

Optimizing the multi-stage claus process: A parametric sensitivity analysis on the sulfur recovery

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ABSTRACT


Hydrogen sulfide (H₂S) is another villainous impurity within the ambiance of natural gas, which upon reaction gives birth to undesirable offspring during gas processing and desulfurization at a refinery. Operational risks include shutdowns and decreased production due to sulfur deposits in gas metering systems. This research is to model and analyze the operating parameters of the sulfur recovery unit via the HYSYS software. The sulfur removal unit was simulated utilizing two models; the first served as a Ping Robinson package, while the second employed Sulsim. The factors influencing the unit are feed circumstances, airflow rate, and catalyst type. Both models show that proper air flow helps turn H₂S into elemental sulfur raising liquid sulfur content also it has been seen that the recovery of sulfur is linear to the flow rate of the reaction gas so an increase in gas flow rate from 450 to 500 kmole/h would enhance sulfur to 0.956 mole fraction. The airflow rate significantly influences the formation of liquid sulfur and diminishes H₂S emissions. The optimization of temperature is noted to bring a striking improvement in the efficiency of SRU. For instance, operation at 20–25°C lower than the design specification also gave very high recovery rates (approx. 99.9% efficiency) without adverse environmental impacts. The Sulsim fluid package model aligns more closely with the actual values of the sulfur removal unit.

Keywords: Claus process, Sulfur recovery unit, Hydrogen sulfide, Sulsim, Sulphur, HYSYS.

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1. INTRODUCTION

As an impurity present in natural gas reserves, hydrogen sulfide is one of the main causes of foul by-products in gas processing and desulfurization units at refineries. It's so toxic that it can't be incinerated to free sulfur oxides that would then damage an ecosystem or be released into the atmosphere. A main stoppage risk to the operation attributable to sulfur depositing in gas metering systems and pipelines is an unpleasant shutdown and/or low production. Specific materials had to be used due to the high corrosion of the foul gas by hydrogen sulfide, which also escalated capital expenses (Adewale et al., 2015; Adewale et al., 2016; Santos et al., 2016). In addition, 2% of the errors caused by solid sulfur depositions in the equipment will be far more critical for accurate production flow rate indications (Pack et al., 2012).

Commonly practiced sweetening techniques for various gas streams include adsorption and absorption of hydrogen sulfide from natural gas pipelines (Santos et al., 2016). As a commercial sulfur removal tool, membranes are gaining increasing use around the world. Ideally designed membranes should be able to separate and purify the produced hydrogen with great selectivity following the conversion of hydrogen sulfide into elemental sulfur and hydrogen (Edlund and Pledger, 1993; Syed et al., 2006).

Therefore, hydrogen sulfide should not be dissociated into the atmosphere once separated from fossil fuels; still, at least not because of stringent environmental regulations. Claus Process has now become a renowned extraction process internationally for converting H₂S into sulfur and hydrogen (Eow, 2002; Bengé and Dew,

2005). The present costing has lower capital costs according to the preliminary economic study case relative to acid gas injection (Li et al., 2013). The conversion process for hydrogen sulfide is very efficient and mature in the sense that the prevailing mode of technology it is presently mostly separated by is the sulfur Recovery Units (SRUs) which will recover it as elemental sulfur (El-Bishtawi and Haimour, 2004). Economically not very feasible to break down H₂S at a temperature above 725°C. Whereas, technically catalytic annealing of H₂S boasts high degree efficiency and, additionally, would give an opportunity for regained hydrogen.

Other techniques like the thermochemical process photocatalytic electrolysis and hydrolysis and reactive adsorption have also been tried and shown great promise for hydrogen recovery and high sulfur recovery rate (Huisman et al., 1994; Reverberi et al., 2016). The Claus process hence remains the most popular means for converting hydrogen sulfide (Lins and Guimarães, 2007; ZareNezhad, 2009). The efficacy of the tail-gas treatment method determines the overall sulfur recovery (Eow, 2002). Recently, a novel approach that combines the Claus process with hydrocarbon reforming for the production of on-site hydrogen extraction from the process, and simultaneously lowering the tail-gas flow rate was reported (Huang et al., 2009; Taghizadeh and Bahadori, 2019).

This study employs a dual-framework approach by utilizing both the Sulsim and Peng–Robinson fluid packages. It allows for any noted differences in phase equilibrium predictions that may occur, particularly about liquid sulfur separation and H₂S slip in the tail gas. Regarding the assumptions taken into consideration by this model, it is operating within realistic limits, such as reactor temperature range and air feed allocation as well as equilibrium limited reactions which can be attained in industrial practice, thus making it more real than most others. These parameters have direct relations with the physical setup of the Claus process-air feed flow rate, and feed temperature as well as other operating conditions. For instance, air feed flow manages the stoichiometric balance of oxygen to H₂S, feed temperature starts reaction kinetics and phase separation, while conditions in a reactor control how much sulfur is made and how much H₂S is left. By clearly linking these physical parameters to what happens in the process, this model has both a wider scope and more detail of sensitivity than earlier studies.

The present study takes into account site-specific operating conditions that practically belong to industrial Claus units. Feed composition for simulation considers the H₂S-rich acid gas stream with CO₂ and minor hydrocarbons (SRU in Iraqi's Field of Badra Reservoir) reflecting reality since these components influence reaction equilibrium and sulfur yield. The air feed flow rate and distribution were also varied to test different stoichiometric ratios between oxygen and H₂S as a reflection of actual operational adjustments. Reactor inlet temperatures, as well as furnace operating conditions, have been set within realistic ranges in the

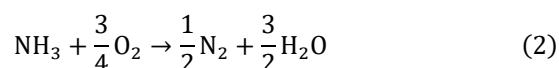
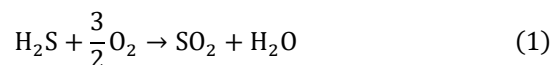
industry so that sensitivity of liquid sulfur recovery, including H₂S slip on thermal and catalytic stage performance can be captured. Such site-relevant conditions which are different from generic assumptions used by most earlier modelling works make our dual-model comparison important and provide reasons to develop a new simulation-based sensitivity analysis.

The Claus multi-stage process has been modelled using two different equations of state: the Sulsim and Peng Robinson fluid packages. Predictive performance with respect to liquid sulfur recovery and H₂S formation in tail gas is compared. Previous works used a single property package, often emphasizing an overall recovery efficiency; thus, our work systematically evaluates model-based differences in predicting the performance of various aspects of detailed steps within the process. This is accompanied by a parametric sensitivity study that provides an explicit quantitative assessment of the impacts that major operating variables-air feed flow rate, feed temperature, and reactor operating conditions-have on both recovery of sulfur and the residual H₂S emission. It gives new insight into the level of confidence of thermodynamic models for Claus process simulation as well as identifies operating parameters that have a significant effect on the performance of Sulfur recovery. This contribution also further clarifies spots where process optimization opportunities lie and supports an even more optimized design of a more efficient sulfur recovery unit.

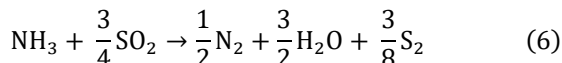
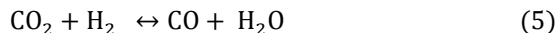
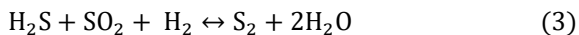
1.1 A DESCRIPTION OF THE SRUS

The modified Claus process consists of the following: (i) an exothermic thermal or combustion operation in a reaction furnace; and (ii) an exothermic catalytic action employing waste heat boilers, converters, and condensers. In the reaction, most of the sulfur dioxide produced in the combustion section is supposed to react with the unburned hydrogen sulfide to produce elemental sulfur (Signor et al., 2010). Now, acid gas and combustion air are introduced into this reaction furnace operating at around 1000°C to achieve a 2:1 molar ratio of H₂S to SO₂ and a 50% conversion to elemental sulfur (ZareNezhad and Hosseinpour, 2008):

- (a) On contact with air, two principal combustion reactions occur in the flame zone.



- (b) These extremely exothermic processes significantly raise the temperature. Multiple side reactions occur. The side reaction eliminates any ammonia that is not oxidized in reaction (2).



(c) Among other flammable impurities, the acid gas stream also introduces some hydrocarbons into the mix, which make carbon monoxide, carbon disulfide, and carbonyl sulfide.

With H₂S:SO₂ 2:1 it is therefore preferable to oxidize only 1/3 of the H₂S feed. Further, the waste heat boiler comes after the reaction furnace for heat recovery and heat integration (El-Bishtawi and Haimour, 2004; Boussetta et al., 2009). This addition of more species then makes the possibility of having an ideal equilibrium reaction difficult since it is not known which of the species' equilibria concentrations will be equal to that of another throughout all process conditions. Further impurities also contribute up to 20%–50% of tail-gas impurities (Gens, 1994; Huisman et al., 1994).

Chardonneau et al. (2015) have shown that even only 1–3% of the impurity of the toluene component results in a 50% loss of efficiency for the Claus process. However, with an enriched supply of oxygen, toluene apparently gets burned in the thermal step (Chardonneau et al., 2015). It is hard to predict the flame temperature and the composition of the gas product from the burner. Precisely measuring the furnace flame temperature and gas product composition is difficult (Ibrahim et al., 2014).

Other methods to enhance the process have been attempted with extra focus on increasing the furnace temperature and the catalytic activity (ZareNezhad and Hosseinpour, 2008; ZareNezhad, 2009). If a 40% H₂S acid gas stream is burned with natural gas, the rise in temperature during the co-firing does not pass the prescribed limit of 1050°C (ZareNezhad, 2009). The other negative impact of the higher concentration of hydrocarbons in the intake feed can, therefore, increase that of carbon disulfide being produced. Preheating the air and acid gas thus augments the temperature of the furnace but at further total cost.

Furthermore, water must not be present in sweetened acid gas streams for the reason that the water causes hydrogen sulfide to interact with iron in construction materials, hence speeding up cracking of the infrastructure (ZareNezhad and Hosseinpour, 2008). Farther from lowering the effectiveness of the furnace, water also enhances undesired aromatics' formation, as showed by Ibrahim et al. (2017).

Unreacted oxygen is allowed to remain in the gas to oxidize SO₂ and SO₃ further before the gas stream reaches the catalytic bed. The SO₃ makes aluminium sulfate which deactivates the catalysts. Craig and Anderson (1995) claim

that sulfuric acid is produced when SO₃ combines with H₂O. It becomes corrosive downstream steel facilities based on various factors like temperature acid concentration. Further, it was also observed that oxygen enrichment enhances the decomposition of polyaromatic hydrocarbons, as well as toluene and benzene-like compounds existing in the acid gas stream (is a possibility) (Ibrahim et al., 2014; Rahman et al., 2016). However high furnace temperatures can have a negative influence on this aspect (Zarei et al., 2016).

The effect of increased air preheat temperature is also assessed from the point of view of the furnace temperature and, hence, the H₂S conversion efficiency in the SRUs for Badra Reservoir Iraqi's Field operating both low and high levels of hydrogen sulfide. The effect of raising the air preheat temperature is investigated in detail, including its potential ramifications for sulfur recapture units also looked into.

The operational conditions were analyzed to assess the contribution of each parameter in terms of performance and the target is to obtain liquid Sulphur in reduced hydrogen sulfide amounts. The optimal operational parameters were selected based on these analyses, and those parameters that had the highest effect on the efficiency of the recovery unit. And lastly, compared with real field data, these selected operational conditions were verified through an actual result comparison (test). Lastly, the process simulation has been validated by comparing actual field data.

2. METHODS

2.1 Conditions of Claus Process

The process of SRU in Iraqi's Field of Badra Reservoir has been simulated by Aspen Hysys Technology (Abdullah et al., 2024; Abdullah et al., 2024; Saud, et al., 2024). Fig. 1 shows a graphical abstract of steps of sulfur recovery unit, where two simulation processes have been conducted using a different fluid package (Ping Robinson, and Sulism). Fig. 2 is a process flow diagram of sulfur recapture unit in Iraq. An inlet stream enters into the Claus process, as shown in. The temperature and pressure of the inlet stream are 35°C and 10 bar, respectively. Pure oxygen enters the process for the first time at a rate of 90 kmol/h and the ammonia that is not wanted also enters the process at 4.7 kmol/h.

The second inlet stream enters the process at a temperature of 120°C and a pressure of 2.4 bar. H₂S, CO₂, CO, H₂, and NH₃ flow rates which equal to 23.9, 16.9, 2.1, 10.2, and 31.6 kmol/h respectively; the conditions of the third inlet stream are 50°C and 2.1 bar; H₂S, CO₂, and N₂ flow rates are 159.1, 174.1, and 31.3 kmol/h. These three streams enter the zone of flame in the section of furnace and are two primary combustion reactions.

2.2 Claus Process Kinetics

The modelling of the flame reactor comprises an oxygen-rich zone with exothermic reactions. Each reactor uses

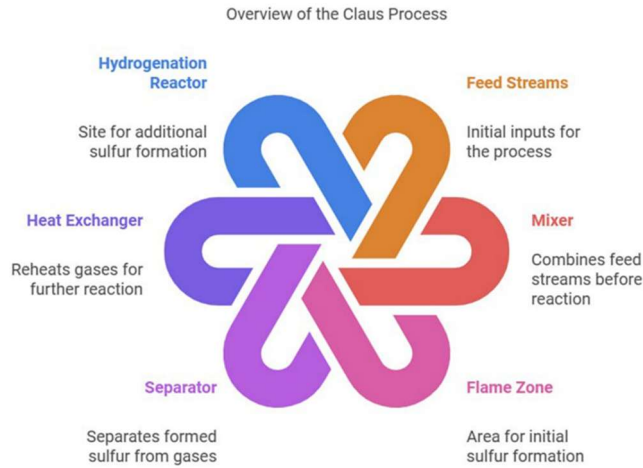


Fig. 1. Steps of Claus process

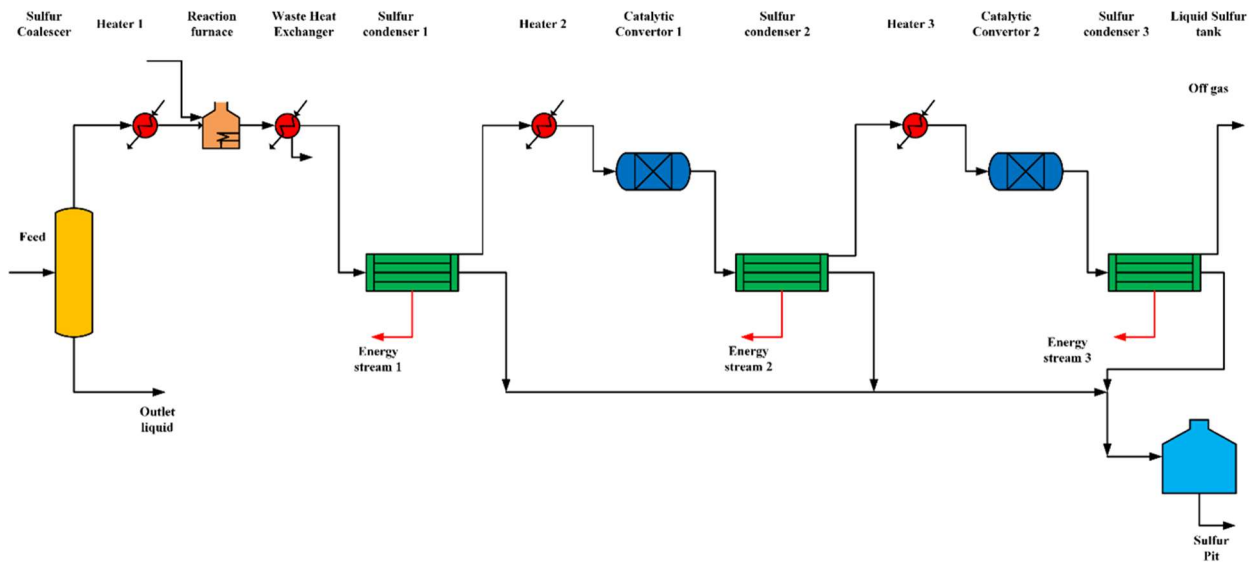


Fig. 2. Sulfur recovery unit in Iraqi's Field of Badra Reservoir

alumina and titanium as catalysts. The highly exothermic fast reactions are then cooled to control the temperature because otherwise sulfur would deactivate the catalyst by depositing on their surfaces. The second is slower and has endothermic reactions requirements. Therefore, the rate equations are (Zahid et al., 2021):

$$-r_i = K_{oi} \exp\left[-\frac{E_i}{RT}\right] P_{H_2S} P_{NH_3} P_{O_2} \quad (7)$$

Where i is the equation number. Whereas r_i is the rate of reaction ($\text{kmol}\cdot\text{s}/\text{m}^3$), P_i is the partial pressure of species i (atm) K_{oi} unit varies depending on temperature and pressure.

$$-r_3 = 3.85 \times 10^7 \exp\left[-\frac{26}{RT}\right] \left(P_{H_2S} P_{NH_3} P_{O_2} - \exp\left[-0.949 - \frac{5840}{T}\right] P_{S_2} P_{H_2O}\right) \quad (8)$$

$$-r_4 = 9.17 \times 10^5 \exp\left[-\frac{45}{RT}\right] \left(P_{H_2S} P_{S_2} - \exp\left[-5.93 - \frac{10,880}{T}\right] P_{S_2} P_{H_2}\right) \quad (9)$$

$$-r_5 = 1.52 \times 10^{12} \exp\left[-\frac{60.3}{RT}\right] \left(C_{CO_2} C_{H_2} - \exp\left[-3.88 - \frac{4166}{T}\right] \frac{C_{CO} C_{H_2O}}{C_{H_2}}\right) \quad (10)$$

$$-r_6 = 2.29 \times 10^4 \exp\left[-\frac{27.5}{RT}\right] C_{NH_3} C_{SO_2} \quad (11)$$

Whereas C_i is concentration of species (kmol/m^3).

$$K_p = \exp\left[-53.67 + \left(\frac{47800}{T(K)}\right)\right] \quad (12)$$

As is evident from Fig. 1 above, the feed enters the process through these three inlets. The first two streams

enter the flame zone after mixing in a mixer, and the other single stream enters an anoxic zone for the chemical reaction zone. Following the flaming zone, some sulfur is formed that collects at the bottom of the separator. After the temperature exchanger, the temperature of unreacted gases moving towards this hydrogenation reactor is 314°C. These travel to the hydrogenation reactor, where a reaction takes place at 314°C under 1.6 atm with 10.5 kmol/h of sulfur passing through the reaction of hydrogenation. The unreacted gases are once again sent to separate hydro generation reaction another hydro generation reactor. More unreacted gas then moved to another hydrogenation reactor. Both reactions are carried out at the same temperature and pressure; 315°C and 1.6 atm, respectively. More sulfur is then produced in the second reactor at a rate of 10.5 kmol/h. All sulfur streams are then mixed together at a common mixer to have a final flow rate of 25.805 kmol/h (Goar et al., 1986; Zahid et al., 2021).

3. Results and Discussion

3.1 Validation of The Model

Two Claus models with three Claus processes were simulated on the basis of given operation conditions. The first model was conducted by applying the Peng Robinson Package and the second one by using Sulsim Package represented in Fig. 3 and Fig. 4, respectively. Results from both models were compared for validation. Validation was done when results achieved are shown to be within an error

of less than 5%. This is as shown in Table 1. From these results and from comparing both packages with actual data, one is able to say that the Sulsim Model is handier, because it is the mode recommended by the methods assistant as a specialized and most suitable fluid package. In our study, we used the Peng Robinson package to show that the earlier methods could not have matched up to the level of perfection as the Sulsim Model.

3.2. Analysis of Sensitivity

The above explained parametric optimization covers the process for operating variables of process plants concentration, temperature, and pressure of chemical equipment. The selection of parameters is dictated by the type of process. In this case, important variables are the feed flow rate, airflow, feed pressure, feed temperature, and type of catalysts used in the reactors and the ratio. The result from the parametric analysis performed revealed that a change in parameter caused an appreciable effect on the efficiency of chemical plants.

3.2.1. Effect of Feed Flow Rate

One of the common practices uses advanced simulation tools like Aspen HYSYS and ProMax to model the effects of varying feed flow rates on sulfur recovery. These simulations can predict changes in the rate of sulfur liquid and overall recovery efficiency under different operational scenarios (Anderson, 1997). The feed flow rate in three-stage Claus process sulfur rehabilitation units imposes a significant influence on the overall recovery efficiency. The

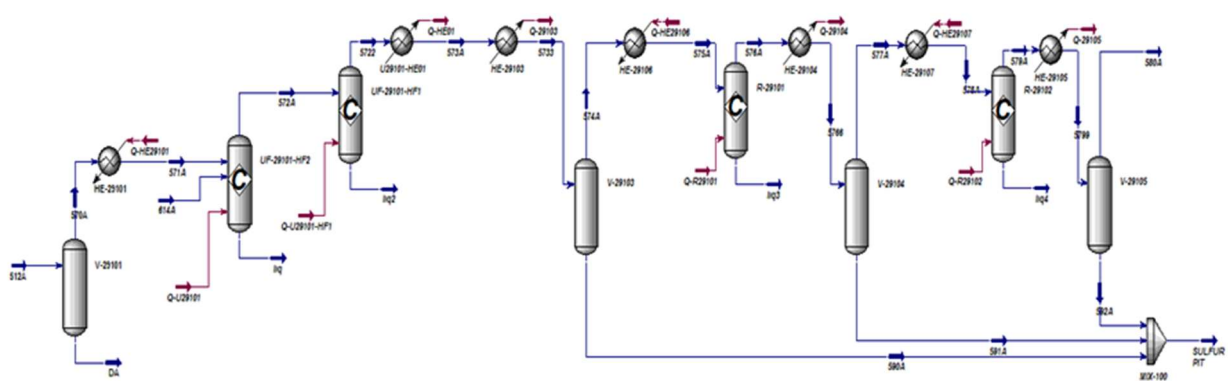


Fig. 3. Three-stage Claus process Sulphur recovery unit using Peng Robinson Package.

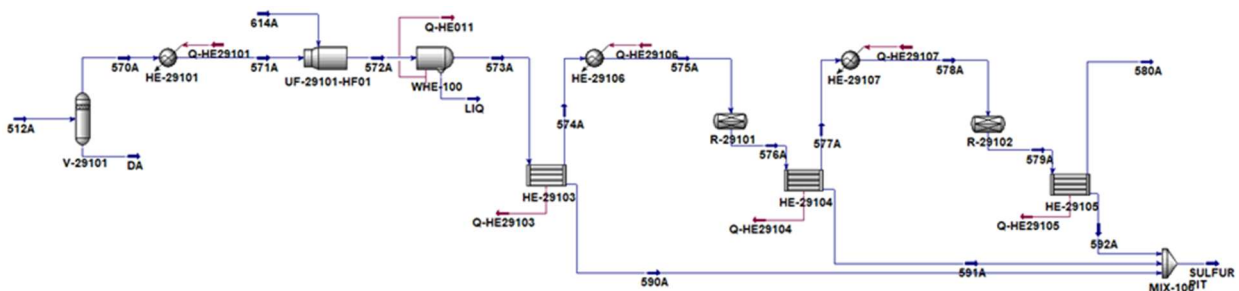


Fig. 4. Three-stage Claus process SRU using Sulsim Package

Table 1. Comparing the model results using two fluid packages with the real values

Stream No.	Property	Actual value	Model 1 (P.R)	Relative error (%)	Model 2 (Slm)	Relative error (%)
512 A	Mole flow rate (kmol/h)	438	438	0	438	0
	Temperature (°C)	40	40	0	40	0
	Pressure (bar)	1.8	1.8	0	1.8	0
570 A	Mole flow rate (kmol/h)	438	438	0	438	0
	Temperature (°C)	40	40	0	40	0
	Pressure (bar)	1.76	2.23	26	1.76	0
571 A	Mole flow rate (kmol/h)	438	438	0	438	0
	Temperature (°C)	240	240	0	240	0
	Pressure (bar)	1.64	1.64	0	1.64	0
572 A	Mole flow rate (kmol/h)	924.8	922.5	0.25	922.5	0.25
	Temperature (°C)	1029	1029	0	1058	2.82
	Pressure (bar)	1.56	1.56	0	1.56	0
573 A	Mole flow rate (kmol/h)	876	863	1.48	871	0.57
	Temperature (°C)	289	289	0	289	0
	Pressure (bar)	1.51	1.51	0	1.51	0
574 A	Mole flow rate (kmol/h)	858	840	2.09	852	0.7
	Temperature (°C)	182	168	7.69	168	7.69
	Pressure (bar)	1.46	1.47	0.68	1.47	0.68
575 A	Mole flow rate (kmol/h)	859.2	840.3	2.2	852	0.83
	Temperature (°C)	225	224.91	0.04	225	0
	Pressure (bar)	1.43	1.43	0	1.43	0
576 A	Mole flow rate (kmol/h)	848.3	844.5	0.44	841.5	0.8
	Temperature (°C)	301	301	0	290.5	3.49
	Pressure (bar)	1.41	1.41	0	1.41	0

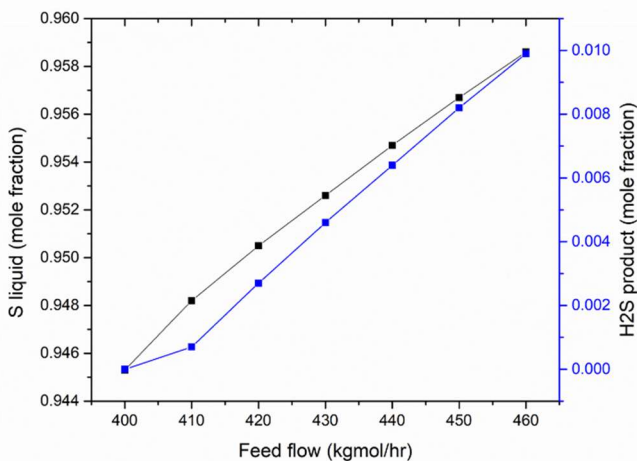


Fig. 5. influencing of feed flow rate on the production of liquid sulfur and H₂S generated using P.R.

efficiency is closely associated with the feed-gas composition and the flow rate. Model 1 produces more H₂S with the Ping-Robinson fluid package (Fig. 5) at higher flow rates, but the concentration of H₂S in the feed is lower and

therefore suboptimal for recovery. The balance between flow rate and concentration is a very important factor since excess flow would result in reduced liquid sulfur phase due to lower hydrogen sulfide concentration, as depicted in Fig. 6 (Polasek and Bullin, 1993; Ibrahim et al., 2023). Secondly, it is of great importance what the ratio between H₂S and CO₂ feed is. This means that it becomes rather difficult to keep an appropriate sulfide/carbon dioxide ratio when the feed flow rate increases. Once this ratio exceeds a certain value, it drops sharply because of an increase in the efficiency of sulfur recovery processes, which then implies that the flow rate has to go into the plant must be controlled so that enough H₂S is available for conversion into sulfur (Polasek and Bullin, 1993; Anderson, 1997).

Interaction of temperature and pressure with feed flow rates is one other interaction. The Claus process operates highly dependent on assigned flow rates, and any fluctuation may ignite improper reactions because it is within the thermal dynamics of the Claus process. Most notably, optimum temperature conditions are very crucial to enhancing sulfur production without adverse environmental effects compared with the results for the two models as shown in Fig. 7 (Ibrahim et al., 2023).

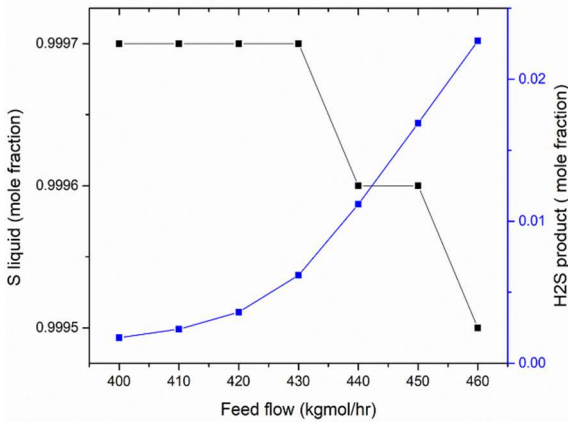


Fig. 6. Impact of feed flow rate on the synthesis of liquid sulphur and H₂S produced via Sulsim

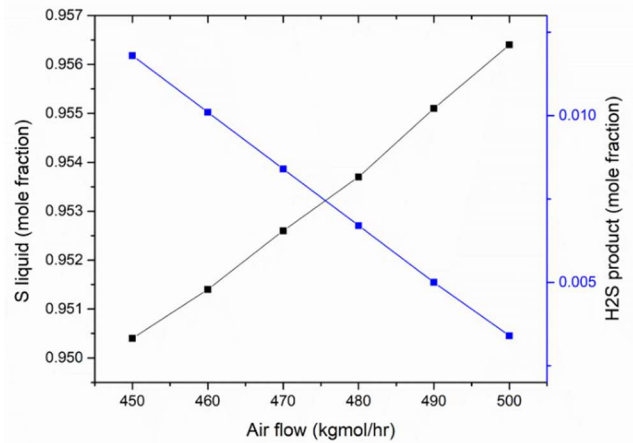


Fig. 8. Effect of airflow rate on sulphur liquid synthesis and H₂S creation using PR.

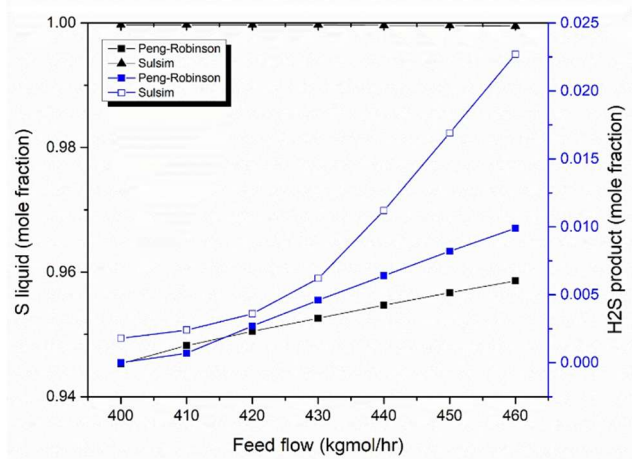


Fig. 7. Correlation between feed flow rate and sulphur liquid production and H₂S generation utilizing two fluid packages.

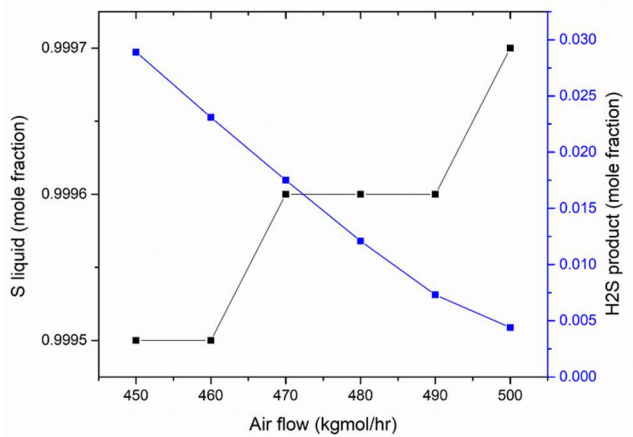


Fig. 9. Impact of air flow rate on sulphur liquid production and H₂S generation utilizing Sulsim.

3.2.2. Effect of airflow

That the flow rate of the gas in the SRU has a significant effect on the sulphur liquid is mainly a relationship which results from the combustion and conversion reactions which take place within this unit. The airflow rates equate to a H₂S to SO₂ ratio of not less than two in the tail-gas, as a stoichiometric requirement for both reaction beds to possess sufficient reactants for total sulphur recovery. In the Claus Process, there are two major reactions as indicated in equations 1 and 2.

For them to react efficiently, air (oxygen) must be available. Otherwise, their sulfur recovery would be hampered; the more unreacted hydrogen sulfide is left in the tail-gas, the less liquid sulfur is produced (Ibrahim et al., 2023). Optimal air flow promotes the conversion of H₂S into elemental sulfur, boosting liquid sulfur content, as apparent in this work for both models in Fig. 8 and Fig. 9. Contrariwise, if air flow is too weak, efficiency hence falls so that there will be less liquid sulfur. Furthermore, it has been noted that the sulfur recovery is linear to the flow rate

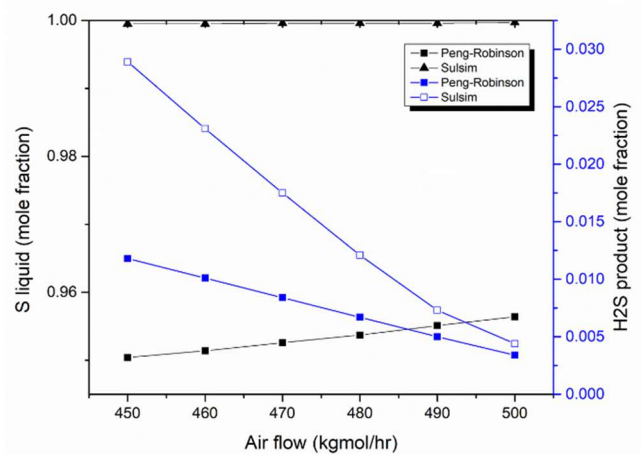


Fig. 10. Impact of air flow rate on sulphur liquid production and H₂S generation in two fluid package processes.

of the reaction gas and hence an increase in gas flow rate would enhance sulfur (Ibrahim et al., 2023). These models can be calibrated as depicted in Fig. 10.

3.2.3. Effect of Feed Pressure

It was observed that as an increasing pressure on sulfur removal units for both models, initially brings about reduced sulfur production because of several kinetic and thermodynamic factors, as seen in Fig. 11 and Fig. 12. Le Chatelier's Principle states that increasing pressure will favor the reaction of those substances producing the least number of gas molecules. Since it is a Claus Process reaction, gaseous reactants are H₂S and SO₂, which produce solid or liquid sulfur. If the reaction is already heavily tilted towards equilibrium, raising the pressure further may not greatly increase the output of sulfur and may even put it under suppression by further shifting the equilibrium toward the reactants if its setting does not suit a high-pressure setting (Abghari et al., 2011; Zahid et al., 2021).

Increased pressure would adversely affect the reaction kinetics. For example, some sulfur-oxidizing bacteria are known to exhibit lowered metabolic activities and rates of sulfur oxidation at elevated pressures. This refers that the rates of reactions may get reduced from increasing the output of sulfur in the case of more concentration of reactants (Osman et al., 2021). Also, the solubility and phases of sulfur matter, too. When the pressure rises, more of the sulfur is soluble in the gaseous phase and less is available for condensation into the liquid phase. This means lower liquid sulfur outputs since not all H₂S available to the system under increased pressure conditions could be converted into sulfur as shown in Fig. 11 (Osman et al., 2021). Analogously, the comparison of the two models in terms of pressure build-up is depicted in Fig. 13.

Higher pressures can complicate the operational dynamics of the sulfur recovery unit, possibly leading to increased equipment friction and the requirement for good quality materials. These may indirectly impact the total efficiency and yield regarding sulfur production.

3.2.4. Effect of feed temperature

As can be seen from temperature dependency temperature affects both the kinetics and the equilibrium involved in the chemical processes. The Claus reaction rates are generally better at higher temperatures for most industrial chemical processes, e.g. the conversion of hydrogen sulfide to elemental sulfur in this case. Operation at high temperatures usually between 200°C and 315°C enhances the conversion of hydrogen sulfide to sulfur, and hence the effect on liquid sulfur production (Zarei et al., 2016). Furthermore, Claus reaction is an equilibrium reaction; that is, the conversion would never be total. The position of equilibrium can be moved by changing temperature too. Higher temperatures will encourage more gas product formation which in itself is a pointer toward a low liquid sulfur rate if not well managed in process design isolation; that is, if left to natural courses constraint(s), as shown in Fig. 14 and Fig. 15 (McIntyre and Lyddon, 1997).

The optimization of temperature is indicated to have a remarkable enhancement in the efficiency of SRU. For

example, operation at 20–25°C lower than the design

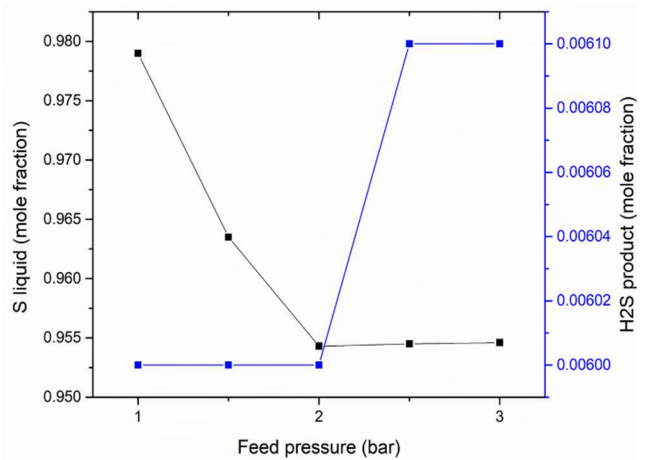


Fig. 11. Influence of feed pressure on sulphur liquid production and H₂S generation utilizing PR.

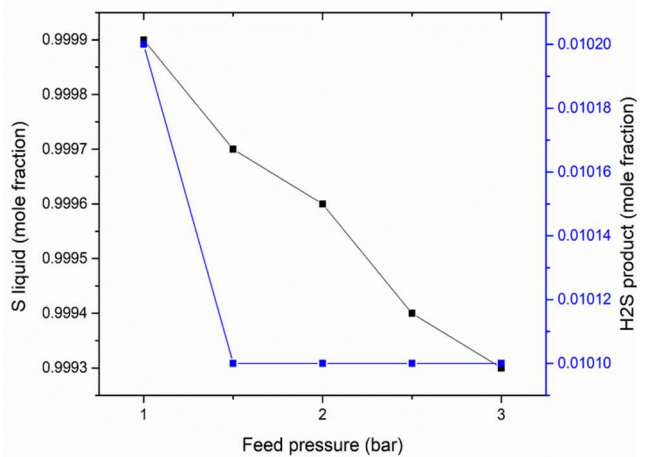


Fig. 12. Effect of feed pressure on sulphur liquid production and H₂S generation using Sulsim.

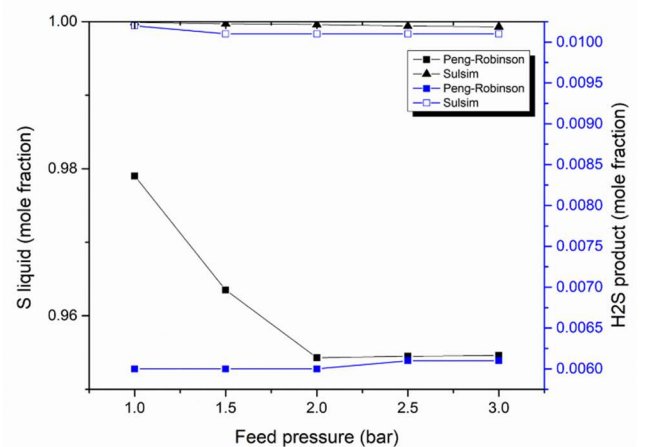


Fig. 13. Comparison of the impact of feed pressure on sulphur liquid production and H₂S generation using two fluid packages.

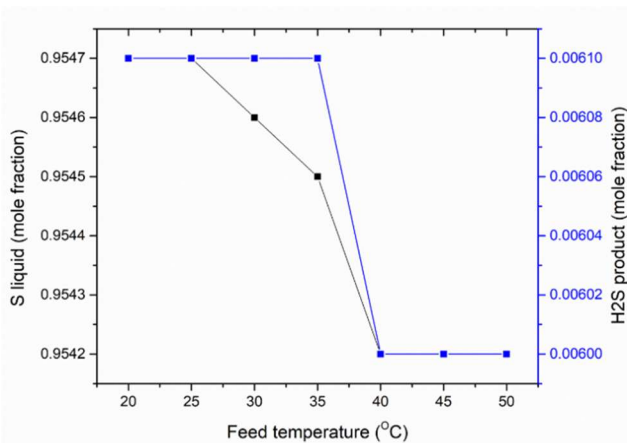


Fig. 14. Influence of feed temperature on sulphur liquid production and H₂S generation using PR.

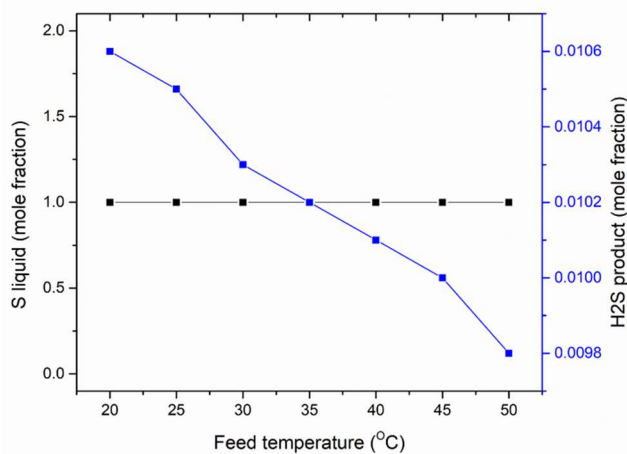


Fig. 15. Effect of feed temperature on sulphur liquid production and H₂S generation using Sulsin

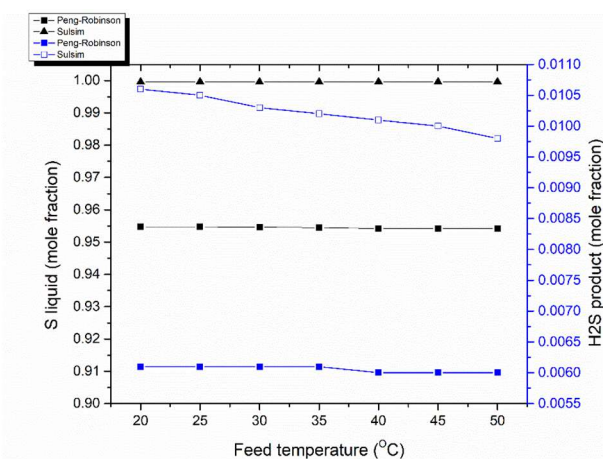


Fig. 16. Analysis of feed temperature effects on sulphur liquid production and H₂S generation using two fluid packages.

specification also gave very high recovery rates (approx.

99.9% efficiency) without adverse environmental impacts; this, therefore, suggests that there is an ambient range at which the process may be effectively managed and a study reported similar to our obtained result (Andarani, 2023). The liquid sulfur will strongly depend on the temperature the sulfur recovery unit is working at. If the temperature gets too high, more sulfur will stay as gas with the liquid sulfur yield decreasing, as shown in Fig. 16. Keeping the temperature too low will make there be incomplete reactions.

3.2.5. Effect of Catalyst Type

It was found that the type of catalyst had a significant effect on the conversion and selectivity to product Fig. 2. Effect of Alumina and Titanium-Based Catalysts. One of the most empirical implications of the Claus process has to do with SRUs' efficiency. The two catalysts affect liquid sulfur produced, which plays a critical role in the optimization of operational performance. Normally, activated alumina is a frequently used catalyst that boasts good initial activity and excellent capacity toward hydrolysing organic sulfur compounds. Nonetheless, its activity degenerates due to sulfation poisoning originating from irreversible adsorption of SO₂ and trace oxygen within it, limiting its useful application especially in catalytic stages of the Claus process (Piéplu et al., 1998; ZareNezhad, 2009).

Promoted alumina catalysts do have a better anti-oxidative capability when iron-containing, but they are not very efficient in the hydrolysis of organic sulfur compared to the titanium-based ones. Such promoted catalysts are often used in dual-bed systems so that sulfate poisoning's impacts can be reduced and the overall conversion rates of H₂S and other sulfur compounds are improved (Piéplu et al., 1998; Mahdipoor et al., 2012).

Ti-based catalysts, particularly those composed of TiO₂, are much better in hydrolysis of COS and CS₂ than the conventional alumina catalyst. For example, the titanium catalyst has been designed to maintain very high rates of conversion of sulfur compounds over extended periods, which would make it especially effective as the first catalyst in the Claus system (Piéplu et al., 1998; Mahdipoor et al., 2012).

The choice of a catalyst directly influences the rate of liquid sulfur and hydrogen sulfide produced. Catalysts based on titanium tend to slightly enhance the conversion efficiency of sulfur species, thus bringing about a higher yield of elemental sulfur and a lower rate of liquid sulfur. This is very important in meeting environmental regulations and optimizing operational costs. The alumina catalyst has sulfur conversion efficiencies of 72.0% and 41.6% for the first and second reactor, respectively as shown in Fig. 17a. The flow rate of hydrogen sulfide is 8.37 kmol/h (Fig. 17b). The titanium catalyst shows sulfur conversion efficiencies of 74.33% and 38.54% for the first and second reactor, respectively as shown in Fig. 18,a. The mole flow rate of H₂S is 11.91 kmol/h, as shown in Fig. 18b.

Design	Rating	OutletSpecs	Worksheet	Performance
Sulfur conversion [kgmole/h]				54.92
Sulfur conversion efficiency [%]				72.04
Inlet sulfur dewpoint temperature [C]				167.5
Outlet sulfur dewpoint temperature [C]				242.2
Inlet sulfur dewpoint margin [C]				57.54
Outlet sulfur dewpoint margin [C]				48.34
COS hydrolysis [%]				74.18
CS2 hydrolysis [%]				40.29
H2S reacted [%]				68.66
COS + CS2 + H2S at outlet [ppmmol]				1.988e+004
Space velocity [1/hours]				1.000
Catalyst bed volume [m3]				2.468e+004

(a)

Design	Rating	OutletSpecs	Worksheet	Performance
Sulfur conversion [kgmole/h]				8.857
Sulfur conversion efficiency [%]				41.57
Inlet sulfur dewpoint temperature [C]				165.4
Outlet sulfur dewpoint temperature [C]				196.6
Inlet sulfur dewpoint margin [C]				44.58
Outlet sulfur dewpoint margin [C]				24.21
COS hydrolysis [%]				26.36
CS2 hydrolysis [%]				6.05
H2S reacted [%]				38.74
COS + CS2 + H2S at outlet [ppmmol]				1.311e+004
Space velocity [1/hours]				1.000
Catalyst bed volume [m3]				2.499e+004

580A		
Temperature	160.0	C
Pressure	1.300	bar
Molar Flow	830.7	kgmole/h
Master Comp Molar Flow (H2S)	8.3765	kgmole/h

(b)

Fig. 17. Reactors using Alumina catalysts, (a) Reactors conversions, (b) H₂S flow rate generated

Design	Rating	OutletSpecs	Worksheet	Performance
Sulfur conversion [kgmole/h]				56.66
Sulfur conversion efficiency [%]				74.33
Inlet sulfur dewpoint temperature [C]				167.5
Outlet sulfur dewpoint temperature [C]				243.1
Inlet sulfur dewpoint margin [C]				57.54
Outlet sulfur dewpoint margin [C]				53.61
COS hydrolysis [%]				99.04
CS2 hydrolysis [%]				98.22
H2S reacted [%]				61.48
COS + CS2 + H2S at outlet [ppmmol]				2.011e+004
Space velocity [1/hours]				1.000
Catalyst bed volume [m3]				2.468e+004

(a)

Design	Rating	OutletSpecs	Worksheet	Performance
Sulfur conversion [kgmole/h]				7.536
Sulfur conversion efficiency [%]				38.52
Inlet sulfur dewpoint temperature [C]				165.4
Outlet sulfur dewpoint temperature [C]				193.8
Inlet sulfur dewpoint margin [C]				44.58
Outlet sulfur dewpoint margin [C]				24.95
COS hydrolysis [%]				12.32
CS2 hydrolysis [%]				5.65
H2S reacted [%]				29.81
COS + CS2 + H2S at outlet [ppmmol]				1.430e+004
Space velocity [1/hours]				1.000
Catalyst bed volume [m3]				2.498e+004

580A		
Temperature	160.0	C
Pressure	1.300	bar
Molar Flow	830.5	kgmole/h
Master Comp Molar Flow (H2S)	11.9156	kgmole/h

580A

(b)

Fig. 18. reactors utilizing titanium catalysts, (a) Conversions in reactors (b) H₂S flow rate

Opposed to alumina catalysts, which show high initial activity but low resistance to deactivation hence the lowest sulfur recovery and worst performance concerning unconverted sulfur compounds. The introduction of titanium catalysts has shown enhanced overall performance

in terms of better sulfur conversion and meeting environmental concerns.

4. CONCLUSION

The feed flow rate to a three-stage Claus sulfur unit of

great importance in determining the rate of sulfur liquid and recovery efficiency. It is not easy to achieve high recovery rates and stay environmentally compliant without careful optimization of operational parameters and feed composition. In brief, our study summarized main conclusions as follows:

- The flow of air plays a major role in keeping the reaction conditions at the required level. Changes in airflow can cause big changes and these underscores having fine control over operating conditions.
- Though higher pressures may improve some aspects of the Claus process, they may result in lower yields of sulfur due to shifts in equilibrium as well as kinetic limitations and certain operational difficulties.
- Reaction kinetics, and the efficiency of sulfur recovery would be better at high temperatures; therefore, caution must be exercised when dealing with gaseous sulfur. Thus, control of system temperature may optimize the performance of the system and is, in fact, an avenue through which economic gains can be realized.
- A proper catalyst will improve sulfur recovery and thereby reduce environmental impact, making it a crucial choice for a sulfur recovery unit operator. Titanium-based catalysts offer hydrolysis activity as well as long-term stability when compared to alumina catalysts which tend to get deactivated notwithstanding their initial effectiveness.
- The results gained validation by checking these two simulations against the actual data wherein the error came out to be less than 2%.

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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