Simulation And Sustainability Assessment Of H₂S Utilization From Acid Gas On Haldor Topse Wet Gas Sulfuric Acid And Claus Processes

Zhihong Zeng, Tien-Jie Tse, and Yu-Fen Liao

ABSTCT: The purpose of this project was to simulate both of these state-of-the-art models were used to generate lots of data 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 profitable (higher profit) in most of the evaluated operating conditions.

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To evaluate which of these two technologies suits beer at which capacities and concentrations, a correct benchmarking metric is needed. 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 [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 "Profit" pillar.

In this work, both Claus and WSA processes are modelled 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 modelled 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 used 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 (S 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.
Applied Materials and Technology

In the WSA process, the feed air and acid gas are fed into a combustor, where there are various reactions occurred in the first reactor.

**Table 2**

<table>
<thead>
<tr>
<th>No</th>
<th>Feed Capacity</th>
<th>H₂O Concentration</th>
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**Table 3**

<table>
<thead>
<tr>
<th>Reactor</th>
<th>Conversion in WSA reactors [4]</th>
</tr>
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<tbody>
<tr>
<td>Reactor 1</td>
<td>S + SO₂ → 2SO₂</td>
</tr>
<tr>
<td>Reactor 2</td>
<td>SO₂ + 1/2O₂ → SO₃</td>
</tr>
<tr>
<td>Reactor 3</td>
<td>SO₃ + O₂ → SO₄</td>
</tr>
</tbody>
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**Figure 2**

In this simulation, the considered elemental sulfur (S) is the final product, which can be sold and taken as part of the annual profit.

**Table 4**

<table>
<thead>
<tr>
<th>No</th>
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<th>x²</th>
<th>dx²</th>
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**Figure 3**

The reactions are conducted under an adiabatic condition. This method was used to minimize necessary calculations.
Fig. 2. Simulation Flow Sheet of WSA process

Fig. 3. Simulation Flow Sheet of Claus process

Fig. 4. Regression model of prot ($/hr) in Claus and WSA processes (a) side view and (b) top view
S concentration ($x^2$) and H$_2$S concentration region, not enough high at the lower concentration range of H$_2$S, which is seen that for most of the H$_2$S concentrations and capacities, respectively. These values are close to 100%, showing their reasonableness. The multiple R values (square root of R²) for these models are shown by their accuracies. For equation 16 and 17 have the values of 97% and 85%, respectively (15). Based on the simulation runs, regression/plant models (in $/hr) for both WSA and Claus processes are developed as function of feed pressure steam to be generated. High Pressure Steam (HPS) at 40 barg (270 ºC) while Claus process is shown in Figure 3.

The outlet stream contained some of S$_2$O to produce sulfur S (its concentration and feed reactor at 215 ºC. This reactor produces elemental sulfur S, as the final product according to the following reaction:

$$2S + 3O_2 \rightarrow 2SO_2$$

Equation 14

Waste from the Claus process is used to calculate the capacity ($x^1$) and H$_2$O capacity ($x^2$) concentrations, respectively. These values are close to 100%, showing their reasonable accuracies. The multiple R values ($\sqrt{R^2}$) for these models are shown by their accuracies. For equation 18 and 19 are 94% and 71%, respectively. For this FEDI criteria, both equations are reasonably good (> 70%). These models are plotted as shown in Figure 5. From these plots, WSA is seen to be more environmentally friendly through its lower GWP, if not the same (the mid - low GWP). These data are researched for the future work.

Toxicity hazard models via TDI are shown as follows.

$$TDI = 0.11x^2 - 0.0167x + 38.32$$

Equation 20

$$TDI = 0.0025x^2 - 1.75x + 40.5$$

Equation 21

For equation 20 and 21, their multiple R values are 80% and 99%, respectively. These values again suggest the reason why the WSA process is more preferable in the Claus process. Nonetheless, a more appropriate model can be developed regression models for FEDI (Fire and Toxicity Index). Due to more efficient conversions of WSA process, the amount of flammable materials in the system is lower and the FEDI index. As a result, WSA has a lower GWP, if not the same (the mid to low GWP). These data are researched for the future work.

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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 and economically viable option among the Claus and WSA processes. These conclusions are based on a comparison of various sustainability indices, which include environmental impact (safety), economic efficiency (people), and social acceptability (prot).

As shown in Figure 7, the WSA process has a higher sustainability index in most of the operating conditions. This is because the production of sulfuric acid occurs in the WSA process, while it is not considered in the Claus process. In this regard, future work on comparing the Claus process with other sulfur recovery processes is needed.

Nonetheless, the current work has shown that in three cases, the WSA process is superior than the Claus process. In the most part of the operating conditions, the WSA process is more profitable, producing lower GWP index, lower FEDI, and higher TDI. Future work on comparing the Claus process with other sulfur recovery processes is needed.

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Dallal. Simulation of a Wet Gas Sulfuric Acid Plant, which can then be compared with the Claus process. In this regard, future work on comparing the Claus process with other sulfur recovery processes is needed.

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