Simulation and Sustainability Assessment of H₂S Utilization From Acid Gas on Haldor Topse Wet Gas Sulfuric Acid and Claus Processes

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ABSTRACT: Haldor Topse Wet Gas Sulfuric Acid (WSA) is an alternative to convert H₂S into elemental sulfur. On the other hand, Haldor Topse Claus process is a widely adopted process to reduce emissions from refineries by converting H₂S into elemental sulfur. The purpose of this project was to simulate both of these state-of-the-art technologies and evaluate their suitability for a new refinery in the Klang Valley. To do this, various acid gas capacities and H₂S concentrations were used as the basis for subsequent development of regression models. The results showed that the WSA process was safer (lower Fire and Explosion Damage Index), more environmentally friendly (lower Global Warming Potential), and more portable (higher production rate) compared to the Claus process. However, the Claus process is more cost-effective. Therefore, a decision matrix was developed using scorecard principle models. The results showed that the WSA process was safer (lower Fire and Explosion Damage Index), more environmentally friendly process, and lastly, it is a safer process, while the Claus process is more cost-effective. Despite the presence of these two state-of-the-art technologies and evaluate their suitability for a new refinery in the Klang Valley. To do this, various acid gas capacities and H₂S concentrations were used as the basis for subsequent development of regression models. The results showed that the WSA process was safer (lower Fire and Explosion Damage Index), more environmentally friendly process, and lastly, it is a safer process, while the Claus process is more cost-effective. However, the Claus process is more cost-effective. Therefore, a decision matrix was developed using scorecard principle models. The results showed that the WSA process was safer (lower Fire and Explosion Damage Index), more environmentally friendly process, and lastly, it is a safer process, while the Claus process is more cost-effective.

INTRODUCTION

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evaluate which of these two technologies suits beer at which capacities and concentrations. To have a correct benchmarking metric, the above-mentioned sustainability pillars are used. In this research, the "People" pillar is indicated by well-known safety indices such as Fire and Explosion Damage Index (FEDI) and Toxicity Damage Index (TDI) via a Hazard Identification and Risk Assessment (HI) study is used [7, 8]. Safety assessment considers the chemicals used and the operating conditions of the process. For the "Planet" pillar, Global Warming Potential (GWP) is selected as the index for the environmental impact. Lastly and obviously, the annual profit of the process is taken as the "Prot" pillar.

In this work, both Claus and WSA processes modeled and simulated using a process simulation software called Symmetry-iCON. Based on the mass balance obtained from the simulations, the indices of FEDI, TDI, GWP, and annual profit are calculated accordingly. Due to the required granularities within the applicable range of capacities and concentrations, running smaller steps of variations is required. In this case, a surrogate approach of merging machine learning and first principles [9] is adopted. Thus, required simulation runs are obtained via a Design Of Experiment (DOE) using Central Composite Design (CCD) [10]. The data is then used to develop the surrogate models, which are then used to create a surface map for each process in each index. Finally, surface maps of both processes are plotted together for each index for comparison.

2. RESEARCH AND METHODOLOGY

Figure 1 shows the overall methodology for this work where both Claus and WSA processes were modeled to calculate FEDI, TDI, GWP, and annual profit. CCD-based simulation runs were then performed for the development of surrogate models. Then surface maps of the models were plotted for each index for comparisons.

The components taken in the simulation were hydrogen sulfide (H₂S), carbon dioxide (CO₂), carbon monoxide (CO), water (H₂O), methane (CH₄), sulfur dioxide (SO₂), sulfur trioxide (SO₃), nitrogen (N₂), oxygen (O₂), hydrogen (H₂), sulfuric acid (H₂SO₄), and elemental sulfur (S₂ and S₈). Typical unit operations used in this simulation were furnaces, conversion reactors, heat exchangers, and separator vessels. In the WSA process, its condenser had three basic functions, namely a place to react (converting SO₃ to H₂SO₄), to reduce temperature and to condense (condensing SO₃ gas and H₂SO₄ gas to H₂SO₄ liquid), and to separate the gas from the condensed phase (separating liquid H₂SO₄ and clean gas) (11). In Symmetry-iCON, there is no WSA condenser unit per se available to do these three functions. Hence, this three equipment (conversion reactor, heat exchanger, and vessel) were used to simulate one WSA condenser.
The reactions that occurred in the combustor are as follows: a highly exothermic reaction, in a step occurring in the reactor is to convert SO\(_2\) to SO\(_3\). The reactions that
took place where the hot sulfuric acid was condensed into liquid phase as the expected product. The clean gas is released at the top of separator. The developed flowsheet of this process achieves current requirement of acid mist emissions of about 20 ppmv without depending on air dilution. The conversions of the reactions are conducted under an adiabatic wise manner. Reactions in the first reactor are as follows:

1. H\(_2\)S + 3/2O\(_2\) \rightleftharpoons S + 3/2O\(_2\)(g)
2. S + 3/2O\(_2\) \rightleftharpoons SO\(_2\) + 1/2O\(_2\)(g)
3. S + 3/2O\(_2\) \rightleftharpoons 2SO\(_2\)
4. 2SO\(_2\) + O\(_2\) + 3H\(_2\) \rightleftharpoons 2SO\(_3\) + 3H\(_2\)O

The vapor sulfuric acid stream was then cooled in a heat exchanger by cooling water at 20 ºC before entering a phase separator. At this point, the condensation of sulfuric acid takes place where the hot sulfuric acid is cooled from 443 ºC to the acid dew point temperature. The sulfuric acid is then condensed into liquid phase.

3. RESULTS AND DISCUSSION

Table 2

| S concentration | Feed Capacity |
|-----------------|--------------|
| Mole %          |              |
| 35.015          | 233          |
| 8.5             | 89.9          |
| 92.4            | 36.63         |
| 4.29            | 392.26        |

In this project, H\(_2\)S is bunt into CO\(_2\) and CH\(_4\) since it was mentioned that in one of our previous works [12]. More details on how to calculate FEDI, TDI, GWP, and annual prot are taken in one of our previous works [12].

Table 3

| Reaction | Conversion fraction |
|----------|---------------------|
| 1        | 0.9107              |
| 2        | 0.947               |
| 3        | 0.947               |
| 4        | 0.947               |

The reactions are converted to SO\(_3\) during the combustion process. The main reaction is the H\(_2\)S reacting in a step occurring in the combustor, where there are various reactions occurred in the combustor. The stream enters three consecutive conversion reactors with different temperatures of inlet streams. The stream is cooled at 430ºC before entering the reactor. The stream is converted to SO\(_3\) before entering the reactor. The stream enters three consecutive conversion reactors with different temperatures of inlet streams. The stream is cooled at 430ºC before entering the reactor. The stream is converted to SO\(_3\) before entering the reactor.

In the WSA process, the feed air and acid gas are fed into a combustor, where there are various reactions occurred in the combustor. The stream enters three consecutive conversion reactors with different temperatures of inlet streams. The stream is cooled at 430ºC before entering the reactor. The stream is converted to SO\(_3\) before entering the reactor.

The developed flowsheet of the WSA process is shown in Table 3. The WSA process is one of the most common processes for sulfur recovery from acid gas generated in oil and gas refining. Elemental sulfur (S) is the final product. The sulfur is S\(_\text{2}+\) since it was produced from the combustion of H\(_2\)S. Further details on the methodology and the indices representing the three pillars of sustainability (3Ps). The regression models were developed as a function of two variables, namely feed capacity (x\(_1\)) and H\(_2\)S concentration (x\(_2\)) to convert SO\(_2\) to SO\(_3\). A general form of a second order regression model was used in this work. It is shown as

\[ Y = ax_1 + bx_2 + cx_1^2 + dx_2^2 + ex_1x_2 + f \]

where Y is the dependent variable (y) and x\(_1\), x\(_2\), x\(_1^2\), x\(_2^2\), and x\(_1x_2\) are the independent variables. The dependent variables (y) obtained were then used to calculate the above indices representing the three pillars of sustainability (3Ps). The dependent variables (y) obtained were then used to calculate the above indices representing the three pillars of sustainability (3Ps).
Fig. 2. Simulation Flow Sheet of WSA process

Fig. 3. Simulation Flow Sheet of Claus process

Fig. 4. Regression model of prot ($/hr) in Claus and WSA processes (a) side view and (b) top view
p zööēp' d'z'x és 'p "šl̂ n̂x" THr és p yu n̂x̂ yōo èx 644. H lyo "p'1'l̂pøó q'x'z ép ̂p'1' e'p'1' "zööēp' e'p'x 2 p ̂p'1' r̂l' e'p'x Thhr "p'pyē èp 'p'uzo" phl n̂ 1' p̂ ŝp̂ ŝl̂ p̂ ép̂ ŝ É 684 H 2H2 Ep ̂t' "phl n̂ 1' "ox̂ p z'q'x'p'1' "zööēp' ZÛ x̂ phl n̂ 1' Thhr "p'ozūn̂ n̂ x̂ 1' p̂ŝ p̂ x'q'x'p'1' "n̂x̂yōo 1' p̂ŝ l̂y o n̂p'1' l̂p̂h tower 1' 664 H "zööōn̂ ty ī'p'z'" Z, 1' x̂ knob 1' èŝp ep q'ŵ Thhr "pl̂n̂ ẑr̂y?

M̂ zh' 5̂3̂6̂ZÛ x̂ 1' M̂ Û / 7̂5̂5̂ 3' Ẑ, 58-

p zööēp' e'p'x n̂ŷd typó ŝzp z'q ZÔ x̂ l̂y o M̂ zh' t̂v̂ èŝp "p'pyē è x̂ 1' sl̂p̂ É 6 1' p̂n̂ p' x̂p'ŷx'1' É ŝl̂p̂ É 6 1' ĵr' Thhr 2̂H2 ép ̂t' "p'ozūn̂ n̂ x̂ 1' p̂ŝ p̂ x'q'x'p'1' "n̂x̂yōo 1' p̂ŝ l̂y o n̂p'1' l̂p̂h tower 1' 669 H 2. x̂ phl n̂ 1' "zööōn̂ ty ī'p'z'" Z, 1' èŝp p ŷŵ z'q'ŵ Thhr "pl̂n̂ ẑr̂y?

M̂ zh' 5̂3̂6̂ZÛ x̂ 1' M̂ Û / 7̂5̂5̂ 3' Ẑ, 59-

*pp p̂r̂p 3̂ q'z' n̂pl̂ m̂ 1' 1'p̂ p̂to 0' p̂pp'p 0' èp x̂n̂ŵ v̂ 3̂ èp f̂l̂ŵ o q'z' q̂n̂x̂p' f̂r̂h 1' "x̂n̂x̂p' 2 N̂ 1' o 1̂ o t̂ûẑx'0 0' èp ŝq̂x 3̂ è 0' p̂r̂p'1' ép̂ l̂o 6 1' ŝl̂ 1' ĵr' Thhr 2̂H2 ép ̂t' "p'ozūn̂ n̂ x̂ 1' p̂ŝ p̂ x'q'x'p'1' "n̂x̂yōo 1' p̂ŝ l̂y o n̂p'1' l̂p̂h tower 1' 669 H 2. x̂ phl n̂ 1' "zööōn̂ ty ī'p'z'" Z, 1' èŝp p ŷŵ z'q'ŵ Thhr "pl̂n̂ ẑr̂y?"

Ĵ R̂l̂tĥ d̂x̂ x̂q' "pl̂ d̂r̂h 1' Ĥŷ o t̂ x̂x̂r̂êŷt̂ŷ "

q̂ p̂x̂l̂ x̂ "zööōn̂ ty x̂ òp̂o è 0' n̂l̂ŵd̂v̂ ï̂p̂ ò 0' "z' d̂ m̂ŵf̂îr̂t̂ ĝm̂ës è 0' "ẑr̂p̂x̂p' 2 1' f̂z ̂m̂ "x̂n̂x̂p' 2 N̂ 1' o 1̂ o t̂ûẑx'0 0' èp ŝq̂x 3̂ è 0' p̂r̂p'1' ép̂ l̂o 6 1' ŝl̂ 1' ĵr' Thhr 2̂H2 ép ̂t' "p'ozūn̂ n̂ x̂ 1' p̂ŝ p̂ x'q'x'p'1' "n̂x̂yōo 1' p̂ŝ l̂y o n̂p'1' l̂p̂h tower 1' 669 H 2. x̂ phl n̂ 1' "zööōn̂ ty ī'p'z'" Z, 1' èŝp p ŷŵ z'q'ŵ Thhr "pl̂n̂ ẑr̂y?".
Fig. 5. Regression model of GWP in Claus and WSA processes (a) side view and (b) top view.

Fig. 6. Regression model of FEDI in Claus and WSA processes (a) side view and (b) top view.

Fig. 7. Regression model of TDI in Claus and WSA processes (a) side view and (b) top view.
4. CONCLUSIONS

The WSA process has been shown to be the more sustainable process for H₂S recovery. The WSA process is more portable, producing lower GWP, lower FEDI, and higher TDI. Future work should consider the Claus process to be integrated with a WSC system to get an apple comparison.

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