Improve sulphur plant performance through simulation

The various units of the sulphur plant are closely connected, creating process dependencies that can be better understood using simulation

JENNIFER DYMENT, CHAD MONDOR and FREDERIC TONNAIRE
Aspen Technology

Meeting product and environmental specifications with changing feed conditions can be challenging. To ensure reliable operation, units are typically operated to over-perform on specifications. Accurate predictions of the sulphur and carbon dioxide content of the sales gas can allow producers to be sure specifications are met, while adjusting the process to minimise energy costs and product quality giveaway.

The goal of the sulphur recovery process is to remove sulphur at an optimal recovery efficiency, while meeting tail gas specifications and opex guidance. Simulation models have shown to be useful tools for design and to troubleshoot operations.

Sulsim has been used in industry for decades, and has been proven to be one of the most accurate simulators of the modified Claus process. When faced with sour feedstocks, Sulsim Sulfur Recovery allows engineering consultancies to make specification guarantees with confidence or engineers at plants to operate reliably while meeting regulations.

The sulphur recovery unit (SRU) is sometimes a bottleneck in refineries by limiting the amount of sulphur that can be accommodated in crude oil and unconventional feedstocks, while still meeting flare specifications. By maximising sulphur recovery using Sulsim Sulfur Recovery, refiners can accommodate more sour crudes in the slate for increased margins. Changing feed conditions can cause variability in operations. Engineers can use the simulator to pre-emptively predict SRU performance, adjust operating conditions to optimise the unit, and to ensure reliable operation and reduce the number of upsets.

The required components for sulphur recovery and the supported components

Required components for sulphur recovery		Additional supported components for sulphur recovery		
Hydrogen	S1_Vapor	Argon	n-Hexane	E-Mercaptan
Oxygen	S2_Vapor	Ammonia	n-Heptane	nPMercaptan
Nitrogen	S3_Vapor	HCN	n-Octane	nBMercaptan
CO	S4_Vapor	Methane	n-Nonane	1Pentanthiol
CO_2	S5_Vapor	Ethane	n-Decane	Methanol
H_2S	S6_Vapor	Propane	Benzene	
COS	S7_Vapor	i-Butane	Toluene	
SO_2	S8_Vapor	n-Butane	m-Xylene	
CS_2	S_Liquid	i-Pentane	E-Benzene	
H_2O		n-Pentane	M-Mercaptan	

Table 1

The sulphur recovery process involves many energy intensive steps. Engineers can minimise opex in existing plants by identifying optimal temperatures for operation with Sulsim Sulfur Recovery. Designers can build the right plant configuration to meet sulphur recovery targets for a given operating window at a minimum capex, while also ensuring that the design is flexible enough for the needs of the plant. The integration of Sulsim Sulfur Recovery into Hysys enables global optimisation in design and for evaluating alternative configurations in strategic studies

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Implementation of Sulsim Sulfur Recovery in Hysys

The functionality available for decades as part of standalone Sulsim has been completely incorporated into Aspen Hysys V9. Aspen Technology and Sulphur Experts have independently validated and verified that all pre-existing functionality works as designed in the Hysys environment.

In Hysys, the Sulsim property package, sub-flowsheet environment, and unit operations can be used to simulate all commercial process configurations for the Claus process with over 30 unit operations.

Standalone Sulsim has been fully integrated into Hysys by implementation of:

- A specialised Sulfur Recovery sub-flowsheet environment.
- A dedicated Sulsim (Sulfur

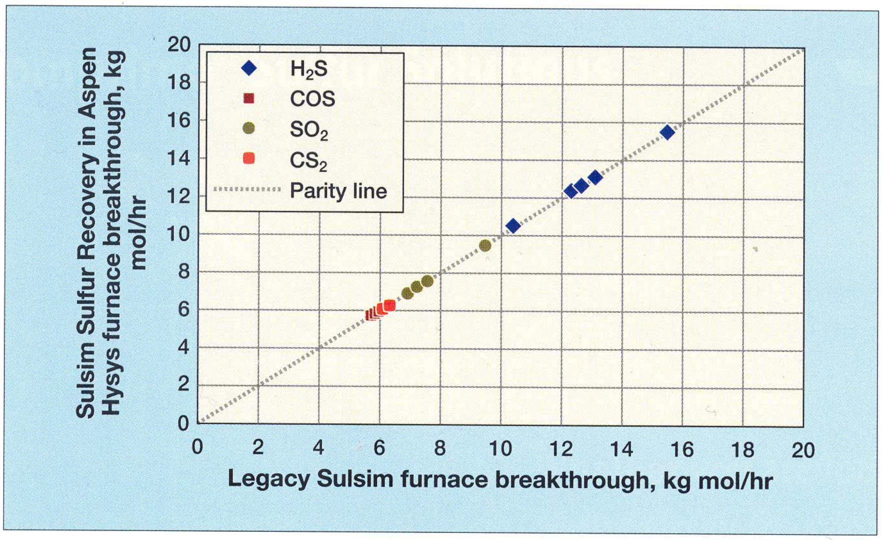

Figure 1 Results from Sulphur Experts' Sulsim compared to Aspen Hysys for reaction furnace breakthrough

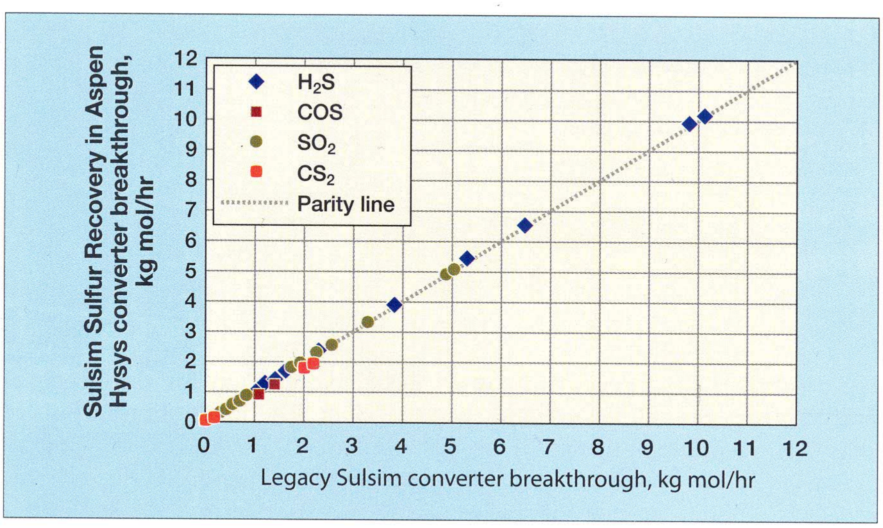

Figure 2 Results from Sulphur Experts' Sulsim compared to Aspen Hysys for catalytic converter breakthrough

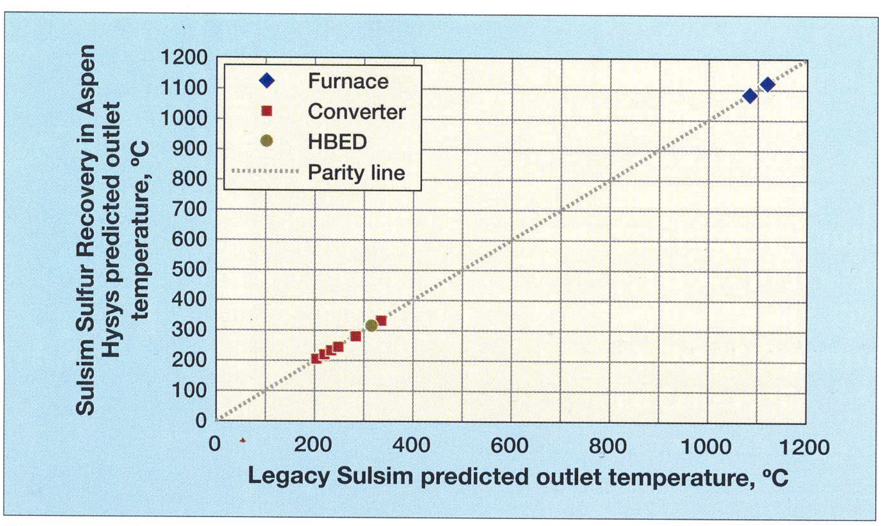

Figure 3 Results from Sulphur Experts' Sulsim compared to Aspen Hysys for outlet temperature prediction of key unit operations

Recovery) property package (see **Table 1** for components required and supported).

- A specialised unit operations palette, including all previously available Sulsim unit operations as well as some new operations introduced in this release.
- A Sulsim-to-Hysys case converter for easy migration.

Lastly, Aspen Technology provides a case converter for easy transfer of legacy Sulsim cases to Sulsim Sulfur Recovery in Hysys. The case converter has been validated across hundreds of customer cases, and is documented.

Validation results

Aspen Technology and Sulphur Experts worked extensively and independently to ensure that the results were sufficiently equivalent. The two companies independently tested hundreds of cases, and no unexpected differences in the results have been observed between the two simulators. Sulsim Sulfur Recovery in Aspen Hysys includes improvements to the underlying models available in Sulsim which results in known differences, as noted in the in-product help.

Sulphur component breakthrough prediction

As part of the validation work between the two simulators, the breakthrough of selected sulphur species following unit operations such as the reaction furnace, waste heat exchangers, catalytic converts and so on has been compared. **Figures 1** and **2** show a subset of that data for the furnace and catalytic converter. Sulsim results are plotted on the x-axis and the results from Hysys are plotted on the y-axis. Results in almost all tested cases were nearly identical.

Temperature prediction

As part of the validation work between the two simulators, Aspen Technology and Sulphur Experts compared the outlet temperature of key unit operations such as the reaction furnace, catalytic converters, HBED, and so on. **Figure 3** shows a subset of that data. Sulsim results are plotted on the x-axis and the results from Hysys are plotted on the y-axis. Results were shown to have been nearly identical in the majority of cases. In some cases, particularly when recycling sulphur from the tail gas section to the reaction furnace, Aspen Hysys results were slightly different due to improvements in the HBED model and tighter solver tolerances.

Sulphur conversion efficiency

Sulphur conversion efficiency is an important metric to optimise the SRU and to understand the effects of operational changes. The two developers compared the sulphur conversion efficiency in each stage of the SRU between the two simulators. **Figure 4** shows a subset of that data. Sulsim results are plotted on the x-axis and the results from Hysys are plotted on the y-axis. Some differences were observed between Sulsim and Sulsim Sulfur Recovery in Hysys. However, these differences were expected as part of the model improvements made with Hysys V9 (differences listed in the in-product help). In cases where significant differences were observed, results were compared against the original plant data and Hysys results were generally found to be more accurate.

Validation work was performed across many more properties and cases; however, for brevity we show the data above to demonstrate the methodology used.

SRU modelling

All previously available functionality in Sulsim is made available in Sulsim Sulfur Recovery in Aspen Hysys V9. In addition to pre-existing functionality, the developers have included a new suite of models and capabilities that cover a wider range of operating conditions and equipment configurations:

- The Sulsim property package contains extended components S1 through S8, with full details of these sulphur species reported to the user in the simulation environment.
- Five new empirical reaction furnace models have been included in this release, extending the total number to nine models. These models were developed from 769 unique plant data sets and have been validated to be more accurate predictors of furnace operation compared to the legacy models.
- A new incinerator model with kinetic correlations predicts break-through of key sulphur species to the flare.
- Catalytic converter unit operations now include a model for simulating titania catalyst (including mixed bed), as well as alumina catalyst.
- A model has been developed for the selective oxidation converter; this now predicts conversion.
- A simplified SO_2 absorber unit operation is included.

In the following section, we will discuss these new options and the validation work done to ensure accuracy.

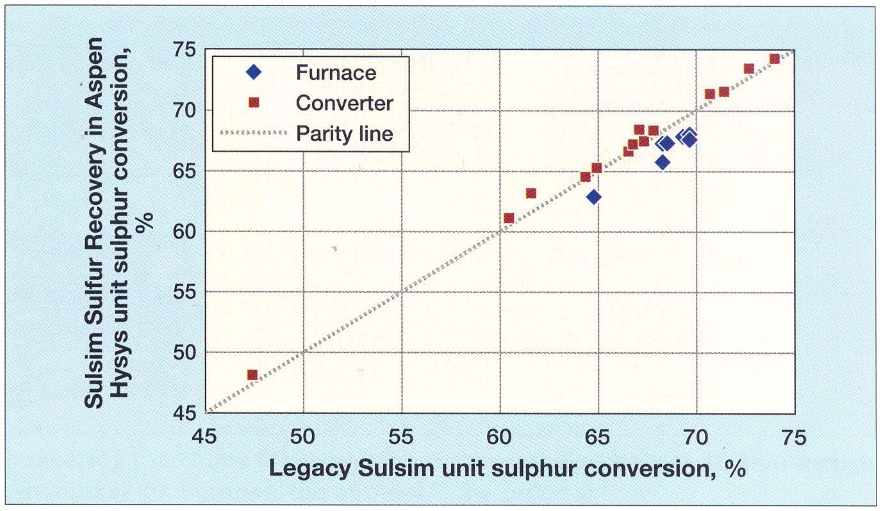

Figure 4 Results from Sulphur Experts' Sulsim compared to Aspen Hysys for sulphur conversion efficiency across the thermal and catalytic stages of the SRU

New furnace models

With Hysys V9, five new furnace models have been developed from 769 unique plant data sets. Aspen Technology and Sulphur Experts regressed the data to create predictive models for conversion, CO, COS, CS_2, H_2, and so on. The new empirical models include support for the following feeds and configurations:

- Straight-through amine acid gas
- Sour water stripper acid gas
- Split flow with lean acid gas
- Oxygen enrichment all acid gas
- Co-firing amine acid gas.

Between Sulsim 5 and Hysys V9, twice as many data points were regressed and the new curve was shifted slightly.

Claus catalytic converter model

Validation work was completed for support for titania catalysts for the Claus catalytic converter model, in addition to alumina. Models were developed for the titania catalysts for systems that reached and did not reach conversion equilibrium.

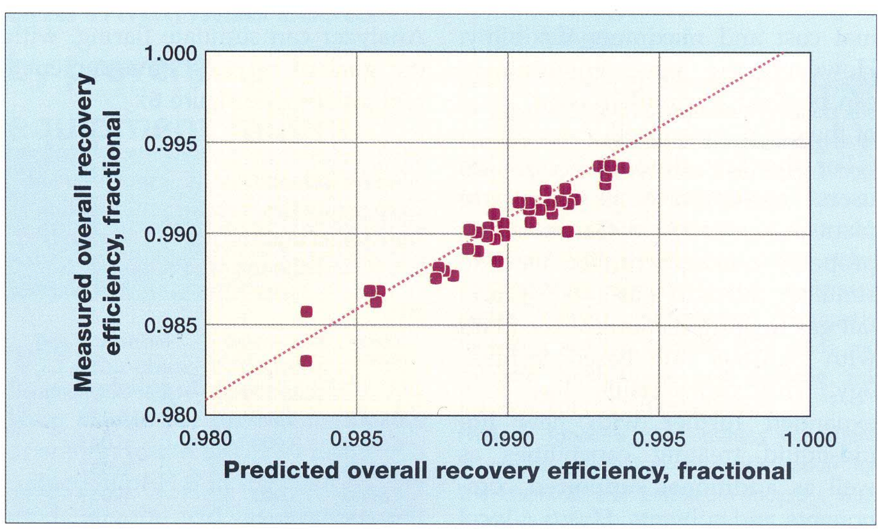

Figure 5 Results from measured recovery efficiency compared to recovery efficiency predicted by Aspen Hysys

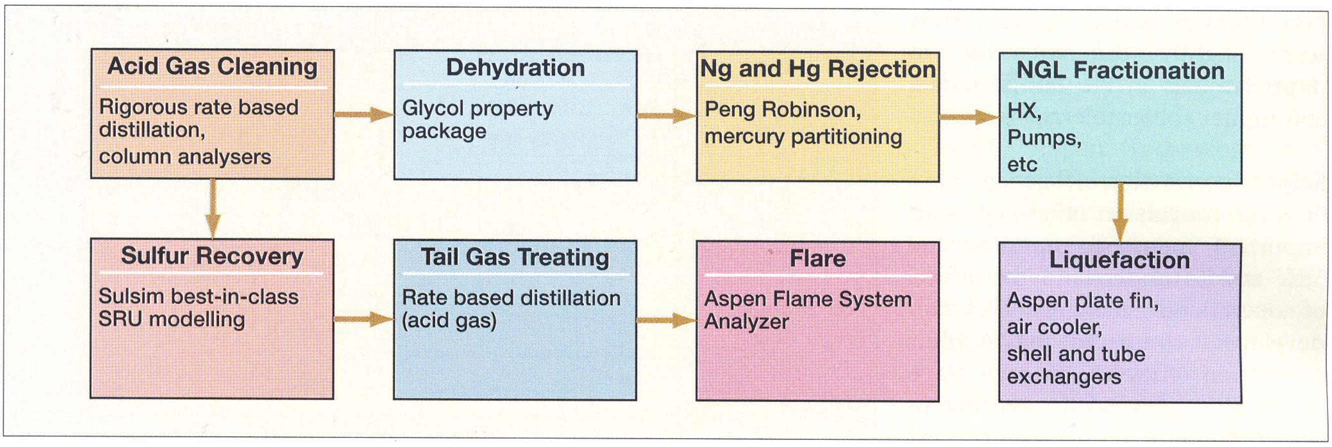

Figure 6 The full aspenONE Engineering Midstream Solution

Selective oxidation converter

With Hysys V9, the overall recovery efficiency can be predicted using the new model for selective oxidation converter, such as the Jacobs Superclaus process. Work was done to compare the prediction to measured plant data. A comparison for a number of sample cases is shown in **Figure 5**.

The benefit of modelling the entire gas plant

The gas plant in midstream and refining industries contains several units, each having specific operational objectives. For a plant to be designed and operated at maximum efficiency, while meeting specifications and yield targets, a simulator is often required for global process optimisation.

Sulsim Sulfur Recovery in Hysys can be used to optimise the sulphur recovery process within the gas plant, and can help in meeting sulphur recovery targets at minimal cost and maximum flexibility. However, the same environment can be used to simulate other areas of the gas plant as well.

For the first time in Hysys V9, users can optimise all major gas plant processes. Acid Gas Cleaning property packages can be used to simulate the acid gas treating and tail gas treating sections of the plant with rigorous rate based technology. This functionality has been expanded further with new liquid-liquid treating capabilities as well as additional supported components and solvents. Hysys Glycol & CPA property packages can be used to model the dehydration process. The Peng Robinson property packages, and other layered functionality such as the mercury partitioning utility, can be used to simulate removal of inerts such as nitrogen and helium, as well as other contaminants such as mercury. Hysys and Aspen Exchanger Design and Rating (EDR) can also be used to simulate gas-liquid fractionation, LNG compression, and LNG regasification processes. Finally, Aspen Flare System Analyzer can simulate flaring, with the goal of meeting environmental regulations (see **Figure 6**).

For a plant to be designed and operated at maximum efficiency, a simulator is often required for global process optimisation

An Air Demand Analyzer tool is added to the air flow rate into the reaction furnace so that the H_2S to SO_2 ratio is at the targeted value

State	Air Demand Analyzer - target value	Incinerator and stack - COS + CS_2 + H_2S at exit, ppmmol
Case 1	1.500	6.115
Case 2	2.000	6.065
Case 3	3.000	6.037
Case 4	5.000	6.059
Case 5	10.00	6.149

Table 2

Layered functionality from other AspenTech products is also available for use in areas of the Hysys gas plant flowsheet, such as Simulation Workbook, Capital Cost Estimator, Energy Analyzer, and other safety environment functionality, such as blowdown technology and relief valve sizing.

Case study: modelling the SRU with the rest of the gas plant

This process contains an acid gas removal step with sulfolane-DIPA, a two stage Claus process, and a tail gas treating unit. In the first task of this case study, we want to see how the regenerator overhead from the tail gas treating unit affects the rest of the unit if it is recycled back to the reaction furnace. The tail gas treating unit is simple in this case, but the rate based distillation modelling technology for acid gas removal could have been used for greater accuracy. We want to see if this will affect the concentration of sulphur (COS + CS_2 + H_2S [mol]) and what can be done to improve the performance of the unit. In this example, let us assume the limit is 6 ppm.

In the second task, we will look at the acid gas removal unit and how a new feed will change the sales gas sulphur concentration. In this example, let us assume the sales gas specification is 3 ppm (H_2S [mol]). We will also evaluate different ways of improving the unit.

Task 1: meet flare specification in the SRU

The sulphur concentration reported in the incinerator is 5.98 ppm, which is under the assumed 6 ppm flare specification. With the addition of the recycle block which circulates the overhead stream from the regenerator to the reaction furnace, the sulphur concentration in the flare increases to 6.07 ppm. The rest of the flowsheet adjusts accommodate this change and convergence is reached in seconds.

Next, a few opportunities can be explored for improving the performance of the unit:

Adjusting the air flow rate into the reaction furnace

Adjusting the air flow into the reaction furnace is one way of improving the process. With the addition of an Air Demand Analyzer tool, a user can adjust the ratio of H_2S to SO_2 by changing the air flow rate and observe the resulting sulphur concentration in the flare. By increasing the ratio from 2 to 3, the sulphur concentration has decreased to 6.04 ppm (see **Table 2**).

Regulating the temperature of the catalytic converter

Another way to improve the process would be to add an adjust block on the second catalytic converter. This adjusts the temperature of the inlet stream so that it is 10°C above the sulphur dewß point. The resulting flare concentration is 5.85 ppm, well below the assumed specification of 6 ppm.

Task 2: meet sales gas specification

Currently, the flow rate of sulphur going to the SRU through the acid gas stream is 760 kgmol/hr and the sales gas H_2S composition is 1.6 ppm.

Changing the feed composition and flow rate

The new feed has a flow rate increase of 5% and the composition is different, with more sulphur. As a result, there is more H_2S going to the SRU, and the H_2S component in the sales gas is too high at 13.3 ppm for the assumed specification of 3 ppm. The amine loading is relatively low at 20.77 ppm (see **Table 3**).

The composition before the feed change (left) and the composition after (right)

	Mole fractions		Mole fractions
H_2O	0.0000	H_2O	0.0000
CO_2	0.0495	CO_2	0.0400
DIsoPAmine	0.0000	DIsoPAmine	0.0000
Sulfolane	0.0000	Sulfolane	0.0000
H_2S	0.2673	H_2S	0.2900
Methane	0.5842	Methane	0.5700
Ethane	0.0693	Ethane	0.0700
Propane	0.0198	Propane	0.0200
Nitrogen	0.0099	Nitrogen	0.0100

Table 3

Increasing the amine make-up rate

An option to improve the process would be to increase the amine make-up rate. This significantly reduces the H_2S composition to 2.5 ppm and increases the amount of H_2S going to the SRU from 760 to 814 kgmol/hr.

Meeting the flare specification in the SRU

If you then go into the SRU, you will find that the adjust block for the H_2S concentration in the flare gas is still within specification at 5.88 ppm, still in range of the assumed specification. This is probably due to the adjust block on the second catalytic converter.

With simulation of the SRU, users can identify problems early and reliably, meet regulations on sulphur emissions, and minimise costs by preventing equipment failure

Benefits

In completing the case study, we were able to see how changing the operation in the SRU can result in a reduction of H_2S in the flare gas. By modelling the acid gas cleaning unit and the SRU in one simulation, we could quickly see how the two units can handle changes to the feed or the process.

Conclusion

With the acquisition and inclusion of Sulphur Expert's Sulsim in Aspen Hysys, users can optimise an entire plant from the hydrotreaters through acid gas recovery, sulphur recovery, and tail gas treating units in one environment, leveraging conceptual tools for economic evaluation, or energy recovery available within the Hysys environment. The three are closely connected and usually operate together, creating process dependencies that cannot be efficiently optimised separately. Engineers can ensure that the plant can handle a variety of changing feed conditions.

With simulation of the SRU, users can identify problems early and reliably, meet regulations on sulphur emissions, and minimise costs by preventing equipment failure. Users can plan for catalyst degradation and optimise the entire facility's sulphur removal needs in a single design.

Jennifer Dyment is the Marketing Manager for Aspen Plus and its associated products and features with AspenTech. She has a degree in chemical engineering from the Thayer School of Engineering at Dartmouth College.

Chad Mondor is a Senior Process Engineer with AspenTech, with broad experiences in global manufacturing support, process equipment design, project management, computer modelling and tool building, fluid solids and catalytic technologies, and applying risk management and business acumen.

Frederic Tonnaire is a Business Consultant in process modelling and optimisation for the chemical and petroleum industry, with particular interest in the technical aspects of creating models and enhancing engineering software applications.