical reactors (or oxidation volume)**: plug flow or CSTR, adiabatic, isothermal or specified output temperature, etc.
- **Nitrous vapors compressors**: one-stage or multi-stage, isentropic or polytropic efficiency, with the ability to provide manufacturers curves, etc.
- **Heat exchangers**, with possibility to take into account oxidation reactions in gas phase.

Pinch analysis features are included (extraction of selected stream data, composite curves...) as well as the ability to run case studies to automatically perform **sensitivity analysis**. Additionally, ProSimPlus HNO₃ is a particularly open software in which users can integrate their own models and specific know-how.

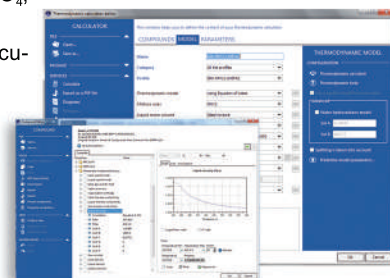


Unit operation configuration windows

A vast know-how in properties and chemical reactions already integrated

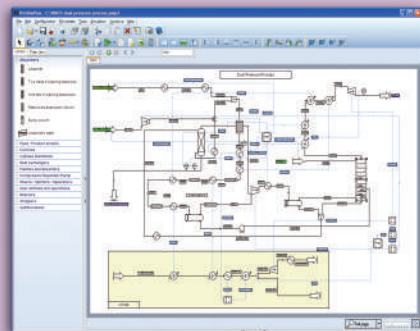
The quality of a simulation relies above all on a good thermodynamic and chemical modeling of the system. ProSimPlus HNO₃ includes physical and chemical models built on many years of research and validated by intensive industrial use. As these elements are readily available in the software, the user can concentrate on other aspects of his process. Among these elements one will find:

- A complete properties database of the components involved in these types of process (H₂O, NO, NO₂, N₂O₄, N₂, O₂, HNO₃, NH₃, N₂O, N₂O₃, HNO₂, CO₂, CO, CH₄, H₂).
- A thermodynamic model based on equations obtained from experimental measurements and able to accurately represent the non-ideality of the liquid phase (liquid fugacity, excess enthalpy, liquid density...).
- A model particularly well suited to strong nitric acid concentrations (concentration or bleaching columns).
- Mass transfer with chemical reactions in liquid phase automatically taken into account: N₂O₄ and N₂O₃ absorption, HNO₃ and HNO₂ hydrolysis or HNO₂ decomposition.
- Chemical reactions in gas phase automatically taken into account, with specific correlations:
 - NO to NO₂ oxidation reaction kinetic model in gas phase: Sherwood's, Koukolik and Marek...
 - NO₂ to N₂O₄ dimerisation equilibrium constant in gas phase: Koukolik and Marek, Bodenstein...
 - N₂O₃ formation equilibrium constant in gas phase: Miller, Beattie and Bell...
 - NOx-H₂O-HNO₃ systems equilibrium constant: Koukolik and Marek, Zhidkov, Carberry...



Definition of the thermodynamic system (component and model)

Unrivalled convergence methods for immediate results



Flowsheet of a dual-pressure unit

Specifically adjusted algorithms, based on the **simultaneous modular approach**, are particularly well adapted to the complexity of these processes. This development, unique in the world of simulators, comprises in particular:

- The **automatic determination of the calculation sequence**: stream initialization and tear streams selection are usually not required.
- The **simultaneous treatment of recycles and design specifications** through proven methods;
- The **multivariable control approach** that allows imposing one or several process outputs by simultaneously adjusting one or several selected parameters.
- The **possibility to simulate the process partially** after a parameter modification, instead of running the full simulation over again.
- A **fast and reliable convergence** at each unit operation level that is ensured by using the best suited method.

The industry reference software, quickly adopted by users

World leading engineering firms in the nitric acid field and fertilizers producers already rely on ProSimPlus HNO₃ to design new units or revamp existing plants. This software is also extensively used in industries dealing with NOx: energy, chemical, nuclear,...



ProSimPlus HNO₃ is very intuitive. Engineers who are accustomed to another simulation tool are surprised how easy to learn it is and how fast they can progress with the software without expensive training. The MS Windows® based graphical environment provides many features to **easily built process flow diagrams**: drag and drop, copy and paste of unit operations, colors, sizing, sub-flowsheets, tree view, images and text insertions, zoom facility, different views of the same process... and to **quickly analyze and understand simulation results** (charts plotting, global material balances calculation directly from the flowsheet, NOx content, oxidation degree...). During and after the simulation, convergence status is shown on the diagram and in the simulation report (along with indications on the source of error). The complete report is generated in HTML and MS-Excel formats and flowsheets and charts can be copied and pasted in other environments or saved in .BMP or .EMF formats.

