The CONTACTOR™
Published Monthly by Optimized Gas Treating, Inc.
Volume 11, Issue 9, September, 2017

Simulating the Waste Heat Boiler in an SRU

(or… Why It's Important to Get the Temperatures Right)

A year or so ago we introduced a simulation tool for design, analysis, and troubleshooting of sulphur recovery units (SRUs) as part of the ProTreat® simulator. Our SRU simulator is based on fundamental chemical reaction kinetics, not on regressions to dodgy plant performance test data. Our approach to all simulation is that *the simulator must be truly predictive*. This means it has to be based on engineering science, not curve fits to limited, gross observations. Curve fits are only really valid in the range of the underlying data. Science is generalizable. Its underlying data are scientific measurement and mechanistic models—plant performance data serve only *to test* the model.

The waste heat boiler (WHB, see Figure 1) is arguably the most fragile part of an SRU and is subject to sudden and very costly failure. The most common failure point is the tube to tubesheet joint where temperatures can become unacceptably

Figure 1 Waste Heat Boiler (courtesy Schmidtsche Schack, Düsseldorf)

high, causing the welds there to fracture and the joints to fail. To provide operability, this region of the WHB is protected by ceramic ferrules (Figure 2) inserted a short distance into the tubes and which usually also cover the complete face of the tubesheet (Figure 3). On the utility side, high and medium pressure steam is generated (heat recovery) by cooling the hot gas on the process side. Sulfur is not usually condensed there except perhaps at turndown conditions. Other interesting reactions taking place in the WHB. Elemental sulfur has three forms: S_2, S_6 and S_8. In the WHB, S_2 is exothermally converted to S_6 and

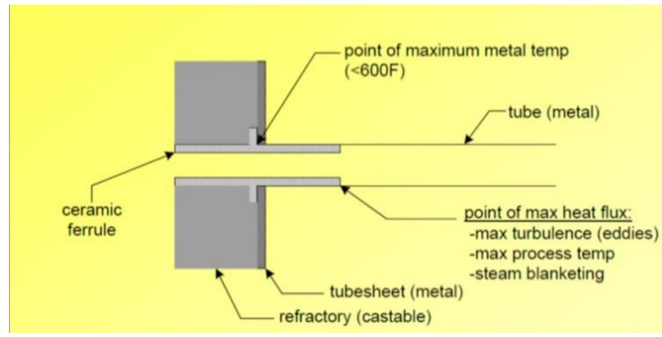
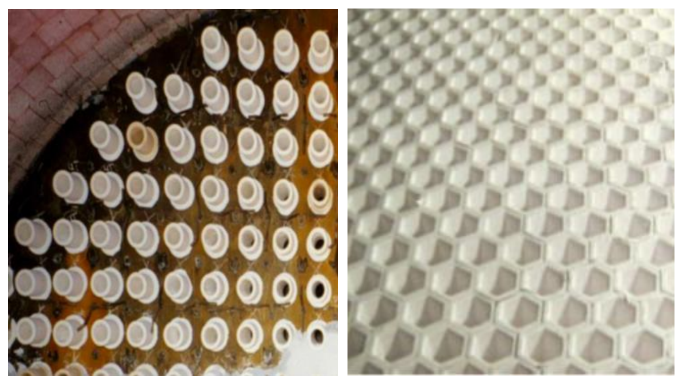


Figure 2 Thermal Protection by Ceramic Ferrules



Round Ferrules before Casting **Hexagonal Ferrules**

Figure 3 Types of Ceramic Ferrules, Seen Installed

S_8. But there are other reactions of equal importance in the present context, namely hydrogen recombination with S_2, and COS formation from carbon monoxide and S_2. These are both exothermic and they take place primarily at the WHB's front end. Radiation also plays a part, too.

Approaches to Recombination Modeling

The recombination reactions can generate significant heat near the front of the WHB, i.e., close to the fragile tube-to-tubesheet joint area, so getting the simulated temperature there as correct as possible is important. The models used by all other SRU simulators either:

- Ignore local recombination and assume the reaction furnace (RF) is at equilibrium, or
- Lump these reactions into RF effluent, or

- Freeze the reactions by assuming they reach equilibrium at a quench temperature.

The fourth approach is to model the reactions fully reaction rate based. It is the one uniquely taken by ProTreat® simulation.

Case Study

The case study is drawn from a Claus unit revamp project proposing a low level of oxygen enrichment (30% O_2, wet basis) to achieve a 25% incremental improvement in unit capacity. The question is what effect various approximations common in other commercial simulators have on performance parameters when oxygen enrichment is considered.

Figure 1 shows a partial flowsheet of the SRU consisting of the reaction furnace and the WHB. When combustion air is enrich by using 30% pure oxygen, more feed can be crammed into the SRU because the gas now contains less nitrogen (an inert component that occupies volume better utilized by Claus feed gas). Thus, the SRU sees a 25% increase in capacity. There are two cases to consider: air operation and operation with 30% O_2 enrichment. Main concerns are percentage sulphur recovery, a key SRU performance parameter and maximum inside tube wall temperature which is critically important in preventing very costly WHB failures.

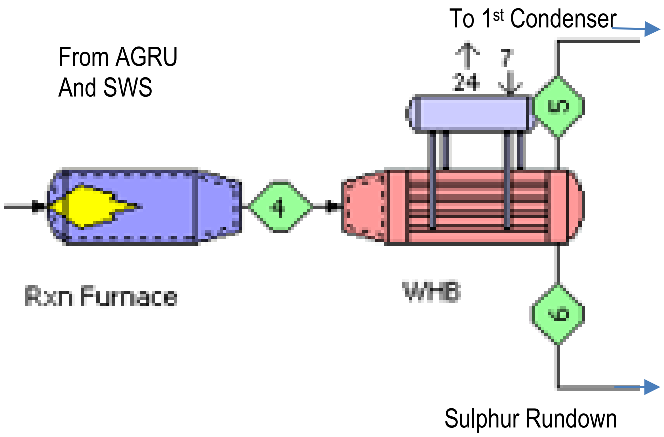


Figure 4 Reaction Furnace and Waste Heat Boiler

Table 1 shows important differences between air-only and 30% oxygen enrichment operations. Numerical values are based on ProTreat® simulation using an assumed steam-side heat transfer coefficient of 350 BTU/h·ft^2·°F. Notable differences include:

- WHB inlet is 319°F hotter when enriched air is used because feed is being processed at a 25% higher rate,
- Effluent from the WHB is 54°F hotter,
- Tube wall temperature (max.) goes from 591 to 634°F,
- Maximum heat flux rises by 26%,
- Ammonia in the effluent from the first condenser almost doubles.

It is interesting to see (Figure 5) how tube wall temperature varies with distance along the WHB. Heat flux behaves similarly.

Table 1 Air Operation Compared with 30% O_2 Enrichment

	Air Only	30% Enriched
% H_2S In/Out	4.4 / 7.0	4.03 / 10.0
RF/WHB Temp. Out (°F)	2360 / 577	2679 / 631
Max Tube Wall Temp (°F)	591	634
Max Heat Flux (BTU/h·ft^2)	37,700	47,700
Sulphur Recovery (%)	97.10	97.34
H_2S in Tail Gas (%, wet)	2.4	2.8
COS in Tail Gas (ppmv, wet)	493	528
1st Condenser ppmv NH_3 Out	36	63
Outlet Pipe Corrosion (mil/yr)	1.6	3

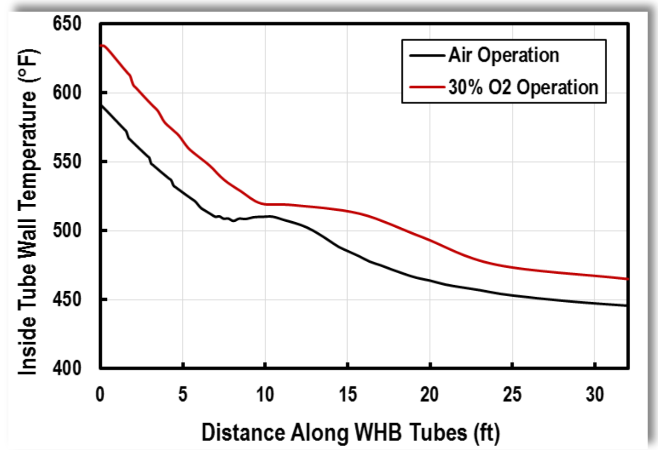


Figure 5 Tube Wall Temperature Profile along WHB

Tube wall temperature (and heat flux) do not decrease steadily along the length of the WHB tubes. Rather, it reaches a point where temperature plateaus between 510 and 520°F. This is the temperature at which S_2 is known to undergo conversion to S_6 and S_8. The polymerization reactions are exothermic and the heat generated keeps the process stream uniformly hot for some distance along the tubes.

What do less rigorous models tell us?

- Lumping recombination reactions into furnace effluent gives a predicted RF outlet temperature 219°F too hot,
- Ignoring radiation heat transfer in the WHB kicks up predicted outlet temperature a further 20°F, from 631°F to 651°F for the worst case, O_2 enrichment
- Just these two oversimplifications alone are likely to cause wrong operating and/or design decisions to be made, costing money.

The ProTreat simulator's SRU model is *completely* reaction kinetics based and is the best and most rigorous available.

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