UniSim-Design Simulation and Analysis of a Sulphuric Acid Manufacturing Plant with Double Absorption Process

Amine Mounaam[1,2], Yasser Harmen[2,4], Younes Chhiti[2,3], Ahmed Souissi[1,2], Mohamed Salouhi[1]
and Mohamed El Khouakhi[2]

[1]*All Laboratory, Ecole Mohammadia d'Ingénieurs, Mohammed V University, Rabat, Morocco*
[2]*Innovation Lab for Operations, Mohammed VI Polytechnic University, Ben Guérir, Morocco*
[3]*Ibn Tofail University, Kenitra, Morocco*
[4]*Science Engineer Laboratory for Energy (LabSIPE), National School of Applied Sciences,*
Chouaib Doukkali University, El Jadida, Morocco

Keywords: Sulphuric Acid, Modelling, Simulation, UniSim-Design, Chemical Reactions, Double Absorption Process, UniSim-Thermo, Peng-Robinson, NRTL.

Abstract: In the sulphuric acid manufacturing industries, plant modelling and simulation is a challenging task to minimize emissions, maximize production performance and revenue. In this context, this study presents the steady behaviour of a double absorption process of an industrial sulphuric acid plant. The closed-loop process is modelled and simulated using UniSim Design R451 simulator and validated with plant data. The model includes principally: conversion reactor, plug flow reactors, absorbers, heat exchangers, pumps and compressors. The parameters of the converter kinetic were fitted to the real plant data, while the other parameters were estimated using conventional correlations. The results show a good agreement for the complete plant, with an accuracy that exceeds 97 %. Besides the optimization aspects, UniSim Design plant model is also useful for operator training, simulation of diverse scenarios and development of processes digital twin.

1 INTRODUCTION

Worldwide, sulphuric acid is the most used chemical products in the basic chemical industry (Moats et al., 2006). Particularly, sulphuric acid plants are very important in the modern processing industry, because of its various applications; by far, in the phosphate fertilizer industry (Kiss et al., 2010). The industrial production of sulphuric acid was started with the combustion of sulphur in the presence of steam and natural nitrate. Nowadays, various technologies are available to produce sulphuric acid. The contact process is the most popular (Oni et al., 2018), overall, sulphuric acid is produced in two main steps: (1) oxidation of sulphur dioxide SO_2 to sulphur trioxide SO_3, and (2) absorption of SO_3 by diluted sulphuric acid to form concentrated sulphuric acid. Indeed, the contact process has passed through two stages: single absorption process, where 97 % of SO_2 is oxidized to SO_3 and the unoxidized SO_2 is emitted to the environment. Next, in 1968, the double contact

process was introduced to achieve 99.5 % or higher conversion rate, whereas the unreacted SO_2 and SO_3 are released to the environment (Moeller & Winkler, 1968). In this context, improving the performance of the double contact process to achieve high energy efficiency and maximize revenues, and minimize environmental impact remain major challenges (Lee et al., 2019).

In such case, two approaches are available: experimental tests and/or simulation and modelling. In fact, the experimental tests exhibit some drawbacks, such as high cost of materials acquisition and maintenance, and validity area of the solution complexity. In contrast, the main benefits of simulation and model-based control and optimization applications for industrial plants can be summarized as: minimization of the experimental tests time and cost, high flexibility in the process flowsheet elaboration with the ability to change and replace equipment (Boschert & Rosen, 2016), and also the development of processes digital twin (Parrott &

91

Warshaw, 2017). Therefore, several stationary and dynamic modelling and simulation studies have been performed to optimize the sulphuric acid manufacturing plant. In particular, numerous studies have been conducted on the steady and dynamic modelling of SO_2 oxidation reactors, which focused on the design and operating conditions. For example, Günther et al. (Günther et al., 2012) developed a mathematical model to describe the dynamics oxidation of SO_2 to SO_3. The results proposed a new design for zero-emission to the environment. Also, Mann et al. (Gosiewski, 1993) proposed a new dynamic simulation based on ordinary differential equations, which describes the behaviour of a single-bed reactor in the contact sulphuric acid plant, thus, several variables have been studied, such as flow start-up and initial fixed-bed reactor temperatures. Interestingly, the results showed that the model can be used for the qualitative analysis of SO_2 oxidation. Recently, Sørensen et al. (Sørensen et al., 2015) validated a dynamic model of SO_2 oxidation using experimental data from a sulphuric acid pilot plant. The results demonstrated that the dynamic simulation can efficiently be used to evaluate operating conditions, equipment sizing with respect to the environmental impact.

In contrast to the previous studies, few studies were conducted for the complete sulphuric acid plant. Notably, Kiss et al. (Kiss et al., 2010) presented a complete model of an industrial sulphuric acid plant using gPROMS tool. The results demonstrated that 40% of SO_x emissions can be reduced by the optimization of the split fraction or feed flow rates. In addition, they developed an excel interface, which simulates the real behaviour of the plant. Also, the results of Oni et al. (Oni et al., 2018) showed that the process can be operated at different optimal conditions, and the ideal conditions was 9.5 ppm of SO_x and 70.9 ppm of acid mist and 143.0 M\$/y of net revenue. Likewise, Rahman et al. (Rahman et al., 2019) developed a new model that offers a cost-effective solution to reduce energy demand and limit emissions of aromatic compounds. In addition to the above-mentioned study, Chowdhury et al. (Chowdhury et al., 2012) simulated and optimized a simplified process for the production of sulphuric acid using Aspen HYSYS simulator. The results exhibited that the process plant simulation is an effective approach to optimizing annual profit. On the other hand, various limitations are noted in the models mentioned, for example, the non-consideration of the thermal kinetics of the conversion reactions, which is a key step in the sulphuric acid manufacturing plant.
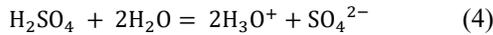
Based on the previous investigations, a considerable effort has been made to improve the performance of the double-absorption contact process. Indeed, these studies were based on multi-objective optimization, which considers environmental impact as a main objective such as sulphuric acid production. In this context, it is important to dispose of more powerful and flexible modelling and simulation solutions, which reflect the experimental plant reality, and resolve the limitations of the existed models. In this study, the closed loop of sulphuric acid process is modelled and simulated using UniSim Design R451 simulator and validated with plant data.

2 PROCESS DESCRIPTION

The simplified bloc-flow diagram of the sulphuric acid manufacturing process with double absorption is presented in Figure 1.

Firstly, moist air is filtered in an air filter to eliminate particles contained in the air. To reduce its moisture content, the air is dried by absorption in a drying tower using the circulating sulphuric acid H_2SO_4. The liquid sulphur that has been prepared in the melting unit is burned with the dry air in the sulphur burner, which forms the sulphur dioxide SO_2. The reaction of sulphur combustion is exothermic; thus, a waste heat boiler is paced at the outlet of the sulphur burner to recover the heat of the sulphur combustion and generate the saturated steam. As the optimal required temperature for the sulphur dioxide SO_2 conversion is 420°C, a by-pass of the sulphur burner is mixed with the waste heat boiler outlet to regulate the desired temperature. The conversion of SO_2 into SO_3 is carried out in a converter formed by four catalytic bed. The vanadium oxide V_2O_5 is used as a catalyst to accelerate the SO_2/SO_3 conversion. In order to reach the high desired conversion on SO_2, the gaseous outlet flow of the 1st converter bed passes through an inter-pass heat exchanger to regulate its temperature before feeding the 2nd converter bed. Between each bed of the four converter beds, heat exchangers and economizers are used for the same raison. After passing the three first beds of the converter, the outlet flow of the 3rd bed feeds the first absorption tower, in which the SO_3 formed reacts with the H_2O presented in the diluted circulating H_2SO_4 98% to form the concentrated H_2SO_4 99%.

The outlet gas flow of the first absorption tower feeds the 4th bed of the converter where the remained SO_2 is converted to SO_3, before feeding the second absorption tower in order to absorb the formed SO_3.

Figure 1: Bloc-flow diagram of the studied process.

The conversion rate of SO_2/SO_3 is 99.99%, and the absorption rate of SO_3 absorption in water is around 99.98%. Also, a sulphuric acid circulation tank is used to feed the drying tower, the first and the final absorption tower with the circulating sulphuric acid. The cold fluid used to cool the sulphur acid in the acid cooler and the product acid cooler is sea water. Boilers at the liquid outlet of the first absorption tower is used to recover the energy produced by the absorption reaction.

3 PROCESS SIMULATION

3.1 Components

In this study, UniSim-Design R451 simulator was used to perform the simulation of the studied sulphuric acid manufacturing process.

The simulation goes through two principal steps: the basis environment configuration and the simulation environment configuration. At the basis environment stage, the necessary components included in the manufacturing process are added, and the appropriate fluid-packages must be chosen to ensure a correct prediction of flow and mixture properties according to their temperature and pressure. At the simulation environment stage, material and energy streams are added and configured. Also, the flowsheet of the studied process is elaborated. Finally, the different reactions that governs the process must be specified. For the sulphuric acid manufacturing process, all the required components are available in the simulator components library, except the raw solid sulphur which has been replaced directly by the liquid sulphur. The components used in this simulation are represented in the following table:

Table 1: UniSim Design components list for the sulphuric acid process simulation.

Component name	Component formula
Oxygen	O_2
Nitrogen	N_2
Water	H_2O
Sulphur liquid	S
Sulphur dioxide	SO_2
Trioxide sulphur	SO_3
Sulphuric acid	H_2SO_4

3.2 Fluid-packages

The UniSim-Thermo was selected as advanced thermodynamics in this simulation. The non-random two-liquid model (NRTL) model was selected for the liquid phase. It is used to correlates the activity coefficients of the different components presented in liquid phase according to their mole fractions. The Peng-Robinson (PR) model was selected for the vapor phase. Henry's Law was selected for the Henry constant and solubility coefficients estimation of gaseous components in sulphuric acid, especially water and trioxide sulphur.

3.3 Reactions

As mentioned above in the process description section, four reactions are involved in the acid sulphuric manufacturing process:

$$S + O_2 = SO_2 \qquad (1)$$

$$SO_2 + \frac{1}{2} O_2 = SO_3 \qquad (2)$$

93

$$SO_3 + H_2O = H_2SO_4 \tag{3}$$

$$H_2SO_4 + 2H_2O = 2H_3O^+ + SO_4{}^{2-} \tag{4}$$

The reaction (1) represents the sulphur combustion within the sulphur burner. The reaction (2) describes the conversion of the sulphur dioxide SO_2 to the sulphur trioxide SO_3 using V_2O_5. The reaction (3) represents the sulphur trioxide SO_3 absorption in water H_2O within the two absorption towers, while the reaction (4) represents the sulphuric acid H_2SO_4 dilution with the water absorbed in the drying tower. All four reactions are exothermic and generate an enormous amount of energy

3.4 Unit Operations Simulation

The combustion of the liquid sulphur was simulated using an adiabatic conversion reactor. The combustion is considered complete with full consumption of liquid sulphur. The mass balance of the sulphur burner is given by the following equation:

$$\dot{N}_{i,out} = \dot{N}_{i,in} + \nu_i . \xi \tag{5}$$

$$\dot{H}_{out} = \dot{H}_{in} + \xi . H_{reaction} \tag{6}$$

$$\dot{H}_{in} = \sum_{i=1}^{4} h_{i,in} \dot{N}_{i,in} \tag{7}$$

$$h_{i,in} = \int_{T_0}^{T_{in}} C_{p,i}(T) . dT \tag{8}$$

$$\dot{H}_{out} = \sum_{i=1}^{4} h_{i,out} \dot{N}_{i,out} \tag{9}$$

$$h_{i,out} = \int_{T_{in}}^{T_{out}} C_{p,i}(T) . dT \tag{10}$$

Where:
- $\dot{N}_{i,in}, \dot{N}_{i,out}$: inlet and outlet molar flow of the component i (mol/h);
- ν_i : stoichiometric coefficient of the component i in the reaction (1);
- $\xi = \dot{N}_{s,in}$.
- $\dot{H}_{in}, \dot{H}_{out}$: inlet and outlet heat flows (kJ/h);
- $H_{reaction}$: molar enthalpy of the reaction (1) (kJ/mole);
- $h_{i,in}, h_{i,out}$: inlet and outlet molar enthalpy of the component i (kJ/mole);
- $C_{p,i}$: specific heat of the component i (kJ/mole. °C);
- T_0, T_{in}, T_{out} : reference, inlet and outlet temperature of the sulphur burner, respectively (°C).

The catalytic conversion of the SO_2 to SO_3 was simulated by a plug flow reactor with as a kinetic heterogenous reaction. In 1997, Froment and Bischoff have proposed a kinetic model to estimate the rate of this conversion by the following equation (Anton A. Kiss et al, 2010):

$$r_2 = \frac{K_1 . P_{O_2} . P_{SO_2} . \left(1 - \dfrac{P_{SO_3}}{K_p . P_{O_2}{}^{\frac{1}{2}} . P_{SO_2}} \right)}{\left(1 + K_2 . P_{SO_2} + K_3 . P_{SO_3} \right)^2} \tag{11}$$

Where:
- r_2 : kinetic reaction rate of the reaction (2) (kmol/kg.cat. s);
- P_i : pressure of the component i (atm);
- K_1 : first rate constant (1/atm1/2);
- K_p : second rate constant (kmol/lh.cat.atm².s);
- K_2 : third rate constant (atm-1);
- K_3 : third rate constant (atm-1).

The rate constants K_1, K_p, K_2, K_3 were calibrated and adjusted using the simulated plant data, and they are given by:

$$K_1 = \exp\left(15.31 + \frac{45501}{RT} \right) \tag{12}$$

$$K_p = \exp\left(41.30 - \frac{93943}{RT} \right) \tag{13}$$

$$K_2 = \exp\left(-71.74 + \frac{71655}{RT} \right) \tag{14}$$

$$K_3 = \exp\left(15.31 + \frac{437269}{RT} \right) \tag{15}$$

The absorption reactions (3) and (4) were simulated using the absorber model integrated in the simulator and based on column theory. The multi-stage absorption towers present a series of equilibrium and non-equilibrium flash stages. At each stage, there can be a mass and heat transfers between the two phases that feed the column in counter current. The following equations show the mass transfer balance between the components i and j in the gas and liquid streams respectively, within an absorption tower:

$$\frac{4}{\pi . D^2} . \frac{d}{dz}(\dot{Q}_G . C_{i,G}) = -\dot{N}_i . A_s \tag{16}$$

$$\frac{4}{\pi . D^2} . \frac{d}{dz}(\dot{Q}_L . C_{j,L}) = -\dot{N}_j . A_s \tag{17}$$

$$\dot{N}_i . \left(\frac{1}{k_L} + \frac{1}{k_G . H_i} \right) = \frac{P_i}{H_i} + \frac{D_i}{D_j} . C_{j,L}; \dot{N}_i = \dot{N}_j \tag{18}$$

Where:

- D: absorber diameter (m);
- $\dot{Q}_G, \dot{Q}_L$: gas and liquid volumetric flow rates (m3/h);
- $C_{i,G}, C_{j,L}$: component i and component j concentration in the gas and liquid respectively (mole/m3);
- $\dot{N}_i$: molar flow rate of the component i (mole/m2.h);
- A_s: specific area (m2/m3);
- k_G, k_L : gas and liquid partial mass transfer coefficients;
- H_i: Henry coefficient of the component i;
- P_i: partial pressure of the component i (Pa);
- D_i: mass diffusivity of the component i.

The simulation of the heat transfer operations within the process was realized using the heat exchanger model presented in the simulator library. This model is based on the material and energy balance equations. The Log-Mean Temperature Difference LMTD method is adopted to calculate the heat transfer flow rate $\dot{W}_{ex}$ exchanged between the two flows:

$$\dot{W}_{ex} = U_{ex}.A_{ex}.\Delta T_{LM}.F_t \qquad (19)$$

$$\Delta T_{LM} = \frac{(T_{tb,out} - T_{tb,in}) - (T_{sh,out} - T_{sh,in})}{\ln \frac{T_{tb,out} - T_{tb,in}}{T_{sh,out} - T_{sh,in}}} \qquad (20)$$

Where:

- $\dot{W}_{ex}$: heat transfer flow rate (W);
- U_{ex}: heat transfer coefficient (W/m². K);
- A_{ex}: heat transfer areas (m²);
- F_t: correction factor.

The pumps used to increase the pressure of liquid streams were simulated using the centrifugal pump model assuming that that fluid is incompressible. The pump simulation is based on the general pump equation that gives the ideal power required to rise the liquid pressure according the inlet and outlet pressures, flow rate and density:

$$\dot{W}_{id} = \frac{(P_{out} - P_{in}).\dot{M}}{\rho} \qquad (21)$$

$$\dot{W}_{ac} = \dot{H}_{out} - \dot{H}_{in} \qquad (22)$$

$$\text{Effenciency } (\%) = \frac{\dot{W}_{ac}}{\dot{W}_{id}} \qquad (23)$$

Where:

- W_{id}: ideal required power (W);

- W_{ac}: actual required power (W);
- P_{in}, P_{out}: inlet and outlet pressure (Pa);
- $\dot{M}$: inlet mass flow rate (kg/h);
- ρ: fluid density (kg/m3);
- $\dot{H}_{out}, \dot{H}_{in}$: inlet and outlet heat flow rates (W);
- Effenciency (%): pump efficiency (%).

The compressors used to increase the pressure of the gas streams were simulated by the centrifugal compressor model based on the isentropic efficiency. The isentropic ideal power and the actual power required for gas compression is defined as follow:

$$\dot{W}_{id} = \dot{M}.\frac{n}{n-1}.\frac{P_{in}}{\rho_{in}}.\left[\left(\frac{P_{out}}{\rho_{in}}\right)^{\frac{n-1}{n}} - 1\right].F_p \qquad (24)$$

$$\dot{W}_{ac} = \dot{H}_{out} - \dot{H}_{in} \qquad (25)$$

$$\text{Effenciency } (\%) = \frac{\dot{W}_{ac}}{\dot{W}_{id}} \qquad (26)$$

Where:

- ρ_{in}: gas inlet density (kg/m3);
- n: volume exponent;
- F_p: correction factor;
- Effenciency (%): compressor efficiency (%).

The following table regroups the different UniSim-Design equipment models used to perform this simulation:

Table 2: UniSim Design equipment models for the studied process simulation.

Equipment model	Description
Conversion reactor	Sulphur combustion
Plug flow reactor	SO_2 conversion
Absorber	H_2O and SO_3 absorption
Heat exchanger	Heat transfer
Cooler	Fluids cooling
Pump	Liquids pumping
Compressor	Gas compression
Splitter	Flows division
Mixer	Flows mixing
Valve	Flows control

4 RESULTS AND DISCUSSION

In order to configure the basis environment of the simulator, the chemical components involved in the

95

sulphuric acid manufacturing process were defined (Table 1). In addition, the necessary fluid-packages (PG for the gaseous phase and NRTL for the liquid phase) were specified. The four principal reactions governing the process (liquid sulphur burning, sulphur dioxide conversion, sulphur trioxide absorption and sulphuric acid dilution) were also defined with their reaction rates. Next, in the simulation environment of the simulator, the equipment models were inserted, and the global flowsheet of the studied process was elaborated including the gas circuit and the acid circuit.

Figure 2. shows the simulation of the sulphuric acid manufacturing plant with double absorption performed under the UniSim-Design R451 simulator. The key streams used to perform this simulation are summarized in Table III. for the liquid sulphur and the wet air properties, Table IV. for the operating key streams of the circulating sulphuric acid, and Table V. for the dilution and cooling water key streams.

Figure 3 presents the simulation results of the sulphuric acid concentration within the drying tower. The circulating sulphuric acid used for air-drying feeds the column from the top at the concentration of 98.6%, and absorbs the water contained in the wet air that feeds the column from the bottom. The sulphuric acid is diluted and leaves the drying column at the concentration of 98.33% as shown in the simulation results. It is observed that the dry air entering the column at 25°C leaves at the temperature of 65.8°C, which is justified by the exothermicity of the sulphuric acid dilution reaction.

The dry air leaving the drying column is compressed before feeding the sulphur burner. An adjustment of the compressor energy stream is used in order to maintains the pressure of the dry air at 153 kPa. The energy required to increase the air
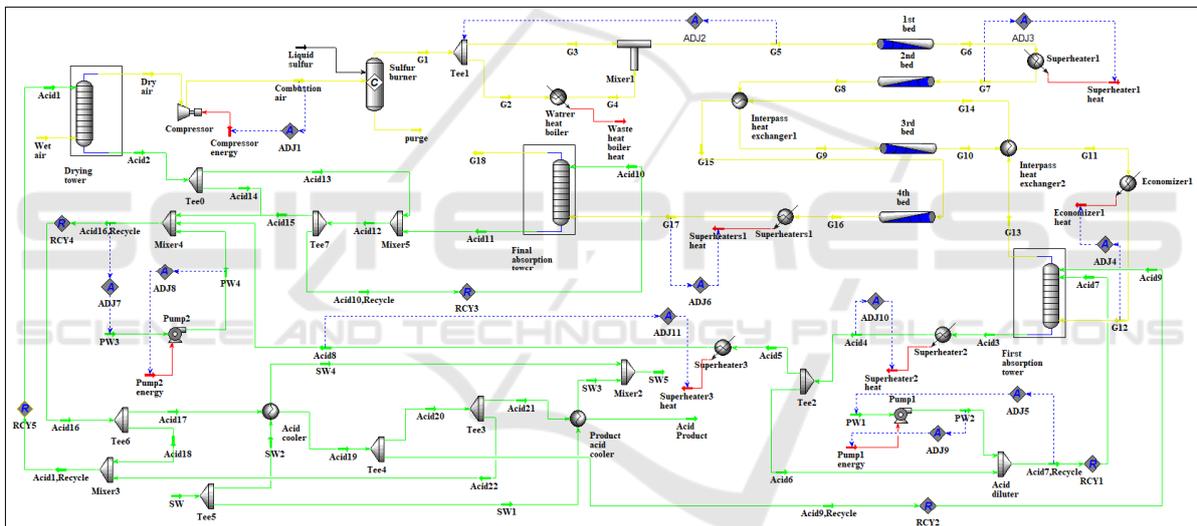

Figure 2: UniSim-Design simulation of the sulphuric acid manufacturing process with double absorption.
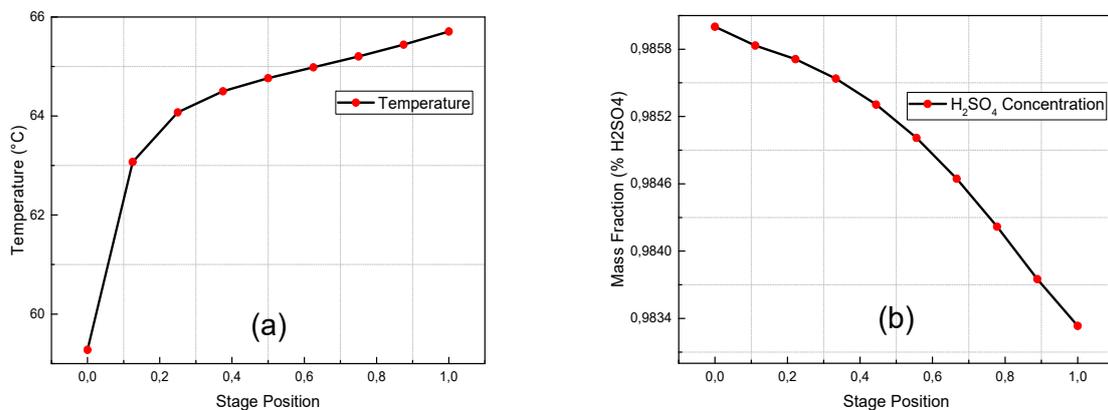

Figure 3: Temperature (a) and sulphuric acid concentration (b) variations in the drying tower stages.

Table 3: Liquid sulphur and wet air properties.

Stream	Wet air	Liquid sulphur
Flow rate (m^3/h)	540	32
Temperature (°C)	25	130
Pressure (kPa)	101.3	1920
O_2 (%)	20.68	0
N_2 (%)	78.04	0
H_2O (%)	1.28	0
S (%)	0	100

Table 4: Sulphuric acid operating key streams.

Stream	Acid 1	Acid 7 + Acid 9	Acid 10
Description	Sulphuric acid in the drying tower	Sulphuric acid in the first absorption tower	Sulphuric acid in the final absorption tower
Flow rate (m^3/h)	1245	2890	1030
Concentration (%H_2SO_4)	98.6	98.97	98.6

Table 5: Water operating key streams.

Stream	SW	PW1	PW3
Description	Sea water for the sulphuric acid cooling	Process water for the strong sulphuric acid dilution	Process water for the circulating sulphuric acid dilution
Flow rate (m^3/h)	2765	28	3

pressure from 98 kPa to 154 kPa (Figure 4) is estimated by the simulator at 8302 kW, with an adiabatic efficiency of 75% and a polytropic efficiency of 76.52%.
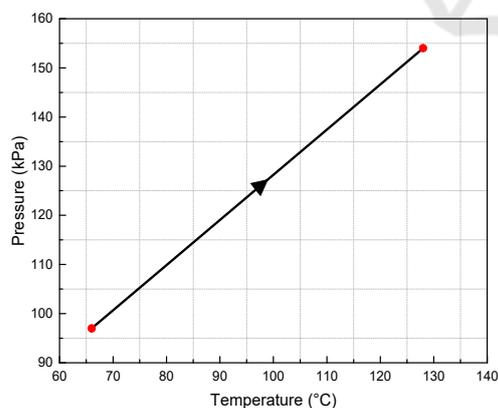
Figure 4: P-T curve of the air compressor.

The liquid sulphur feeds the sulphur burner at 130°C and 1920kPa and reacts with the dry air to form the SO_2. The combustion gas mixture produced at the sulphur burner leaves at the temperature of 1216 °C with a complete combustion of the liquid sulphur. The reaction heat of liquid sulphur

combustion is calculated at 25°C as 298190 kJ/mole. A small amount of the SO_3 is also produced because of the high temperature within the sulphur burner. The molar composition of the combustion gas is: 9.7% of O_2, 79.16% of N_2, 10.87% of SO_2 and 0.27% of SO_3. The hot combustion gas passes through a waste heat boiler to recover a part of the combustion heat and to promote the required temperature of the SO_2 conversion. An adjustment of the by-pass fraction at the inlet of the waste heat boiler is used to maintain the desired temperature.

As mentioned in the process description section, the converter is formed by four catalytic bed, and each bed is simulated by a plug flow reactor. The temperature at the inlet of the three first beds is adjusted to 440°C by superheaters and inter-pass heat exchangers, and at 400 °C for the last bed. As illustrated in the SO_2 conversion-Temperature curve (Figure 5), the four operating lines represents progress of the conversion rate within the four beds of the converter. The SO_2 conversion rate is accompanied with a temperature increase since the conversion reaction is exothermic. Once the conversion rate riches the equilibrium curve, a cooling step is required to achieve a higher conversion rate. Several conversion stages and inter-
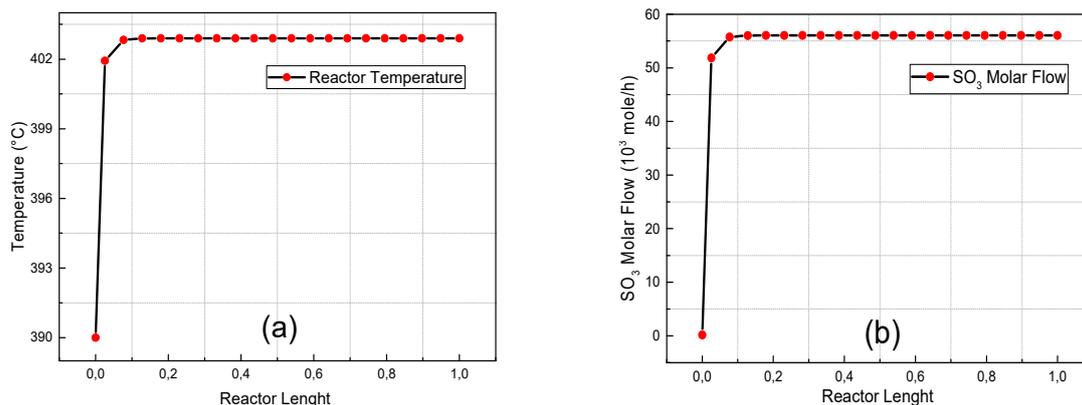
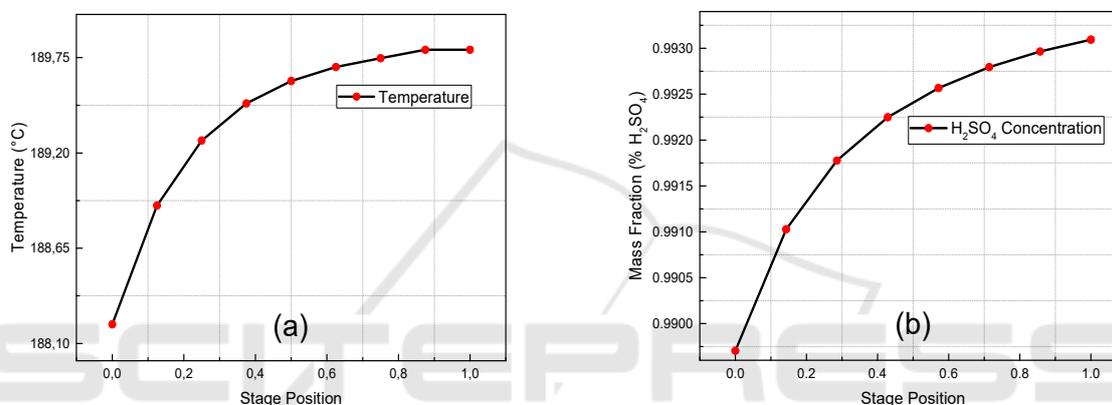Figure 5: Temperature (a) and SO_3 molar flow (b) variations in the 4th catalytic bed.

Figure 6: Temperature (a) and sulphuric acid concentration (b) variations in the first absorption tower.

step cooling are necessary. The outlet temperatures are 643°C, 527°C, 462°C and 404°C for the converter stages, respectively. The SO_2 conversion rates in the three first beds are 63.43%, 89.95%, 96.54% respectively.
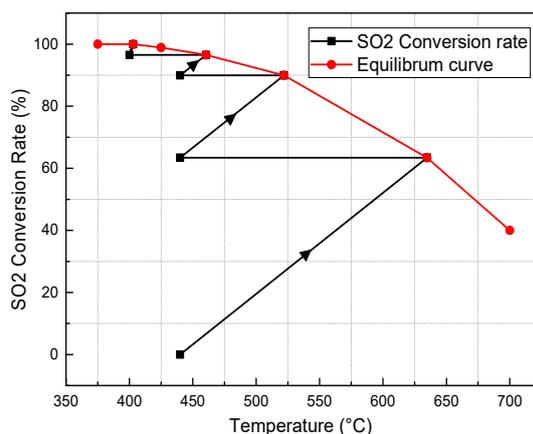

Figure 7: Conversion-Temperature curve of the catalytic converter.

The outflow gas of the 3rd bed is cooled and sent to the first absorption tower in order to absorb the SO_3 produced by the SO_2 catalytic conversion, then gone back to the 4th bed in which the remaining SO_2 is converted into SO_3. Figure. 6. Shows the temperature and the SO_3 mole flow variations along the 4th bed. The SO_2 conversion rate at the last bed achieves 99.97%. However, the conversion of the SO_2 into SO_3 is accompanied with a temperature increase due to the heat generated by the reaction as illustrated in Figure 6. The molar enthalpy of this reaction is given by the simulator as 98925 kJ/mole.

The absorption rate of SO_3 is around 99.98% in the first absorption tower and 100% in the second absorption tower. As shown in the simulation results of the first absorption tower of Figure 7, the absorption of SO_3 is an exothermic reaction that generates 97333kJ/mole. The circulating sulphuric acid 98.97% feeds the first absorption tower at 189°C, and leaves at the concentration and temperature of 99.30% and 173°C, respectively. However, it feeds the second absorption tower with a concentration of 98.60% and a temperature of 65°C,
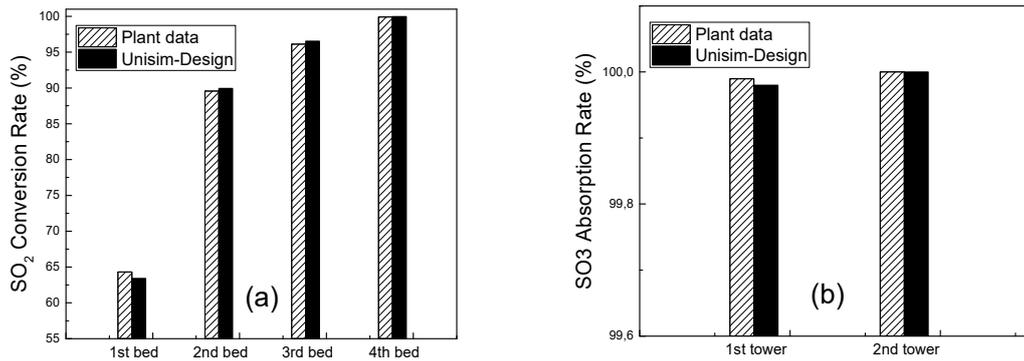
Figure 8: UniSim Design converter (a) and absorption towers (b) simulation results versus plant data.
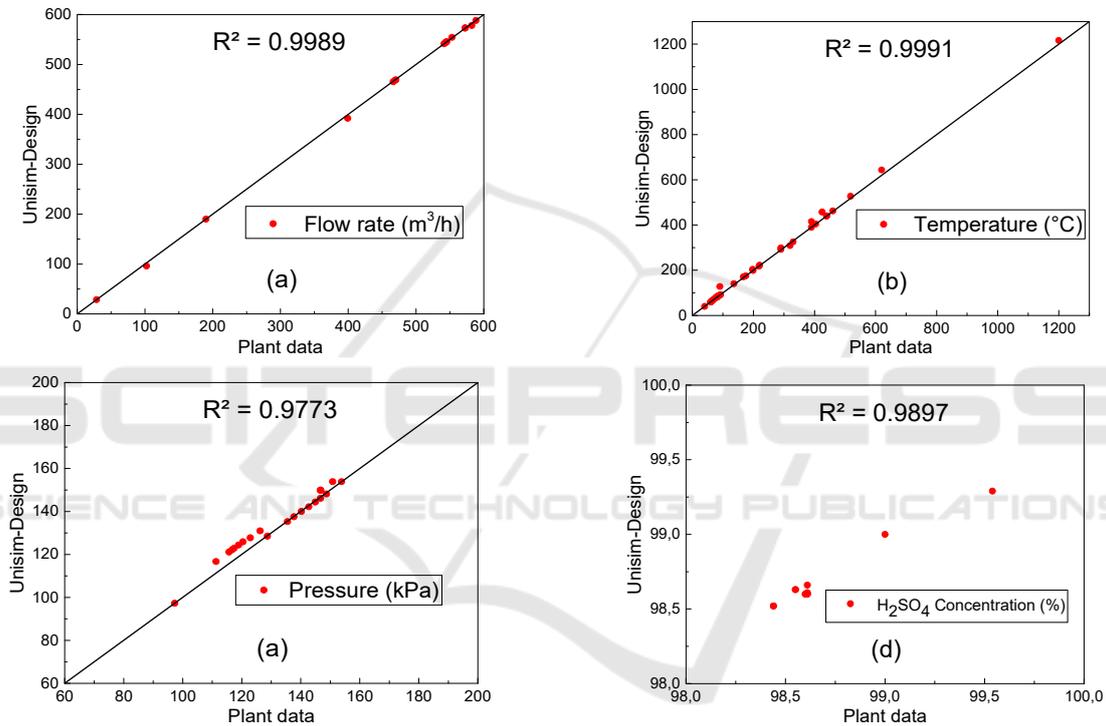

Figure 9: Simulation results versus plant data correlation for the flow rates (a), temperatures (b), pressures (c) and sulphuric acid concentrations (d).

and leaves the tower at a concentration of 98.67% and the temperature of 82.76°C (after absorbing the SO_3 generated in the 4th catalytic bed).

In order to validate the process simulation, the simulation results of the SO_2 conversion rate within the four catalytic beds of the converter, and the SO_3 absorption rate within the two absorption towers were compared to the plant data as shown in Figure 8. In addition, the temperature, pressure, flow rate and sulphuric acid concentration values found in the simulation were compared to the real plant measurement and have shown a high accuracy (Figure 9) between 97% and 99%. The comparison of

the results indicates that the simulations performed under UniSim Design R451 simulator represent a high level of validity to accurately describe the industrial process.

5 CONCLUSIONS

In this study, a steady-state simulation of a double absorption sulphuric acid plant was conducted using Honeywell UniSim-Design R451 simulator. The simulated process includes gas and acid circuits, with a SO_2 conversion rate of 99.9%, and a SO_3 absorption

rate of 99.98%, and an average of 140 ppm of SO_2 gas sent to the atmosphere. The developed model and simulation includes the different manufacturing process units: drying tower and air compressors, sulphur burner and heat recovery boiler, SO_2 converter and heat exchangers, first absorption tower and energy economizers, second absorption tower, acid and water pumps, acid diluter systems, acid cooling systems and acid circulating tank. The results obtained were validated using the real data extracted from the manufacturing plant under the same operating conditions, and a considerable accuracy of 97% was observed. Thus, the plant modelling and simulation using UniSim Design R451 simulator can be used to efficiently calculate mass and energy balances. Furthermore, it can be used to improve the manufacturing process, test advanced process control methods and develop digital twins to facilitate the digital transformation of industries.

REFERENCES

Boschert, S., & Rosen, R. (2016). Digital twin-the simulation aspect. In *Mechatronic Futures: Challenges and Solutions for Mechatronic Systems and Their Designers*.

Chowdhury, N. B., Hasan, Z., & Biplob, A. H. M. (2012). HYSYS Simulation of a Sulfuric Acid Plant and Optimization Approach of Annual Profit. *Journal of Science (JOS)*.

Gosiewski, K. (1993). Dynamic modelling of industrial so2 oxidation reactors part I. model of "hot" and 'cold' start-ups of the plant. *Chemical Engineering and Processing*.

Günther, R., Schöneberger, J. C., Arellano-Garcia, H., Thielert, H., & Wozny, G. (2012). Design and modeling of a new periodical-steady state process for the oxidation of sulfur dioxide in the context of an emission free sulfuric acid plant. In *Computer Aided Chemical Engineering*.

Kiss, A. A., Bildea, C. S., & Grievink, J. (2010). Dynamic modeling and process optimization of an industrial sulfuric acid plant. *Chemical Engineering Journal*.

Lee, J., Cameron, I., & Hassall, M. (2019). Improving process safety: What roles for digitalization and industry 4.0? *Process Safety and Environmental Protection*.

Moats, M., Davenport, W. G., & King, M. J. (2006). Sulfuric Acid Manufacture. In *Sulfuric Acid Manufacture*.

Moeller, W., & Winkler, K. (1968). The double contact process for sulfuric acid production. *Journal of the Air Pollution Control Association*.

Oni, A. O., Fadare, D. A., Sharma, S., & Rangaiah, G. P. (2018). Multi-objective optimisation of a double contact double absorption sulphuric acid plant for cleaner operation. *Journal of Cleaner Production*.

Parrott, A., & Warshaw, L. (2017). Industry 4.0 and the digital twin. *Deloitte University Press*.

Rahman, R. K., Ibrahim, S., & Raj, A. (2019). Multi-objective optimization of sulfur recovery units using a detailed reaction mechanism to reduce energy consumption and destruct feed contaminants. *Computers and Chemical Engineering*.

Sørensen, P. A., Møllerhøj, M., & Christensen, K. A. (2015). New dynamic models for simulation of industrial SO2 oxidation reactors and wet gas sulfuric acid plants. *Chemical Engineering Journal*