

# Jump Start Guide: Sulsim™ Sulfur Recovery in Aspen HYSYS® V9

Using and Optimizing Your Sulfur Recovery Unit in Aspen HYSYS

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## Introduction to Sulsim™ Sulfur Recovery in Aspen HYSYS®

This jump start guide will elaborate on the benefits of using Sulsim Sulfur Recovery in Aspen HYSYS to optimize your Sulfur Recovery Unit (SRU) design and operational performance. Sulsim technology, the leading sulfur recovery process simulator developed by Sulphur Experts, has been fully integrated in V9 of Aspen HYSYS, allowing users to optimize the entire gas plant in one simulator. Additionally, Sulsim Sulfur Recovery in Aspen HYSYS V9 includes new functionality, models and unit operations, enabling prediction of a much wider range of operating conditions and process configurations at high fidelity.

## Scope of this Document

### Process & Industry Overview

We will cover an overview of the sulfur recovery industry and the sulfur recovery process, including the benefits of using a simulator to meet process goals and operate efficiently.

### Using Sulsim Sulfur Recovery in Aspen HYSYS

We will cover how Sulsim Sulfur Recovery in Aspen HYSYS can be used to meet these needs and how users can migrate their files from standalone Sulsim formats to Sulsim Sulfur Recovery in Aspen HYSYS. We will also cover an introduction on how to get started using the Sulsim property package and functionality in Aspen HYSYS.

### Self-Guided Demonstration

We will provide a self-guided demonstration showing the process of importing a standalone Sulsim file to Aspen HYSYS, integrating the Sulsim functionality with other processes, such as Acid Gas Cleaning in Aspen HYSYS, and a brief example on new Sulsim functionality.

### Optimize the Entire Gas Plant in Aspen HYSYS

We will conclude with a summary of how Aspen HYSYS can be used to optimize the entire gas plant in a single environment, as well as share resources to help you get started using Aspen HYSYS today.

## Process & Industry Overview

Sulfur emission standards are becoming increasingly stringent. Predicting and properly managing sulfur recovery units in gas plants and refineries can help you avoid the consequences of not meeting standards while improving the monetization of the unit.

Obstacles for predicting the performance of the unit include changing feedstocks, including compositions and temperatures, degrading equipment and catalysts, suboptimal operations due to inadequately controlled airflows or temperatures, and controllability.

## Gas Treating Industry – Why Does Gas Need to be Treated?

Before natural gas and associated gases can be sent to the sales pipeline and used in commercial and residential applications, they must first be treated to remove contaminants and harmful substances such as H<sub>2</sub>S, SO<sub>2</sub>, NH<sub>3</sub>, and other sulfur containing compounds.

Acid gas needs to be treated for safety considerations and to meet environmental regulations which protect against H<sub>2</sub>S toxicity. Acid gases must be removed to reduce equipment corrosion. SO<sub>2</sub> emissions must be kept at a minimum to protect against acid rain and other environmental impacts. Liquid product qualities can be impacted from dissolved acid gases, and in particular, the copper strip test is used to ensure acceptable levels of these dissolved acid gases. Lastly, inerts and other compounds with low heating values must be removed to meet the heating value specifications of commercial and residential products.

## Typical Gas Plant Configuration: Many Processes Require Global Optimization

A typical gas plant configuration consists of many different processes that are configured specifically for the plant’s feed conditions and operational objectives. Global plant optimization enables a more efficient greenfield/brownfield design and enables margins to be maximized while ensuring reliability in operations.

At a high level, there are two major objectives of a gas plant. The first is to maximize production of sales products with minimal product quality giveaway at minimum OPEX. This objective is facilitated through a series of processes that can include acid gas treating, dehydration, inerts removal (such as nitrogen & helium), liquids fractionation, and LNG compression. The second major objective is to meet environmental and regulatory requirements on emissions. This objective is typically facilitated with an acid gas treating step, sulfur recovery step, tail gas treating step, and an incinerator/flare. Figure 1 shows all the possible steps within a gas plant.

Prior to the release of aspenONE® V9, a unit or design engineer would need to employ multiple simulators to ensure that a given process could meet emissions specifications across the operating window. The acid gas treating and tail gas treating processes could be rigorously simulated using Acid Gas Cleaning, but the user would need to export and import results to standalone Sulsim to optimize the sulfur recovery unit. Now in aspenONE V9, a user can optimize all of these processes in a single Aspen HYSYS environment. In other words, the Acid Gas Cleaning property package can be integrated with the Sulsim Sulfur Recovery property package in a single flowsheet environment, enabling global optimization of the process. The integration of Sulsim into Aspen HYSYS V9 enables a complete end-to-end accurate modeling solution.

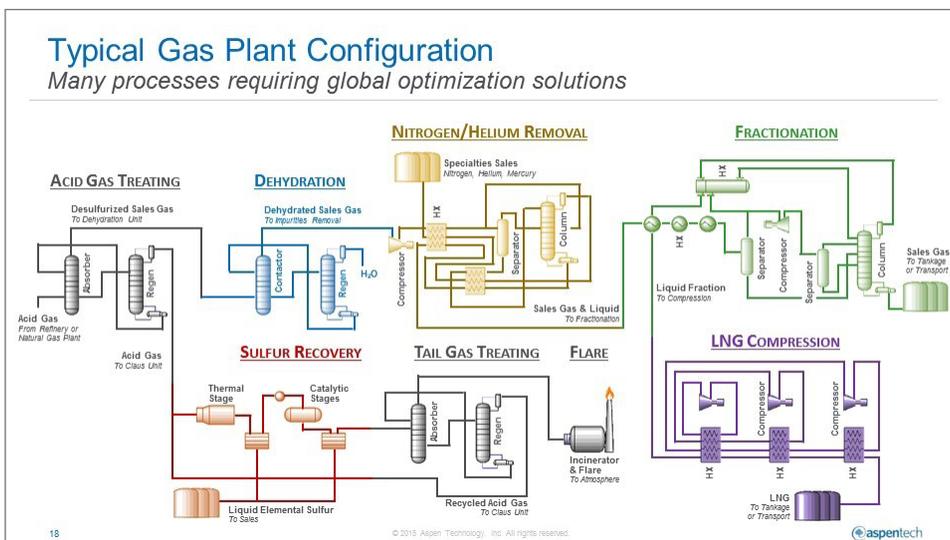
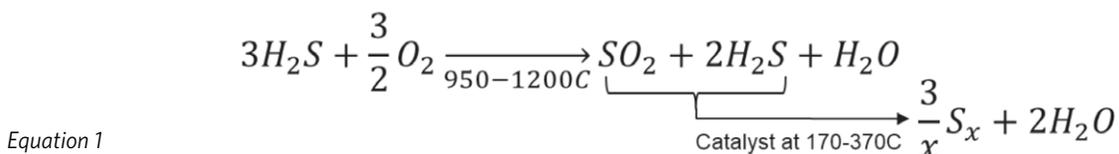


Figure 1:  
A typical gas plant flow diagram.

## The Sulfur Recovery Process

The sulfur recovery process employs a modified-Claus reaction that captures elemental sulfur from hydrogen sulfide, carbonyl sulfide, carbon disulfide, sulfur dioxide and other sulfur-containing species in a series of thermal and chemical reactions. Typically, acid gases from the acid gas treating process and other refinery off-gas streams, such as sour water strippers, are combined and sent to a reaction furnace with air at high temperature. Reactions take place in about 2 seconds at 1000-1400°C, with the goal of converting 1/3 of the total H<sub>2</sub>S in the inlet to SO<sub>2</sub> at the outlet. Following heat recovery, elemental sulfur produced in the furnace is drawn out of the system using a low temperature condenser at about 130°C. The remaining gaseous effluent is sent through several catalytic sections in series, which continue to convert the remaining SO<sub>2</sub> and H<sub>2</sub>S to elemental sulfur and water.



Typically, a cumulative sulfur recovery of > 98% is targeted in refining and midstream applications. The gaseous effluent from the last catalytic stage condenser is low in sulfur-containing compounds, but may require some additional treating to meet flare gas specifications. This gas is sent to tail gas treating processing, which can contain unit ops such as a hydrogenation bed, reducing gas generator, quench tower, amine absorber, incinerator and flare. In short, the sulfur recovery process is a key enabler to process sour feeds and meet emissions specs, while producing elemental sulfur for sales.

Next, we will cover the functionality of Sulsim Sulfur Recovery, and how it can be used to simulate and optimize this process in operations, troubleshooting and design.

## Using Sulsim Sulfur Recovery in Aspen HYSYS

### Need for Accuracy

The goal of the sulfur recovery process is to remove sulfur from process streams at an optimal recovery efficiency, with attention to tail gas specifications and costs. An accurate simulation model can be used for this purpose, in both design and operations.

Sulsim Sulfur Recovery can be used to meet regulations and avoid penalties. Sulsim has been used in the industry for decades, and has been proven to be one of the most accurate simulators of this process. Sulsim Sulfur Recovery gives users confidence when making guarantees on specifications or meeting targets in operation. Sulsim Sulfur Recovery can be used to operate reliably and process sour feedstocks.

The sulfur recovery unit (SRU) can sometimes be a bottleneck in refining in terms of limiting the amount of sulfur that can be accommodated in crude oil and unconventional feedstocks, while still meeting flare specifications. By maximizing sulfur recovery using Sulsim Sulfur Recovery, refiners may be able to accommodate more sour crudes in the slate for increased margins. Changing feed conditions can cause variability in operations. Users can use Sulsim Sulfur Recovery to pre-emptively predict sulfur recovery unit performance, ensure reliable operation and reduce the number of upsets.

The sulfur recovery process involves many energy-intensive steps, where process streams must be heated and cooled to achieve conversion and sulfur removal. Users can minimize OPEX in existing plants by identifying optimal temperatures for operation with Sulsim Sulfur Recovery. Designers can use Sulsim Sulfur Recovery to build the right plant configuration to meet sulfur 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.

## Simulate the Sulfur Recovery Process in Aspen HYSYS

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

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

Standalone Sulsim has been fully integrated into Aspen HYSYS by implementation of:

- A dedicated Sulsim (sulfur recovery) property package
- A specialized sulfur recovery sub-flowsheet environment (Figure 2)
- A specialized unit operations palette, including all previously available Sulsim unit operations, as well as some new operations introduced in this release (Figure 3)
- A Sulsim-to-HYSYS case converter for easy customer migration

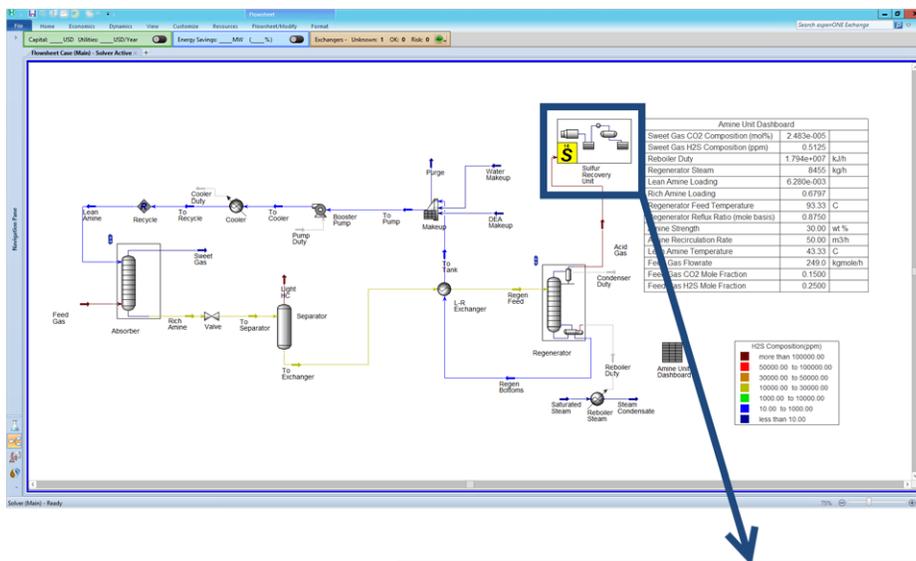
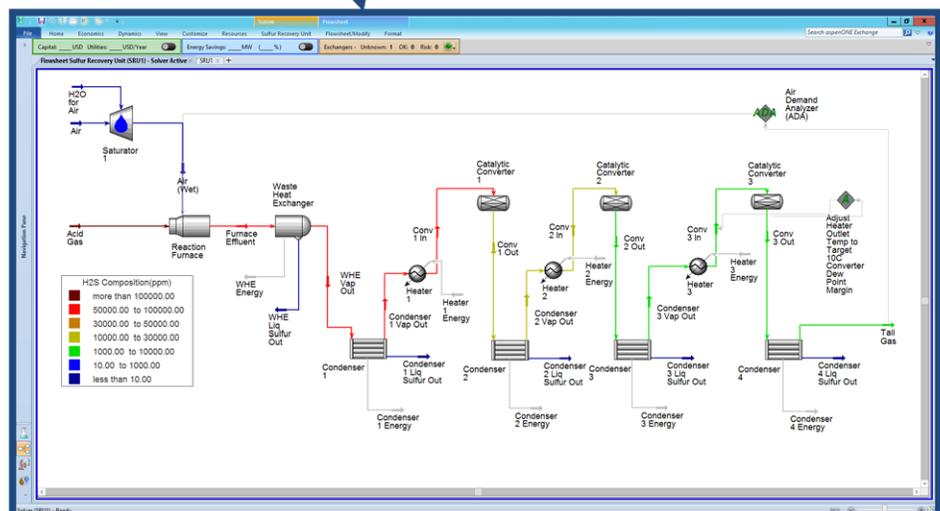


Figure 2: Sulsim Sulfur Recovery is available in Aspen HYSYS as a sub-flowsheet with a specialized model palette and property package.



Additionally, for the first time in Aspen HYSYS V9:

- The Sulsim property package contains extended components S1 through S8, with full detail of these sulfur 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 that cover a wide range of process configuration and feed compositions.
- A new incinerator model with kinetic correlations is now available, which predicts breakthrough of key species to and out of the flare.
- The catalytic converter unit operations now include a model for simulating mixed-bed titania catalyst, as well as alumina.
- A new model has been developed for the selective oxidation converter.
- A new simplified SO<sub>2</sub> absorber unit op is included for simulating tail gas treating.

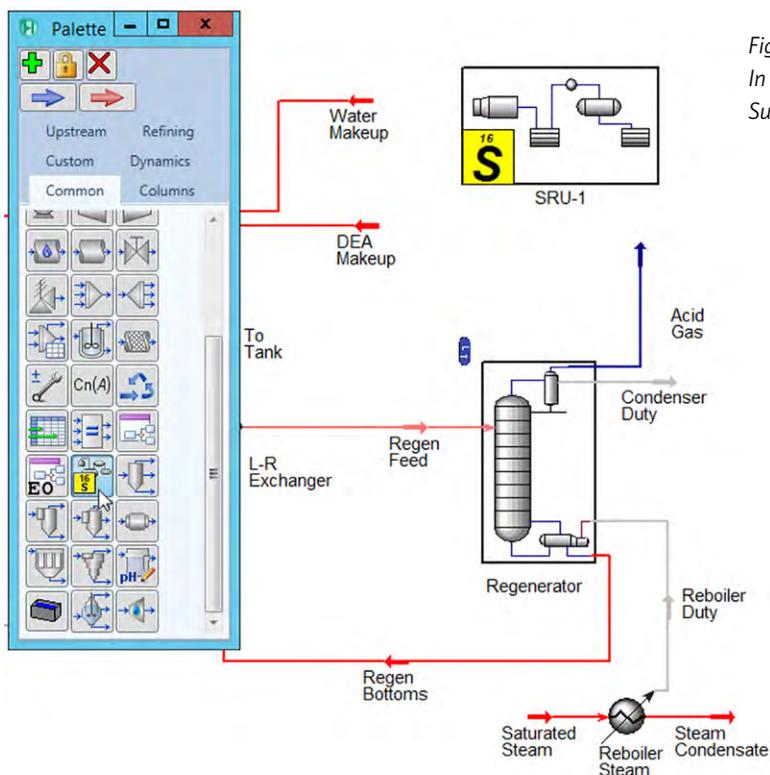


Figure 3:  
In the common tab of the model palette of Aspen HYSYS, the Sulfur Recovery Unit (SRU) sub-flowsheet can be found.

Lastly, AspenTech provides a case converter for easy transfer of legacy Sulsim cases to Sulsim Sulfur Recovery in Aspen HYSYS. The case converter has been validated across hundreds of customer cases, and additional details on the converter functionality can be found by pressing F1 to access the help section in Aspen HYSYS or the Sulsim case converter.

### Sulsim Sulfur Recovery in Aspen HYSYS

To get started using Sulsim Sulfur Recovery in Aspen HYSYS, you will need to:

- Set up the Sulsim (Sulfur Recovery) property package.
- Set up the associated component list.
- Add an SRU operation to the Aspen HYSYS flowsheet.
- Connect any relevant streams to the SRU operation.
- Enter the SRU sub-flowsheet environment to configure your sulfur recovery process.
- View the performance reporting.

## Set up the Fluid Package and Associated Component List

The implementation of Sulsim into Aspen HYSYS is made possible through the inclusion of a brand new property package, called Sulsim (sulfur recovery) in the properties environment. Certain components are required for simulating the SRU, while others are unsupported in the SRU sub-flowsheet. See a list of the required components and additional supported components in Figure 4.

There are a few different ways to add the new fluid package and associated component list:

1. **Creating a blank SRU flowsheet:** When a user adds a new SRU and chooses to create a blank flowsheet, Aspen HYSYS will create a new Sulsim Fluid Package with a component list with all of the required and additional supported components.
2. **The traditional way:** Users can add a Sulsim property package in Aspen HYSYS in a similar manner to any other property package used for simulation. Once the Sulsim (Sulfur Recovery) package has been added, click the simulation environment and add the required components for Sulsim, removing any unsupported components.
3. **Using a Template:** A property package and a corresponding component list is imported if an SRU is added to the flowsheet and a pre-existing template is chosen as the source (such as a template created using the Sulsim-to-HYSYS case converter).

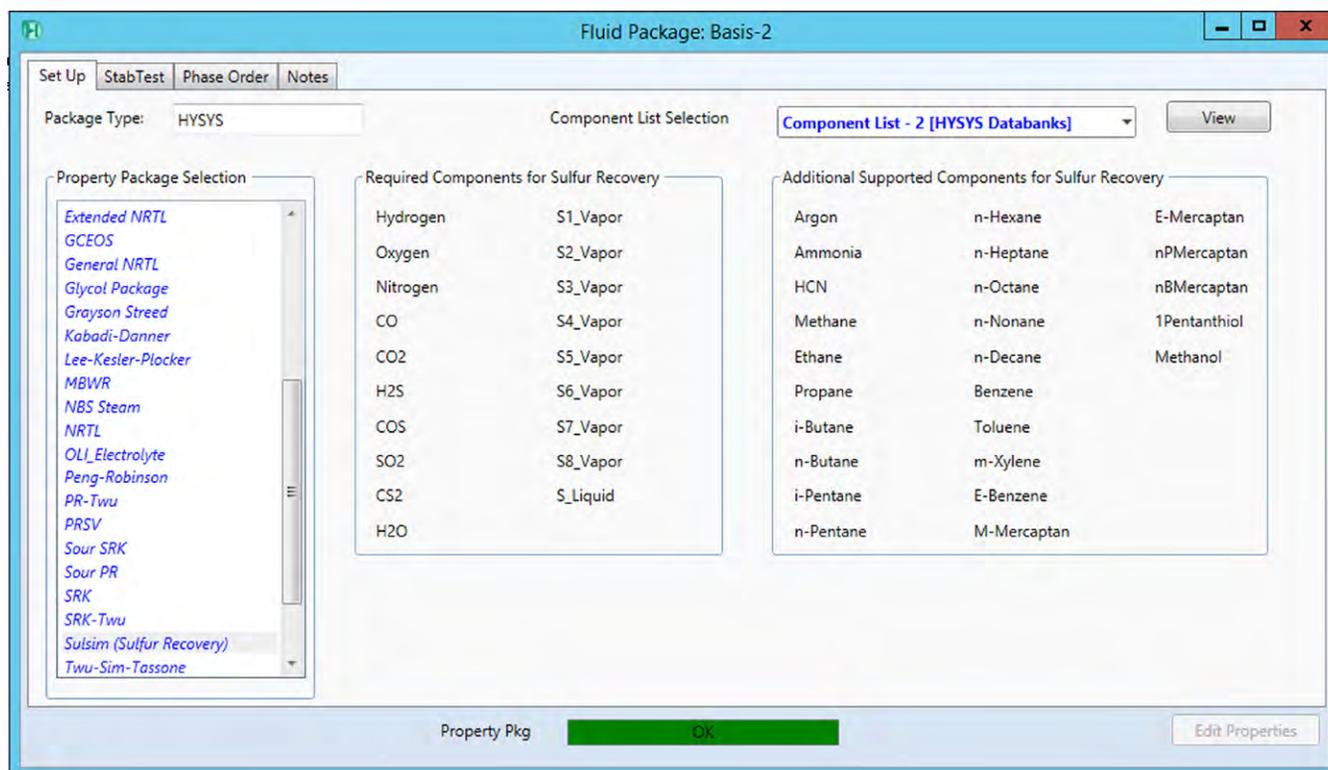


Figure 4: The required components for sulfur recovery and the unsupported components.

## Add an SRU Operation and Connect it to the Rest of the Flowsheet

After set up of the properties environment is complete, users can navigate to the simulation environment to begin configuration of their Claus plant. For users that wish to simulate their Claus plant in a pre-existing Aspen HYSYS case file, such as alongside an Acid Gas Cleaning process, users can simply click on the Sulfur Recovery Unit operation on the Aspen HYSYS palette and place the icon on the Aspen HYSYS flowsheet.

Aspen HYSYS will give you a few options: use a template, create a blank flowsheet, or paste exported objects.

Treat the SRU sub-flowsheet as you would any unit and connect any relevant streams to it. Those streams will appear in the subflowsheet.

The Sulsim Case Converter can also import pre-existing standalone Sulsim flowsheets directly into a pre-existing Aspen HYSYS case file. Simply configure the converter to target the pre-existing Aspen HYSYS case file as output and your Sulsim flowsheet will be directly added to this Aspen HYSYS case file.

## Configure Your Sulfur Recovery Process

Sulsim Sulfur Recovery functions within this “Sulfur Recovery Unit sub-flowsheet”. Click the “Enter Sub-Flowsheet Environment” button in the Sulfur Recovery Unit form to begin.

### Explore the New Sulsim Sulfur Recovery Sub-flowsheet Environment

The Sulsim Sulfur Recovery palette, available in the sub-flowsheet, contains 33 unit operations. All pre-existing Sulsim unit operations are fully supported, as well as some select unit operations from the Aspen HYSYS palette, and new unit operations made available first in Aspen HYSYS V9. To bring up the Sulsim Sulfur Recovery palette in the sub-flowsheet, press F4 on the keyboard. Special “Combination” options are also available on the palette and ribbon to quickly build thermal, catalytic and tail gas stages in your flowsheet.

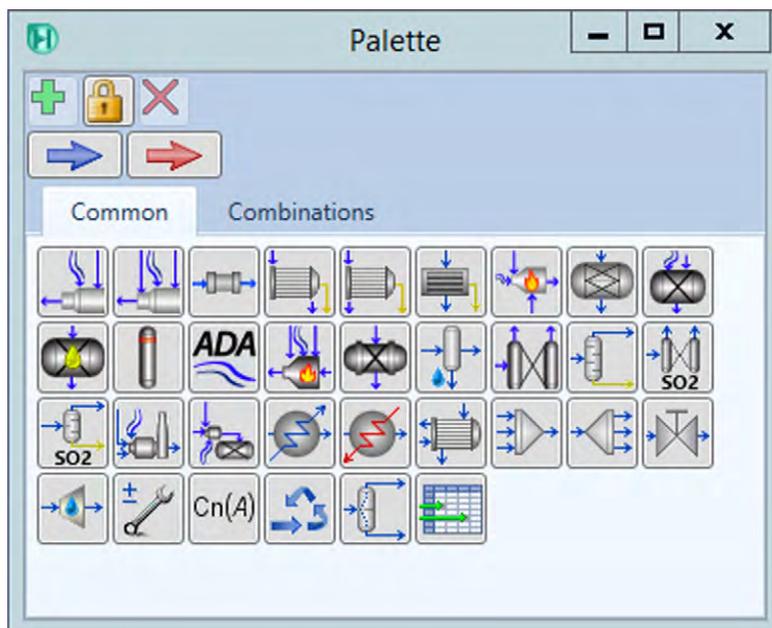


Figure 5:  
The model palette in the SRU sub-flowsheet combines the unit operations available in Sulphur Expert’s Sulsim with several from Aspen HYSYS.

### Set up the Sulfur Plant Thermal Section

1. Add an acid gas stream and a furnace air stream matching your plant's furnace inlet stream compositions, temperature, pressure and flow rate.
2. Add a single chamber reaction furnace unit op to the flowsheet using the palette.
3. Configure the FUR-100 unit by double-clicking and navigating through the various tabs on the form:
  - a. Connect the acid gas and furnace air streams to the furnace unit op.
  - b. Add a furnace effluent outlet gas stream (the unit op should converge).
  - c. Explore the various options for empirical models on the Furnace | Parameters ply. You can press "F1" to get additional guidance on which model to select.
  - d. Specify a reasonable pressure drop.
4. Add a single pass waste heat exchanger unit op to the SRU flowsheet.
5. Configure the WHE-100 unit:
  - a. Connect the furnace effluent stream as inlet.
  - b. Add streams for the WHE outlet gas, liquid sulfur outlet and the energy stream.
  - c. Specify a temperature for the WHE outlet gas.
  - d. The unit op should converge.
6. Add a condenser unit op to the flowsheet.
7. Configure the COND-100 unit:
  - a. Connect the WHE outlet gas stream as inlet.
  - b. Add streams for the gas outlet, liquid sulfur outlet and energy stream.
  - c. Specify a temperature for the gas outlet stream.
  - d. The unit op should converge.

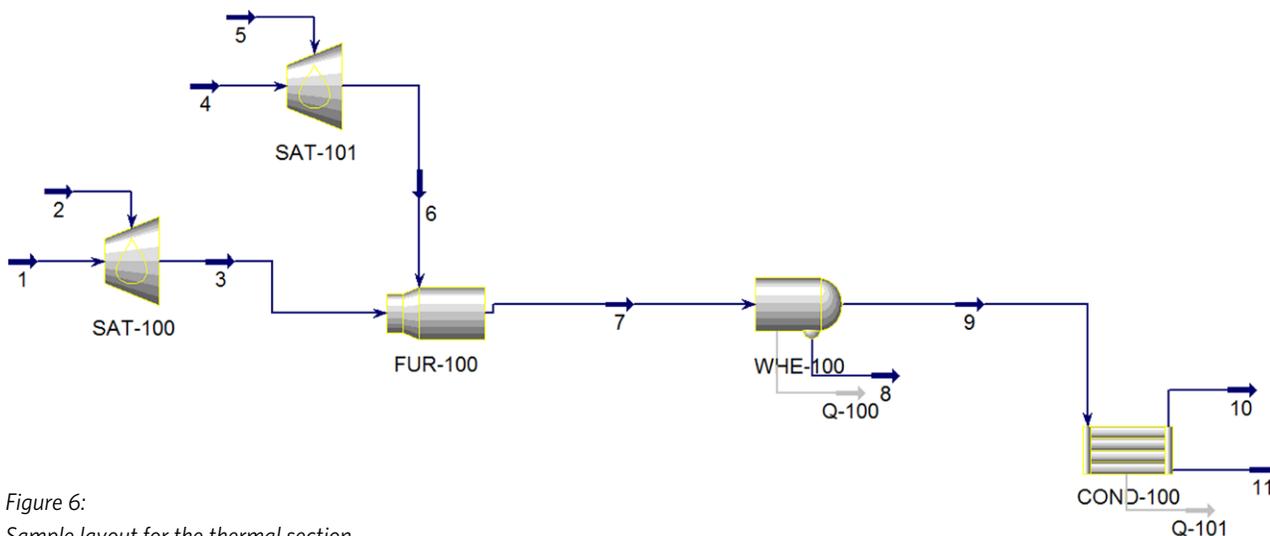


Figure 6:  
Sample layout for the thermal section

### Set up the Sulfur Plant Catalytic Section

1. After the set up of the thermal section has been completed, add a heater or a direct fired heater to the flowsheet.
2. Connect the condenser gas outlet as inlet to the heater.
3. Configure the heater with an energy stream and/or any other material streams that may be required:
  - a. Direct fired heater will require an air stream and a fuel gas stream.
  - b. Specify either an outlet temperature or all flow rates (as in the case with the direct fired heater). You may also use an adjust block to solve any required objective function.
4. Add one of the three catalytic converter unit ops to the flowsheet.
5. Attach the heater outlet as the inlet to a catalytic converter.
6. Configure the catalytic converter as per the form guidance:
  - a. Note the availability of alumina and titania catalyst options on the "Parameters" page of the form.
7. Add a condenser section, similar to the process defined in the previous task.

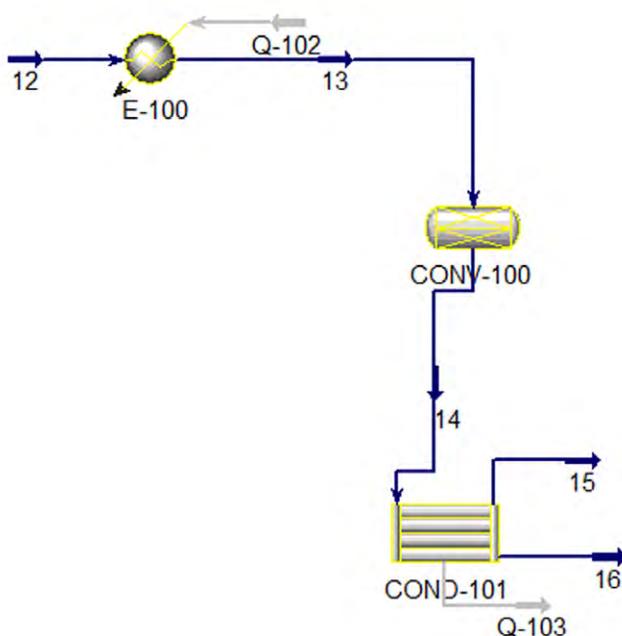


Figure 7:  
Sample layout for the catalytic section.

### Use the Combinations Option

For quick and easy set up of a thermal, catalytic, or tail gas treating section of your Claus plant, you can either:

- From within the SRU sub-flowsheet environment, navigate on the ribbon to the Sulfur Recovery Unit | Add Combinations.
- Navigate to the "Combinations" button on the palette within the SRU sub-flowsheet environment.

### Refer to Provided Example Files to Get Started

If you wish to become familiar with Sulsim Sulfur Recovery in Aspen HYSYS using our provided example files, navigate to the Aspen HYSYS ribbon | Resources | Examples button. Open the folder corresponding to Sulsim (Sulfur Recovery) to find the provided Sulsim example files. The examples below are provided as high-level guidelines on how to simulate and review the performance of your sulfur recovery unit.

## View Performance Reporting

Performance information specific to Aspen HYSYS Sulsim is viewable on most unit ops and streams within the Sulfur Recovery sub-flowsheet environment. Enter the stream or unit op form and navigate to the “Performance” tab or ply to view important sulfur recovery metrics specific to this operation.

To view an overall sulfur recovery unit performance summary:

- Enter the sulfur recovery unit sub-flowsheet environment
- On the ribbon, navigate to Sulfur Recovery Unit | Performance Summary

A cumulative performance summary will be displayed, showing key metrics to this process across sequential unit operations in the flowsheet, as shown below in Figure 8.

Efficiency		Thermal: Reaction Furnace	Catalytic: Catalytic Converter	Catalytic: Catalytic Converter	Catalytic: Catalytic Converter
Stage					
Conversion (Unit) [%]		65.72	69.94	71.83	60.08
Conversion (Cumulative) [%]		65.72	89.70	97.10	98.84
Recovery (Unit) [%]		99.81	99.48	98.27	92.85
Recovery (Cumulative) [%]		65.60	89.57	96.97	98.71
COS Hydrolysis [%]		N/A	90.92	39.21	60.33
CS2 Hydrolysis [%]		N/A	74.35	11.20	25.66
Overall Recovery Efficiency [%]		---	---	---	98.71

Production		Thermal: Reaction Furnace	Catalytic: Catalytic Converter	Catalytic: Catalytic Converter	Catalytic: Catalytic Converter
Stage					
Conversion (Unit) [kg/h]		1301	474.7	146.6	34.54
Conversion (Cumulative) [kg/h]		1301	1776	1923	1957
Recovery (Unit) [kg/h]		1299	474.6	146.5	34.47
Recovery (Cumulative) [kg/h]		1299	1774	1920	1954
Total Inlet Sulfur [kg/h]		---	---	---	1980

Figure 8: The performance summary form shows the efficiency and production throughout the SRU.

## Optimize the Entire Gas Plant in Aspen HYSYS

In summary, the gas plant in midstream and refining industries contains many different processes, 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 optimization.

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

For the first time in Aspen HYSYS V9, users can optimize all major gas plant processes in Aspen HYSYS.

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 in Aspen HYSYS V9, with new liquid-liquid treating capabilities, as well as additional supported components and solvents. Aspen 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 in Aspen HYSYS to simulate removal of inerts such as N2 and He, as well as other contaminants such as Hg. Aspen HYSYS and Aspen Exchanger Design and Rating (Aspen EDR), can also be used to simulate gas-liquid fractionation, LNG compression, and LNG regasification process. Finally, Aspen Flare System Analyzer™ can simulate flaring with the goal of meeting environmental regulations.

Layered functionality from other AspenTech products are also available for use in areas of the Aspen HYSYS gas plant flowsheet, such as Aspen Simulation Workbook™, Aspen Capital Cost Estimator™, Aspen Energy Analyzer™, and other safety environment functionality, such as BLOWDOWN™ Technology and PSV.

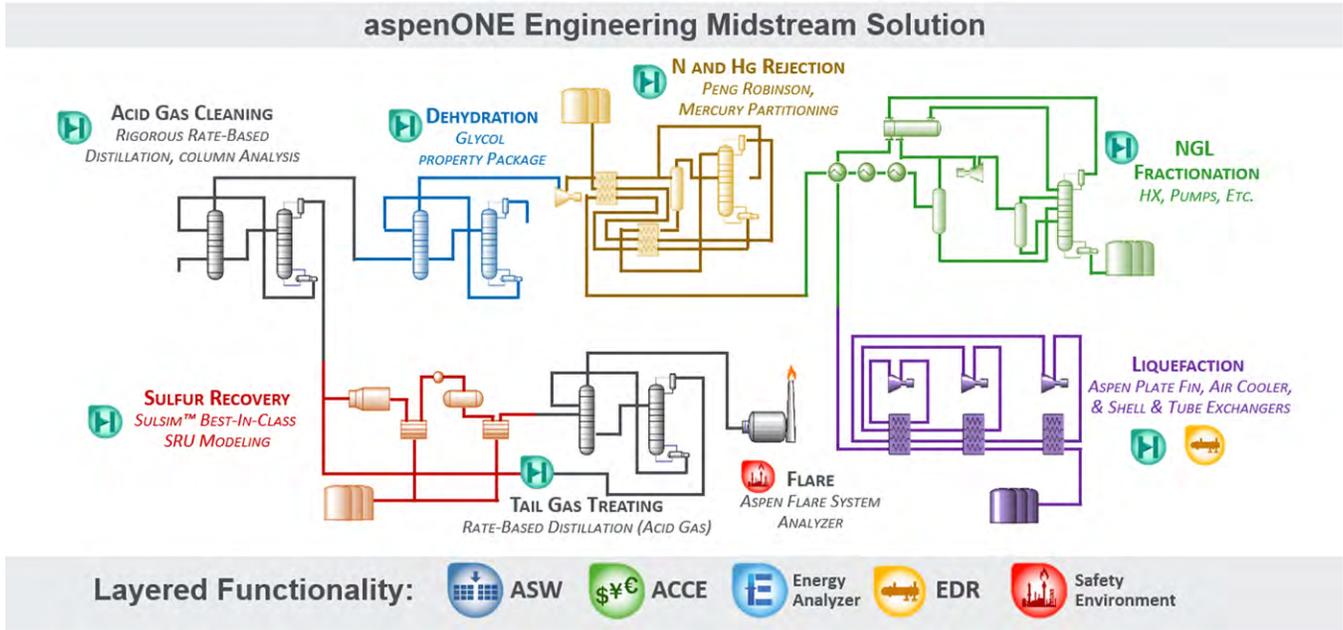


Figure 9: The full aspenONE Engineering midstream solution.

## Self-Guided Demonstrations

We have several self-guided demonstrations of Sulsim Sulfur Recovery in Aspen HYSYS on the support center website. These will show you:

1. How you can use the Sulsim Case Converter to convert a standalone Sulsim flowsheet to an Aspen HYSYS format.
2. How to connect this process to a pre-existing Acid Gas Cleaning flowsheet.
3. How to utilize the major new features available for the first time in V9 alongside examples of how you can use Sulsim Sulfur Recovery to optimize your process.

To complete the self-guided demonstration, you need a computer meeting the minimum software and hardware requirements for the aspenONE Engineering suite and a copy of Aspen HYSYS V9 installed. You will also need the *2 Stage Claus Process for Demo.s70* and *Acid Gas Cleaning Using DEA for Demo.hsc* starter files made available on the AspenTech support site in a knowledge base item. Search for these files at <http://support.aspentech.com>. To complete the self-guided demonstration, use the starter files in combination with the instructions.

For more information or help, please press F1 within Aspen HYSYS, or reach out to AspenTech via the contact information at the end of this training.

AspenTech is a leading software supplier for optimizing asset performance. Our products thrive in complex, industrial environments where it is critical to optimize the asset design, operation and maintenance lifecycle. AspenTech uniquely combines decades of process modeling expertise with machine learning. Our purpose-built software platform automates knowledge work and builds sustainable competitive advantage by delivering high returns over the entire asset lifecycle. As a result, companies in capital-intensive industries can maximize uptime and push the limits of performance, running their assets faster, safer, longer and greener.

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