

## Jump Start Guide: Acid Gas Cleaning in Aspen HYSYS®

A Brief Tutorial (and supplement to and online documentation)

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## Introduction

The new Acid Gas Cleaning capability in Aspen HYSYS allows users to more rigorously simulate gas processing from beginning to end, including the removal of acid contaminants. This new feature allows users to model:

- Amine treating for gas sweetening
- Sulfur removal, including hydrogen sulfide, mercaptans, COS, and CS<sub>2</sub>
- Carbon dioxide removal
- Amine regeneration
- Amine degradation
- Tail gas treating
- Gas-liquid and liquid-liquid treating
- Systems with physical solvents

This feature is a part of Aspen HYSYS, which allows users to seamlessly integrate it with existing models for gas processing, making modeling easier and more accurate.

## Scope of this Document

This document is intended as a “getting started” guide. It will cover the process of creating a new case for Acid Gas Cleaning, setting up component lists, fluid packages, and working in the simulation environment to build the model. It is not meant as a standalone reference document. We recommend pairing this guide with a range of other resources, including:

- AspenTech knowledgebase items, training and sample models available in Aspen Exchange
- AspenTech Online Training modules available from within the product
- AspenTech support website ([esupport.aspentech.com](https://esupport.aspentech.com))
- AspenTech courseware available in online and in-person versions
- AspenTech business consultants

Knowledge of Aspen HYSYS V10 is assumed for this guide. Aspen HYSYS V10 and Aspen Plus® V10 need to be installed for access to the functionality. If you do not know how to build a flowsheet in Aspen HYSYS, you should first consult reference material on this subject. We recommend the following:

- Jump Start: Getting Started with Aspen HYSYS
- Getting Started with Aspen HYSYS Computer-Based Training module
- Aspen HYSYS training course

## Example Cases

A number of example Acid Gas Cleaning cases are available in Aspen Exchange and through the Samples folder within Aspen HYSYS V10. These sample cases can serve as a starting point for your modeling, as they have a completed setup Properties Environment and a completed flowsheet in the Simulation Environment. You can start with one of these example files and edit some basic input parameters to have a case ready for simulation. The following example cases are available:

- Acid Gas Cleaning Using a Physical Solvent (DEPG)
- Acid Gas Cleaning Using DEA
- Acid Gas Cleaning Using DGA
- Acid Gas Cleaning Using DIPA
- Acid Gas Cleaning Using MDEA
- Acid Gas Cleaning Using MDEA + DEA
- Acid Gas Cleaning Using MDEA + DEA + MEA
- Acid Gas Cleaning Using MDEA + MEA
- Acid Gas Cleaning Using MDEA + Piperazine
- Acid Gas Cleaning Using MEA
- Acid Gas Cleaning Using PZ
- Acid Gas Cleaning Using SULFOLANE-DIPA
- Acid Gas Cleaning Using SULFOLANE-MDEA
- Acid Gas Cleaning Using SULFOLANE-MDEA-PZ
- Acid Gas Cleaning Using TEA
- Effect of H<sub>3</sub>PO<sub>4</sub> on Acid Gas Cleaning Using MDEA
- Effect of Heat Stable Salts on Acid Gas Cleaning Using MDEA
- Liquid-Liquid Treating Using MDEA
- Acid Gas and COS-CS<sub>2</sub>-Mercaptans Cleaning Using MDEA

For this guide, we will show the basic workflow for creating a model for Acid Gas Cleaning using MDEA.

## Properties Environment

The first step in building any Aspen HYSYS flowsheet is setting up the Properties Environment. In this environment, the user selects the components that will be used in the simulation and groups them into Component Lists. The user must also select one or more Property Packages, which are models for the calculation methods for physical properties. The combination of a Component List and a Property Package is called a Fluid Package, and the user must define a complete Fluid Package before they can move on to the Simulation Environment.

## Component List

When modeling an Acid Gas Cleaning process, the first step in building the Aspen HYSYS model is to create a component list including all the components used in the process. In this case specifically, the following components must be added in order to simulate gas cleaning.

- Methane (main component in natural gas)
- Ethane
- Amine or amine blend
- Carbon dioxide (CO<sub>2</sub>)
- Hydrogen sulfide (H<sub>2</sub>S)
- Water (H<sub>2</sub>O)

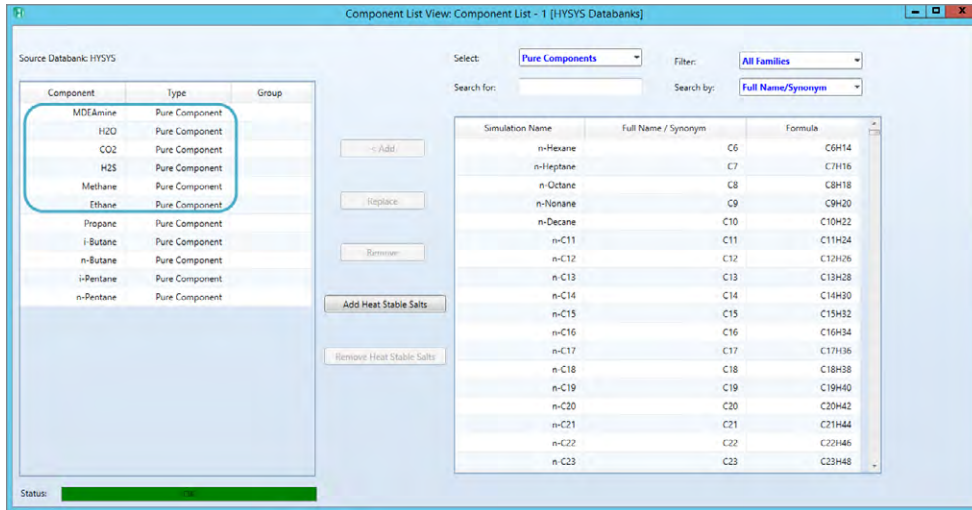


Figure 1: The Component List populated with all necessary components for Acid Gas Cleaning. On the right, the option to “Add Heat Stable Salts” appears.

Other common components, such as lighter hydrocarbons, can be added depending on the characteristics of each individual process scenario.

The following amines and amine blends are supported by the Acid Gas - Chemical Solvents package:

- Methyldiethanolamine (MDEA)
- Piperazine (PZ)
- Diethanolamine (DEA)
- Diglycolamine (DGA)
- Monoethanolamine (MEA)
- Diisopropanolamine (DIPA)
- Triethanolamine (TEA)
- Blend of any two supported amines listed above
- Sulfolane + MDEA
- Sulfolane + DIPA
- Sulfolane + MDEA + PZ
- MDEA + MEA + DEA

The following amines and amine blends are supported by the Acid Gas - Liquid Treating package:

- MEA
- DEA
- MDEA
- DGA
- MDEA + PZ

The following solvent is supported by the Acid Gas - Physical Solvent package:

- DEPG



After selecting Acid Gas as a Property Package, you can then move into the Simulation Environment. If the required components have not been added, when you click the button to switch to the Simulation Environment, a pop-up reminder shows the option to add the components automatically (Figure 4).

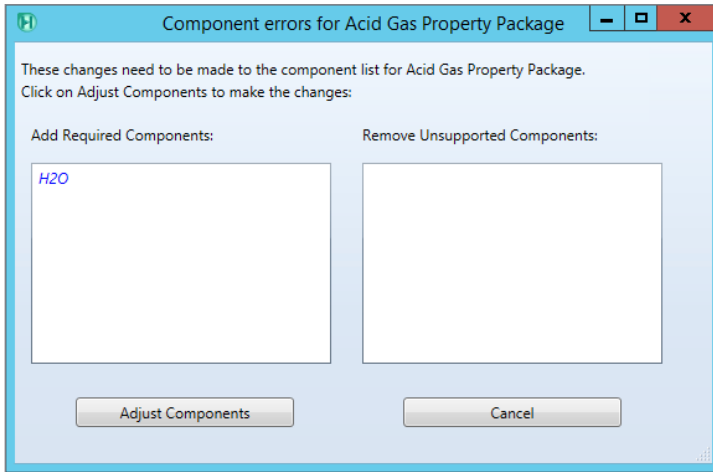


Figure 4: If not all required components are added to the Component List, Aspen HYSYS can add them automatically before moving to the Simulation Environment.

## Reactions

The reactions and chemistry for this case are automatically generated by Aspen HYSYS using the underlying thermodynamics and calculation models in the Acid Gas Property Package, and the component list associated with the Property Package. You don't need to make any edits to this part, and can proceed straight to the Simulation Environment. However, if you would like to analyze the underlying reactions in the process, they are available in the Properties Environment under the "Reactions" tab, as shown in Figure 5.

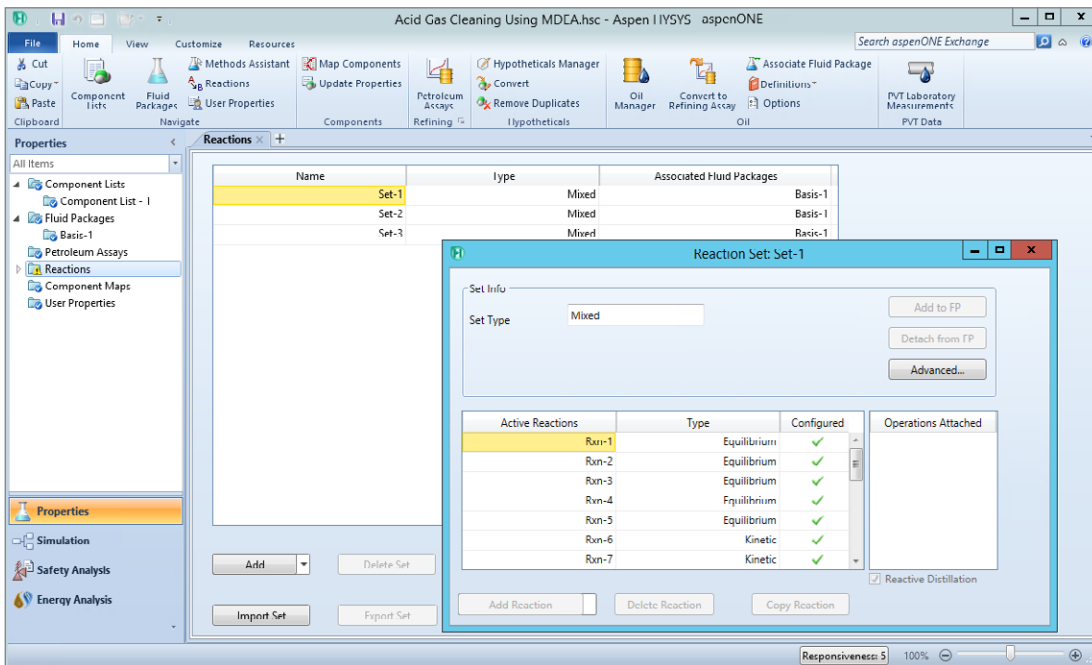


Figure 5: Reaction list for the Acid Gas Cleaning process generated automatically when Components and Properties related to Acid Gas Cleaning are entered.

## Simulation Environment

### Flowsheet

In the Simulation Environment, you will find a blank page on which to build your model. The necessary Unit Operations that can be added to the flowsheet for the process simulation, including Columns and Streams, can be found under the “Flowsheet/Modify” tab in Aspen HYSYS, by clicking the “Models and Streams” button. For reference, Figure 6 displays an example flowsheet of the Acid Gas Cleaning process and how it appears in Aspen HYSYS.

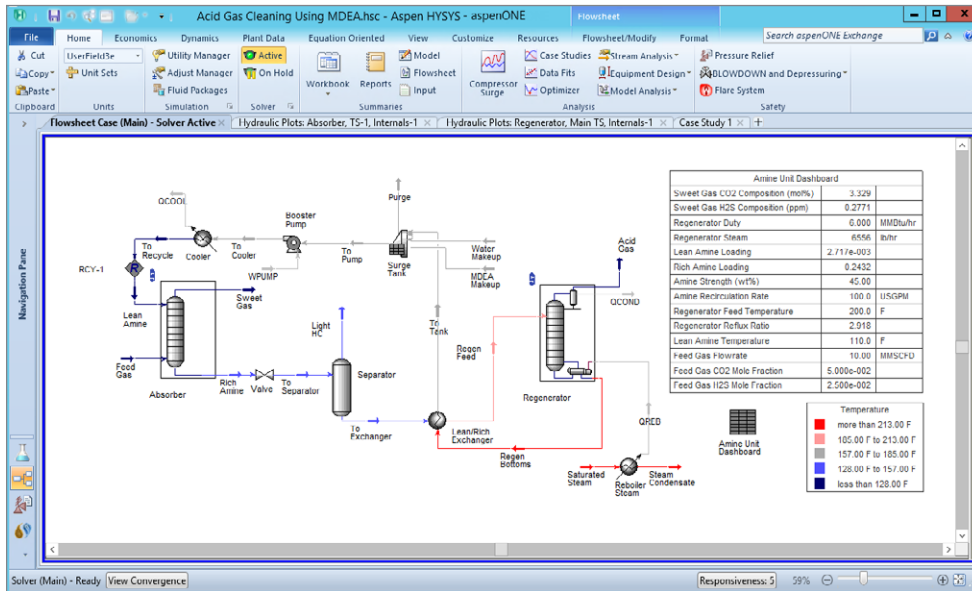


Figure 6: An example flowsheet of the Acid Gas Process in Aspen HYSYS.

## Unit Operations

The Unit Operations required for the simulation of the Acid Gas Cleaning process include, but are not limited to, several columns, streams, heat exchangers, a valve, pump and makeup unit. The Unit Operations needed for a basic process are outlined below.

### Columns

In the Simulation Environment flowsheet, add the three most important columns for the Acid Gas Cleaning process. These include the Absorber, Regenerator (which will be defined from a Distillation Column) and Separator, which can be found in the Palette, as shown in Figure 7. These columns are necessary for the gas cleaning and amine regeneration portions of the process, and should be added first. For the Absorber column, you can make one of the following selections from the palette: Absorber, Reboiled Absorber, Refluxed Absorber, or Custom Column. For the Regenerator, you can pick the Distillation column from the palette. For the separator, a simple Separator block will do.



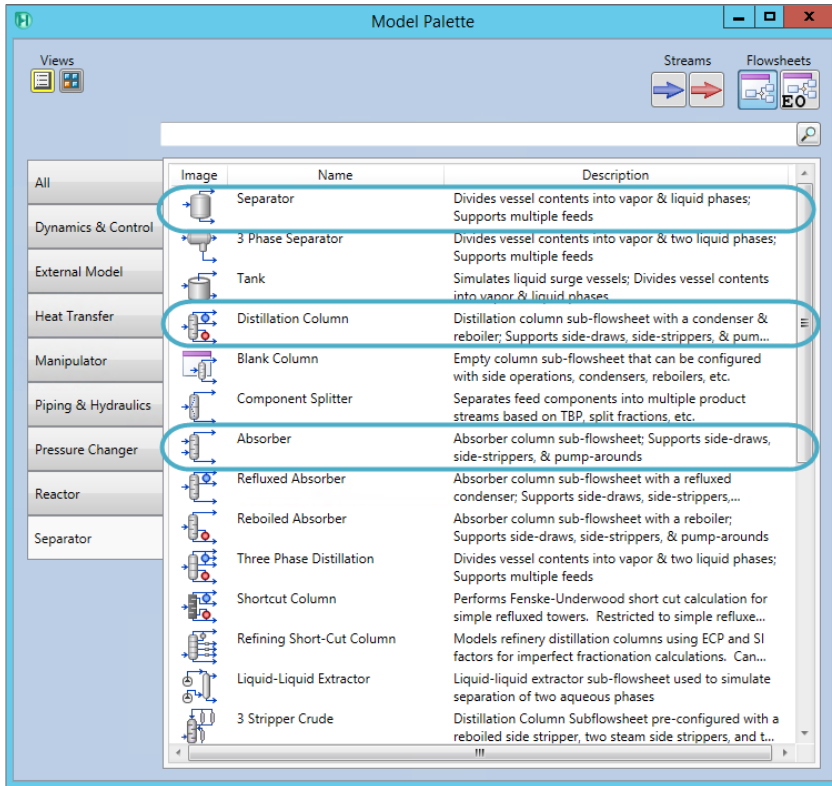


Figure 7: The basic equipment necessary for the Acid Gas Cleaning simulation model: the Absorber, Regenerator (Distillation Column) and Separator.

## Absorber

The Absorber should be set up first, with the help of the Absorber Column Input Expert, shown in Figure 8. On the first page, the connected streams, total number of stages, and inlet stage are selected. On the second page, enter the top and bottom stage pressures, and on the third, the estimated top and bottom temperatures, which are optional. The bottom pressure will usually be the pressure of the feed gas stream entering at the bottom of the column and the top pressure will reflect a small pressure difference of about 3-5 psi.

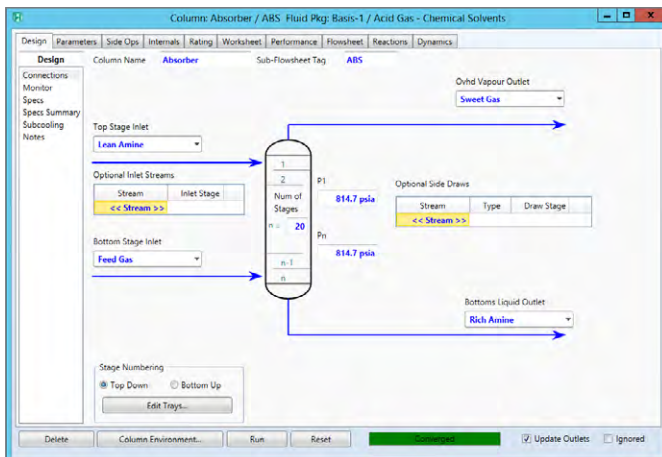


Figure 8: The Absorber Column Input Expert, which helps with the setup of the Absorber column. The first page, where the connected streams are selected, is shown.

When setting up different parameters for the Absorber column, Aspen HYSYS V10 provides smart defaults to converge your column more quickly. However, there are also several different options to customize your design, including multiple column options for the Absorber column, which can be selected in the “Parameters” tab, under the “Acid Gas” ply on the left, as seen in Figure 9. Under that same ply, there are also options available for different types of tray or packing internals, shown in Figure 10.

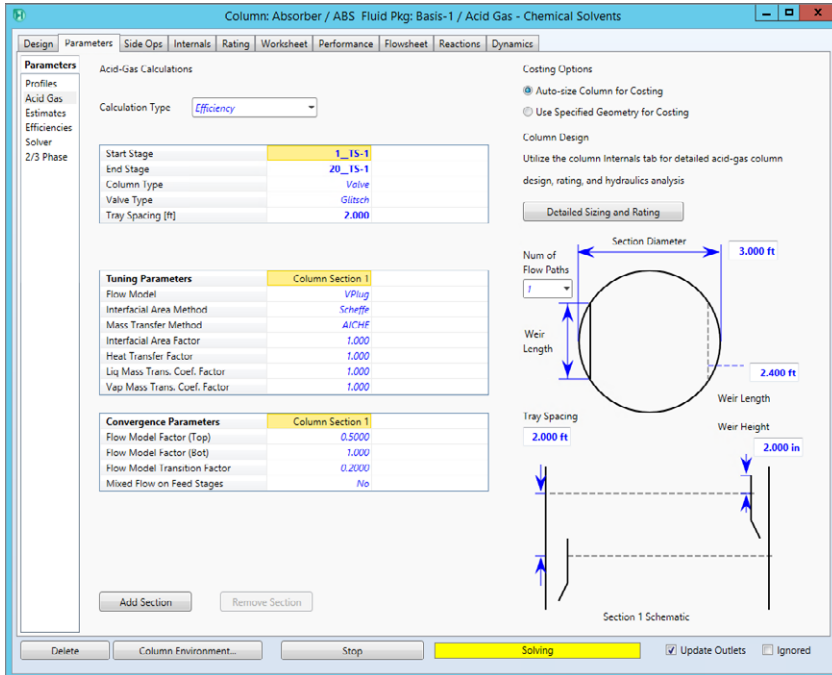


Figure 9: Column types available under the “Acid Gas” ply in the “Parameters” tab in the Absorber column.

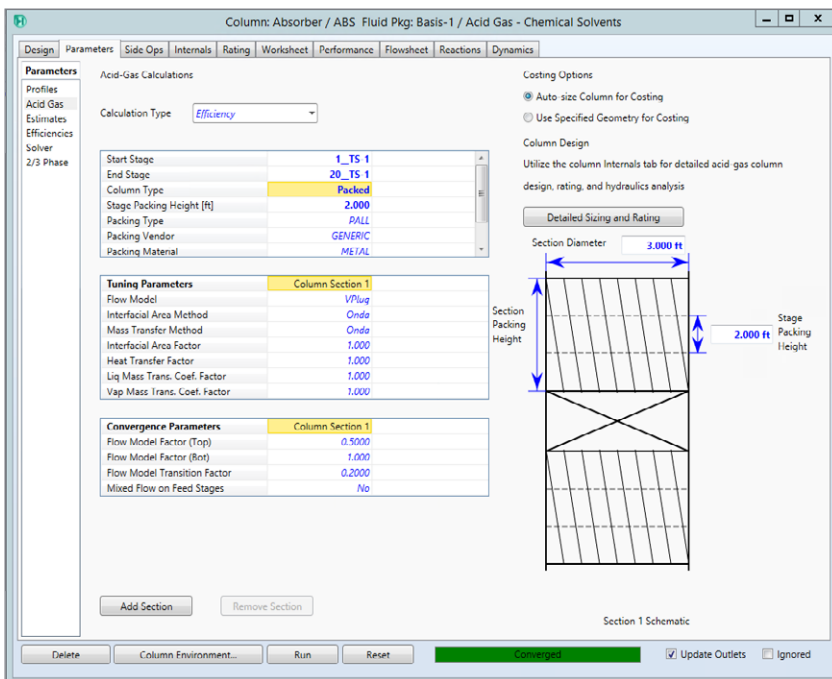


Figure 10: Options for column packing calculations in the “Acid Gas” ply in the “Parameters” tab in the Absorber column.

With Aspen HYSYS V9, the Column Analysis functionality was added to allow for interactive insight into the operation of the distillation column. This functionality is compatible and recommended for Acid Gas Cleaning.

Click “Detailed Sizing and Rating” or the “Internals” tab to use this functionality. If any information was added in the previous screen, it will be transferred here (Figure 11). Click “add new” to add an additional section of tray or packing, export and import section templates and then click “Run” and the “View Hydraulic Plots” to view the results.

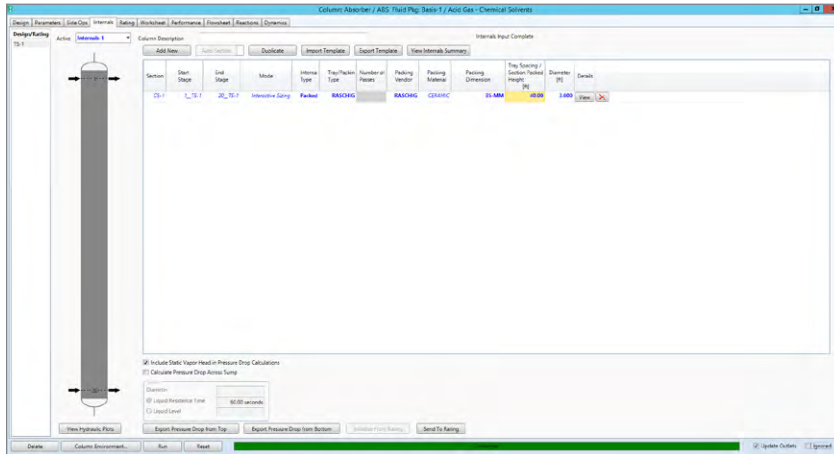


Figure 11: Add new column sections, duplicate sections and save and use section templates.

The Hydraulic Plots (Figure 12) shows, for each stage, the operating point and the larger operating window to the column. This plot will differ for trays and packing. See where operational issues like flooding or weeping may occur.

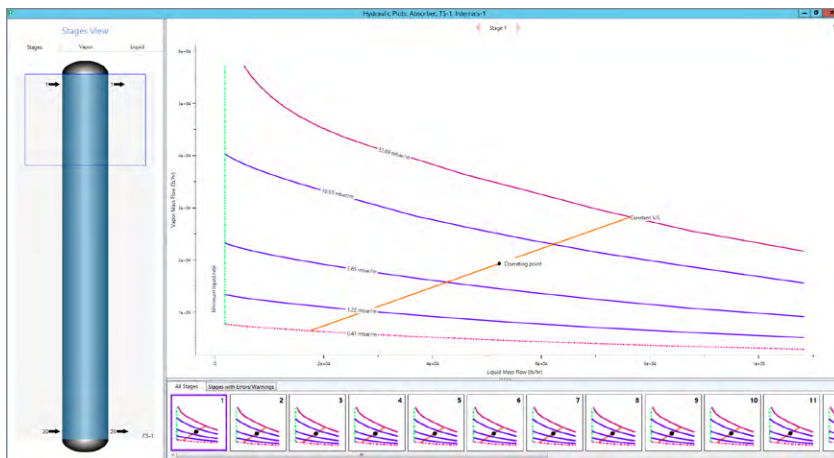


Figure 12: See the operating point and potential operating issues.

It is also possible to select the type of calculation being done on the column for the Acid Gas process, choosing between the more rigorous rate-based “Advanced Modeling” option and the quicker “Efficiency” option, as seen in the close-up in Figure 13. The “Efficiency” option is the one most commonly used; it is a highly rigorous method that uses rate-based calculations in the background to calculate stage efficiencies of  $H_2S$  and  $CO_2$ , and then uses these values to solve the column. The accuracy and ease of use of this method is enough for most user cases. In some expert cases, however, the user has the option of switching to the more rigorous Advanced Modeling type that uses rate-based calculations to calculate the column itself. This type can be used for specifying or monitoring a larger number of variables, or for modeling mercaptans, COS, and  $CS_2$ .

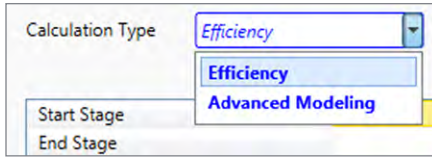


Figure 13: Close-up of the Calculation Type options in the “Acid Gas” Ply. The “Efficiency” option yields faster results, while “Advanced Modeling” should be used for more rigorous calculations.

When the column is set up and the streams connected are specified, the column will converge, giving the results of the first step of the Acid Gas Cleaning process. To see the resulting H<sub>2</sub>S and CO<sub>2</sub> compositions, as well as the H<sub>2</sub>S and CO<sub>2</sub> loading in the Amine streams, select the “Performance” tab, and the “Acid Gas” ply on the left, as shown in Figure 14.

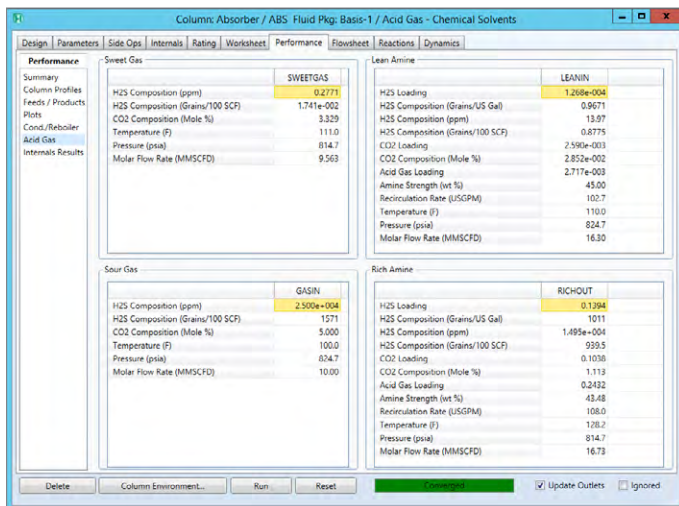


Figure 14: Results of the Acid Gas Cleaning process, as shown in the Absorber column results.

## Separator

After the Absorber has been set up, the rich amine stream is connected to a valve to flash the amine solution. The mixture is then split in the Separator, which can be set up by specifying an inlet stream (Depressurized Rich Amine stream “To Separator”) and two outlet streams: Light Hydrocarbons (“Light HC”) and the liquid Rich Amine mixture (“To Exchanger”), as shown in Figure 15.

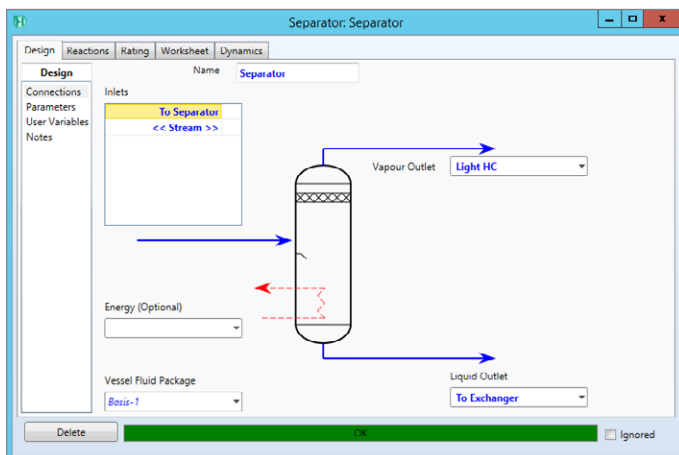


Figure 15: The setup of a Separator in the Acid Gas Cleaning process.

## Regenerator

After the Separator, the liquid Rich Amine mixture gets sent through a heat exchanger and into the Regenerator. In this example, a Distillation Column Subflowsheet was used. To set up the Column, there is a Distillation Column Input Expert. First, the inlet stream and output streams need to be defined, as well as energy streams for the condenser and reboiler, as shown in Figure 16. We have selected a Full Reflux Condenser as an example.

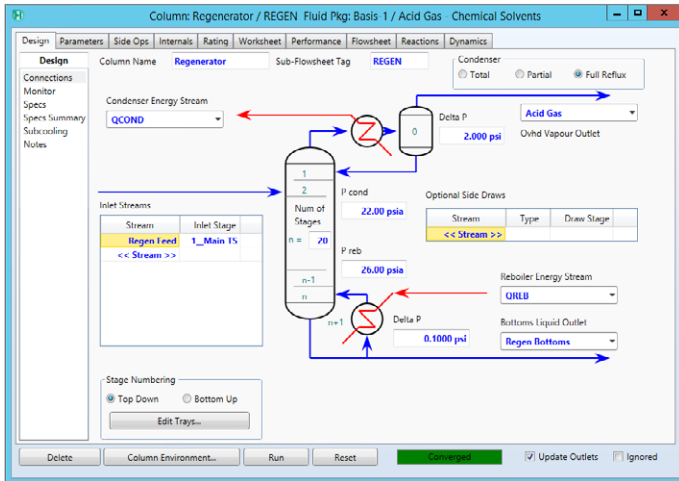


Figure 16: First page of the setup for a Distillation Column with the Input Expert.

On page 2, you can configure the reboiler. In this example, we used a Once-through, regular Aspen HYSYS Reboiler. On page 3, pressure was added to the Reboiler and Condenser, as well as any pressure drops across the equipment. On page 4, the option is available to input the estimated temperatures for the Condenser and Reboiler, and on page 5, you can setup a Vapor Rate and Reflux Ratio for the Condenser.

Once the Input Expert is done, all the information necessary to converge the Regenerator will be defined. As with the Absorber, the Regenerator has Acid Gas-specific options under the Parameters tab for the type of column, tray packing, etc.

## Valve and Pump

In addition to the columns, a valve is necessary to drop the pressure of the Rich Amine stream coming out of the Absorber to flash separate it from lighter hydrocarbons in the Separator. Downstream, before the amine stream, is recycled into the Absorber. It is important to add a pump to make up the pressure difference so that the absorption in the column happens at a higher pressure.

## Heat Exchangers

Two heat exchangers should be added to the simulation for the Acid Gas Cleaning process, in addition to those already included in the column Unit Operations. One exchanger should be included after the pump to cool down the pressurized amine stream, and the other should be between the Separator and the Regenerator to warm up the Low Pressure Rich Amine stream with energy left over from the Lean Amine coming out of the Regenerator.

## Makeup Block

In the Acid Gas Cleaning process there are losses of amines and water in the system with outgoing streams of Sweet Gas, Sour Gas, and other areas of the process. To make up for those losses, you can add a "Makeup Block", which avoids convergence issues by calculating necessary makeup and purge streams to the system. The overall overview of the Makeup Block in the flowsheet can be seen in Figure 17. You only need to specify the inlet and outlet amine streams, amine concentration and total flow of the outlet stream, which eliminates the need for adding spreadsheet operations.

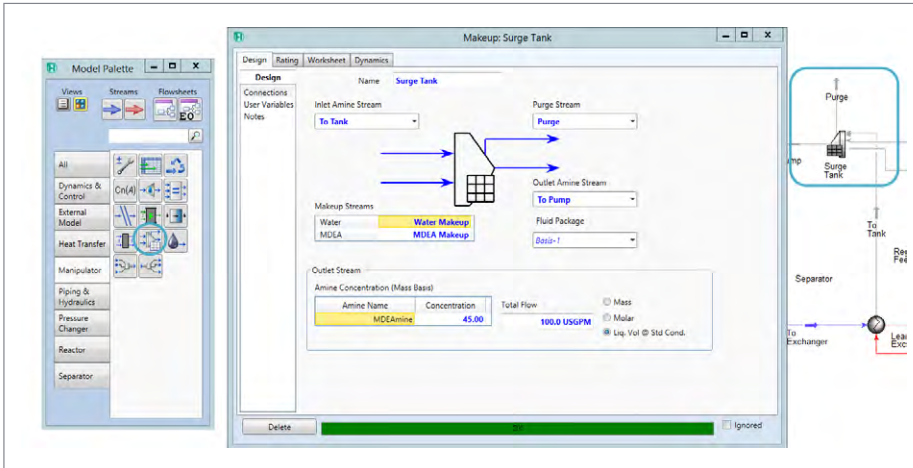


Figure 17: On the left, the Makeup Block in the "Manipulator" palette. Top right, the inputs (Amine Concentration, Total Flow) and connections (Inlet and Outlet Amine Streams, Amine Makeup, Water Makeup, and Purge Stream) necessary for the Makeup Block to converge. On the bottom right, the Makeup Block as it appears in the flowsheet, connected to the Amine input and output, Makeup streams, and purge stream.

## Streams

As these pieces of equipment are added, it's necessary to add the streams connecting them as well. The most important streams are:

- **Gas**
  - Feed Gas into the Absorber
  - Sweet Gas out of the Absorber
  - Acid Gas out of the Regenerator
  - Light Hydrocarbon out of the flash separation process
- **Amines**
  - Lean Amine between the Regenerator and the Absorber:
    - Gives up some heat in the Lean/Rich Exchanger
    - Gets additional amines and water in the Makeup Block
    - Pressurized in the Pump
    - Cooled in the Cooler
  - Rich Amine between the Absorber and the Regenerator:
    - Flashed to a lower pressure through a Valve
    - Separated from lighter hydrocarbons in the Separator
    - Heated up before Regenerator



## Stream Setup

After the unit operations are properly set up, some of the streams need to be characterized between the simulation converges. To set up a stream, the Temperature, Pressure, and Flow Rate need to be specified, as shown in Figure 18. In addition, the Composition of some streams needs to be specified. For the Acid Gas Cleaning process specifically, information about Heat Stable Salt content can be entered in the composition by clicking the Composition ply, then “Edit”, and entering the HSS Composition Wizard, shown in Figure 19.

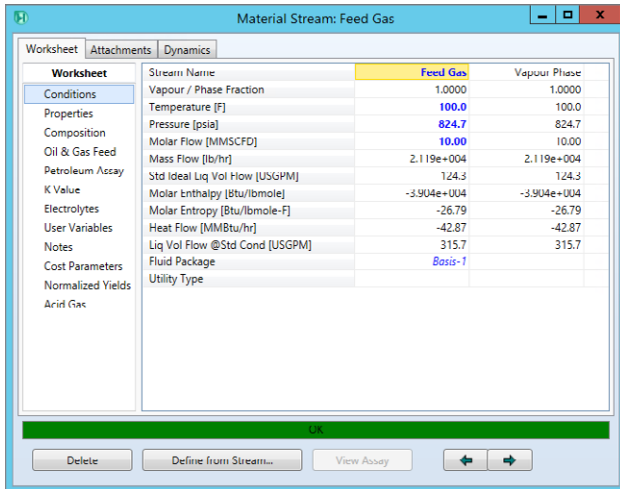


Figure 18: Basic stream specifications.

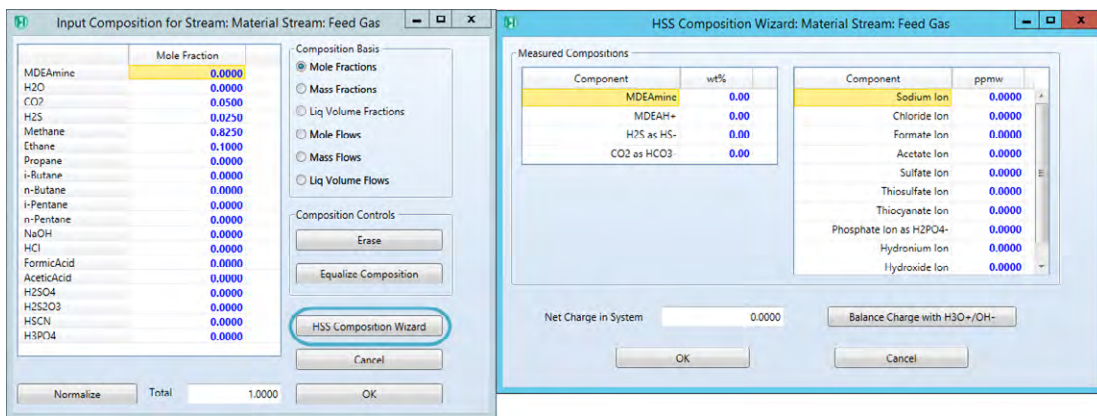


Figure 19: The Heat Stable Salt Composition Wizard, where the amount of heat stable salts in the stream can be specified.

When all basic streams and columns are connected, the flowsheet should look like the one in Figure 20, which includes from left to right: an Absorber, Separator, Regenerator, two heat exchangers (Cooler and Lean/Rich Exchanger), Booster Pump (increases pressure before the Absorber), Valve (decreases pressure before the flash separation), and a Makeup Block with incoming water, Amine Makeup streams and a purge stream.

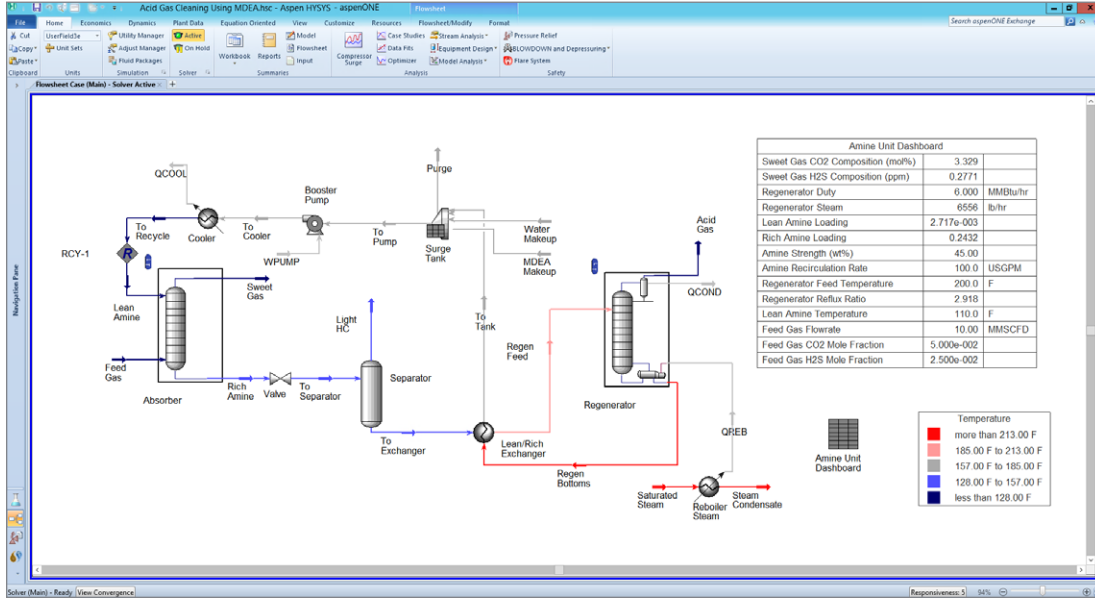


Figure 20: Acid Gas Cleaning using the MDEA example in Aspen HYSYS V10.



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