Available online at www.sciencedirect.com
ScienceDirect
Procedia Engineering 83 (2014) 215 – 224
Procedia Engineering
www.elsevier.com/locate/procedia

"SYMPHOS 2013", 2nd International Symposium on Innovation and Technology in the Phosphate Industry

Dynamic operator training simulators for sulphuric acid, phosphoric acid, and DAP production units

Coral Siminovich[a], Sergio Joao[a]*

Global Training & Simulation Services, Division of SNC-Lavalin Inc., 360 St-Jacques Street West., Suite 800, Montreal, Quebec H2Y 1P5, Canada

---

Abstract

Dynamic process simulators are widely used in the chemical and petrochemical industries for operator training, plant design, and optimization; but there is a lack of rigorous simulators in the phosphate fertilizer industry. Some of the many difficulties encountered in phosphate fertilizer simulation include: lack of knowledge of thermodynamic properties, presence of many phases (gas, liquid, and solids), high levels and variation of impurities in phosphate rock producing unknown effects, complexity in modeling particle size distribution, etc. Dynamic training simulators were successfully developed for sulphuric acid, phosphoric acid, and DAP production units of OCP Group's Jorf Lasfar complex using a commercial simulation platform. A new thermodynamic property package was developed for sulphuric acid and oleum to correctly predict vapor pressure, density, enthalpy, and SO_2 solubility. Also, a rotary drum granulator was developed to consider the reaction chemistry of DAP production and the stochastic nature of solids created. The granulator can accurately predict particle size distribution, moisture content, ammonia and dust losses, and gas/solid temperatures. It was shown that the simulators could precisely reproduce control room and field operations to model plant start-ups, emergency or normal shutdowns, process upsets, and normal operations.

Peer-review under responsibility of the Scientific Committee of SYMPHOS 2013

Keywords: Operator Training Simulator; simulation; sulphuric acid; phosphoric acid; DAP

---

1. Introduction

It is estimated that in the U.S. alone, $10 billion are lost annually in the process industries due to plant operator error when faced with process upsets [1]. Operator training is therefore the key to reducing losses as well as incidents. Operator Training Simulators (OTS), are dynamic representations of the plant particularly beneficial for improving operator response when faced with critical process upsets, training operators faster, and achieving quicker startups. Operators are given full access of their virtual plant, allowing them the ability to learn as well as make mistakes without exposing anyone to any danger or cutting down on the plant's operational time. The operator can practice and master his response to high risk situations which require outstanding performance under high amounts of stress and pressure.

A typical OTS project consists of a model, the graphics, and the simulation user interface. The model is based on reliable physical phenomena, kinetics, mass, heat and momentum transfer, and thermodynamics, allowing precise reproduction of plant behavior during all operating situations; transient and steady state [2]. The simulation environment is composed of basic unit operations such as pumps, valves, and vessels, combined with a user specified fluid package, which will determine the equations of state for the calculation of thermodynamic and physical properties such as enthalpy, density, and compositions [3]. For the

---

* Corresponding author. Tel.: +1-514-845-2166x2250; fax: +1-514-845-2073.
E-mail address: sergio.joao@snclavalin.com

1877-7058
Peer-review under responsibility of the Scientific Committee of SYMPHOS 2013
doi:10.1016/j.proeng.2014.09.041

projects which will be discussed, the plant controls, logic, and emergency shutdown system are all simulated within the model and mimic the functionality of the actual DCS. The DCS graphics are replicated and communicate with the model through the simulation user interface. Training scenarios and exercises, which are accessible through the simulation user interface, are configured to represent process upsets, plant start-ups and shutdowns, and equipment and transmitter malfunctions. Manual operations such as manipulation of field valves or sampling and lab analysis are included in the model and are accessed from the simulation user interface through a set of graphics specially conceived for such purpose. Changing ambient temperatures or raw material composition can also be simulated and set by the instructor.

Even though dynamic simulation has become increasingly essential for plant design, optimizing costs, productivity, ensuring safety [4], and is widely used in chemical and petrochemical industries, there is a lack of rigorous simulators in the phosphate fertilizer industry. Phosphate fertilizers have become central to the agricultural market. With an increase in production over the past forty years of 31 million metric tons and production expected to reach 55 million metric tons by 2030 [5], it is a vital industry that should not be overlooked. Some of the many difficulties encountered in phosphate fertilizer simulation include: lack of knowledge of thermodynamic properties, presence of many phases (gas, liquid, and solids), high levels and variation of impurities in phosphate rock producing unknown effects, complexity in modeling particle size distribution, etc.

Three OTS were successfully developed for OCP Group's Jorf Lasfar sulphuric acid, phosphoric acid, and DAP production units using commercial software (Honeywell's Unisim Operations Suite R410). The simulators were developed as part of the OCP Skill program , a large training program aimed at developing the skills of new hires and subsequently its existing workforce. This article will discuss each simulator and the results achieved by these models.

Nomenclature

DAP	Di-ammonium phosphate
DCS	Distributed Control System
MAP	Mono-ammonium phosphate
NP	Nitrogen-Phosphorus
NPK	Nitrogen-Phosphorus-Potassium
OTS	Operator Training Simulator
PSD	Particle Size Distribution

2. Developed simulators

The simulators were developed jointly by SNC-Lavalin and OCP Group, hereafter named OCP, and are based on the corresponding units of OCP's Jorf Lasfar complex. They were built according to design (mainly equipment datasheets and P&IDs), heat and mass balances (provided by OCP or calculated based on design/plant conditions), and operating data (DCS and historians). All relevant DCS, ESD, local controls and logic were simulated to replicate control functionality. The graphics were all built to represent the DCS graphics and local panels with a high level of detail.

The simulators not only incorporate process and control functionality, but also additional features such as being able to run the model at least three times faster than real time, giving the operator trainee the ability to fast forward trivial steps (i.e. filling a tank with water) and concentrate on the more demanding tasks of a start-up. This feature is also useful to be able to quickly see the final process response to a step test, especially for processes such as DAP production units where residence times are significant.

The exercises and training modules included a scoring system, which allows to evaluate the trainee's response to abnormal situations, start-up and shutdown, based on pre-defined criteria (i.e. the ability of the operator to maintain key process variables in a certain range). The instructor can then choose to evaluate the trainee himself or let the simulator do the evaluation, adding flexibility to the models and saving resources since the instructor's presence is not necessarily required.

Throughout model development, reviews and tests were performed with experienced plant operators and engineers from OCP. This validation not only reviewed the model scope and steady-state conditions, but ensured that all three simulators accurately respond to normal and abnormal operating situations. Tests included plant start-up, shutdown, step tests, as well as process upsets. The acceptance criteria for all three simulators was a maximum of 5% deviation between the model and actual plant/design data for key parameters, and directionally correct behavior with less than 10% deviation for transient scenarios. The percent deviation was based on the variable's transmitter range.

2.1. Sulphuric acid OTS

The sulphuric acid model contains the main areas in a sulphuric acid production plant which are: combustion, conversion, and absorption, excluding the sulphur fusion area. A high-level process schematic can be seen in Fig.1.

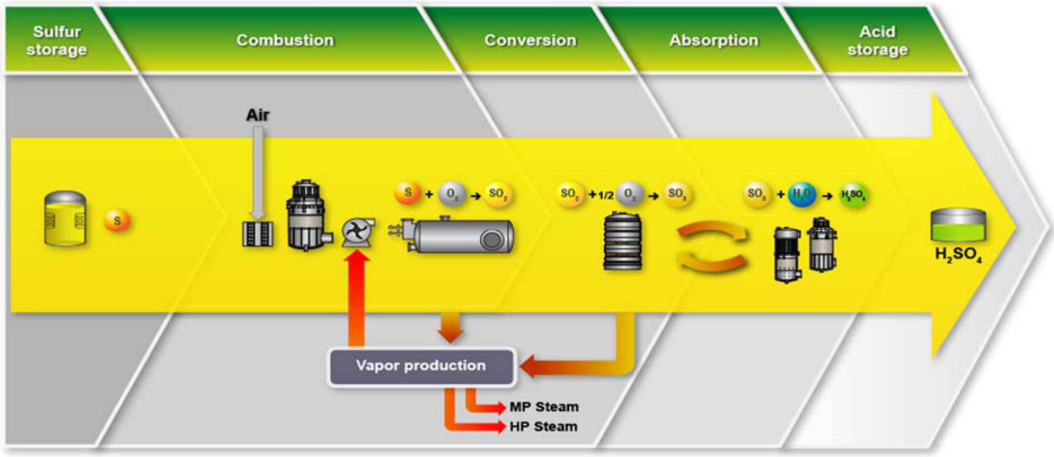


Fig.1 General overview of sulphuric acid production process

In the combustion section, liquid sulphur will react with oxygen present in air to produce mainly sulphur dioxide. The hot gases leaving the burner are used to produce high and medium pressure steam from feed water. In the conversion section, sulphur dioxide will oxidize in the presence of a catalyst to product sulphur trioxide. The sulphur trioxide will then be absorbed to produce sulphuric acid in the absorption section. In this section, the sulphur trioxide gas and 98.5% sulphuric acid are fed counter-currently to absorption towers where the gas will react with the water present in the sulphuric acid to produce more sulphuric acid.

The non-ideal and electrolytic nature of the system and the lack of a fluid package in the simulation platform that could correctly predict the interactions of sulphuric acid with water, sulphuric trioxide, and sulphuric dioxide, made it necessary to develop a specific fluid package robust enough to model transient behavior and maintain faster than real time requirements. The development of this fluid package concentrated on addressing the following for the aqueous sulphuric acid system: vapor pressure, density, enthalpy, and solubility of sulphur dioxide. Fig. 2-3, and Tables 1-3, show a comparison of some of the results obtained with the model against literature [6-7] and design data for aqueous sulphuric acid systems. It is important to note the versatility of the fluid package developed, since it can not only predict very well the system's properties (the deviation between the model and literature being less than 5%), but do so for a range of sulphuric acid concentrations and temperatures. In addition, the same fluid package was also developed to handle solutions of sulphur trioxide in sulphuric acid (i.e. oleum).

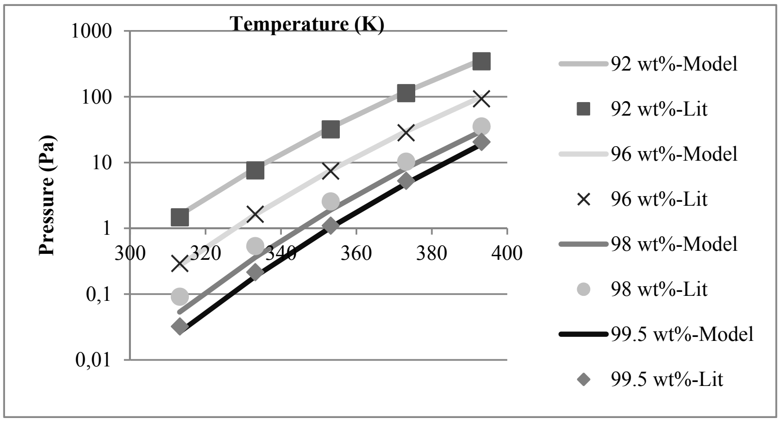


Fig. 2. Model total vapor pressure results for strong sulphuric acid aqueous systems against literature data [6].

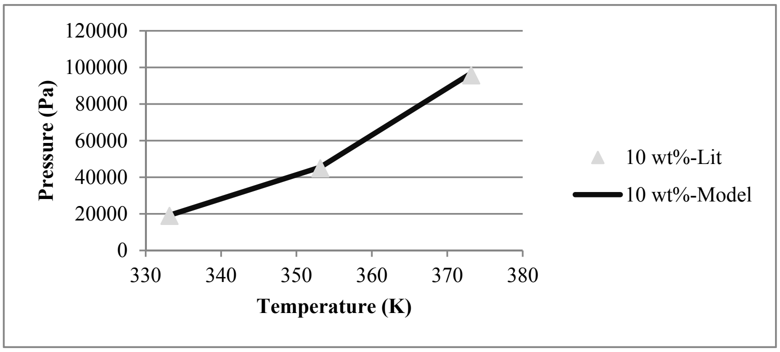


Fig. 3. Model total vapor pressure results for weak sulphuric acid aqueous system against literature data [6].

Table 1. Model density results for sulphuric acid aqueous systems against literature data [6].

		Model	Literature	
H_2SO_4 wt%	Temperature (K)	Density (kg/m3)	Density (kg/m3)	% Error
10	313	1056	1056	0.01
10	333	1040	1045	0.49
92	313	1832	1802	-1.71
92	333	1818	1781	-2.05
96	313	1848	1814	-1.90
96	333	1834	1795	-2.19
98	313	1847	1815	-1.78
98	333	1832	1796	-2.04
98.5	313	1844	1814	-1.65
98.5	333	1831	1795	-2.00
99.5	313	1839	1811	-1.55
99.5	333	1828	1792	-1.97

Table 2. Model sulphur dioxide solubility results for sulphuric acid aqueous systems against literature data [7].

		Model	Literature	
H_2SO_4 wt%	Temperature (K)	Concentration of SO2 in solution (g/100 g solution)	Concentration of SO_2 in solution (g/100 g solution)	% Error
92	313	2.16	2.08	-3.79
92	353	0.76	0.75	-1.27
96	313	2.25	2.16	-4.35
96	353	0.79	0.78	-1.46
98	313	2.30	2.20	-4.66
98	353	0.81	0.80	-1.59
98.5	313	2.31	2.21	-4.76
98.5	353	0.81	0.80	-1.61
99.5	313	2.34	2.23	-4.96
99.5	353	0.82	0.81	-1.68

Table 3. Model duty prediction against design data for common process heat exchangers.

Exchanger	Design Duty (J/s)	Model Duty Prediction (J/s)	Error %
Dry Cooler	1.89E+07	1.97E+07	-3.96
Product Cooler	3.08E+06	3.00E+06	2.34

It was possible to not only match plant design conditions, but to also model transient conditions with high accuracy. In addition, equipment itself was modeled based on literature data as much as possible. For example, absorption towers incorporated factors affecting efficiency into calculations, such as acid to gas ratios that could affect contact between phases; and conversion rates in the converters were accurately calculated based on equilibrium curves and catalyst activity. Table 4 shows results between predicted converter temperatures and plant design data. There are small temperature differences due to enthalpy errors (see Table 3) and the fact that, contrary to the simulator, plant design considers perfect SO_3 absorption in the towers and no SO_2 in acid, as well as no equipment heat losses.

Table 4. Model converter temperatures against design data.

Converter temperatures (K)		
	Design data	Model
Bed 1 in/out	693 / 877	693 / 874
Bed 2 in/out	727 / 818	724 / 812
Bed 3 in/out	722 / 757	716 / 749
Bed 4 in/out	698 / 728	693 / 723

The complex start-up, including long tasks such as pre-heating of the sulphur burner, was shown to reproduce the actual plant behavior all throughout its duration. The ability to run the model 25 times faster than real time was shown particularly advantageous for the start-up of this process, since it can take approximately 6 days to completely start the plant. For an easier and more convenient training, the start-up was divided into 6 training exercises; which also allowed the trainee to repeat and focus on specific and more challenging scenarios during the start-up without having to spend additional time in other sections.

The model was not only able to perform well under transient conditions encountered during start-up and shutdown, but also during process upsets. Some of the process upsets that were considered and included in the training scenarios were: high acid concentration, heat exchanger fouling, valve plugging, and loss of feed water. The latter process upset would entail an emergency shutdown which would require the utmost operator alertness and critical skills; emphasizing the importance of adequately training operators to be prepared for such situations.

2.2. Phosphoric acid OTS

The phosphoric acid production process considered is carried out in the following stages: thickening, attack and filtration, storage of weak acid, acid concentration, and storage of strong acid. A high-level overview of the process is shown in Fig. 4. The scope included two OTS models for phosphoric acid. The first one included storage of weak acid, acid concentration, and storage of strong acid. The second OTS dedicated to thickening, attack and filtration is currently in the early stages of development; however a heat and mass balance was performed and shown to closely match design data but will not be discussed here.

After weak acid (29% P_2O_5) is produced in the attack and filtration units, the content of impurities in the acid is reduced in the storage section by precipitation due to a decrease in temperature. In the concentration section, water and some volatile impurities will then evaporate from the 29% P_2O_5 clarified acid. Acid concentration is carried out under vacuum conditions and in a continuous manner in the evaporator. Gases from the evaporator are then condensed by direct contact with water, and non-condensables are removed through a vacuum pump. The final storage unit receives the concentrated strong acid (54% P_2O_5) from the evaporator. The strong acid storage section is very similar to the weak acid storage and impurities will be further removed by precipitation.

In the phosphoric acid industry, the different components coming in with the phosphate rock are analyzed and expressed as various theoretical (lab) but not real components [8]. A rigorous heat and mass balance, which is needed to accurately model the process and calculate fluid properties, cannot be performed using lab components. Since the model uses real components, a method was developed in order to convert simulation components to those used in the industry and vice-versa. For example, the simulator could either show concentrations based on H_3PO_4 (real) or P_2O_5 (lab). This was also helpful to display lab analysis results, which are available to the operator not only live, but with terms they are familiar with (i.e. P_2O_5, CaO, SO_3, F, SiO_2, Fe_2O_3, Al_2O_3, etc.).

Modeling the concentration section required special attention due to the very low operating pressure of the system (<10 kPa). An activity coefficient thermodynamic fluid package was selected and the vapor pressure of water was adjusted so that the right amount of evaporation could be obtained. Dynamic instabilities were nonetheless observed in the evaporator. In Fig. 5, small composition changes to the evaporator caused the flash to predict sudden and very rapid condensation of the vapor phase causing a large pressure drop. To overcome this issue and increase the robustness of the model, thermodynamic flash adjustments in the evaporator were found to be a good solution. Fig. 6 shows the improved process response and increased stability.

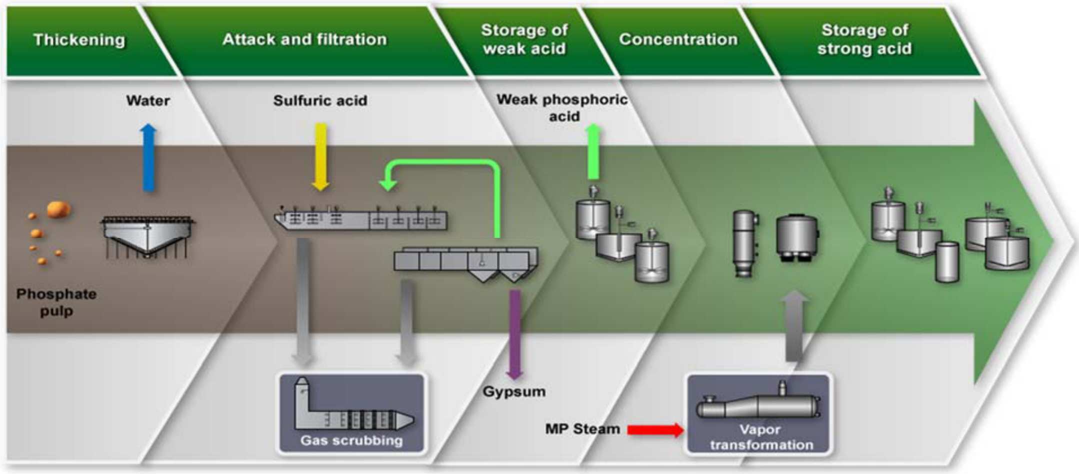


Fig. 4. General overview of phosphoric acid production process.

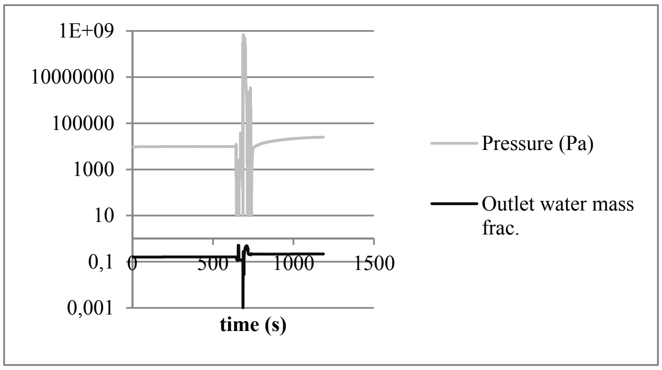


Fig. 5. Dynamic instabilities in evaporator.

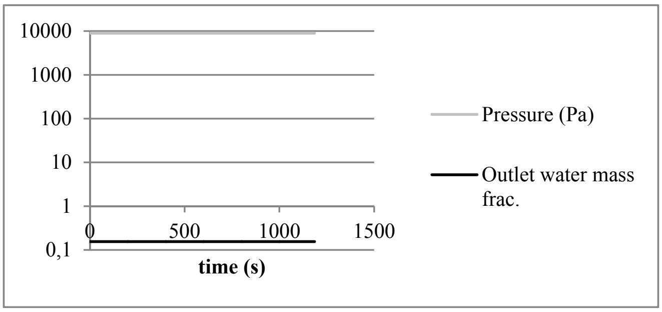


Fig. 6. Improved stability and robustness of evaporator.

The model can accurately predict P_2O_5% and solids% in all sections. The steady state values for not only the aforementioned parameters, but also for critical variables such as evaporator temperature and steam consumption, were shown to represent the plant with less than 5% deviation. In addition, the model was successfully able to reproduce start-up, shutdown, and process upset scenarios, such as power failure and loss of vacuum due to mechanical failure of the vacuum pump. Insufficient heating of the acid in the concentration section due to partial obstruction of the evaporator heat exchanger filter is an important training scenario that was also included. This is a common situation that may arise from solids accumulating and would require a shutdown. For that reason, it is essential that the operator learns to recognize the signs leading to such conditions and identifies the actions to be taken. In this case, the simulator showed a lower P_2O_5% production, which concurs with experienced operators observations.

2.3. DAP fertilizer OTS

The main steps in a typical DAP production process are: reaction, granulation, and drying; particle screening and crushing; and product cooling and coating. An illustration of this process is shown in Fig. 7.

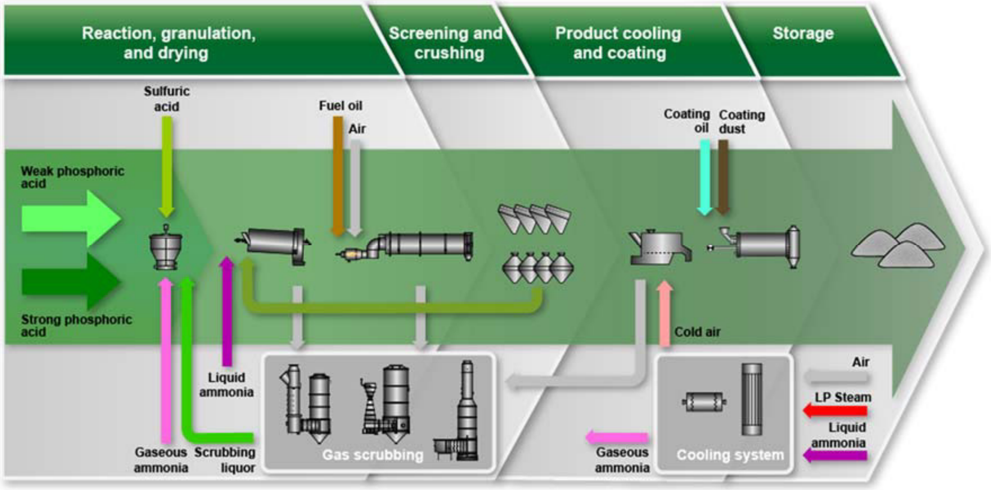


Fig. 7. General overview of DAP fertilizer production process.

The DAP production process begins in the pre-neutralizer, where part of the reactions to produce DAP will take place. Phosphoric acid, sulphuric acid, ammonia, and scrubbing liquor containing phosphoric acid and MAP/DAP from the gas scrubbing section, are all fed to the pre-neutralizer where ammonia will react with phosphoric acid to produce MAP. Once all phosphoric acid is depleted, MAP will react with any remaining ammonia to form DAP. Sulphuric acid will also react with ammonia to form di-ammonium sulphate; its main use being to reduce the amount of P_2O_5 in the product. The MAP/DAP slurry is then fed to the rotary drum granulator where recycled solids and ammonia are injected to increase the DAP formation reaction. Besides acting as a reactor, the granulator will also agglomerate the slurry and form humid phosphate fertilizer granules. These granules are then dried in a rotary drum dryer, where the water content of the particles is decreased. The solids are then screened according to their size; fines and part of the on-spec product are recycled directly to the granulator, while coarse particles are crushed before being recycled back into the process. On-spec product is then cooled and coated before being sent for storage. Gases out of the pre-neutralizer, granulator, and dryer, as well as dust collected throughout the solids loop, are scrubbed with phosphoric acid to recover most of the ammonia.

Even though particle size distribution (PSD) is rigorously calculated in the model in equipment such as screens and conveyors and propagated throughout, there were no existing unit operations in the software that could predict PSD, while taking into account the reaction mechanism and the many factors affecting granulation. The approach taken to address this issue was to partner with a third party company specializing in mathematical modeling of granulation equipment, to develop a high fidelity module to represent the granulator. The granulator takes into account particle formation by agglomeration, as well as the effects of the NP ratio and humidity content on the DAP formation reaction, amongst others.

The granulator module was able to predict PSD, moisture content, ammonia and dust losses, and gas/solid temperatures accurately in steady state and transient modes. Fig. 8 and 9 show the granulator response to an increase in recycled solids flow; the results show a decrease in product humidity due to the change in the solids to liquid ratio in the granulator, which causes a decrease in mean particle size. The opposite effect is seen in Fig. 10 and 11, as a consequence of an increase in slurry flow to the granulator. The reaction in the granulator was also shown to be correctly represented. As shown in Fig. 12, 13, and 14, a decrease in ammonia flow to the granulator will cause a decrease in temperature which will increase the moisture content and the mean particle size, as well as decrease ammonia losses.

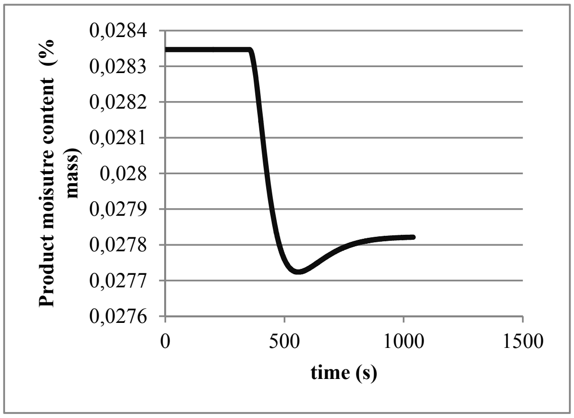


Fig. 8. Product moisture response to an increase in recycled solids to granulator.

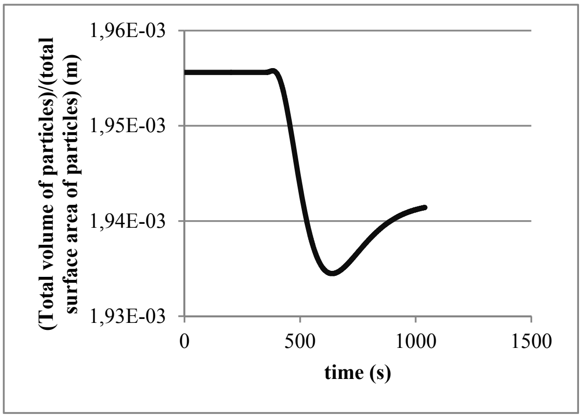
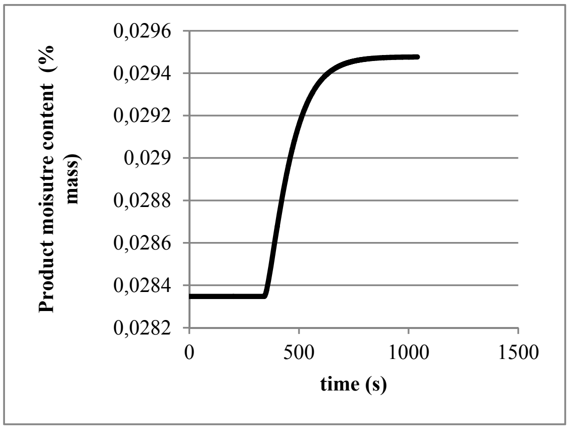


Fig. 9. Particle size response to an increase in recycled solids to granulator.



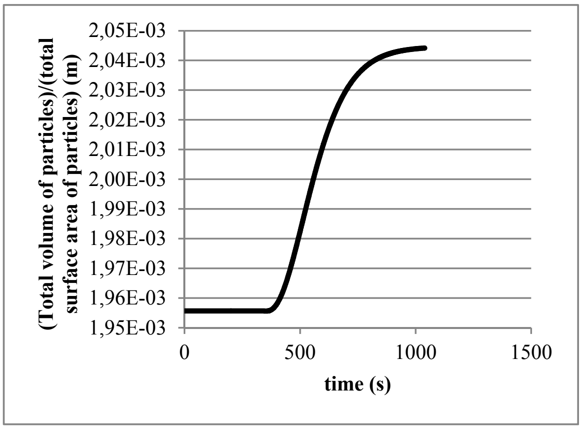


Fig. 10. Product moisture response to an increase in slurry flow to granulator.

Fig. 11. Particle size response to an increase in slurry flow to granulator.

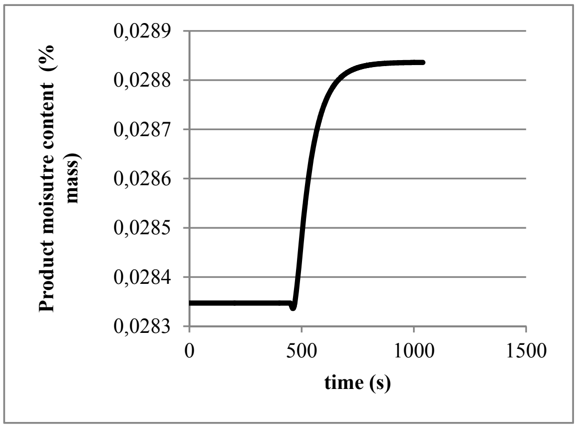


Fig. 12. Product moisture response to a decrease in ammonia flow to granulator.

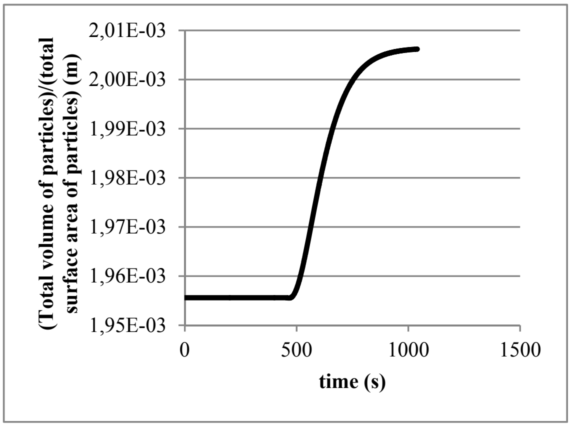


Fig. 13. Particle size response to a decrease in ammonia flow to granulator.

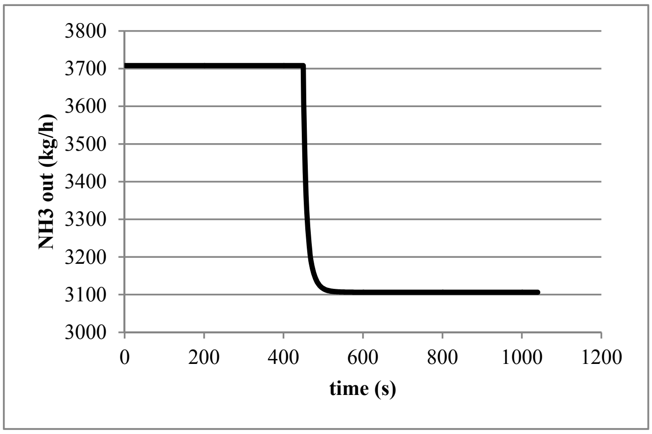


Fig. 14. Ammonia outlet flow response to a decrease in ammonia flow to granulator

A very important and characteristic feature of this process is also the constant change of phosphoric acid quality. The changes in composition for this raw material introduce instabilities and therefore require constant manipulation of process variables to maintain the desired operating conditions. This feature was successfully incorporated into the model by allowing the instructor to vary the composition of boundary streams and thus creating the desired effect.

The process intrinsic operating challenges were also successfully represented. For instance, slurry crystallization in the pre-neutralizer was considered and was based on solubility curves dependant on temperature and NP ratio. This allowed to represent the very narrow operating range in the pre-neutralizer, which must be carefully maintained by the operator to preserve maximum fluidity of the slurry. Additionally, the ammonia vapor pressure dependence on temperature and NP ratio was incorporated in the pre-neutralizer and granulator modules, so that the DAP formation reaction could be accurately represented, making it difficult for the operator, for instance, to increase the NP ratio beyond its normal operating value without having to very significantly increase the amount of ammonia injected and deal with a considerable amount of nitrogen loss to the environment.

Some of the most common process upsets were also incorporated to the model as training exercises. Conveyor and crusher mechanical problems, poor distribution of ammonia and slurry in the granulator, as well blockage of screens, are amongst the most common upsets. Equipment's current (amps) indicators were also modeled and shown to be accurate during failures. Obstruction of lines downstream of the granulator due to very coarse particle production, and which would lead to a fast shutdown, was also configured as a training module. By implementing these upsets on the model, the operator is faced with real and common issues occurring at the plant, exposing, training, and reducing reaction times in such high pressure situations.

This model was able to closely match the current steady state operating conditions for key parameters, such as those shown in Tables 5-6.

Table 5. Model results for pre-neutralizer key variables against plant data.

Pre-neutralizer		
	Plant data	Model
NP ratio	1.41 – 1.54	1.52
Temperature (K)	391 – 394	393
Density (kg/m3)	1510 - 1545	1540

Table 6. Model results for finished product key variables against plant data.

Product		
	Plant data	Model
N %	17.45 – 18.54	17.89
P %	45.53 – 47.97	47.1
Water mass %	1 – 2.2	1.1

The start up behavior was shown to be directionally correct even in the most critical start-up scenarios, such as the pre-neutralizer ammoniation for which correct reaction rates, densities, temperatures, and NP ratio were obtained. Dynamic behavior was validated by experienced operators and demonstrated to be correct throughout transient conditions.

3. Conclusion

It has been proven that OTS is an effective tool for cutting losses as well as incidents related to human error [1]. Operators are trained using a hands-on approach, leading to better and quicker operator response during abnormal situations. The growing phosphate fertilizer industry lacked OTS models because of the challenges encountered in phosphate related processes, including complex thermodynamics, composition of phosphate rock and levels of impurities, stochastic nature of granulator, etc.

High-fidelity simulators were developed for the sulphuric acid, phosphoric acid, and DAP units of OCP's Jorf Lasfar complex to train operating personnel on start-ups, shutdowns, and respond to process upsets in a safe way. In order to face previous challenges, a thermodynamic fluid package was developed to represent the non-ideal behavior of the sulphuric acid system. For phosphoric acid, a method was developed to easily convert between lab analysis and real components so a rigorous heat and mass balance could be performed. A granulator module was developed to properly predict and display particle properties and size distribution in DAP production.

All three simulators were shown to accurately represent the plant and were validated by OCP's operating personnel. The deviation between the models' steady state and design/plant operating conditions was shown to be less than 5%, and dynamic behavior shown to be directionally correct with less than 10% error. Start-ups, shutdowns, and process upsets, were all incorporated as part of training modules and exercises. The success of these new simulators in such a fast growing industry is predicted to decrease human (operator) errors, increase profits, and decrease accidents.

Future work will be done to expand the scope of the simulators to include other phosphate fertilizers (MAP, NPK) and processes, such as phosphoric attack tanks, filtration and beneficiation plant. It will also be investigated how simulator models can be reused to identify process bottlenecks and to validate process and control changes prior to implementation.

Acknowledgements

We would like to thank OCP for all the resources and technical contribution. The project would not have been possible without the assistance of Mr. Amine Louali, Mr. Hicham El-Habti, Mr. Youssef Lahmiti, Mr. Alaoui Driss, Mr. Mabrouk Kamal, Mr. Noufoussi Hassan, and Mr. Abdelouahed Tari. We would also like to thank SNC-Lavalin's E-learning and OTS teams for their help in the development of the project.

References

[1] Roe, A., Mason, J., Alamo, J., 2010. "The Role of Simulator Technology in Operator Training," Consulting-Specifying Engineer.
[2] Le Floc'h, J.G., Parmentier, F., 2005. Consider dynamic simulation for successful training, Hydrocarbon Engineering 84, p. 52.
[3] Delisle, M., Alamo, J., 2009. "High Fidelity Dynamic Simulation for the Mining and Metallurgical Industry," COM2009 – Conference of Metallurgist.
[4] Dissinger, G.R., 2008. Studying Simulation: A case for dynamic simulation as an important factor in the design and operation of a plant, Hydrocarbon Engineering 13, p. 113.
[5] Vance, C., Uhde-Stone, C., Allan, D., 2003. Phosphorus acquisition and use: critical adaptations by plants for securing a non renewable resource, New Phythologist 157, p. 423.
[6] Perry, R.H., Green, D., 1997. Perry's Chemical Engineers' Handbook, 7th Edition, McGraw Hill, New York, USA.
[7] Louie, D., 2008. Handbook of Sulphuric Acid Manufacturing, 2nd Edition, DKL Engineering, Richmond Hill, Canada.
[8] OCP Group Project: Internal Report for H_3PO_4 Conversion of Lab to Real Components, SNC-Lavalin div. GTS, July 2012.