The CONTACTOR™

Published Monthly by Optimized Gas Treating, Inc.
Volume 14, Issue 01, January, 2020

Assess Claus Unit Performance by Simulation – Part I

Whether at the level of an individual piece of equipment or an entire plant, optimization is usually done using simulation tools. The first step, however, is to verify that the tools chosen are able to reproduce the measured performance of this or a similar unit under its present operating conditions. This article benchmarks the SulphurPro® simulator against the measured performance of a sulphur recovery unit (SRU) processing an ammonia-rich acid gas using low-level oxygen enrichment. The process forms and recycles a significant concentration of COS back to the Reaction Furnace (RF). This provides a fairly stringent test of a model that relies on fundamental chemical reaction kinetics and heat transfer rate calculations to predict performance, rather than one that uses curve fits to forecast performance.

This Part I installment presents a Base Case study of a refinery SRU producing about 125 tonnes per day of sulphur from 3.4 MMscfd of amine acid gas (AAG) with 91% H_2S plus 6.8% CO_2, balance nitrogen on a dry basis, comingled with a SWS acid gas (SWAG) flow of 0.6 MMscfd that is 45 mol% H_2S and 55 mol% ammonia on a dry basis. Simulation includes SRU feed gas preparation, the main body of the Claus SRU, and the front-end of the tail gas treatment unit (TGTU) through the quench tower.

Base Case

Figure 1 shows the flowsheet for the base case. Pure oxygen is used to enrich the oxygen content of the intake air to 28.5%. The total *combined* (enriched) air flow is adjusted using the Solver block marked ADA (Air Demand Analyzer) to ensure the total air flow rate from the flow multiplier (marked MULT) in the figure results in a H_2S to SO_2 molar ratio of 1.9 as measured in the gas leaving the final sulphur condenser during performance testing.

Our purpose is to use simulation to quantify the effect of oxygen enrichment on the sulphur processing capacity of the plant as well as on ammonia destruction and WHB performance parameters in the same processing unit. To this end, an addition computational (Solver) loop was added to the flowsheet in order to calculate the plant feed sulphur flow necessary to have the same total molar flowrate of gas exiting from the first thermal condenser (Stream 26 in Figure 1). The flow rate of this stream is conventionally taken to represent the SRU's gas handling capacity, as discussed more fully later. For the base case study, however, this Solver block was left disabled. The gas flow calculated from the first condenser (but with the COPE® recycle removed) formed the capacity basis for other levels of oxygen enrichment.

To ensure simulator credibility, the first task was to compare simulated versus measured performance indicators. Table 1 shows the *relative* percentage deviation of simulated results from measured data for some 25 of the parameters for which measurements were made. *Every parameter is **predicted** within a few percent of measured!*

Table 1: Simulation vs. Measured Data: Base Case

Parameter Measured	Measured	Simulated	% Deviation
Enriched Air + O_2 Flow (MSCFH)	284.4	267.4	-6.0
Enriched Air O_2 Content (dry mol %)	28.5	28.4	-0.35
Reaction Furnace Outlet Temp, (°F)	2300	2385	3.7
WHB Steam Production Flow (lb/h)	32000	30398	-5.0
WHB Process Outlet, (°F)	512	510.9	0.2
Condenser-1 Steam Production (lb/h)	3042	2871	-5.6
Condenser-1 Process Gas Out (°F)	329	325.6	-1.03
Converter-1 Outlet Temperature (°F)	602	604.1	0.35
Condenser-2 Steam Production (lb/h)	3138	2911	-7.24
Condenser-2 Process Gas Out (°F)	332	332.06	0.02
Converter-2 Outlet Temperature (°F)	471	472.3	0.27
Condenser-3 Steam Production (lb/h)	1409	1467	4.09
Condenser-3 Process Gas Out (°F)	317	312.3	-1.5
Converter-3 Outlet Temperature (°F)	412	409.2	-0.7
Condenser-4 Process Gas Out (°F)	261	260.6	-0.2
H_2S in Condenser-4 Vapor Outlet (mol %)*	0.49	0.54	9.96
SO_2 in Condenser-4 Vapor Outlet (mol %)*	0.26	0.27	3.55
TGU RGG Burner Air Flow (MSCFH)	31.7	30.2	-4.7
RGG Burner Natural Gas (MSCFH)	3.3	3.1	-4.7
RGG Burner Tempering Steam (lb/h)	164	156	-4.6
Hydrogen Makeup for Hydrogenation Reactor (MSCFH)	7.4	7.6	3.3
Hydrogenation Reactor Inlet (°F)	570	562.0	-1.4
Hydrogenation Reactor Outlet (°F)	603	614.7	1.9
Quench Tower OH Temperature (°F)	85	86.4	1.7

***Measured ratio of H_2S to SO_2 is 1.88**

The SulphurPro® simulator can also provide a little more detailed picture of the operation of the catalytic converters by breaking the reactors into discrete, incremental depths of catalyst bed in order to assess temperature and conversion profiles across the beds. This can be done in both design and rating modes. SulphurPro allows the catalyst beds to have varying levels of activity relative to the fresh catalyst.

Figure 2 shows temperature profiles across the catalyst beds in the three converters. Points are the average of two thermocouple readings at opposite ends of a bed width. Converters-2 and -3 were simulated as having fresh catalyst beds. When Converter-1 was simulated this way, it was obvious that the catalyst was to some degree aged or deactivated. When simulated as just under 60% deactivated the solid black line was obtained, so in an overall sense the bed does indeed appear to have a little over half of its original activity remaining. It is interesting to note that, as measured, the temperature profile in the first converter actually has two rather flat sections joined by a rapid transition from one to the other. This is a classic profile for what one would expect for a catalyst being poisoned by a feed contaminant. However, the contaminant, whatever it is, seems to be readily adsorbed onto the catalyst and deactivation will move through the converter's catalyst bed like a wave. Possible contaminants (poisons) might include BETX or even the soot formed from their decomposition.

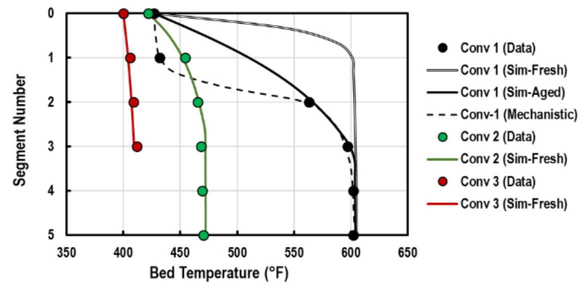

Figure 2. Calculated (Solid Lines) vs. Temperatures Measured Through the Catalyst Beds

SulphurPro® gives a faithful rendition of what was actually observed in the operating unit; therefore, one can conclude that at least in this instance it is a highly reliable model. It is important to emphasize that model calculations are *pure predictions* done completely without tuning of any kind. The predictions rely upon fundamental laboratory measurements of chemical reaction kinetics combined with well-founded models for heat transfer. There is no direct reliance on tuning any parameters to plant performance data; thus, SulphurPro is solidly placed to predict the performance of individual units and the SRU as a whole, both robustly and with good accuracy.

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To learn more about this and other aspects of gas treating and sulphur recovery, plan to attend one of our training seminars. For details, visit www.ogtrt.com/seminars.

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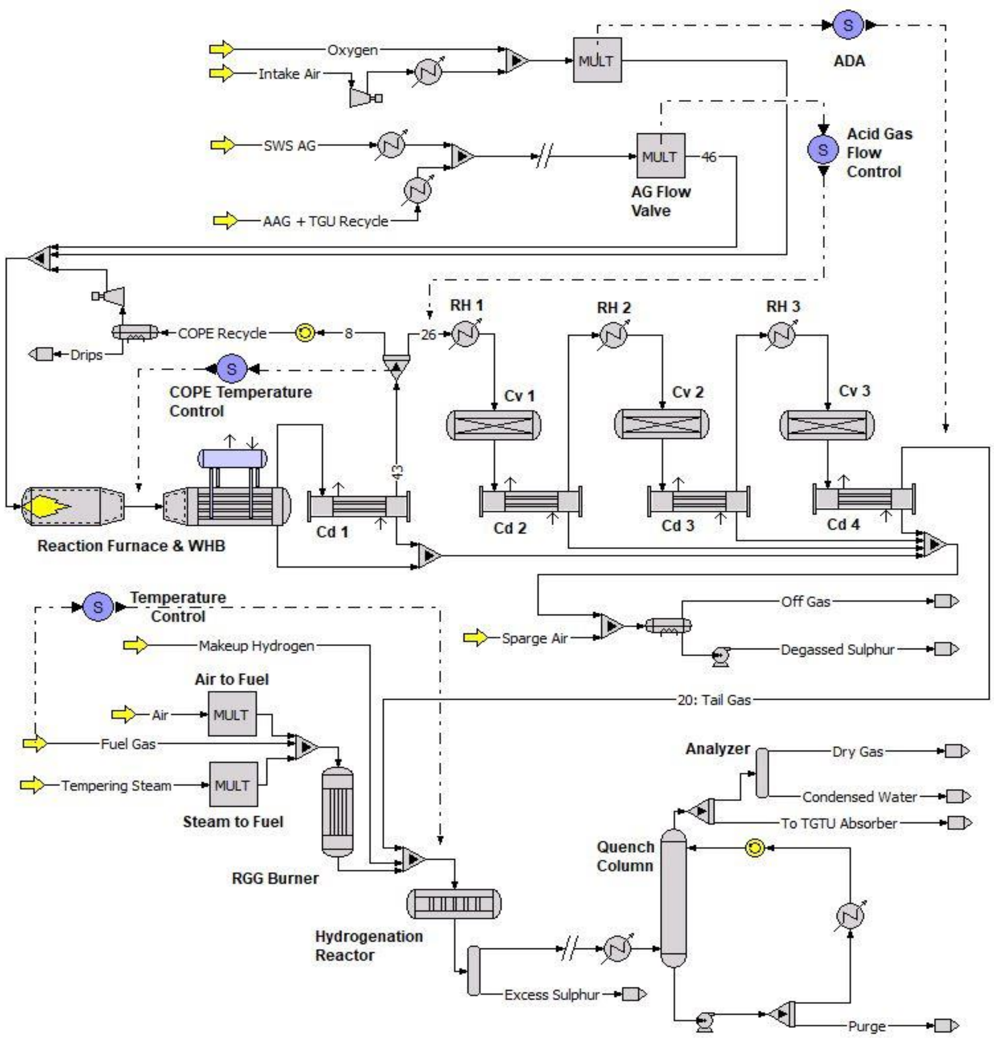

Figure 1. Refinery SRU with Partial TGU Flowsheet