The CONTACTOR™

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SRU Thermal Oxidizer

Tail gas oxidation is the last processing step in an SRU before unrecoverable material and contaminants are discharged to the plant's stack, thence to atmosphere. This is where sulfur emissions are measured and compliance with emission regulations is assessed. Thermal oxidation is indeed the tail of the dog and it can end up wagging the dog.

The unit's purpose is to oxidize anything that will react with oxygen in a reasonable length of residence time so that what is discharged to the stack and the atmosphere is N_2, CO_2, water vapor, and a very small amount of SO_2. Oxidizer performance is dictated by the three Ts: Time, Temperature, and Turbulence.

The oxidizer consists primarily of a burner and a reactor space or volume. A hydrocarbon fuel is burned with considerable excess air. The excess air is then partially consumed by various oxidation reactions in the reactor volume. The thermal reactor performs several important functions:

- Contaminant destruction;
- Dilution of emitted species with inert species to reduce the concentration of regulated compounds;
- VOC destruction;
- Conversion of potentially dangerous chemical species such as H_2S to a relatively safer ones such as SO_2 before emitting to atmosphere;
- Energy recovery via waste heat boiler.

Model

SulphurPro®'s model for the thermal incinerator is a hybrid of reaction kinetics for individual species and Gibbs Free Energy Minimization. It uses fundamental reaction kinetics for all reduced sulfur species (regulated), hydrogen, carbon monoxide, and ammonia. Gibbs Free Energy Minimization is applied to all remaining species for which reaction kinetics data are unavailable, for complex free radical and exotic species chemistry, and for the diversity of fuel gas sources.

Design is often done using rules of thumb, without detailed models to support the approach, the calculations, or the design itself. These and other factors provide ample motivation for model development, including:

- Opportunities for optimization. For example, optimization through saving fuel gas by combusting only what is required to drive the oxidation reactions to completion. This minimizes the free oxygen emanating from the thermal oxidizer, and it minimizes the size of the equipment necessary to meet emission regulations;
- Confidence in design. Design confidence can be improved by ensuring that contaminant destruction will take place to the extent desired (especially with CO where destruction is highly sensitive to residence time);
- Better accuracy. Greater accuracy can be had by kinetically modeling the oxidation of the most important species. This captures residence-time or space-velocity effects, which are not accounted for in an equilibrium or fractional-conversion type of model.

Case Study

Figure 1 shows a typical Thermal Oxidizer arrangement with Burner, feed streams and Oxidizer. Inlet-1 is the

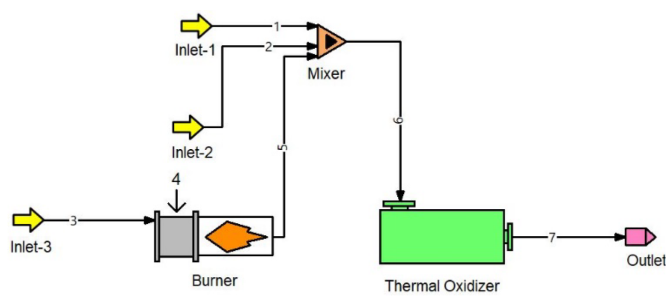

Figure 1 Thermal Oxidizer with Feeds and Burner

TGTU Contactor overhead, Inlet-2 is effluent from the sulfur pit degasser (containing air plus trace H_2S, S_X, etc., Inlet-3 is fuel gas for the burner (in this case, methane), and Stream 4 is l burner combustion air (130% of stoichiometric air required for combustion.)

The reactor data used in the simulation are its volume (5 m^3) and its diameter (3 m) leaving the length calculated as 1.416 m. Reactions calculated by chemical kinetics require the reactor length to be divided into segments, in this case 10.

Species modeled kinetically include all reduced sulfur species (H_2S, COS, CS_2), H_2, CO, NH_3 (with multiple competing pathways) together with all their assumed reaction products as shown in the dialog of Table 1. Other species (except Argon) are handled via Gibbs Free Energy Minimization, and all reactions are solved simultaneously. Gibbs components reach equilibrium in the first Oxidizer segment while kinetically controlled species continue to react throughout the reactor volume.

Table 1 Kinetically Controlled Reactions

Select All / Select None		Kinetic Factor
☑ H2S Oxidation	2H2S + 3O2 <--> 2SO2 + 2H20	1.0
☑ COS Oxidation	2COS + 3O2 <--> 2CO2 + 2SO2	1.0
☑ CS2 Oxidation	CS2 + 3O2 <--> CO2 + 2SO2	1.0
☑ H2 Oxidation	2H2 + O2 <--> 2H2O	1.0
☑ CO Oxidation	2CO + O2 <--> 2CO2	1.0
☑ Sour NH3 Oxidation	2NH3 + SO2 <--> N2 + 2H2O + H2S	1.0
☑ NH3 Oxidation	4NH3 + 3O2 <--> 6H2O + 2N2	1.0
☑ NH3 Decomposition	2NH3 <--> N2 + 3H2	1.0

Table 2 presents details of the vapor inlet stream to the thermal oxidizer, i.e., to Segment 1.

Table 2 Details of Reactor Inlet Stream

Temperature (°F)	1,386.025		
Pressure (psia)	14.700		
Mass Flow Rate (lb/h)	44,549.704		
Composition (mol%)			
Water	26.816	NH_3	1.589e–07
CO_2	4.286	SO_2	3.203e–05
H_2	1.832	C1	1.219e–08
O_2	2.340	COS	3.437e–04
Ar	0.327	CS_2	4.748e–07
S_2	1.534e–03	CO	2.658e–02
S_6	7.677e–06	N_2	64.251
S_8	7.923e–07	NO	0.114
MDEA	1.104e–05	NO_2	8.791e–05
H_2S	5.520e–03		

Table 3 shows the profile of species molar flow rates (lbmol/h) along the flow path of the thermal reactor

Table 3 Species Flow Profiles (lbmol/h) along Reactor

	From 1†	From 2	From 4	From 7	From 10
Water	497.16	497.16	497.16	497.16	497.16
CO2	74.82	74.82	74.82	74.82	74.82
H_2	3.84e-3	4.46e-7	5.3e-15	4.3e-27	8.1e-40
O_2	25.22	25.22	25.22	25.22	25.22
Ar	5.67	5.67	5.67	5.67	5.67
S_2	0	0	0	0	0
S_6	0	0	0	0	0
S_8	0	0	0	0	0
MDEA	0	0	0	0	0
H_2S	4.63e-5	2.16e-8	4.1e-15	2.2e-25	2.6e-38
NH_3	1.17e-9	4.75e-13	6.9e-20	2.4e-30	2.8e-45
SO_2	0.156	0.156	0.156	0.156	0.156
C1	0	0	0	0	0
COS	1.80e-5	5.26e-8	3.9e-13	5.1e-21	1.5e-29
CS_2	1.21e-7	1.72e-9	3.0e-13	4.5e-19	1.6e-25
CO	3.35e-4	2.43e-7	1.0e-13	1.8e-23	7.4e-34
N_2	1115.73	1115.73	1115.73	1115.73	1115.73
NO	6.36e-2	6.36e-2	6.36e-2	6.36e-2	6.36e-2
NO_2	3.38e-4	3.38e-4	3.38e-4	3.38e-4	3.38e-4

This is a hybrid kinetic model that weds reaction kinetics for the species important in determining sulfur emissions with Gibbs Free Energy Minimization for non-critical species (and for which kinetic data are unavailable). No simulator other than SulphurPro® is capable of modeling a thermal oxidizer to this level of completeness and accuracy. It is certainly far more accurate than an equilibrium-only model or with assumed conversions. Note that kinetically determined species rapidly decline to immeasurably small values as they progress through the oxidizer. SO_2 is the only emergent sulfur species.

In the design phase, one can experiment with thermal oxidizer size, burner residual oxygen and temperature to ensure sufficient conversion of critically-restricted, permitted pollutants such as H_2S, SO_2, CO, etc. In operations, because SulphurPro's Thermal Oxidizer model is fully-predictive, it can be used to evaluate the effect of process changes (tail gas flow and composition, sweep and degassing feeds to the Oxidizer) with a high degree of reliability.

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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. Visit www.protreat.com/seminars for details.

† From 1 indicates From Segment 1 (at front of Oxidizer). From 10 means Oxidizer effluent.