Solving Three Common Problems Through SRU Simulation

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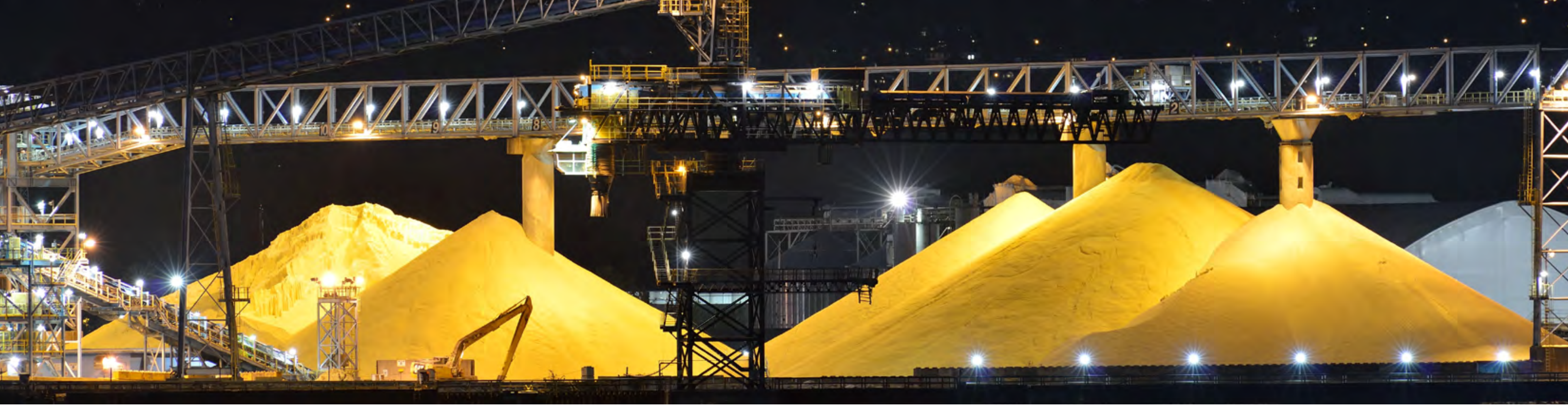
Small operational issues in the sulphur recovery unit (SRU) can lead to higher emisisons — or worse, a frustrating and costly shutdown. Simulation of the SRU can enable more reliable operations and fewer shutdowns through the prevention of issues and quick and effective troubleshooting.

In this paper, we present three common operational issues and show how simulation was used to prevent or quickly resolve the situation.

Introduction

Sulfur emission standards are important for protecting our environment, but keeping the SRU running efficiently and without additional expense can be challenging. Predicting and properly managing SRUs in gas plants and refineries can help you avoid the consequences of not meeting standards while also improving the capacity of the unit.

Obstacles for predicting the performance of the unit include changing feedstocks (including compositions and temperatures), degrading equipment and catalysts and suboptimal operations due to inadequately controlled airflows or temperatures. In this paper, we will discuss the three common problems in the SRU and examine how the innovations in SRU simulation can provide ways to optimize your operation.



Solving Common Operational Problems

Problem 1: Optimizing First Bed Claus Reaction Versus Hydrolysis Reaction

Carbonyl sulphide (COS) and carbon disulphide (CS_2) are two common contaminants observed in the acid gas. COS and CS_2 are converted to elemental sulphur or hydrogen disulfide (H_2S) through equilibrium reactions. H_2S and elemental sulfur can be recovered to avoid loss in recovery efficiency. These equilibrium reactions are typically referred to as hydrolysis reactions and are kinetically limited.

There are two approaches to overcome the limitation: raising the catalyst bed temperature to boost hydrolysis rate and promoted alumina or titanium dioxide catalysts. Both of these options incur additional costs to the SRU, and accurate simulation can provide insights for better decisions.

The empirical correlation for the amount of the COS and CS_2 hydrolysis reactions developed by Sulphur Exeprts was fit against more than 200 experimental results to ensure accurate representation of the plant performance. The correlation is used in the catalyst bed model. As shown in Figure 1, an increase in first bed temperature can boost hydrolysis rate.

Typical bottom bed temperature in operation is between 310 degrees Celsius (590 degrees Fahrenheit) and 340 degrees Celsius (644 degrees Fahrenheit). However, the first bed efficiency will decrease due to less Claus reaction. The overall efficiency is also shown to improve with increasing bed temperature because of lowering COS and CS_2 breakthrough, allowing for increased conversion in subsequent converter(s).

Titanium dioxide (TiO_2), commonly referred to as titania, has higher activity for hydrolysis of COS and CS_2 at lower temperatures compared to alumina. Titania catalyst can be used to treat high amounts of COS and CS_2 if the feed contains more contaminants or if more of these species are created in the reaction furnace. While the the industry typical lifespan of alumina catalyst in the first converter is five years, titania can survive more than 10 years if there is no irreversible damage.

The higher performance comes with a higher cost. Titania catalyst can often cost two to seven times more than the alumina catalyst. Common practice is to protect the titania by placing a layer of alumina on top of the of it to act as an active guard layer while preserving the higher performance of the titania from run to run.

A new titania catalyst model is available in Aspen HYSYS® V9. Extensive regression and validation work was done for the development of this model to ensure that the results were in line with commercial expectations. The model was developed from more than 100 complete plant data sets.

The titania catalyst model was determined to be valid for mixed catalyst beds if the titania volume was at least 25 percent of the total catalyst. The titania catalyst model also predicts whether equilibrium conditions are achieved based on the catalyst volume or space velocity. For this reason, the titania catalyst model requires the user to input either the catalyst volume or space velocity to determine whether equilibrium was reached and if it accurately predicted the breakthrough of components such as COS and CS_2.

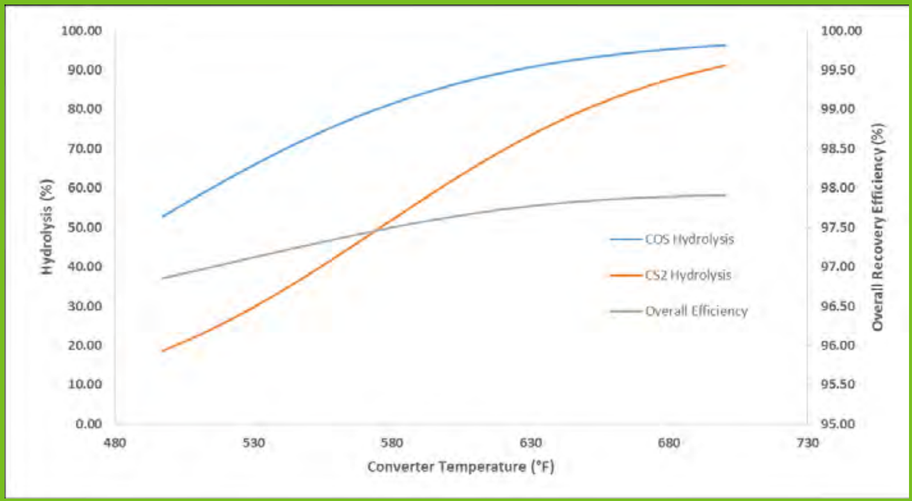


Figure 1:
Effect of first bed temperature on COS/CS_2 hydrolysis and overall efficiency.

In one of the case studies, we examined a three-stage Claus process without a tail gas treating unit. Figure 1 shows the key parameters, including furnace effluent temperature, overall recovery efficiency and third-condenser-outlet COS and CS_2 flow rates. The process was designed to operate at 65 percent H_2S acid gas feed and achieve a recovery efficiency of 97.6 percent (Case 1). However, as the feed quality flunctuates, simulation was used to investigate the lowering acid gas quality at 50 percent H_2S in the feed.

Without fuel gas co-firing, the reaction furnace temperature dropped to 970 degrees Celsius (1,778 degress Fahrenheit), which can potentially cause BTEX breakthrough. Evaluation was performed with 6 percent fuel gas co-firing, which raises the furnance effluent temperature above 1,080 degrees Celsius (1,976 degrees Fahrenheit) and yields an efficiency of 96.1 percent (Case 3). As Figure 1 shows, the CS_2 level has nearly doubled from the design case.

The first bed temperature inlet temperature was raised to 250 degrees Celsius (482 degrees Fahrenheit) to avoid COS and CS_2 breakthrough, which brings up the efficieny to 96.5 percent (Case 4). Finally, titania catalyst was considered in the first bed to further boost hydrolysis reaction. This allows the efficiency to be restored to 98.0 percent (Case 5). Without the titania catalyst, the process was unable to retain the recovery efficiency when acid gas quality significantly lowers in the feed.

With the tools available in the simulator, it is much easier to optimize the first catalyst bed temperature to balance hydrolysis reaction. It can also help to identify when or if titania catalyst should be chosen to improve performance based on current or expected acid gas quality over the life of the plant.

Case	Furnace Effluent Temperature °C (°F)	Overall Recovery Efficiency (%)	Condenser 3 Outlet COS (kgmol/hr)	Condenser 3 Outlet CS_2 (kgmol/hr)
1	1076 (1969)	97.6	0.13	0.27
2	970 (1778)	96.8	0.07	0.40
3	1080 (1976)	96.1	0.10	0.49
4	1081 (1978)	96.5	0.08	0.40
5	1084 (1983)	98.0	0.01	0.07

Table 1:
(Case Study of Three-Stage Claus Process With Lowering Acid Gas Quality)

Simulation Results From Sulsim Sulfur Recovery in Aspen HYSYS

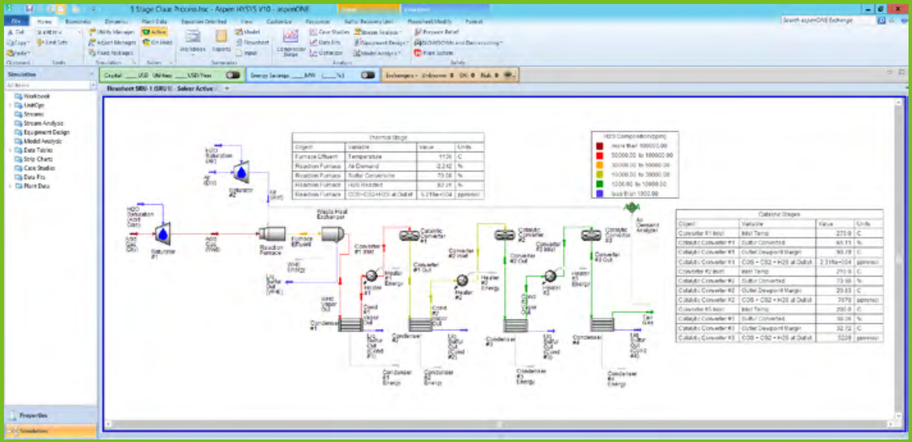


Figure 2:
Three-stage Claus process in Sulsim Sulfur Recovery in Aspen HYSYS

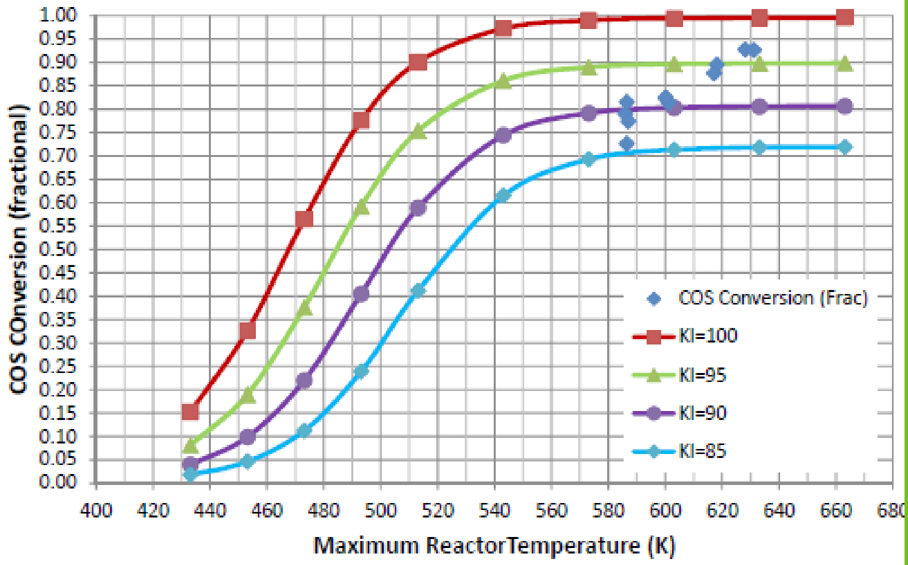


Figure 3:
Example results: titania COS conversion versus temperature and catalyst activity

Problem 2: Running Claus Bed Too Hot — Optimizing Dew Point Margin

In the second or third converter bed, it is suggested to operate as cold as feasible to maximize the equilibrium efficiency. These temperatures are limited by the sulfur dew point, because formation of liquid sulfur will deactivate the catalyst, which is another operation problem that will be discussed. The determination of the sulfur dew point is heavily dependent on simulator or laboratory tests due to its variance with acid gas quality, upstream conversion and other factors.

Sulsim™ Sulfur Recovery in Aspen HYSYS offers a specialized property package in which the parameters have been refined over years of industry experience to ensure a match with plant performance. It allows for accurate prediction of sulfur dew point. Ideally, the Claus bed should be operated at the dew point to maximize conversion across each bed. However, a safety margin, also referred to as sulfur dew point margin, is recommended to allow for heat losses, errors in calculation or capillary condensation of sulfur in the catalyst. The suggested dew point margins are 5 to 15 degrees Celsius, or 9 to 27 degrees Fahrenheit, to minimize efficiency loss to 0.1 to 0.5 percent.

In the model shown in Figure 2, a three-stage Claus process has the second and the third converter dew point margins at 20.8 degrees Celsius (37.5 degrees Fahrenheit) and 32.7 degrees Celsius (58.9 degrees Fahrenheit). At these operating conditions, the overall recovery efficiency is 97.8 percent. Figure 3 shows the efficiency improvement with smaller dew point margin. In this case, a 0.4 percent efficiency improvement can be achieved with a tighter dew point margin.

Case	Second Bed Dew Point Margin °C (°F)	Third Bed Dew Point Margin °C (°F)	Overall Recovery Efficiency (%)
Base	20.8 (37.5)	32.7 (58.9)	97.8
1	15.0 (27.0)	32.7 (58.9)	97.8
2	15.0 (27.0)	15.0 (27.0)	98.2

Table 2:
(Overall Recovery Efficiency Improvement With Dew Point Margin) Simulation Results From Sulsim Sulfur Recovery in Aspen HYSYS

Figure 4 shows how much dew point margin can affect efficiency loss. Due to utility side limitations, it is not unheard of in the industry to find dew point margins as high as 50 degrees Celsius. For large dew point margins, the efficiency loss can be as high as 3 percent. With the accuracy of prediction Sulsim Sulfur Recovery provides, process engineers and operators can determine optimal dew point margins to avoid efficiency loss and to determine the new optimal operating condition when feed changes.

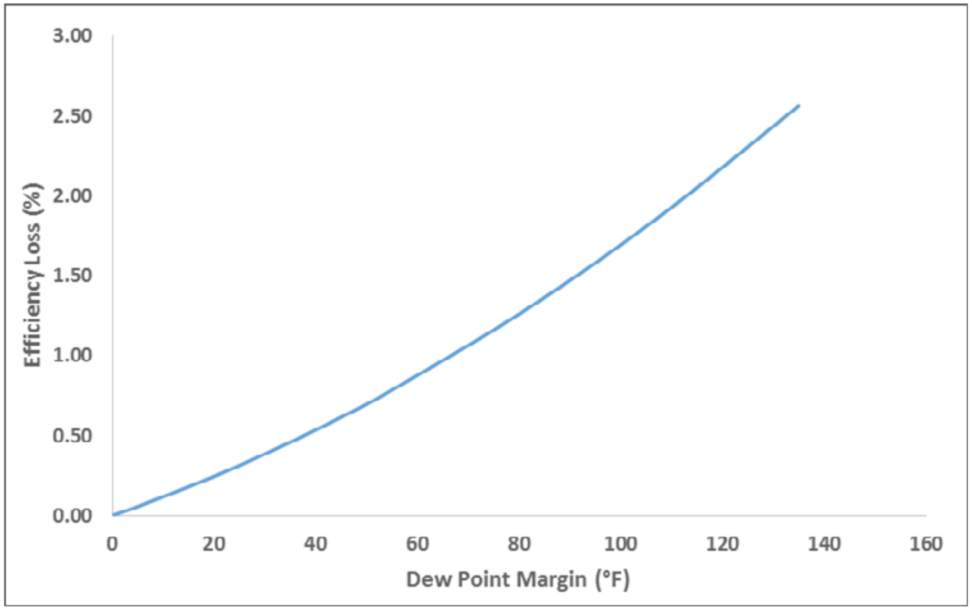


Figure 4: Recovery efficiency losses versus dew point margin

Problem 3: Catalyst Deactivation

Replaced at planned turnarounds, catalyst beds must be able to provide high conversion over their lifespan with varying operating conditions. Replacing still-active catalysts or upgrading without real need to more expensive specialty catalysts (when the real issue is deactivation) leads to high capital costs. Understanding catalyst deactivation through the use of simulation can help engineers reduce unneccesary change-outs of alumina or excessive use of expensive specialty catalysts or even failing to select the right specialty catalyst that could prevent deactivation.

Catalyst deactivation can be caused by thermal aging, hydrothermal aging, carbon contamination and sulfur contamination. Some of the damages can be reversible, while others, such as thermal aging, can cause permenant damage to the catalyst. Understanding if and when deactivation is occurring allows the engineer to make the right catalyst selction and choose the right change-out intervals.

The Claus catalytic converter model in Aspen HYSYS performs an isenthalpic equilibration using free energy minimization while inhibiting certain components to represent the reactions present. The inputs to the unit are the approaches to equilibrium of the reactions that take place in the converter (Figure 6). With a given approach to equilibrium of the Claus reaction, an empirical correlation developed by Sulphur Experts will be used to determine the extent of the COS and CS_2 hydrolysis reactions over an alumina (Al_2O_3) catalyst.

In addition, titania catalysts can be modeled in Aspen HYSYS. The correlation uses the reactor temperature and the catalyst activity to determine defaults for the approach to equilibrium for the COS and CS_2 hydrolysis reactions. By default, Sulsim assumes a fresh, active and sufficient catalyst bed with an approach of 100 percent. Changing the approach to equilibrium of the Claus reaction can be used to indicate different levels of activity of the catalyst — a lower value can be used to represent a slightly deactivated catalyst.

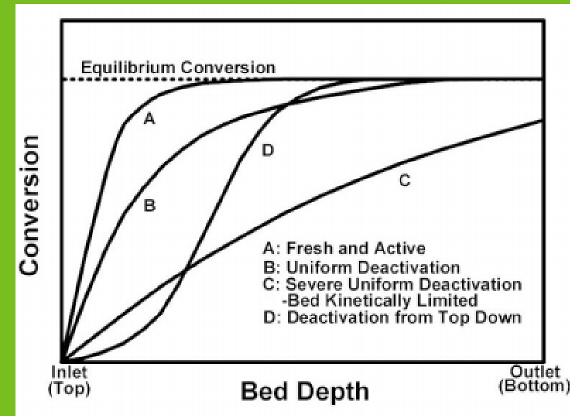


Figure 5:
Catalyst deactivation[1]

Approach to equilibrium (%) of:

H2S/SO2 reaction	100.00
COS hydrolysis	45.00
CS2 hydrolysis	8.07

Figure 6:
Tuning factors available in the Claus catalytic converter model

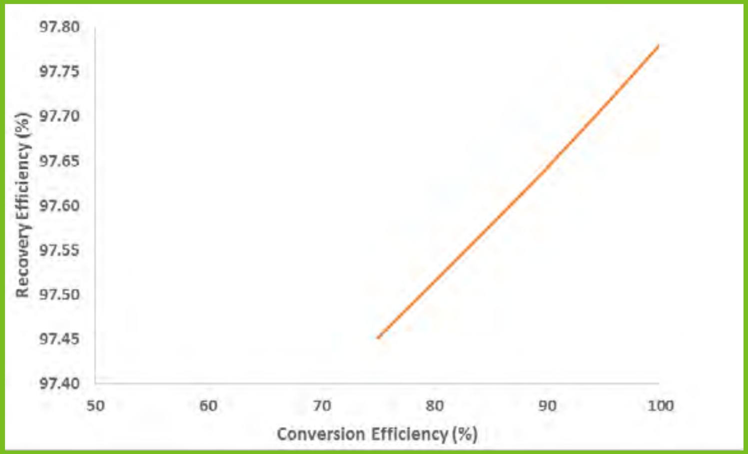


Figure 7:
Effect of equilibrium approach on overall recovery efficiency

As discussed in Problem 1, Sulsim can accurately predict the hydrolysis reaction based on the approach to equilibrium. This allows the process engineers and operators to understand the effect of deactivated catalyst on downstream units, meet environmental standards and avoid unnecessary catalyst replacement to save capital costs. Coupled with field analysis, Sulsim can be used to better guide the operators when a catalyst bed is deactivated and needs to be rejuvenated or replaced.

With the Sulsim Sulfur Recovery in Aspen HYSYS, the evaluation can be performed on the effect of deactivated catalyst. Figure 7 shows that a 20 percent decrease in equilibrium in the second converter can result in 0.3 percent of overall recovery efficiency loss..

Conclusion

The improvements made in Sulsim Sulfur Recovery in Aspen HYSYS V9 and V10 increase the accuracy of modeling the sulfur removal process and extend the applicability to a wider range of feed conditions, unit operations and catalyst types. Sulsim Sulfur Recovery is used widely in the industry to ensure sulfur recovery targets are met at minimal cost and that maximum flexibility is given to both operations and process design.

Extensive validation work has been done to ensure an accurate representation of the plant performance. In the three case studies, we showed how Sulsim Sulfur Recovery can be used to identify operational problems common to the industry, and how Sulsim Sulfur Recovery can be used to easily provide solutions to avoid missed targets.

Reference

[1] The Seven Deadly Sins of Sulphur Recovery, Gerald E. Bohme, John A. Sames, Sulphur Recovery Sixteenth Edition, p. 315.

Technology That Loves Complexity

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