# a Digital Twin

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nitric acid is manufactured from ammonia in the form of a solution of HNO_3 in water, following the well-known Ostwald process. Concentrations of $55 - 60\%$ HNO_3 are necessary to be used in the fertilizer industry, while azeotropic concentrations ($65 - 70\%$) are required by general procedures in the chemical processing industry, mainly for organic nitration.

Espindesa developed its high pressure process during the 1970s in Europe and, since then, has continuously updated this technology to deal with the most severe regulations and the increasing cost of energy by developing a dual pressure process. In the actual scenario of high cost energy and metals, there is a clear benefit of the dual process for nitric acid manufacturing compared to the mono pressure process,
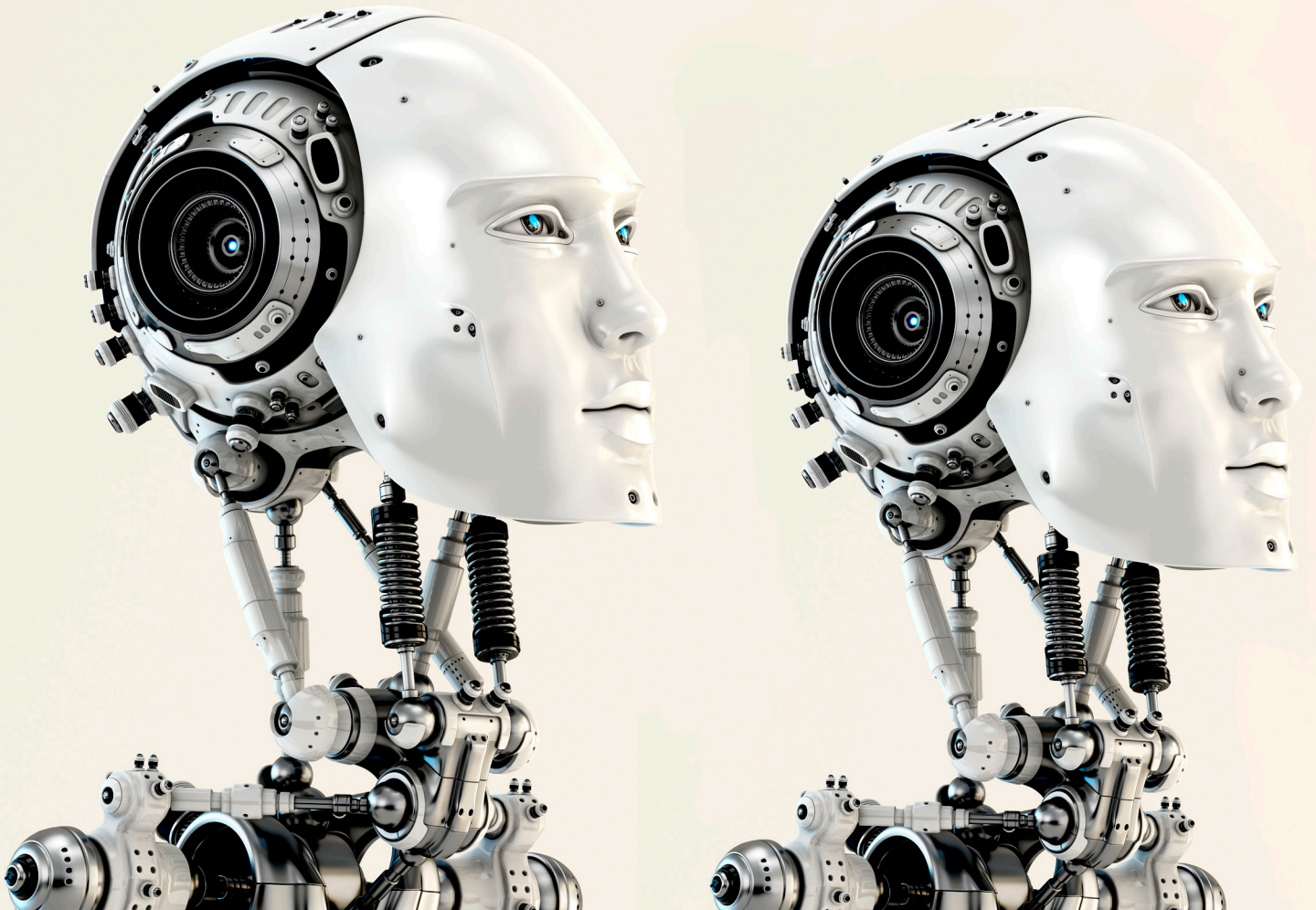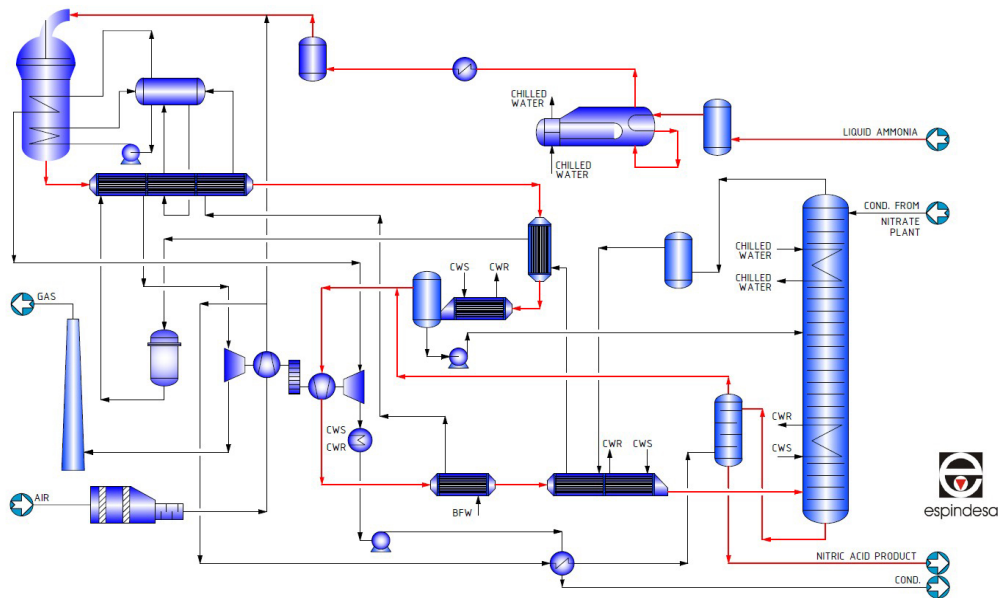
Figure 1. Process flow diagram of Espindesa's weak HNO_3 nitric acid dual process.
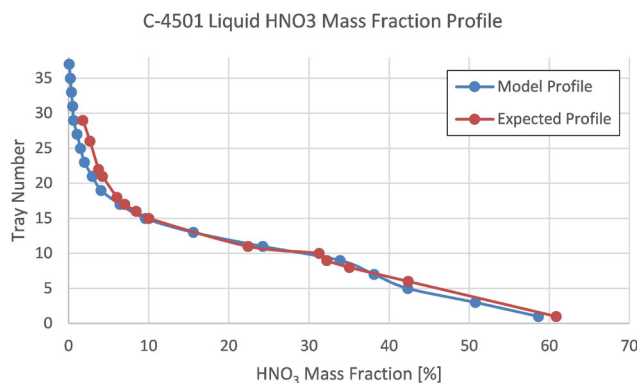

Figure 2. Comparison of simulated results in front of real data for liquid nitric acid concentration in absorber trays.

mainly for large plants. This is mainly due to the operating costs related to ammonia and the catalyst, platinum. In the early 2000s, Espindesa improved its dual pressure process, featuring azeotropic acid concentrations, low N_2O and NO_x tail emissions, extremely efficient raw material and energy consumptions, and pollution prevention at plant startup and shutdown.

Process deployment

As a process licensor and technology provider, Espindesa is often in charge not only of the engineering, procurement and construction (EPC) project stages, but also of the commissioning, plant startup and operating support service stages. To better cover the needs of its clients and final users of its technology, Espindesa was in need of a tool that could simplify the commissioning and startup stages. The company specified the requirements for a software tool; a digital twin of the processing plant that could be used to demonstrate both to engineers and plant operators how the new facility was built and how it was expected to behave once in operation. Furthermore, through integration with existing process control human machine interfaces (HMI), it also had to be an excellent tool to train both control room and field operators on the plant operating procedures, as well as on the implemented control system.

Inprocess was asked to develop the Espindesa Nitric Acid Digital Twin (ENADT) due to its experience in building dynamic simulation models with commercially available technology, as well as its proven skills in the development of software extensions to be run from inside such commercial process simulators, and also because of its long list of successfully deployed operator training systems (OTS).

Espindesa's requirements for ENADT were established during the project definition stages. ENADT had to be a portable, high fidelity, dynamic, training instrument capable of accurately representing the behaviour of the equipment, the instrumentation and the implemented control strategy in the nitric acid plants, interacting with the user with a series of operator screens, specifically selected among the HMIs available in the control system databases.

Associated benefits

ENADT, once deployed, would be used primarily to train control room operators on various aspects of the plant operations. It has been demonstrated that model-based training tools can provide operators with the equivalent of approximately six years of on-the-job training, and that periodic training, especially on critical emergency scenarios, brings operator skill levels to their highest level. Real-time dynamic simulators are recognised as the ultimate training tool because they allow experience to be gained in every type of operating condition in a virtual 'hands-on manner', including the following:

- Normal operation: various conditions around design.
- Unusual operating scenarios.
- Startup from cold conditions.
- Restart from tripped conditions.
- Shutdown, both normal and emergency.
- Equipment malfunctions.
- Emergency conditions and process upsets.
- Communication with field operators.

Moreover, simulator training is also one of the most cost-effective tools for operator training. A high fidelity simulator allows the operator to experience more operating situations in a relatively short period of training time, usually just before the plant is commissioned. An OTS therefore represents the best method for conducting supervised training exercises, which help to reduce personnel errors and consequently maximise plant availability. Consequently, the use of such training tools results in an increase in plant productivity and an improvement of product quality.
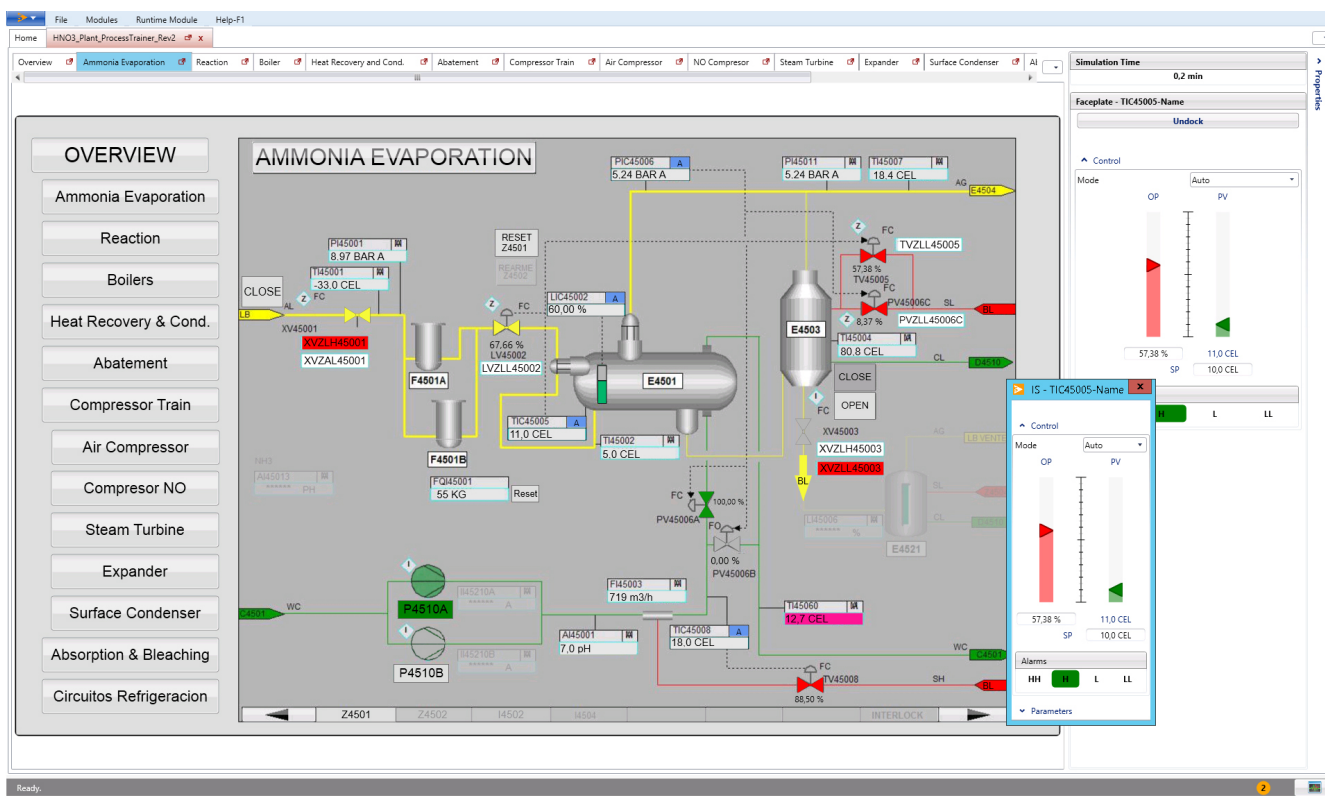
Figure 3. Human machine interface (HMI) with the mimic of the control room operators' interfaces.
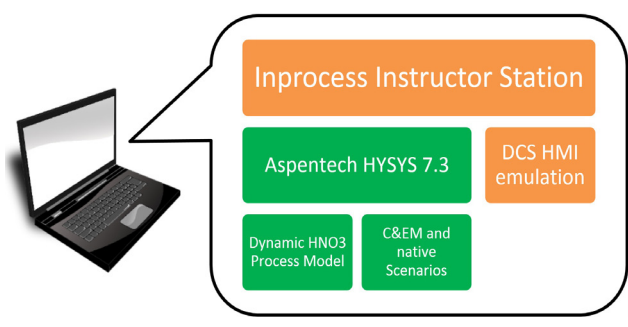

Figure 4. Architecture of the training tool.

Therefore, the following benefits can be achieved by proper operator training based on a dynamic simulation tool:

- Minimisation of startup time and therefore achieving steady production within a shorter time.
- Achievement of easier, more stable, on going production.
- Reduction or prevention of operating incidents, unnecessary trips and emergencies, which lead to an increased on stream production rate and a reduction in risk of equipment damage.
- Increase of operator confidence, which allows operation of the plant closer to the product specifications and process constraints.

In the present case, the nitric acid process, especially in dual pressure process technology, is mostly a continuous process. Startup and shutdown operations are infrequent but still very important. These transients may take a long time and the incorrect operation may lead to high emissions of NO_x in atmosphere. Few control room operators have the opportunity to experience those activities on the field. Consequently, most of them have little or no direct

experience with such procedures. The tool developed by Inprocess fills this gap and provides insight into the process outside of the normal operating conditions.

The process

Ammonia oxidation
The process air is filtered and compressed up to 3 − 4 bar in the first stage of the compression system.

The evaporated ammonia is reheated, filtered and mixed with process air before entering the ammonia burner where Pt-Rh catalyst and getter gauzes are placed. Temperature reaches 870 − 890°C. The reactor can include a N_2O abatement catalyst to reduce N_2O levels lower than 50 ppm in the tail gas.

The process heat is recovered in a series of heat exchangers, where temperature is decreased from reaction temperature to 145°C. At this point, the gases enter the low pressure cooler-condenser, which cools them below dew point, so most of the water produced in the ammonia oxidation reaction condenses in the form of a 30% nitric acid stream. This is separated from the gas and pumped to the appropriate tray of the absorber.

Process gas compression and cooling
The dry cool process gases are mixed with the secondary air after it has been used in the bleaching tower to strip most of the free NO_x remaining in the product acid. Then, they are compressed to 8 − 11 bar, with a temperature increase to 200°C.

In the pipes downstream of the compression system, the NO contained in the process gas reacts with the oxygen of the secondary air and it is oxidised to NO_2. Two further heat exchangers lower the process gases temperature down to 50°C before entering the absorption tower.

Absorption

By the time the gases reach the absorption tower inlet, the oxidation of NO to NO_2 has been completed. Absorber internals are sieve trays with integral cooling coils. The required number of trays depends on the allowed NO_x content in the exhaust gas. If values below 200 ppm are required, then a catalyst for $DeNO_x$ abatement would probably be necessary.

The nitric acid solution leaving the bottom of the absorber is of reddish colour due to the presence of free dissolved NO_2. The colour is eliminated by counter-current bleach with the secondary air in a small sieve tray column. After bleaching, the acid product is colourless and contains less than 20 ppm of NO_2.

Tail gas leaves the absorber at approximately 10 bar and 20°C before being reheated to 420°C in a series of three heat exchangers. Gases are sent to the gas turbine, which recovers approximately 70% of the power required to drive the compression system. The rest of the power is provided by a steam turbine.

Dynamic modelling challenges

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, etc.) and the specificity of the equipment used in these units (absorption columns for nitrous vapours by aqueous nitric acid solutions: autocatalytic chemical reactions in gas phase, mass transfer with chemical reaction in liquid phase, plate or packing towers, spray columns, plate coolers, etc.) make the dynamic simulation of these processes very complex with general purpose dynamic simulation software.

However, Aspen HYSYS®, a general purpose process simulator, has the advantage of being easily extensible (through object-oriented programming), although it is much better recognised for its emphasis on the hydrocarbon processing industry. On top of that, the Inprocess staff has a history of success using the dynamic capabilities of Aspen HYSYS in more than a hundred projects related to engineering design studies or, as in this project, to create a dynamic replica of the operating plant, with the associated emergency shutdown (ESD) and programmable logic controller (PLC) systems, incorporating the operating procedures, capable of shutting down and starting up the plant.

To successfully overcome some of the known modelling limitations of Aspen HYSYS for chemically complex processes, Inprocess applied the following tailored solutions:

- Development of a dynamic stage-by-stage absorption column (the standard absorber block did not allow all of the phenomena occurring in the real NO_x absorber to be combined). Figure 2 shows the match between simulated results obtained with Inprocess approximation and real plant data.
- Combination of thermodynamic packages (equation of state (EOS) and activity models) with properly tuned binary interaction parameters, and reverse calculation of densities.
- Programming of a dynamic kinetic reaction extension to model the autocatalytic type of reaction occurring in the absorption area.

- Model discretisation by the implementation of continuous stirred tank reactor (CSTR) cascades to describe dynamic pressure-flow behaviour inside pipes with reactions.
- Implement heuristic equations beside first principle equations to improve the efficiency of the dynamic model and increase the speed of the simulation.

Simulation tuning

The high level of detail included in the simulation allows for a precise dynamic representation, but the tuning of the model was a fundamental step to achieve the required level of accuracy.

The tuning required the comprehensive optimisation of the following:

- Thermodynamic parameters.
- Kinetic parameters.
- Discretisation of reaction areas.
- Equipment tuning.
- Heuristic relationships tuning.

This optimisation was not only aiming to reach a good representation of the steady state conditions, but had the main goal of being able to reproduce accurate representations of the dynamic transients.

The capability of capturing the transient behaviour of the system in the dynamic model was key in ensuring the future success of the whole project. This was not an easy task. Just to give a clue on how complex the system was, the whole of the plant downstream the oxidation reactor (piping, exchangers, vessels, etc.) was also behaving like an oxidation reactor, with kinetic limitations in the gas phase. Such a situation makes the nitric acid production (and the NO_x emissions) strongly dependant on the residence time of the gases in these pipes and equipment, a physicochemical phenomenon that was necessary to be well captured by the model. Additionally, and due to environmental limitations, the amount of NO_x (in the level of ppm) was one of the key and sensitive variables in the process and thus, to represent it well enough, the simulation model needed to achieve high precision, having to reach an accuracy of few ppm in a stream of several metric tonnes of flow.

An appropriate tuning was possible only through a detailed and extensive dynamic testing of the model over a wide variety of tests covering the interaction between all the major variables. The following provides a set of scenarios used for testing purposes (not comprehensive):

- Turndown operations.
- Ammonia evaporation and chilling loss on absorption column.
- Condensate loss on absorption column.
- Cooling loss on the absorption column.
- Change on the distribution between primary and secondary air flows.

Each test was validated by the licensor of the process, which also helped to improve the simulation quality and flexibility. Through these enhancements, the ENADT tool was mathematically robust and accurate enough to run normal plant operating conditions and emergency scenarios, as well as shutdown and startup procedures.

Evolution to a training tool

Once the dynamic simulation model was ready and capable of reproducing known real plant behaviours, it was improved by incorporating the real control strategy, the safety system logics and the associated operating procedures. To provide an agile training tool, the architecture was kept as simple as possible with logics and automated procedures integrated with the process simulation inside the Aspen HYSYS software. Inprocess combined its own software product, Inprocess Instructor Station (IIS), to reproduce a series of HMI screens, starting from the distributed control system (DCS) snapshots, with the aim of mimicking the behaviour of the control room operators' interfaces.

The communication between the emulated HMI and the Aspen HYSYS process variables and logics is also handled through the IIS software, providing the framework and end-user interface of the application.

In order to incorporate automatic sequences and manual operations carried through the IIS HMI emulation, Inprocess developed Aspen HYSYS user variables, which were used to manage the priorities on an event-based logic preventing conflicts between embedded sequences and end-user actions.

The ENADT resulted in a tool that:

- Holds all of the basic meta-functionalities of an OTS (start/stop the simulation, save and load snapshots, etc.).
- Allows the interaction of the user with the dynamic simulation through custom-made HMIs.
- Permits the execution of complex automated scenarios with the interaction of the user (startup and shutdown).

- Provides monitoring and gathering on simulation data.
- Provides an alarm management system for training purposes.
- Accurately simulates the behaviour of the nitric acid plant under emergency conditions.

Inprocess' technology approach was thoroughly validated by Espindesa, ensuring that a training experience based on dynamic simulation could accurately (based on its proprietary criteria) represent the behaviour of its nitric acid plants.

Conclusion

Espindesa is now in possession of a tool that is able to provide final users and owners of its nitric acid technology with a training tool valid for engineers and operators. It also owns a portable instrument capable of providing process demos directly on potential clients' facilities.

Although not the most common tool for such applications, Aspen HYSYS dynamics has demonstrated rigour and flexibility when simulating the unit operations, the control strategy, and the instrumentation involved in nitric acid plants.

The collaboration between Inprocess and Espindesa was the key element of success of the project. Inprocess' experience in the development of a customised dynamic simulation model, in developing simulator extensions, in implementing control strategies, in creating HMIs, in transferring its knowledge to its clients, and the deep knowledge of the process carried by Espindesa, allowed the creation of a flexible and rigorous digital twin for the nitric acid process. **WF**