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Research Article

Modeling, Evaluating and Scaling up a Commercial Multilayer Claus Converter Based on Bench Scale Experiments

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Abstract

Industrial scale reactors work adiabatically and measuring their performance in an isothermal bench scale reactor is faced with uncertainties. In this research, based on kinetic models previously developed for alumina and titania commercial Claus catalysts, a multilayer bench scale model is constructed, and it is applied to simulate the behavior of an industrial scale Claus converter. It is shown that performing the bench scale isothermal experiments at the temperature of 307 °C can reliably exhibit the activity of catalytic layers of an industrial Claus converter operating at the weighted average bed temperature (WABT) of 289 °C. Additionally, an adiabatic model is developed for a target industrial scale Claus reactor, and it is confirmed that this model can accurately predict the temperature, and molar percentages of $\rm H_2S$ and $\rm CS_2$. Based on simulation results, 20% of excess amount of Claus catalysts should be loaded to compensate their deactivation during the process cycle life. Copyright © 2020 BCREC Group. All rights reserved

Keywords: Sulfur recovery plant; Claus converter; Catalyst evaluation; Kinetic modeling; Scale up

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1. Introduction

H₂S (hydrogen sulfide) and carbon-sulfur components (such as CS₂ and COS) are toxic byproducts of refining natural gas and crude oil, and therefore, their entrance in any exhaust gas is under stiff environmental regulations [1,2]. To tackle with this issue, the modified sulfur re-

covery unit (SRU) is cherished to convert H_2S and carbon-sulfur compounds coming from the exhaust of those industries to the elemental sulfur [3,4]. The modified Claus process is conducted at two steps including thermal and catalytic stages [5]. The catalytic reactors of a SRU is usually loaded by alumina (Al_2O_3) and titania (TiO_2) Claus catalysts (combined bed or multilayer configuration) to promote the following reactions [6,7]:

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$$2H_2S + SO_2 \leftrightarrow 2H_2O + \frac{3}{n}S_n$$
, $\Delta H = -11.85 \frac{kcal}{mol}$ (1)

$$CS_2 + 2H_2O \rightarrow 2H_2S + CO_2$$
, $\Delta H = 4.54 \frac{kcal}{mol}$ (2)

$$CS_2 + SO_2 \to CO_2 + \frac{3}{n}S_n$$
, $\Delta H = -12.9 \frac{kcal}{mol}$ (3)

Industrial scale reactors usually work adiabatically, and they are essentially different from bench or even pilot scale reactors. In the former, there is a temperature profile along the catalytic bed whereas in the latter a constant temperature governs the whole bed. There are many literatures that tried to model a laboratory or bench scale and an industrial scale Claus reactor (called catalytic converter). Kerr et al. devoted a research on developing a kinetic model for the modified Claus reaction (Equation 1) in a laboratory scale device, and they estimated kinetic parameters for the Arrhenius form of its reaction rate [8]. In the other works, these researches developed a kinetic model for COS and CS₂ hydrolysis reactions [9], and then tried to find a deactivation mechanism for the Claus catalysts in a laboratory scale reactor [10].

Mendioroz et al. studied the kinetic of modified Claus process on γ-alumina at low temperature (100-200 °C) in a bench scale device [11]. To develop Langmuir type expression for the main Claus reaction, experiments were carried out at the different SO2 and H2S concentrations. The results showed the chemical reaction between adsorbed species, such as H₂S as the controlling step of the process. Nedez and Ray tried to comprehend mechanisms involved in the deactivation of Claus catalysts based on the bench scale experiments [12]. In this research, a feed containing H2S, SO2, H2O and CS2 was used, and O₂ was injected as a deactivation agent. They discovered that the main cause of the deactivation for the Claus alumina catalyst was the sulphation of its surface, and it could tremendously affect the activity of the catalyst versus time of the operation. Zagoruiko and Matros [13] proposed a mathematical model for the main Claus reaction carrying out in a catalytic reactor under conditions of sulfur condensation. To construct the model, a Langmuir type expression was successfully used, and based on simulation results, a reverse flow was recommended to regenerate the catalytic bed which was deactivated by the accumulation of sulfur inside pores of the catalyst.

Gemmingen and Lahne developed a kinetic model for a Linde Clinsulf process for the sulfur recovery, and they only included main

Claus reaction and hydrolysis of COS in their model [14]. The required kinetic parameters were estimated from chemical equilibrium of each reaction according to the mass conservation law and temperature-dependent equilibrium constants. In the other research, Abedini et al. proposed a model for rapid estimation of the produced sulfur in converters of Claus process. To simplify the model, they only considered the main Claus reaction [15]. Nabikandi and Fatemi developed a kinetic model for an industrial scale SRU unit in which main Claus reaction and hydrolysis of CS₂ and COS compounds were included [16]. They recommended that using kinetic based equations for simulating SRU was more accurate than using equilibrium (Gibbs free energy minimization) modeling approach. Ghahraloud et al. built a thermal model and catalytic sections of a commercial scale SRU loaded with alumina catalyst based on kinetic parameters reported in the literature. They concluded that s kinetic model could be successfully used to simulate the output variables of the target SRU.

Moreover, in the other research accomplished by these authors, this proposed kinetic model was utilized to simulate the sulfur emission of a SRU [18]. Based on simulations results, it was recommended that by implementing isothermal reactors instead of adiabatic convertors, less H₂S emission (about 1.8%) was achievable. In this respect, Sadighi and Mohaddecy used the solid package of Aspen plus for simulating and optimizing inlet temperatures of SRU convertors [19]. By comparing simulation results with data obtained from the under study unit, it was confirmed that using Aspen plus was reliable for optimizing temperatures of Claus convertors, especially when the corresponding kinetic constants of the loaded commercial catalysts in the convertors of SRU were not available.

The aim of this research is to evaluate the performance of an industrial Claus converter by using data obtained from isothermal bench scale experiments. To emulate behaviors of a Claus converter in terms of H₂S and CS₂ conversions, a multilayer Claus model is developed. Next, by using this combined bed model, the bed temperature for carrying out bench scale experiments is proposed such that the behavior of the Claus converter can be imitated. Thereafter, an adiabatic model is developed, and it is applied to scale up a bench scale reactor to an industrial Claus convertor. Outputs of this model are validated versus the actual data gathered from a commercial SRU.

2. Materials and Methods

2.1 Process Description of the Understudy Industrial Scale Claus Unit

A block flow diagram of the understudy Claus process unit is presented in Figure 1. As seen, the acid gas from the upstream is directed to the acid gas KO drum D-101. The exhaust gas from this drum is warmed up to 220 °C in the E-106 by using HP steam, and then it is conducted through the reaction furnace (H-101). The following reaction is carried out in this unit:

$$H_2S + \frac{3}{2}O_2 \to SO_2 + H_2O$$
 (4)

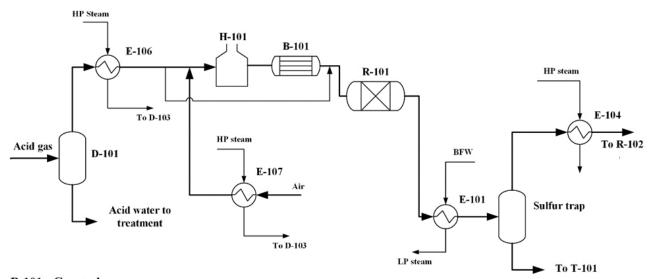
The process gas leaving the gas cooler (B-101) is entered to the first catalytic reactor (R-101) with the temperature and pressure of about 250 °C and 1.34 barg, respectively. In this reactor, sulfur is produced, and thereafter it is trapped. Due to the exothermic nature of Claus reactions, the temperature increases across the catalytic bed. However, the inlet temperature of the reactor should be adjusted such that its outlet temperature reaches about 310 °C for hydrolyzing COS and CS2 compounds. The hot gases leaving the first reactor are cooled in a condenser (E-104) by generating LP steam. The condensed sulfur is also sent to the sulfur degassing pit (T-101). The output stream of the first Claus reactor is conducted to the second and third converters to further conversion of H_2S and SO_2 . The first Claus reactor is loaded with separate layers of Al_2O_3 and TiO_2 catalysts at its top and bottom, respectively. The gas hourly space velocities (GHSV) of these layers are about $1050\ h^{-1}$ and $2100\ h^{-1}$, respectively. For the understand Claus converter, the mass of Al_2O_3 and TiO_2 catalysts loaded in the top and bottom layers of the catalytic bed are equal to $17900\ kg$ and $12780\ kg$, respectively.

2.2 Experiments in the Bench Scale System

Experiments were carried out in a bench scale plant designed and constructed by Research Institute of Petroleum Industry (RIPI, Iran) for the purpose of studying the catalytic section of the Claus process. The flow diagram of this unit is presented in Figure 2. The reactor is a tube with the inside diameter of 16 mm and total length of 2160 mm. For both Al_2O_3 and TiO_2 catalysts, the first layer (length of 30

Table 1. Specifications of the Claus catalysts studied [20].

Specification	Unit	Al_2O_3	${ m TiO_2}$
Color	-	white	white
Shape	-	Pellet	Bead
Size	mm	3-6	3-4
Density	kg/m^3	680	980
Strength	N/cm	>12	>70
Specific surface	m^2/g	300-400	>100



B-101: Gas cooler BFW: Boiler feed water

D-101, D-103: Acid gas knock out drums E-101, E-104, E-106, E-107: Heat exchangers

HP steam: High pressure steam

H-101: Reaction furnace LP steam: Low pressure steam R-101: First catalytic reactor R-102: Second catalytic reactor

Figure 1. Block flow diagram of the target Claus unit.

mm) is filled with inert $\alpha\text{-}Al_2O_3$ beads to obtain a uniform flow and temperature. The middle layer is loaded with the catalyst mixed with the equal volume of quartz particles, and the remained volume of the reactor is charged with $\alpha\text{-}Al_2O_3$ particles. The specifications of the Claus catalysts are presented in Table 1. It should be mentioned that catalysts studied in this apparatus were the same types as used in the commercial scale Claus converter.

In this unit, temperature along the catalytic bed is adjusted by using five temperature indicators and controllers (TIC). Additionally, a gas chromatograph (GC) with the thermal conductivity detector (TCD) and using helium as a carrier gas is applied to analyze the various species in the feed and product (i.e. N2, H2S, SO₂ and CS₂). By using mass flow controllers (MFCs) and a micro pump for injecting water, feed ingredients of the bench scale reactor are set on values similar to those of a Claus converter. However, due to limitations in the gas analyzing system, carbonyl sulfide (COS) and carbon disulfide (CS2) are lumped into a single compound i.e. CS2. Similarly, CO2 and N2 are lumped into N₂ component. According to the mentioned assumptions, the feed composition is adjusted to the values close to the industrial scale plant (Table 2).

To carry out experiments, the bench scale reactor is loaded with $26.5~\text{cm}^3$ and $13.5~\text{cm}^3$ of Al_2O_3 and TiO_2 catalysts, respectively. To mitigate the effect of the wall and diminish the axial dispersion and back mixing phenomena, both catalysts were diluted with the equal volume of quartz. It is obvious that the GHSV of the catalytic bed can be regulated by manipulating the rate of the gases and water injected by MFCs and micro pump, respectively.

2.3 Developing Kinetic Models for the Claus Reactor

2.3.1 Kinetic model of the bench scale Claus reactor

Kinetic models of the studied Claus reactor were previously described in detail [20], and it

Table 2. Feed composition of the multi-layer catalytic bed.

Compound	Mol%
$\mathrm{CS}_2\mathrm{+COS}$	2.05
$\mathrm{H}_{2}\mathrm{O}$	25.24
$\mathrm{H}_2\mathrm{S}$	3.61
SO_2	2.86
N_2	Balanced

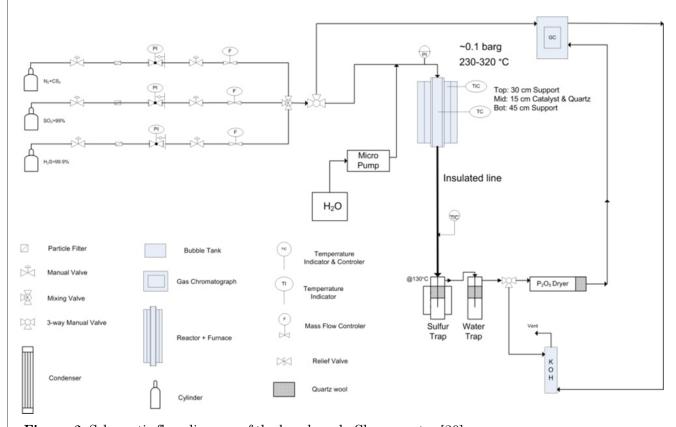


Figure 2. Schematic flow diagram of the bench scale Claus reactor [20].

was confirmed that with an acceptable error, it could certainly predict the H_2S and CS_2 conversions. The following assumptions were presumed in this model: the reactor works in plug flow regime, activity of Claus catalysts do not vary, the reactor is isotherm, and both feed and product streams behave such an ideal gas.

Therefore, rate constants for Equations (1) to (3) were written as follows [12]:

Forward path of the main Claus reaction:

$$r_{H_2S}(1) = -k_1 \frac{C_{H_2S} C_{SO_2}^{0.5}}{\left(1 + K_5 C_{H_2O}\right)^2}$$
 (5)

Backward path of the main Claus reaction:

$$r_{H_2O}(1) = -k_2 C_{H_2O} C_{sn}^{ns1} (6)$$

And, second & third reactions corresponding to CS₂ conversion:

$$r_{CS_2}(2) = -k_3 C_{CS_2}^{0.5} C_{H_2O} \tag{7}$$

$$r_{CS_2}(3) = -k_4 C_{CS_2} C_{SO_2} \tag{8}$$

Besides, kinetic constants of the model were expressed as follows:

$$k_1 = k_{01} \exp\left(\frac{-E_1}{RT}\right) \tag{9}$$

$$k_2 = \frac{k_1}{K_p} \tag{10}$$

$$k_3 = k_{03} \exp\left(\frac{-E_3}{RT}\right) \tag{11}$$

$$k_4 = k_{04} \exp\left(\frac{-E_4}{RT}\right) \tag{12}$$

$$\log K_p(T) = \frac{5910}{T} + 1.13 \times 10^{-3} T - 1.038 \times \ln(T) \quad (13)$$

By considering an infinitesimal volume of catalyst inside the reactor, the mass conservation was expressed as:

$$QC_i\big|_{V+dV} - QC_i\big|_V \pm R_i \cdot \partial V = \frac{\partial (\partial V \cdot C_i)}{\partial t_r}$$
 (14)

And consequently, this equation can be asserted as follows:

$$\frac{\partial C_i}{\partial V} = \frac{R_i \rho_{ave}}{m_f} \tag{15}$$

$$\frac{1}{\rho_{ave}} = \sum \frac{x_{m,i}}{\rho_i} \tag{16}$$

$$\frac{\partial P_i}{\partial V} = R_g T \left(\frac{R_i \rho_{ave}}{m_f} \right) \tag{17}$$

In Equation (17), R_i is the reaction rate of all components *i.e.* CS_2 , H_2O , SO_2 , H_2S , N_2 and sulfur through the catalytic bed which was formulated as:

$$R_{CS_2} = r_{CS_2}(2) + r_{CS_2}(3) \tag{18}$$

$$R_{H,O} = 2r_{CS_2}(2) - r_{H,S}(1) + r_{H,O}(1)$$
(19)

$$R_{SO_2} = r_{CS_2}(3) + 0.5r_{H,S}(1) - 0.5r_{H,O}(1)$$
 (20)

$$R_{H,S} = -2r_{CS_2}(2) + r_{H,S}(1) - r_{H,O}(1)$$
(21)

$$R_{N_2} = 0 \tag{22}$$

$$R_S = -\frac{3}{n} r_{CS_2}(3) - \frac{1.5}{n} r_{H_2S}(1) + \frac{1.5}{n} r_{H_2O}(1)$$
 (23)

$$R_{CO_2} = -r_{CS_2}(2) - r_{CS_2}(3) (24)$$

Kinetic coefficients corresponding to the studied Al₂O₃ and TiO₂ catalysts (Table 2) are presented in Table 3 [20]. Moreover, XRD analysis of the sulfur produced by Claus catalysts proved that sulfur allotropes have eight atoms of sulfur (S8) which is consistent with the other research [21]. Therefore, the stoichiometric coefficients of sulfur in the kinetic model of Al₂O₃ and TiO₂ catalysts (*i.e. n* in Equations 1 and 3) are equal to eight.

In the current study, to develop the multilayer model for the bench scale reactor, two distinguished subroutines were constructed for Al₂O₃ and TiO₂ layers. These functions were named Alumina_model and Titania_model, respectively. Hence, Equations (5) to (24) for each layer in conjunction with its corresponding kinetic parameters (Table 3) were implemented and solved in MATLAB programming interface (MathWorks, 2013). As seen in Figure 3, the feed of the Claus converter (Table 1) is injected to the Alumina subroutine. The product of the Al₂O₃ bed is calculated by the Alumina model, and then it is introduced to the Titania section. Finally, the output of the multilayer catalytic bed is determined by the Titania model.

Table 3. Kinetic parameters estimated for the Al_2O_3 and TiO_2 commercial catalysts [20].

Kinetic parameter	$\mathrm{Al_2O_3}$	${ m TiO_2}$
k_{01} (m 3 /(cm 3 cat.h.kmol $^{0.5}$))	1.36×10^{-7}	15.94×10^5
E_1 (kcal/mol)	7.64	25.05
k_{03} (m 3 /(cm 3 cat.h.kmol $^{0.5}$))	123.17×10^3	97.49×10^{3}
E_3 (kcal/mol)	12.12	8.68
$k_{04} \ (ext{m}^3/(ext{cm}^3 ext{cat.h.kmol}))$	29.13	16.81
E ₄ (kcal/mol)	3.5	3.5
K_5	87.05	218.69
ns1	0	0

2.3.2 Kinetic model for the industrial scale reactor

To develop an adiabatic model in this research, by assuming a variable cross section area (*A*) along the x-direction of the horizontal reactor (see Figure 4), Equation (17) can be expressed as below:

$$\frac{\partial P_i}{\partial x} = A \times R \times T \left(\frac{R_i \cdot \hat{\rho}}{m_f} \right) \tag{25}$$

But, the area cross section of the reactor is sum of the area of the cylindrical (AI) and torispherical (A2) sections of the reactor. According to the Figures 5 and 6, these variables are expressed as follows [22]:

$$\theta = \cos^{-1}\left(1 - \frac{x}{R}\right) \tag{26}$$

$$l = 2R\sin\theta\tag{27}$$

$$A_1 = LR \times l \tag{28}$$

$$z = R_C - \sqrt{(R_C - R_k)^2 - \left(\frac{D_{ext}}{2} - t - R_k\right)^2}$$
 (29)

$$D_{ext} = 2 \times R + t \tag{30}$$

$$R_{\nu} = 3 \times t \tag{31}$$

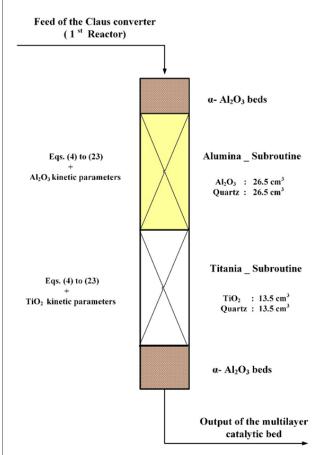


Figure 3. Diagram of the multilayer Claus bed model.

$$\tan \alpha_1 = \frac{z}{R} \tag{32}$$

$$z_1 = x \times \tan \alpha_1 \tag{33}$$

$$z_1 = (2R - x) \times \tan \alpha_1 \tag{34}$$

$$A_2 = z_1 \times l \tag{35}$$

$$A = A_1 + 2A_2 \tag{36}$$

For the understudy Claus reactor, the values of fixed variables including R, LR, and t, are 1.925 m, 6 m and 0.15 m, respectively. Finally, to find the temperature profile along the catalytic bed, the heat balance equation is expressed as follows:

$$\frac{dT}{dV} = \frac{UA_{ext} \left(T_{ext} - T \right) + \sum_{i=1}^{m} \left(-r_i \right) \left(-\Delta H_{r_i} \right)}{\sum_{i=1}^{n} m_{f,i} C_{p,i}}$$
(37)

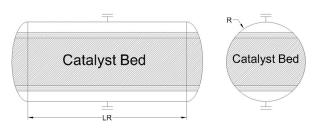


Figure 4. Horizontal view of the industrial scale Claus reactor.

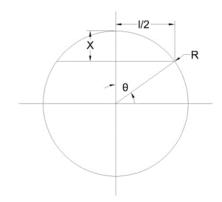


Figure 5. Cross-section of the industrial scale Claus reactor.

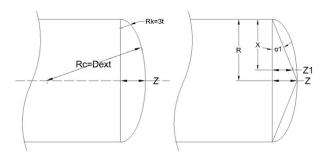


Figure 6. Torispherical head of the industrial scale Claus reactor.

Because of insulating the Claus reactor, it is assumed that the overall heat transfer coefficient (U) is equal to zero. Therefore, there is no heat transfer between the wall of the vessel and the environment, and the converter can be modeled as an adiabatic reactor. To develop the industrial scale adiabatic model, Equations (5) to (37) were implemented in Matlab environment (MathWorks, 2013a), and similar to the bench scale multi-layer (combined bed) model, they were sequentially solved for Al₂O₃ and TiO₂ catalytic layers using the corresponding kinetic parameters (Table 3), fixed variables of industrial scale Claus Converter (dimensions of converter and volume of catalysts), and actual operating conditions (GHSV and composition and temperature of feed).

3. Results and Discussions

3.1 Evaluating the Bench Scale Claus Reactor

The temperature of the bench scale reactor is set on the weighted average bed temperature (WABT) of the industrial scale plant (equal to 289 °C). The GHSVs of Al₂O₃ and TiO₂ catalytic beds are set on actual values equal to 1051.9 h-1 and 2105.5 h⁻¹, respectively. According to results obtained from the proposed combined bed model, it is found that molar percentages of H₂S and CS₂ in the output stream of the bench scale reactor are 1.28% and 0.14%, respectively. Based on data gathered from the industrial scale reactor, these values should reach 1.61 mol\% and 0.02 mol\%, respectively in the product of the first converter. Therefore, it is discovered that evaluating a multilayer Claus bed (isothermal reactor) at the WABT of an adiabatic converter cannot accurately reveal the behavior of Claus catalysts in a combined bed configuration. It is supposed that this discrep-

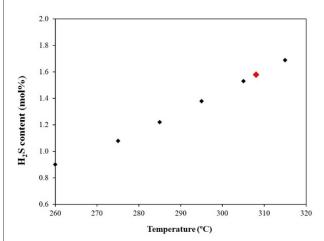


Figure 7. H₂S content of product versus temperature of the bench scale reactor.

ancy can be related to the difference in hydrodynamic regime and non-linearity of the system.

To find a better temperature for the bench scale equipment, variations of H2S and CS2 contents of the product versus bed temperature are presented in Figures 7 and 8, respectively. As seen, by increasing this variable, the H₂S content increases due to the exothermic and reversible nature of the main Claus reaction (Equation 1). Conversely, temperature has a negative effect on the CS₂ content of the product. Furthermore, as observed in Figure 8, CS₂ is effectively converted at the temperatures higher than 290 °C because of high activity of titania layer at the elevated temperatures [23]. In this layer, CS₂ conversion is corresponded to the reactions with both SO₂ and H₂O (Equations 2 and 3), and therefore both reactions are active over the titania catalyst.

It is supposed that the relation between the CS₂ conversion and temperature of the catalytic bed is nonlinear due to the different activities of titania catalyst at low and high temperatures. Hence, if evaluation of the multilayer catalyst is carried out at the WABT (equal to 289 °C), the titania catalyst is not effectively active, and the CS2 conversion is definitely lower than the actual value observed in an industrial scale reactor. In contrast, in this layer due to the exothermic nature of the main Claus reaction (i.e. Equation 1), H₂S is efficiently converted to sulfur, and therefore its conversion is obviously higher than the expected value in a commercial scale converter. Thus, as seen in Figures 7 and 8, at the bed temperature of about 307 °C (higher than WABT), H₂S and CS₂ contents of the outlet stream can meet their actual values expected in a commercial scale SRU at the start of run (SOR).

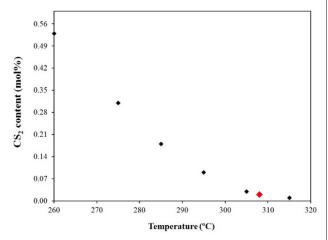


Figure 8. CS₂ content of product versus temperature of the bench scale reactor.

In Figure 9, variations of CS₂ and H₂S mole percentages along the multilayer catalytic bed at the temperature of 307 °C is depicted. As seen, the slope of the curve for TiO2 layer (from 26.5 cm³ to 40 cm³) is larger than that of Al₂O₃ catalytic layer (from 0 to 26.5 cm³). This phenomenon proves that TiO2 catalyst has considerably higher affinity to convert and hydrolyze carbon-sulfur compounds than Al₂O₃ catalyst, and if the converter is totally loaded with the latter catalyst, the carbon-sulfur content of the tail gas will not meet the requirements. Additionally, Figure 9 illustrates the generation of H₂S through TiO₂ layer because of promoting the reverse Claus reaction (see Equation 1). Therefore, to compensate the H₂S production through this layer, implementing at least a reactor after the first converter is essentially needed. It should be recalled that approximately all carbon-sulfur compounds are depreciated through the first converter, and therefore the temperature of the second reactor can be reduced up to the dew point of the elemental sulfur. Therefore, H2S conversion increases because of the exothermic nature of the main Claus reaction. However, if the temperature reaches the values lower than sulfur dew point temperature, it is cultivated, and fills the pores of the catalyst. Consequently, Claus catalysts are encountered with an accelerated deactivation [24,25].

3.2 Scale Up the Bench Scale Claus Reactor

The adiabatic model is run by using actual operating conditions (*i.e.* feed temperature of 235 °C, feed composition of Table 1, and feed flow rate of 1225.06 kmol/h), dimensions of Claus converter and actual volume of catalysts

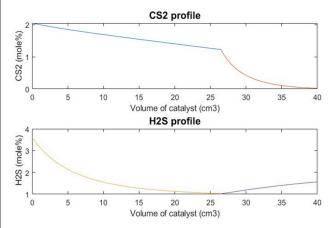


Figure 9. CS_2 and H_2S profiles through the catalytic bed of bench scale Claus reactor at T = 307 °C.

(belongs to R-101). Based on results presented in Table 5, one can conclude that the developed adiabatic model is able to calculate the gas concentrations and the output flow temperature of the target reactor with a reliable accuracy. Moreover, it is observed that mole percentages of CS2 and H2S in the exhaust gas, obtained by the model, is lower and higher than the actual values, respectively. It is supposed that the main source of this error is soaring the activity of catalyst at the initiation, causing a higher conversion for CS₂ compound. As the result, the temperature rises, and the backward path of main Claus reaction is strengthened due to its exothermic nature. Thus, H2S is generated through TiO₂ catalytic layer [20]. Another reason for this deviation is to model Claus reactor as an adiabatic system. Hence, due to transferring heat from the surface of the converter to the environment, there is an inevitable positive error for the outlet temperature computed by the adiabatic model.

Besides, the mole percentages of H₂S and CS₂ through the catalytic bed (x-direction) are presented in Figures 10 and 11, respectively. As seen, H₂S content of the feed decreases through the first layer of the catalytic bed (*i.e.* Al₂O₃); however, through the second layer (*i.e.* TiO₂), it goes up due to rising the bed temperature and promoting the backward main Claus reaction (see Equation 1). Hence, it is essential to implement another catalytic converter after the first one working at the lower temperatures to efficiently convert H₂S in SRUs for satisfying the environmental regulations of gas

Table 4. H_2S and CS_2 content of the product stream.

Component (mol%)	Industrial scale	Bench scale @ 289 °C	Bench scale @ 307 °C
H_2S	1.61	1.28	1.58
CS_2	0.02	0.14	0.02

Table 5. Comparison between the actual values and model outputs for the target industrial scale Claus reactor.

Parameter	Actual value	Adiabatic model
Reactor temperature (°C)	307.6	315.1
H ₂ S in product (mol%)	1.61	1.99
CS ₂ in product (mol%)	0.118	0.002

emission. Furthermore, Figure 10 demonstrates that at the SOR, a part of Al_2O_3 catalytic layer (from 158 cm to 196 cm) does not play a significant role in boosting H_2S conversion. However, commercial Al_2O_3 Claus catalysts, hastily lose their activity versus time [26], and therefore this excess volume of catalyst is reserved to repay the loss of catalyst activity versus process time (life of the commercial Al_2O_3 catalyst is about three years).

As presented in Figure 11, the CS₂ conversion is mainly boosted by the second layer of the catalytic bed (about 195 cm to 240 cm), and converting carbon-sulfur compounds will not promote without providing TiO₂ catalyst at the bottom of the Claus converter. Additionally, similar to the Al₂O₃ catalyst, an excess amount of TiO₂ catalyst is granted for this layer; however, the deactivation rate of TiO₂ catalyst is lower (life of the commercial TiO₂ catalyst is about seven years). Therefore, the height of the excess layer is less than 15 cm (from about 225 cm to 240 cm).

In Figure 12, variations in the profile of the temperature along the length of the catalytic

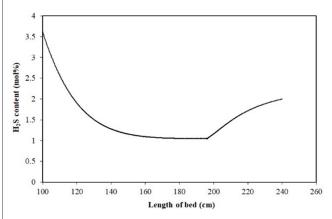


Figure 10. H₂S profile through the catalytic bed of Claus converter.

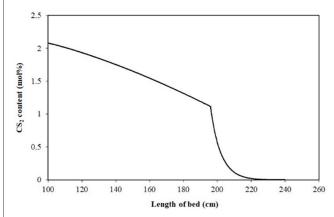


Figure 11. CS₂ profile through the catalytic bed of Claus converter.

bed is presented. As seen, through the Al₂O₃ layer, the temperature increases versus xdirection because of the exothermic nature of the main Claus reaction. Then, as seen in Figure 11, at the start of the titania layer (length of 196 cm), by promoting Equations (2) and (3), CS₂ of the feed which is mostly unconverted in the previous layer (alumina catalyst has low affinity to convert CS₂) is exceedingly converted to H₂S, CO₂, and elemental sulfur. Thus, the temperature sharply increases due to the exothermic nature of Equations (1) and (3) (see Figure 12), and the probability of collision between molecules or diffusion of molecules towards active sites of the catalyst is intensified [27]. Afterwards, the rate of the backward Claus reaction (an endothermic reaction, see Equation 1) increases due to the elevated bed temperature (at the length of 210 cm), and after reaching a peak, the temperature slightly decreases along the length of the Claus converter.

4. Conclusions

Carrying out isotherm bench scale experiments under the linearly weighted average temperature of a commercial Claus converter (i.e. WABT) imposed inaccuracy to assess activities of those catalysts. A kinetic-based multilayer Claus model confirmed that to compromise between H₂S and CS₂ conversions of the isothermal bench scale reactor and those of an adiabatic Claus converter, experiments should be done at the temperature of 307 °C instead of the WABT of 289 °C. Moreover, the industrial scale adiabatic model developed for a real Claus converter was able to calculate the temperature, and molar percentages of H2S and CS₂ of the product equal to 315.1 °C, 1.99%, and 0.002%, respectively. Based on data gathered from the target SRU, the actual values of

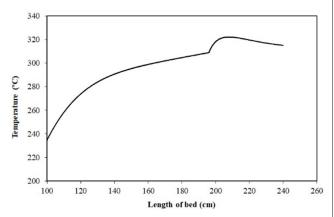


Figure 12. Temperature profile through the catalytic bed of Claus converter.

those variables were 308 °C, 1.61 mol%, and 0.118 mol%, respectively. It was supposed that the main source of above deviations was the high activity of Claus catalysts during bench scale experiments. Additionally, the negligence of the heat transfer from the surface of the converter to the environment (*i.e.* to consider adiabatic process) exacerbated the heat increase through the catalytic bed. About 20% of the total catalyst volume was regarded to compensate the loss of catalyst activity during cycle life.

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Nomenclatures

ciatures
Reactor cross section, (m ²)
Reactor external area, (m ²)
Concentration of component i ,
(kmol.m ⁻³)
Heat capacity of components j ,
(kcal.kmol ⁻¹ .K ⁻¹)
Reactor external diameter, (m)
Activation energy of $i^{\rm th}$ reaction,
(kcal.mol ⁻¹)
Coefficient of the adsorption term in
the main Claus reaction
Frequency factor of $i^{\rm th}$ reaction
Reaction rate constant of component i
Equilibrium constant of Claus reac-
tion, (-)
Catalyst bed length, (m)
Mass flow rate, (kg.h ⁻¹)
Reaction order, (-)
Number of experimental data points,
(-)
Partial pressure, (atm)
Volume flow rate, (m ³ .h ⁻¹)
Reaction rate of component i ,
(kmol.h ⁻¹ .kg cat ⁻¹)
Radius of the reactor, (m)
Reactor inside crown radius, (m)
Gas constant, (kcal/kmol.K)
Summation of reaction rate of all com-
ponents, (kmol.h-1.kg cat-1)
Reactor inside knukle radius, (m)
Reaction temperature, (K)
Thickness of vessel, (m)
Reaction time, (h)

$T_{ m ext}$	Ambient temperature, (K)
U	Overall heat transfer coefficient,
	(kcal. m ⁻² .K ⁻¹ .h ⁻¹)
V	Catalyst bed volume, (m³)
WABT	Weighted average bed temperature
	(°C)
$oldsymbol{x}_{ ext{m,i}}$	Mass fraction of component i , (-)
Z	Depth of the reactor head, (m)
ΔH	Reaction heat, (kcal.h-1)
$ ho_{ m i}$	Density of component i , (kg.m ⁻³)
∂V	Volume element of catalyst bed, (m ³)
$ ho_{ave}$	Average density of the flow through
	the catalytic bed at the reaction tem-
	perature, (kg.m ⁻³)

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