Hindawi
Journal of Sensors
Volume 2020, Article ID 8873039, 10 pages
https://doi.org/10.1155/2020/8873039

Research Article

A Computer Simulator Model for Generating Sulphuric Acid and Improve the Operational Results, Using Operational Data from a Chemical Plant

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Received 12 March 2020; Revised 6 August 2020; Accepted 28 August 2020; Published 8 September 2020

Academic Editor: Bin Gao

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The integration of both sensors and simulation in some industrial processes has received a large increase in the recent years, thanks to results such as increase in production indices or improvement in economic indicators. This document describes the development and validation of a simulation-based computer process for generating sulphuric acid. For this process, the data generated by simulation between the fixed beds of a catalytic reactor versus the results obtained using real data from a sulphuric acid production plant in the Antofagasta Region, Chile, have been used. This sulphuric acid production plant is designed for producing 720,000 tons of sulphuric acid annually, with a production capacity of 26 MW, which is used for both its own consumption and the Big North Interconnected System (SING, for its acronym in Spanish) and a sulphur consumption of 240,000 tons/year. For the simulation process, converter input variables such as temperature and gas flow to later observe the oxidation behavior under different operational scenarios were considered. To do it, a working method has been proposed and the software Aspen HYSYS® was used for the simulation. The simulation result was validated using design operational data provided by the company. The real results show a 99.9% of adjustment concerning the values obtained using the simulation. Based on the findings, a new operational scenario was created, and the economic indicators of the simulator implementation were determined: NPV = CLP 161,695,000 and IRR = 53% with a 6% monthly production increase.

1. Introduction

In copper mining production by leaching, one of the most important inputs is sulphuric acid. Recently, the production of sulphuric acid has increased, particularly in the last few decades, owing to the creation of leaching piles, as an attempt to make copper mining more sustainable and a respectful activity for the environment. In a typically industrial process, the sulphuric acid production usually consumes great amounts of energy. As an alternative for this energy consumption and as a kind of circular economy, in some specific production plants, electric energy production is currently being implemented in conjunction with the same sulphuric acid production cycle.

One way of producing sulphuric acid is using solid sulphur as input. In northern Chile, particularly in Antofagasta Region, an elemental sulphur combustion process is being used to produce sulphuric acid and electric energy, which is utilized for its own consumption (about 30% of the electric energy produced annually), the rest being incorporated into the electric network in the called Big North Interconnected System (SING, for its acronym is Spanish). The company is obtaining good profits with this process; nevertheless, it is far from achieving optimal performance, according to its installed capacity. The plant is designed for producing 720,000 tons of sulphuric acid annually and, due to the heat generated by sulphur combustion, it can also produce 26 MW of electric energy. Previous experiences as those described in [1–4] indicate that the plant design allows producing input for a profitable activity such as copper mining.

According to the plant design, production amounts approximately to 2,060 metric tons of sulphuric acid per day, representing 24,720 metric tons per year (about 5% of

its capacity). To do this, about 680 tons of sulphur must be used daily. On the other hand, by means of an efficient cogeneration process, the company injects SING with about 145 GWh per year, efficiently using the heat produced during the sulphuric acid production process. The company reports 240,000 tons/year of sulphur consumption for both products. This kind of work enables the company to generate both products, partially meeting the needs of the market requiring sulphuric acid and obtaining additional profits by selling electric energy. In this context, the company set the following objective: improving the plant performance through the optimization of the production processes involved.

To achieve this objective and follow the authors as [5–11], a simulation process for study the sulphuric acid and electric energy production was proposed. This paper focuses on the relevance of the simulation conducted with a software specialized for simulating chemical process plant operations and the conclusions obtained after comparing simulation results with the real results obtained from the plant operation. Using this way of working, an operational scenario that allows increasing production and improving the company profitability was identified. According to the above, a proposal was made to conduct the catalytic converter simulation by using the software Aspen HYSYS® Educational license provided by Aspen Technology, Inc., which has been widely used for an in-depth analysis and optimization of various productive processes [12–18]. This tool allows analyzing performance by means of operational changes and simulating the process using design data provided by the company.

The purpose of the simulator is to evaluate the operational parameters previously in order to optimize the oxidation in each bed and, in this way, produce a greater amount of sulphuric acid. In brief, the aim is to implement a simulator for the catalytic converter using the software Aspen HYSYS® (version 9.0–educational software license), validate and establish the simulator ranges for the catalytic converter, and finally, economically evaluate the impact of applying the simulator to new operational scenarios.

In previous works like [11, 19], the use and validation of results of the Aspen HYSYS® software has been presented, and other previous studies use some similar simulation process to learn and improve the results on chemical plants. For example, in [20], a model based on the simulation and analysis results of real operational cases in a Chilean plant is described. For this case, the process and operational conditions were analyzed to improve the conversion of the system. Some works such as those described above incorporate sensor signals and data processing techniques in order to improve the precision capacity of simulation and the results. Examples of this kind of work are described in [21, 22] where the distributed control system (DSC) is used in conjunction with simulation for the aforementioned purposes.

2. Materials and Method

This study used simulation data obtained from the plant production process. The processes involved are liquid sulphur filtration and storage, sulphur combustion and SO_2 generation, catalytic oxidation from SO_2 to SO_3, sulphur acid production, high- and low-pressure steam production, and electric energy generation.

The main input for this production process is liquid sulphur. Liquid sulphur production consists of the following operations: solid sulphur reception, smelting, filtration, and storage. Figure 1 shows the sulphur acid and electric energy production process described below.

Solid sulphur is received by an ATS tower (Figure 1) and then sent by conveyor belts to the stockpile area close to the melting and filtration sections. The melting tank consists of two sections. The first one receives the solid sulphur and melts it by means of steam coils, sending it later as liquid sulphur to the second section. There are two alternatives for controlling liquid sulphur temperature. In the first one, steam coils submerged in the tank provide it with sulphur condensation heat. The second alternative is to use a sulphur recirculation pump that makes part of the liquid sulphur pass through a heat exchanger (IC, for its acronym in Spanish). This increases the sulphur temperature and returns it to the tank to facilitate smelting.

The second section of the melting tank containing liquid sulphur operates as a precapped zone. Here, a submerged impure sulphur pump feeds sulphur from the tank to the primary sulphur filter, which is a kind of sheet filter.

The following systems are involved in SO_2 generation: sulphur combustion, boiler, air drying, and diesel supply.

In this stage of the process, the following reaction occurs:

$$S_{(l)} + O_{2\,(g)} \rightarrow SO_{2\,(g)} + \text{calor} \tag{1}$$

The liquid sulphur from the storage tank acts as a primary fuel. The main function of the boiler is to transfer the heat from the sulphur combustion gases to the water that will be used in the steam cycle. As a result, the gas flow cools down to 420°C and then goes into the converter. The drying air is obtained from the atmosphere and sent by a blower to the drying tower, to later enter as dried air into the combustion stage. If humidity is present, unwanted secondary reactions damaging the burner or the furnace take place. Drying occurs in the drying tower when wet air gets in contact with sulphur acid.

The drying tower (DT) is a piece of equipment coated inside with acid-resistant ceramic bricks. It has a dome of the same material where the filling, also made of ceramics, is supported. The filling is 3.5 m high and is used for increasing the gas-liquid exchange surface. On top, the tower has irrigation systems that allow a uniform distribution of the acid and mesh filters catching acid fog drops dragged by the upward gas flow.

In changing SO_2 to SO_3, the following systems are involved:

(i) Catalytic converter

(ii) Economizer 1, overheater 1, and overheater 2

(iii) Gas-gas IC

In this stage of the process, the following reaction occurs:

$$SO_2 + \frac{1}{2} O_{2\,(g)} \leftrightarrow SO_3 + \text{calor} \tag{2}$$

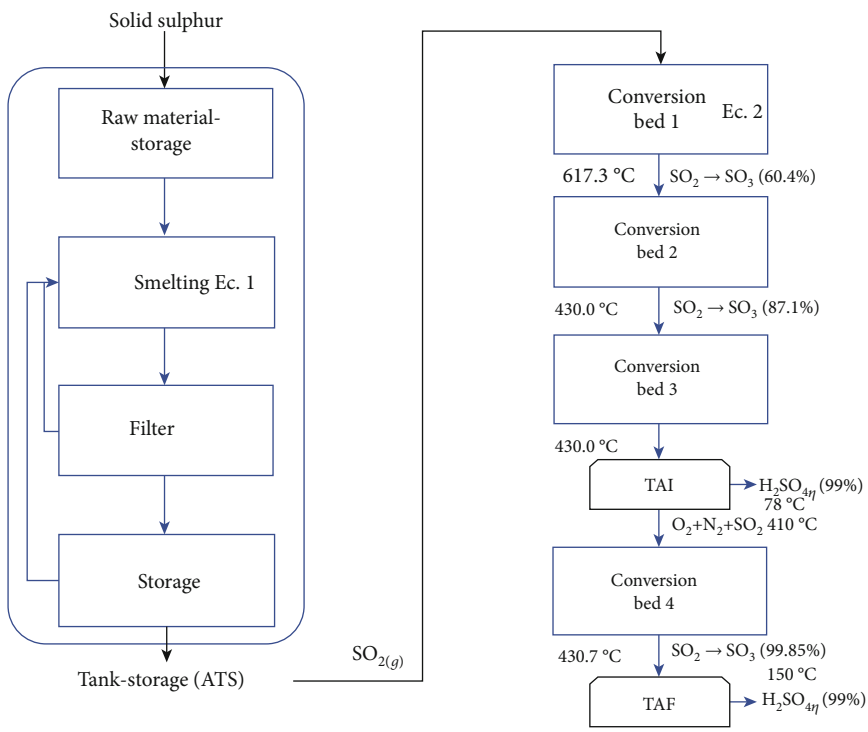

Figure 1: Flowchart of the process to convert $SO_{2(g)}$ into $SO_{3(g)}$ and $H_2SO_{4(l)}$ production.

SO_2 from the combustion furnace enters the 4-step catalytic convertor at a flow close to 167,000 Nm^3/h and 420°C. The converter is made of 304H stainless steel to support the high operational temperatures. Three ranges for temperature used in the process have been defined; labels of high, medium, and low have been assigned to ranges as detailed in Table 1.

The separation plates between individual racks are soldered. The catalyst, vanadium pentoxide (V_2O_5) in the form of pellets, is supported in stainless steel racks with spaced holes and covered with a layer of intalox ceramic saddles.

The thermal insulation of the converter meets the following requirements: optimizing high-level energy recovery, minimizing losses due to high-level energy radiation, protecting equipment at temperatures lower than the dew point and its subsequent corrosion, and keeping the heat within the system.

After entering the catalytic converter, sulphur dioxide (SO_2) reacts into the first bed, reaching a 60.4% conversion. This gas containing sulphur trioxide (SO_3) goes out at medium temperature label, due to the heat liberated during the reaction and must be cooled down before going into bed 2. Overheater 2 fulfills this task, like the other IC since the heat liberated during oxidation is transferred to the steam cycle. Once the gas is cooled down to low temperature label, it goes into the converter again through bed 2, where oxidation continues and SO_2 reaches an 87.1% cumulative conversion. Again, the gas goes out and exchanges heat with overheater 1, cooling down from medium to low, the temperature at which it goes into bed 3. Here, SO_2 reaches a 95.2% conversion and the gas goes out at medium to the gas-gas exchanger.

This IC cools down the gas to low label, the temperature at which it feeds the intermediate absorption tower (TAI, for its acronym in Spanish). SO_3 reacts in this tower by changing into sulphuric acid, while the gas in it goes out at low temperature label. This gas contains only oxygen, nitrogen, and SO_2 that did not react. For this reason, the gas goes to bed 4, previously passing through the gas-gas exchanger where it heats up to medium label. In bed 4, SO_2 reaches a 99.85% conversion. The gas goes out at medium temperature label, to the economizer, which cools it down to low label, the necessary temperature for feeding the final absorption tower (TAF, for its acronym in Spanish).

The gas-gas IC consists of a vertical and a horizontal section, which are considered separate pieces of equipment. Its function is to cool down the gas going out of bed 3 toward TAI (Figure 1), putting it in countercurrent contact with the gas from the same tower that needs to be heated to return to the converter.

Industrial SO_2 oxidation must be conducted in catalyst beds because oxidation in the gaseous phase of sulphur dioxide is kinematically inhibited, making it virtually impossible without a catalyst at a certain temperature. At normal temperature the reaction is so slow that, in practice, it does not occur. Currently, catalysts available in the market are daisy-shaped ring, simple ring, and ball-shaped catalysts. Of all the types in the market, the company uses the daisy-shaped ring since it has a bigger contact surface and less resistance to the gas flow.

Table 1: Temperature ranges and labels defined for the simulation process.

Temperature label	Ranges (°C)
Low	(100-450)
Medium	(451-520)
High	(521-750)

The reaction occurring at ionic level in the catalyst is as follows: SO_2 oxidation consists of smelting one layer on the catalyst surface. SO_2 oxidation occurs with dissolved complexes of vanadium, sulphur, and oxygen, as shown in

$$\begin{gathered}(VO)_2O(SO_4)_4^{-4} + O_{2\,(g)} \leftrightarrow (VO)_2O(SO_4)_4O_2^{-4} \\ (VO)_2O(SO_4)_4O_2^{-4} + SO_{2\,(g)} \leftrightarrow (VO)_2O(SO_4)_4O^{-4} + SO_{3\,(g)} \\ (VO)_2O(SO_4)_4O^{-4} + SO_{2\,(g)} \leftrightarrow (VO)_2O(SO_4)_4SO_3^{-4} \\ (VO)_2O(SO_4)_4SO_3^{-4} \leftrightarrow (VO)_2O(SO_4)_4^{-4} + SO_{3\,(g)}\end{gathered} \tag{3}$$

The reactions described above must be conducted efficiently. To do this, the bed temperature must remain over low temperature label because, below this temperature, the catalyst is deactivated, and oxidation does not occur. The following systems are involved in sulphur acid production: absorption tower, common acid tank and pumps, common acid coolers, product acid tank, and funnel.

In this stage of the process, the following reaction occurs:

$$SO_{3\,(g)} + H_2O_{(l)} \rightarrow H_2SO_{4\,(l)} + \text{calor} \tag{4}$$

The process is conducted in packed bed towers with a concave bottom and coated inside with at least two acid-resistant brick layers. The biggest amount of sulphur acid is produced in TAI. The gas from bed 3 enters through the lower side of the tower at a flow close to 157,600 Nm^3/h at 205°C and 11.49% of SO_3 volumetric concentration. This gas gets in contact with the sulphur acid sprayed from the upper part and reacts to form more sulphur acid, which reaches the bottom of the tower at a greater concentration. To make the acid go out at 98.5% again, it is necessary to regulate its concentration with water and acid from the ATS. This is done automatically by means of control links. The output flow then goes into the common sulphur acid tank.

TAF receives gas with SO_2-SO_3 at a low concentration from the last bed of the catalytic converter. Its packing is different so that it can absorb all the SO_3. Due to the acid concentration at the output not increasing too much, thus, it is discharged directly into the storage tank. The final gas in this tower is discharged into the atmosphere through a funnel. An SO_2 automatic analyzer is installed at the outlet to monitor the gas emitted. Additionally, the oxygen content is measured, being used as an indicator for calculating the SO_2 content at the converter inlet.

To avoid damaging other pieces of equipment and unwanted atmospheric effluents, there is a gas filter on top of the three towers. In TAI and TAF, acid fog is created by condensation. Therefore, the particles are smaller than in the first tower. It is possible to filtrate these particles with candle filters whose efficiency is higher than 95% and are located on the acid distribution systems. All the sulphuric acid circuits are connected to a common pump tank coated with two acid-resistant brick layers. This is recirculated to the towers by means of acid pumps. The tank is kept at high temperature since exothermic reactions occurring during the process heat the acid going into the tank. However, in order to use it, its temperature must be decreased by means of coolers.

In steam production, the following systems are involved: water treatment, heat exchangers, and waste heat absorption. The heat produced by sulphur combustion and SO_2 oxidation is recovered to produce high-pressure overheated steam necessary for generating electric energy. The pieces of equipment in charge of recovering this heat are the boiler, overheater 1, overheater 2, and economizer.

The plant uses seawater that first passes through a reverse osmosis plant and then a demineralization plant. After each treatment, the water is stored in tanks and then treated to be used for different purposes in the plant. The demineralized water is fed to a deaerator tank, which removes gases that do not condensate to avoid corrosion of the overheaters, IC, or the boiler. In addition, this tank receives condensates and low-pressure steam from other stages. Table 2 contains a brief description of the equipment used in the process and their function: heaters 1 and 2, economizer, and boiler.

Economizer 1 is used for cooling down the gas going out of bed 4 to TAF. This is done because it receives demineralized and water. The water goes to the steam dome, where it loses some of its pressure and is heated, going out as saturated steam to overheater 1. The steam going out of this device is enough to make the turbine work. In passing through the turbine, part of the steam goes to an overheater which, owing to water injection, changes it into low-pressure steam. Part of this steam is used for heating the melting tank, while the rest returns to the deaerator. Most of the steam used by the turbine goes to a series of condensers and then returns as a condensate to the deaerator, where the cycle starts again.

The equipment in charge of recovering the heat generated in the combustion furnace is the boiler and the steam dome. Most of the high-pressure steam from the plant is sent to the turbine to generate electric energy. A small part of the steam is extracted from the turbine and returned to the plant to be used at the melting and heating area. The turbine, designed for generating 26 MW, is the main equipment in this stage and is used for changing the rotating mechanical energy obtained from high-pressure steam into electric energy. The steam going out of the turbine is condensed in a condenser cooled by water. The condensate is recycled in the water-feeding tank of the plant.

3. Methodology

The methodology consists of four stages. The following variables are considered in the process: the temperature and

Table 2: Equipment used to transport and use gas flows between the different beds and other equipment for electric energy production.

Name	Description
Overheater 1	Overheater 1 is an IC (heat exchanger). It is a piece of equipment consisting of a shell and tubes, whose function is to transfer gas from bed 2 to bed 3, by overheating the gas
Overheater 2	Overheater 2 is also an IC. It is used for transferring overheated steam going out of bed 1 to the turbine
Economizer 1	Economizer 1 is a vertical IC, used to cool down the gas going out of bed 4 to TAF
Boiler	1,700 m2 surface, 167,000 m3/hr. output flow
Turbine	Vapor pressure 60 bar and medium temperature label, connected to a 26 MW generator

outlet and inlet flow of each bed (4 beds are considered in both the simulation and real operation); SO_2, SO_3, O_2, and N_2 volumetric percentage; and cumulative conversion.

(i) Process Study. In this stage, a study to know how the plant works to obtain sulphuric acid and electric energy is conducted. The goal is to learn about it and prepare experimentation properly

(ii) Simulation. In this stage, data are generated and prepared in accordance with the simulation characteristics

(iii) Model Visualization and Validation. In this stage, simulation results are observed and the values of the parameters of interest and the process output (sulphuric acid and electric energy) are compared with the values of the real operation to check their validity. To define a parameter for determining the validation of results, the r^2 linear regression coefficient was obtained among the values provided by the simulator, by comparing them with data provided by the company. To validate results, the values were adjusted for each variable greater or equal to 0.95, as agreed with the company

(iv) Result Analysis. In this stage, the analysis is aimed at establishing if results are interesting for the company. This was done by analyzing whether the results of the simulations in the different beds do or do not result in a production increase or whether the use of resources is or is not optimized in these processes

The methodological steps are further described below. Stage 1 begins with the study of the company production process, particularly the study of the catalytic converter to later develop a simulator. For systems where only gases interact, several models such as SRK, APL, and Peng-Robinson equations were examined, as shown in Equation (5).

The simulation model is based on equations that are highlighted below. First on our work, the general process is based on the thermodynamic model described in Equation (5). This model of Equation (5) is the most suitable because it is the less erratic for obtaining pressure and temperature results, according to the specific chemical process. A simulation strategy was used for the catalytic converter and the different heat exchangers taking part in the process. Each bed was addressed independently, that is, each bed was simulated as a continuous stirred tank reactor (CSTR) and the different heat exchangers as shell and tube IC.

$$P = \frac{\mathrm{RT}}{(v_m - b_m)} - \frac{a_m ai}{\left(v_m{}^2 + 2v_m - b_m{}^2\right)}. \tag{5}$$

Additionally, for the simulation of the mathematical model, the balances of matter, energy, and pressure drop were made. For this purpose, Equations (6)–(8) were used.

$$F_{AO}\frac{dX}{dW} = -r_A, \tag{6}$$

$$\frac{dT}{dW} = \frac{r_A \Delta H_{rx}(T)}{F_{AO}\left(\Sigma\theta_i C_{pi} + \Delta C_p X\right)}, \qquad \frac{dP}{dZ} = . \tag{7}$$

To simulate the reactor beds, first, the following velocity constants, activation energy (E_a) and the preexponential factor (A), must be solved to introduce them in the program and then select the most suitable reactor, according to the characteristics of the simulation. The reaction conducted in these reactors must be programmed in HYSYS®, based on the velocity constant, as shown in

$$r = \frac{K_1 P_{O_2} P_{SO_2}\left(1 - P_{SO_3}/\left(P_{SO_2}\sqrt{P_{O_2}}K_p\right)\right)}{22{,}414\left(1 + K_2 P_{SO_2} + K_3 P_{SO_3}\right)^2}, \tag{8}$$

$$K_1 = e^{(12{,}160-(5473/T))}, \tag{9}$$

$$K_2 = e^{(-9{,}953+(8619/T))}, \tag{10}$$

$$K_3 = e^{(-71{,}745+(52596/T))} \tag{11}$$

$$K_p = e^{(-10{,}68+(11300/T))}. \tag{12}$$

To enter these data into Aspen HYSYS®, the reaction parameters must be thermodynamically consistent, the velocity constants being given by Equation (13). Following as is summarized in Equation , the activation energy (E_a) and the preexponential factor (A) are processing and

incorporated to the simulation.

$$K = AT^n * \exp\left(\frac{-E_a}{RT}\right), \tag{13}$$

$$K_1 = \exp\left(12{,}160 - \frac{5473}{T}\right), \tag{14}$$

$$K_1 = \exp\,(12, 16) * \exp\left(\frac{-5473}{T}\right), \tag{15}$$

$$K_1 = 190995 * \exp\left(\frac{-5473}{T}\right), \tag{16}$$

$$A_1 = 190995, \tag{17}$$

with $n = 0$ and $T = 698\,\mathrm{K}$

$$\begin{gathered} K_1 = 19448 \\ Ln(K_1) = Ln(A_1) * \left(\frac{-E_a}{RT}\right) \end{gathered} \tag{18}$$

Follow with the ideal gas constant $R = 8{,}314(\mathrm{J/mol\,K})$ and $T = 698\,\mathrm{K}$, data known is replaced as shown in

$$\begin{gathered} \mathrm{Ln}(19448) = \mathrm{Ln}(190995) * \left(\frac{-E_a}{5803, 17}\right), \\ E_{a1} = -4712, 93(\mathrm{J/mol}). \end{gathered} \tag{19}$$

This process is conducted for all speed constants, resulting in

$$\begin{gathered} A_2 = 0, 000048 \rightarrow E_{a2} = 6455, 01\left(\frac{\mathrm{J}}{\mathrm{mol}}\right) \\ A_3 = 6{,}942 * 10^{-32} \rightarrow E_{a3} = 992{,}763\left(\frac{\mathrm{J}}{\mathrm{mol}}\right), \\ A_p = 0, 000023 \rightarrow E_{ap} = 1715, 44\left(\frac{\mathrm{J}}{\mathrm{mol}}\right). \end{gathered} \tag{20}$$

There are two reaction models in Aspen HYSYS®. In this study, the reaction model utilizing kinetic parameters was used. They involve the flow pattern and geometric characteristics of the reactor in the simulation. In addition, the expression of the reaction velocity must be selected. In this case, it was catalytic heterogeneous. The configuration of the reaction process simulation is shown in Figure 2; the process flow is from left to right.

For the reactor simulation, the most suitable is the continuous stirred-tank reactor (CSTR), since it calculates the conditions of the reactor output currents, considering that it is perfectly mixed and the concentration in each point of the reactor is the same. This type of reactor can be used for reactions in the liquid or gaseous phase, though it must be determined. In this case, it was used in the gaseous phase. To determine CSTR, it is necessary to associate one or several reactions and define the following: reactor volume, product output temperature or heat transferred, product output pressure or pressure decrease inside, reaction stoichiometry, and reaction velocity parameters for each reaction. As to dimensions, one of the following measures must be determined: volume, diameter, and height (specified in a horizontal tank).

If the cylindrical tank volume is defined, then the relationship Length/Diameter of the reactor is 3 : 2, by default. To simulate the whole converter, each bed was divided and simulated separately, that is, each bed was dealt with as an independent reactor (CSTR). For the fourth bed, the simulation had to be adjusted and work was done with constants different from the first three since this bed only oxidizes 4% of the total and, more than used for getting a bigger final production, this bed is utilized for complying with law no. 19,300, which sets the rules for establishing the environmental quality norms and those concerning SO_2 emission into the atmosphere.

To study the simulator behavior, the following variables were manipulated at the reactor input current : temperature, gas flow. The input current must be manipulated because it is the only one that has to be specified. The output currents of each reactor are calculated by the simulator. In the last bed, where the input current must also be specified, a 100% efficiency is assumed in the absorption tower. In other words, SO_3 going into the tower is changed into acid. For this step, the control variable is the reactor efficiency in SO_2 oxidation, that is, the SO_2 percentage going out at the end of the oxidation process.

Finally, an economic analysis was made by comparing the plant production with the new production that could be obtained based on the new operational scenario using the simulator and, in this way, to analyze the extent to which production can be increased. To accomplish the validation (the last part of stage 3) and the last stage of the methodology, the design data provided by the company were compared with the results provided by the simulator. By using the validated simulator, tests were made to estimate the best operational configurations and/or parameters to optimize the process.

4. Results and Discussion

A total of 603 sets of simulation data were obtained from 21 simulation cycles. As stated above, the variables and parameters used in the simulator for each bed were compared with the ones described in the plant design report, which shows the temperature and input and output flow of each bed; SO_2, SO_3, O_2, and N_2 volumetric percentage; pressure; and accumulated conversion. Table 3 shows an example of the input process (on the left) and the output values of the variables; molar flow; and SO_2, SO_3, O_2, and N_2 (on the right) for each simulation cycle moment.

Table 4 summarizes the r^2 values and error percentage in the simulation of each of the variables of interest in the simulation process. One of the most important variables in SO_2 oxidation is temperature since this one depends on the catalyst activation or deactivation. A big decrease results in less oxidation and, as a result, a smaller amount of the product. With the equations programmed in the simulator, a 0.99 r^2 regression coefficient was obtained for this variable, as shown

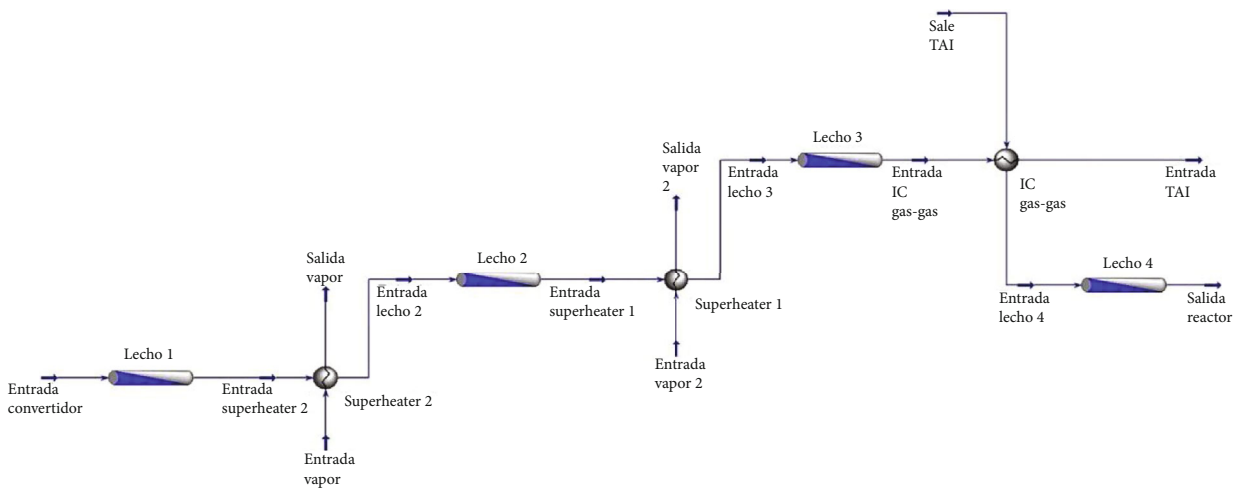

Figure 2: Configuration of Aspen Hysys® modelling.

Table 3: An example of the input and output values of a simulation cycle.

Operational ID	Bed-1 feeding						Bed-1 output				
	Flow [Nm3/Hr]	fluid mixture			Temperatura °C	Presión [bar]	Flujo molar [Nm3/Hr]	fluid mixture			
		SO2	O2	N2				SO2	SO3	O2	N2
1	140000	11.5	9.24	79.26	420	1.25	134880.072	4.33	7.6	5.79	82.28
1	140500	11.5	9.24	79.26	420	1.25	135373.235	4.34	7.6	5.79	82.27
1	141000	11.5	9.24	79.26	420	1.25	135866.398	4.35	7.59	5.8	82.26
1	141500	11.5	9.24	79.26	420	1.25	136337.144	4.36	7.58	5.8	82.26
1	142000	11.5	9.24	79.26	420	1.25	136830.307	4.36	7.57	5.8	82.27
1	145000	11.5	9.24	79.26	420	1.25	139766.868	4.41	7.53	5.82	82.24
1	145500	11.5	9.24	79.26	420	1.25	140237.615	4.41	7.52	5.83	82.24
1	146500	11.5	9.24	79.26	420	1.25	141223.941	4.43	7.5	5.84	82.23
1	146500	11.5	9.24	79.26	420	1.25	141223.941	4.43	7.5	5.84	82.23
1	147000	11.5	9.24	79.26	420	1.25	141717.104	4.44	7.49	5.84	82.23
1	147500	11.5	9.24	79.26	420	1.25	142187.85	4.44	7.49	5.84	82.23
1	148000	11.5	9.24	79.26	420	1.25	142681.013	4.45	7.48	5.85	82.22
1	148500	11.5	9.24	79.26	420	1.25	143174.176	4.46	7.47	5.85	82.22
1	149000	11.5	9.24	79.26	420	1.25	143644.923	4.46	7.46	5.85	82.23
1	149500	11.5	9.24	79.26	420	1.25	144138.086	4.47	7.46	5.86	82.21
1	150000	11.5	9.24	79.26	420	1.25	144631.249	4.48	7.45	5.86	82.21

Table 4: Description of variables used in simulation and related r^2 and Error values.

Variable	r^2	Error (%)
Temperature	0.99	0.60
Molar flow	0.99	0.04
SO_2	0.99	0.50
SO_3	0.99	0.50
O_2	0.99	0.40

in Figure 3. The error in the input and output temperatures of the different converter beds was 0.6%.

Another important variable to be validated is molar flow since it represents the amount of final product, thus providing the amount of flow circulating through the converter, considering losses between beds. Figure 4 shows that the adjustment value is 0.99, with a 0.04% error for all the input and output flows of the different beds, So, the variable can be accepted as validated. Once the molar flow was validated, its components were validated separately to make sure that the data obtained were reliable. The validation began with sulphuric dioxide because when it oxidizes it becomes the raw material of SO_3 sulphuric acid; its monitoring making it possible to control proper oxidation. It also allows detecting the amount of SO_2 liberated into the environment since, when it goes out of the fourth bed, it cannot be eliminated. In this case, the value of the r^2 linear regression coefficient is 0.99 with a 0.5% error.

As stated above, SO_3 is the raw material for producing sulphuric acid. Therefore, it is essential that the simulator provides accurate values of the percentage of this component

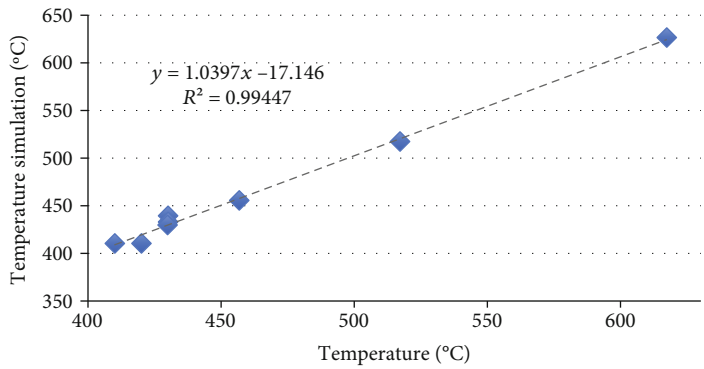

Figure 3: Converter temperature validation.

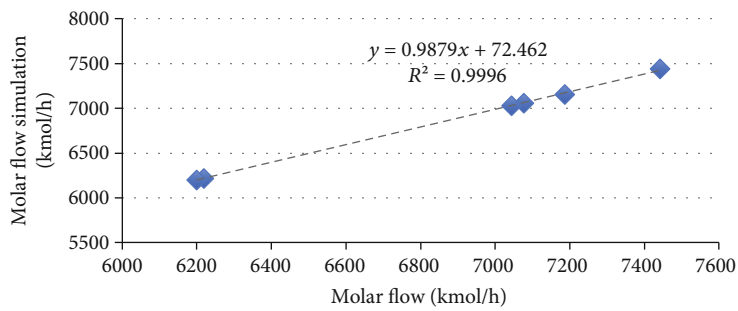

Figure 4: Molar flow validation.

in the gas. To check the validity of the values provided by the simulator, a linear regression was performed, resulting in a 0.99 r^2 coefficient and a 0.5% error.

The O_2 component plays a fundamental role in changing SO_2 to SO_3, thus, knowing the amount of it in the converter facilitates oxidation control. The validation of this variable in the simulator and the resulting accurate values of the amount of oxygen in the flow provide valuable data to the operator. Checking the values provided and knowing if the equations proposed and entered to the simulator are correct, the linear regression is performed, resulting in a 0.99 r^2 regression coefficient and a 0.4% error, thus validating the variable. From the values described above and shown in Table 4, it is possible to conclude that the simulation model is valid since the results obtained show a 0.99 r^2 mean regression coefficient. In this way, this component is validated, and the gas composition is also thoroughly validated.

Figure 5 shows that, at constant temperature, the greater the oxidation, the lower the gas flow and, on the contrary, the greater the gas flow, the less the oxidation. This may happen because there is a lower amount of gas flow, and therefore, it has a greater surface in contact with vanadium pentoxide, thus producing greater oxidation. Figure 5 shows the oxidation behavior when different gas flows are kept constant and the reactor input temperature is manipulated, showing that the lower the temperature, the greater the oxidation. Thus, the temperature used must produce enough SO_3 so that the process can be viable, the catalyst is at activation temperature, and the reaction velocity is high enough.

5. Conclusions and Future Work

In the copper industry, one of the most used inputs to recover copper is sulphuric acid, which can be produced using solid sulphur as input. But frequently, the sulphuric acid production process is usually expensive, due to both energy consumption and solid sulphur and other resources such as water consumption.

In this work, a technique to simulate and evaluate the catalytic conversion process for the production of sulphuric acid has been proposed and developed, and its practical utility has been validated. Additionally, as a result of this process, the production of electrical energy has also been monitored and suggestions to improve the energy generation have been provided, based on simulations and visualization of the results.

In order to achieve the above described, operational data obtained from the operation of a plant in Antofagasta have been used. Real data generated during approximately 3 months has been used to generate appropriate data that was used as input to the simulation, visualization, and validation process.

A concrete conclusion is that the simulation process generates results very close to the real process, since the error is less than 1%, with a converter input temperature in low value (in the range between 300°C and 460°C) and a gas flow between 140.00 and 180.00 Nm^3/h. Other highlight conclusions are as follows:

(i) The simulation process has allowed the identification of process characteristics that could affect

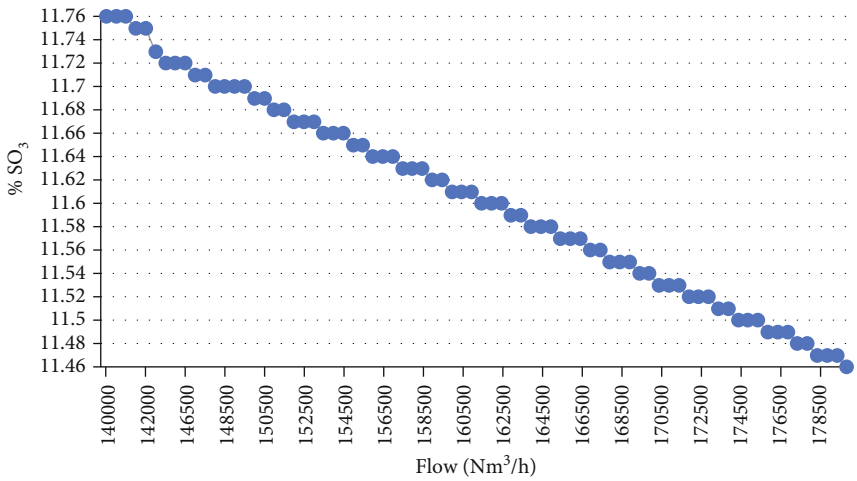

Figure 5: Oxidation behavior at different input flows.

greater production and better use of inputs. For example, tests made in the simulator show that the optimal input temperature is low, and the recommended gas flow is 150.50 Nm^3/h, using these new operational parameters configuration, sulphuric acid production should increase in 4 metric tons/day

(ii) A quantitative analysis of the average daily production of the plant was carried out using the simulation software. The results obtained with the simulator contrasted with the operational results over a period of 6 months. In this analysis, a new operational scenario was defined, and the temperature, pressure, and flow parameters were the most relevant to improve the results. The company has proposed to monitor these parameters according to the simulation results, to obtain a daily increase of 0.2% in the production of sulphuric acid. According to this scenario at CLP 161,695,000 NPV and 53% IRR could be obtained. These results represent an increase of 6% on the monthly production of sulphur acid, with respect to the previous real operational results

(iii) The simulation using Aspen HYSYS® considered the contact stage of the process. This was conducted with 4 CSTR reactors and 3 shell and tube heat exchangers to evaluate and validate the system. After validating the simulator and using the plant design data, it was observed that the error between the design variables and the values obtained from the simulator is lower than 1%. During the simulation process, it was proved that the greatest conversion occurs when the temperature and the flow are at low and 150,500, respectively.

Data Availability

All raw data remains the property of the company that allowed this study. The input data (anonymized data) used to support the findings of this study could be available from the corresponding author upon request.

Conflicts of Interest

The authors declare no conflict of interest.

Authors' Contributions

All the authors collaborated in the design, experiments, result analyses, and paper writing.

Acknowledgments

The authors wish to acknowledge Carolina Aguilar for contributing materials from her undergraduate thesis and Universidad Católica del Norte for the use of the educational license of Aspen HYSYS® software.

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