DESIGNING A ROBUST REACTION FURNACE

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ABSTRACT

Sulfur plant reliability is greatly influenced by the reliability of two interconnected pieces of equipment, the thermal reactor (TR) and the waste heat boiler (WHB). Over the past fifteen years, PMI's engineers have developed performance metrics that must be satisfied to ensure robust WHB operations [1], defined as successful operation between planned turnarounds, without failures. Alongside these metrics is an analysis framework that allows quantification through the use of complex numerical models. Rules-of-thumb (lightly defined metrics) for robust TR operation, such as flame shape and stability, O_2 enrichment level and reactor retention time, have been developed within the industry. To this point, most complex numerical models developed to study these metrics for TRs have been necessarily limited in scope due to the computing requirements required to study these phenomena. With the knowledge that TR operations can have a significant impact on WHB reliability, the authors set about to develop an analysis framework to allow quantification of TR metrics in engineering rather than research time scales.

This paper introduces this framework to the industry for the first time through the analysis of a TR with known problematic operations. Through a series of analyses, the TR was studied at different rates and in different geometric configurations, to investigate possible methods to achieve successful operation. The framework successfully predicted the cause of the problematic operation. It is also capable of quantifying the effect of changes on the reactor's chemical operation, primarily through ammonia destruction. The paper also demonstrates how this analysis framework can be used to not only study problem TRs, but also to optimize throughput without modifying the reactor's steel.

1.0 INTRODUCTION

Reliable sulfur recovery from process streams has become more critical over time, both from increasing environmental regulations and from the need to process higher sulfur content streams (sour gas). In addition, since most regulatory bodies now allow flaring only during emergency operations, processing of the H_2S-containing stream directly impacts refinery throughput [2].

Thermal reactors (TRs), as the first step in the Claus recovery process, are an essential component of most SRUs. Within the reactor, two (2) process streams are mixed and reacted: a stream containing an acid gas mixture (AG)[1] and an oxidizer stream usually consisting of air, or air enriched with O_2 (a few units use pure O_2 for the oxidizer stream [3]). The purpose of the thermal reactor is to convert a percentage of the H_2S in the incoming stream to elemental sulfur in the reactor. As a primary component in the Claus recovery process, TR performance has a direct impact on the reliability of the sulfur block. Problems affecting the TR's performance include:

1. Flame shape / stability
2. Burner noise / induced vibrations
3. Chemical performance, and
4. Refractory reliability

Current state-of-the-art application of CFD to evaluate the performance of TRs addresses, to some extent, problems associated with flame shape and refractory reliability. At this time, to minimize computational effort, it is common to use steady-state analysis techniques. Using these techniques results in no time-history data from the analysis. This lack of time-history data explicitly precludes addressing burner noise and greatly simplifies chemical performance predictions.

This paper addresses the use of CFD to study a TR with known vibration issues at high operational rates. In operation, these vibrations were reduced or eliminated by turning down to lower operational rates. Since that time, additional steps were taken to address the TR's vibration.

The analyses presented within this paper were conducted as part of the author's internal R&D to answer the question: What additional information can CFD, as an engineering tool, provide for TR design and/or operations guidance? Two metrics were established to answer this question, which had heretofore been impossible to explore with industry-accepted CFD techniques:

- Burner noise (frequency and magnitude), and
- Chemical performance

To allow a full presentation of the results of this investigation, "similar" geometry and process flow conditions, rather than the exact actual TR conditions, were used for the analyses.

Four (4) primary analyses were performed on the TR:

1. Operation at problematic (high) rate
2. Operation at turndown where vibrations were not present
3. Operation at high rate without a choke ring
4. Choke ring position exploration

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[1] Stream usually contains H_2S, H_2O, CO, CO_2 and possibly ammonia (NH_3), HCs and BTX

1.1 Burner Noise Metrics

Acoustic characterization of a system is a complex subject with most topics outside of the scope of this paper. To simplify the presentation of results only two metrics were evaluated:

- That the noise should be broadband, i.e., not concentrated at a single frequency, and
- That the noise magnitude should be low enough to not cause undue equipment vibrations

1.2 Chemistry Metrics

The Claus reaction is complex, exothermic, and reversible. As with most chemical reactions, the conversion rate occurring in the TR is highly dependent on the temperatures local to the reacting molecules. Nasato, et al. [4], Kaloidas and Papayannakos [5] and Dowling, et al. [6], indicate that the chemical reformation and removal of H_2S in the reactor is significant, because it:

- Provides a portion of the elemental sulfur and a majority of the H_2 for other reactions, and
- Consumes the portion of H_2S required for successful operation of the complete plant.

Hawbolt, et. al. [7] demonstrated that at temperatures below 1,000 °C and residence times below 0.5 second (s), the H_2S reformation rate is insignificant. Below 950 °C, the overall conversion of H_2S is low even with long residence times.

There also exists a retention time requirement for the oxidation of NH_3, which competes for O_2 with the HCs and H_2S in the reactor. This retention time requirement was reported by Monnery, et. al. [8], based on work performed in ASRLs quartz reactor, as:

- $>$ 1s at 1,200 °C, or
- $>$ 0.5 s at 1,250 °C

Comparing the retention time requirements for proper H_2S conversion and NH_3 destruction, above, shows that the retention and temperature requirements for the destruction reaction are controlling, when NH_3 is present in the TR’s process feed stream. Therefore, for successful operation from a chemistry standpoint, a TR must minimize the amount of incoming process stream that does not meet the destruction retention time requirements delineated above.

1.3 TR Description

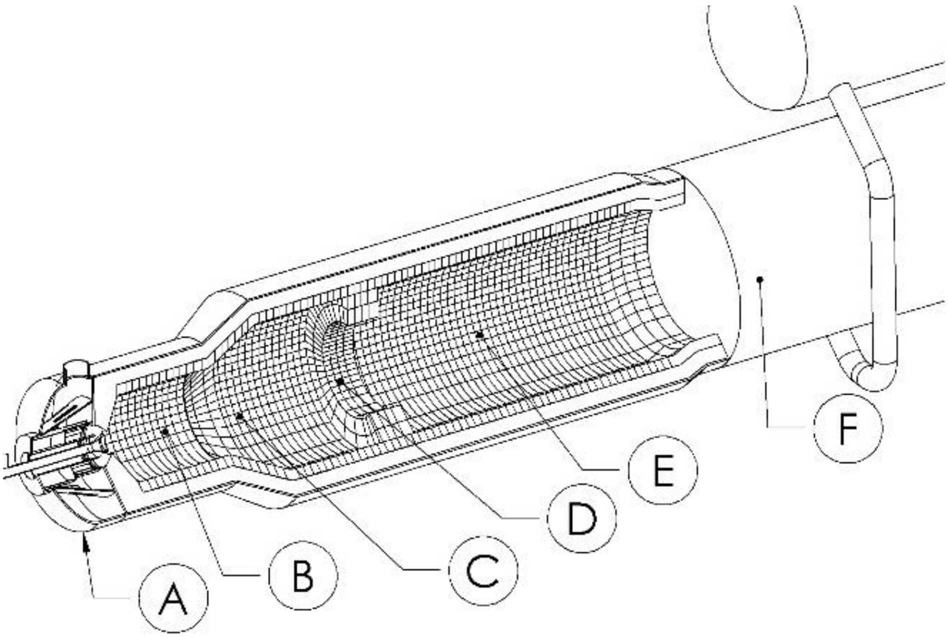

Figure 1 – Cut-away General TR Layout

A typical reactor consists of two primary zones, the combustion zone (C) and the reactor zone (E). The two incoming process streams are combined within the TR's burner bustle (A) before entering the combustion zone. This bustle typically imparts high spin to the incoming process flows before injection into the burner can (B), to promote vigorous mixing for the sub-stoichiometric thermal step of the Claus reaction. The reactor zone is designed to operate as a plug flow reactor to provide enough residence time for the destruction and reformation reactions to complete. How these sections are operated together (flow splits) in a plant is a complex discussion, outside of the scope of this paper.

These two zones are typically separated by a choke ring or perforated wall (separator) (D). The design purpose of this separator is to break up and disperse the jet flow introduced by the burner, thus causing the reactor zone to mimic plug flow reactor behavior. The selection and placement of a ring or perforated wall is currently based on past experience, instead of detailed studies performed on the actual flow and temperature conditions within the TR. As such, many approaches exist within the industry. In addition to the type/placement discussions that occur, there are now arguments within the industry that - with the latest "high-intensity" burner designs - the separator is not needed. To the reader, it should be understood that the separator's type, location and whether it is placed within the reactor are the only reasonable changes that can be made to a reactor once the steel is fabricated. This is because this component is a part of the reactor's brickwork, which is periodically replaced during the reactor's lifetime.

2.0 CFD ANALYSES

To understand the application of CFD to this problem, a brief discussion of CFD as a tool is provided below, followed by the procedures and results for this TR.

2.1 What is CFD?

CFD should be considered a tool that has the ability to simulate complex flow phenomena without the constraints of prototype feasibility. Proper CFD requires highly trained specialists and what most would consider massive computational resources (10^5 cpu-hours is a moderate sized industrial class problem).

CFD can be thought to come in three distinct “flavors”:

- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES), and
- Reynolds Averaged Navier-Stokes (RANS)

which reference how turbulence is solved in the model. A hybrid turbulence treatment technique, detached eddy simulation (DES), combines the features of LES and RANS analyses, as described below.

2.1.1 DNS Analyses

In a DNS analysis the grid spacing (mesh size) and time-steps are chosen to resolve the Kolmogorov scale. This is the scale where turbulent eddies are dissipated as heat within the bulk flow. These scales are very small, on the order of micrometers, and any solution scheme that attempts to resolve these scales must have a compatible mesh and time-step, i.e., very small. A DNS model of this TR would have the following characteristics:

- Number of grid points 10^{45}
- Memory required 10^{36} Tb (not possible)
- CPU hours required (if possible) 10^{43}

Available computing hardware precludes the use of DNS on industrial scale problems.

2.1.2 LES Analyses

LES techniques are typically used in academia to study acoustics. LES models are designed to only consider much larger turbulent length scales than those considered for DNS analyses. Additionally, the time-step is chosen to only be pressure-stable, rather than eddy-stable. These two (2) changes significantly reduce the computing requirements for an LES analysis, such that an LES model of this TR would have the following properties.

- Number of grid points 10^8
- Memory required 10^2 Tb

- CPU hours required, 10^7

As can be seen from the information above, LES analyses are possible, although extremely expensive, for this class of industrial problems.

2.1.3 RANS Analyses

RANS techniques are a method of accounting for the turbulent energy in the flow without explicitly modeling the turbulent eddies. Instead, the eddies' energy is **Averaged** into quantities representing the turbulent energy and dissipation. This averaging technique significantly reduces the computational effort required to solve for flows, but negatively impacts the ability to capture the energies associated with noise in the system. Therefore, pure RANS methods are not suitable for acoustic analyses with CFD.

2.1.4 DES Analyses

From the discussion of CFD techniques above, it is obvious that a hybrid method that combines features of LES and RANS analysis techniques is necessary to model the turbulence in the TR. This hybrid method is known in the industry as DES. In DES certain portions of the domain are treated as LES zones and certain portions as RANS zones. The inclusion of each turbulence treatment method is user controlled, through both the computational grid and the solution methods used in the analysis. This makes DES the most difficult type of CFD analysis to perform, as the analyst must be well versed in the requirements for both turbulence treatment techniques. This is the turbulence treatment method used for the analyses in this paper.

2.2 CFD Procedures

Discrete steps that must be taken in a proper CFD analysis [9]. Specifically:

- Selection of computational volume
- Creation of computational grid
- Physics modeling
- Boundary conditions, and
- Solution

The implementations of these steps are detailed in the appendix.

2.3 CFD Results

The following subsections contain the results for the four (4) analyses conducted on the TR:

- High rate operation with choke ring (high vibrations occurred)
- Turndown operation with choke ring (vibrations were minimal)
- High rate operation with no choke ring, and
- Choke ring position exploration

2.3.1 High Rate with Choke Ring

The analysis at high rate operation with the choke ring indicated two modes of operation, as shown in Figures 2 and 3 below. In the first mode of operation, the flame extends to the front face of the choke ring. It is shown in this mode’s animation that the thermal step reaction continues through the choke ring – shown by “pockets” of reacting gas passing through the ring. In the second mode of operation the high acoustic pressures force the flame into the burner can. In this case it would be expected that significant refractory damage could occur at this location.

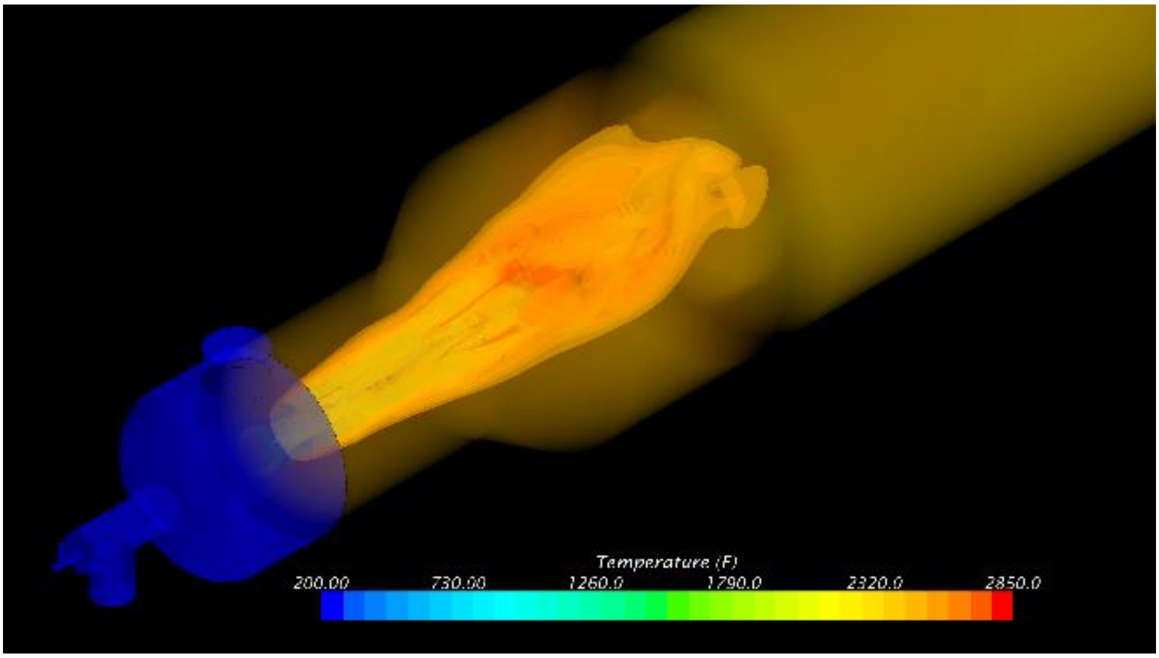

Figure 2 - TR Flame Patterns at High-Rate with Choke Ring, Flame near Choke Ring

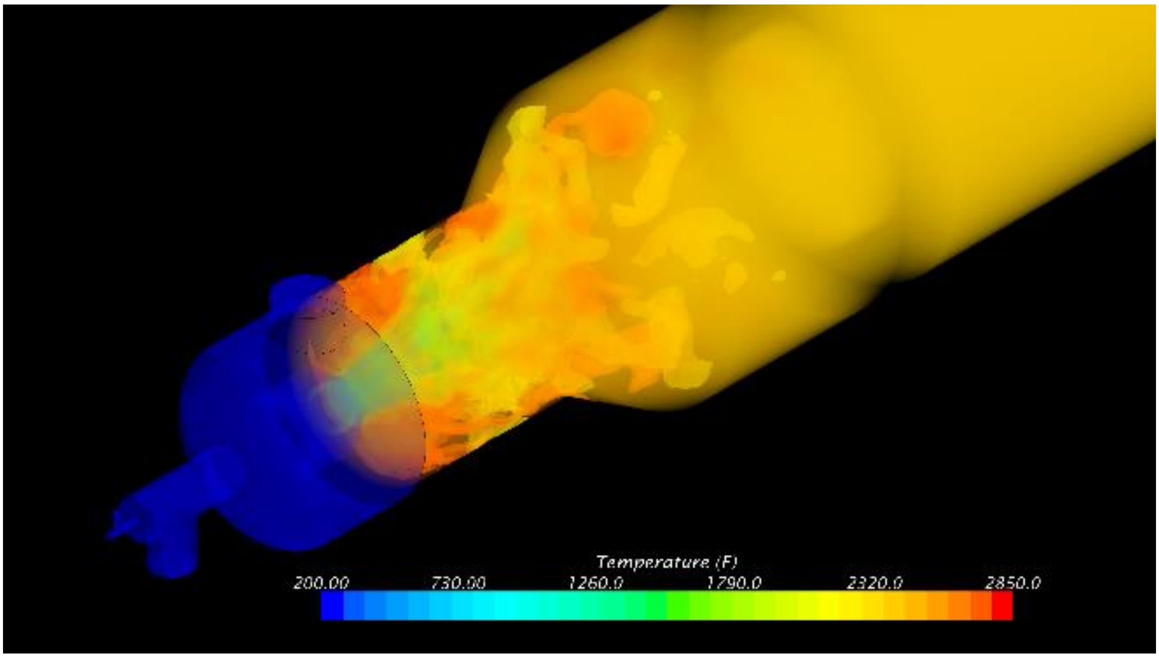

Figure 3 - TR Flame Patterns at High-Rate with Choke Ring, Flame in Can

The Power Spectral Density (PSD) of the acoustic pressure developed in the model is shown in Figure 8. Note the very prominent peak in the PSD at a discrete frequency. While the actual vibration measurements are not presented in this paper, there was less than 5% difference between the CFD predicted frequencies and measured vibrations. It should be noted that the pressure energy associated with this spike is an order of magnitude greater than the other cases examined.

Figure 4, below, shows the results from a single step in the tracer test performed on the TR. When the results of the tracer analysis were queried to determine the percentage of incoming AG flow that was not over 1,250 °C for at least 0.5 seconds it was found that 5.1% of the flow did not meet this requirement. The results of the tracer analyses are shown in Figure 9.

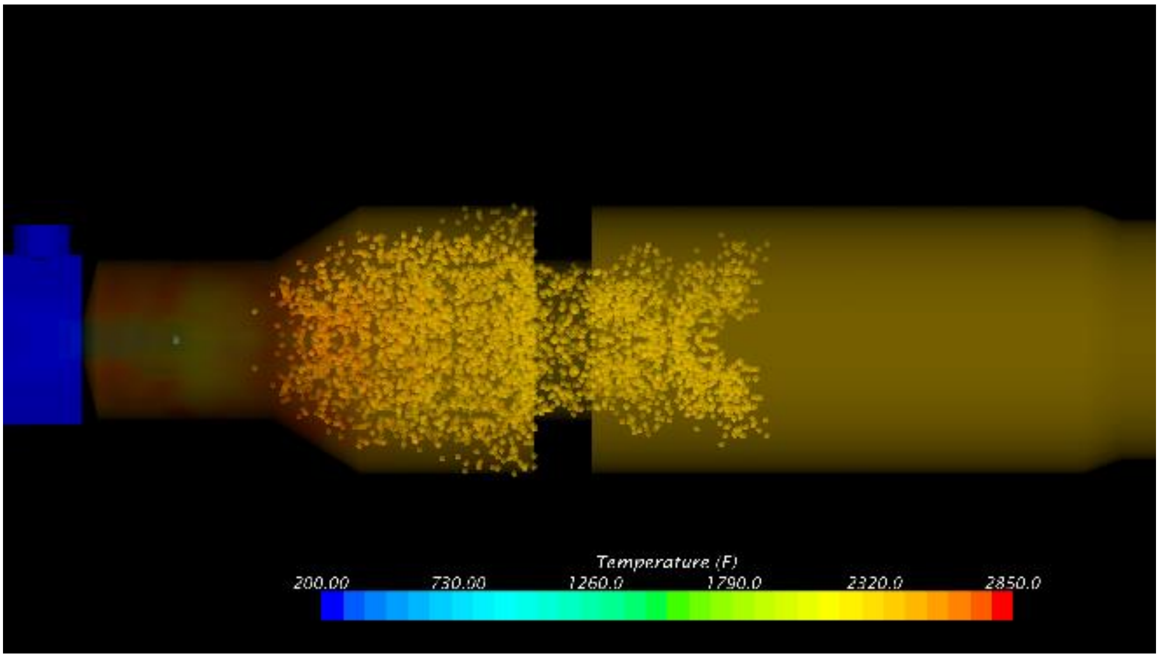

Figure 4 – Sample Tracer Results for High Rate with Choke Ring

2.3.2 Turndown Operation with Choke Ring

During the turndown case, the flame still extends to near the choke ring, as shown in Figure 5, below. From this case's animation it can be seen that the reaction does not proceed through the choke ring, as occurred in the high rate case.

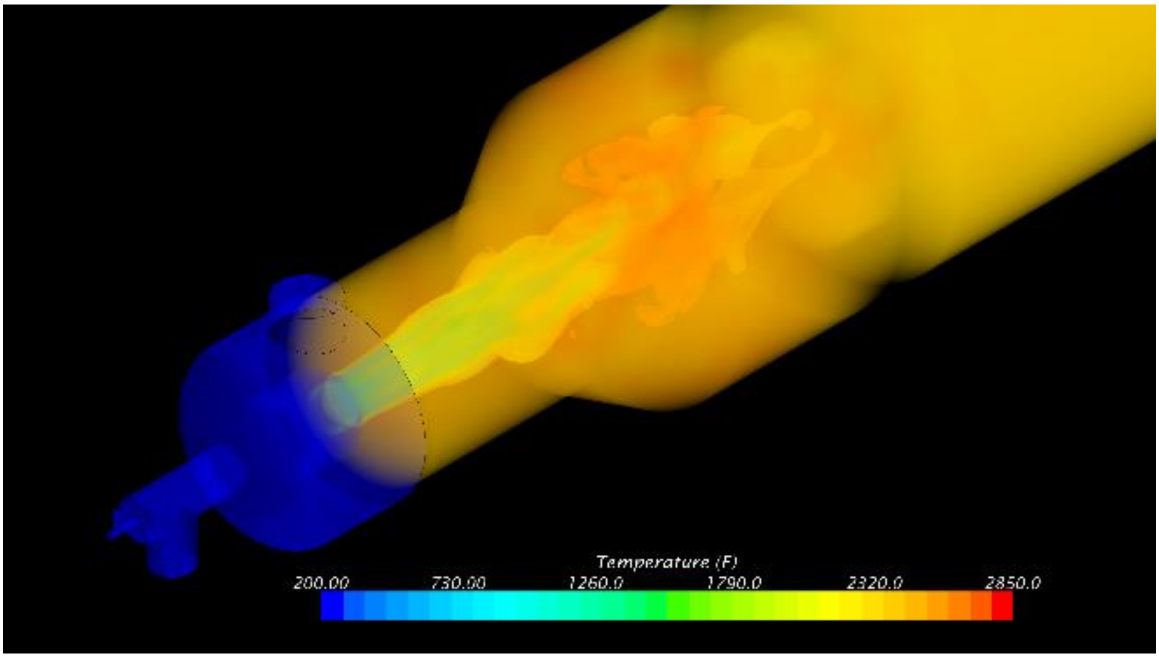

Figure 5: Typical TR Flame Pattern at Turndown with Choke Ring

The results of the acoustic pressure query performed on this model are presented in Figure 8. In Figure 8, a minor rise in the PSD level over a range of frequencies is shown. In summary for this case:

- No coherent signals were evident from the acoustic analysis, indicating that all TR noise could be considered broadband, and
- The predicted acoustic noise within the TR was an order of magnitude less than the noise predicted for the High Rate Operation with Choke Ring case.

Figure 6, below, shows sample results from a single step in the tracer test performed on the TR. When the results of this tracer analysis were queried for retention times less than 0.5 s at 1,250 °C it was found that 3.9% of the AG flow does not meet this criteria.

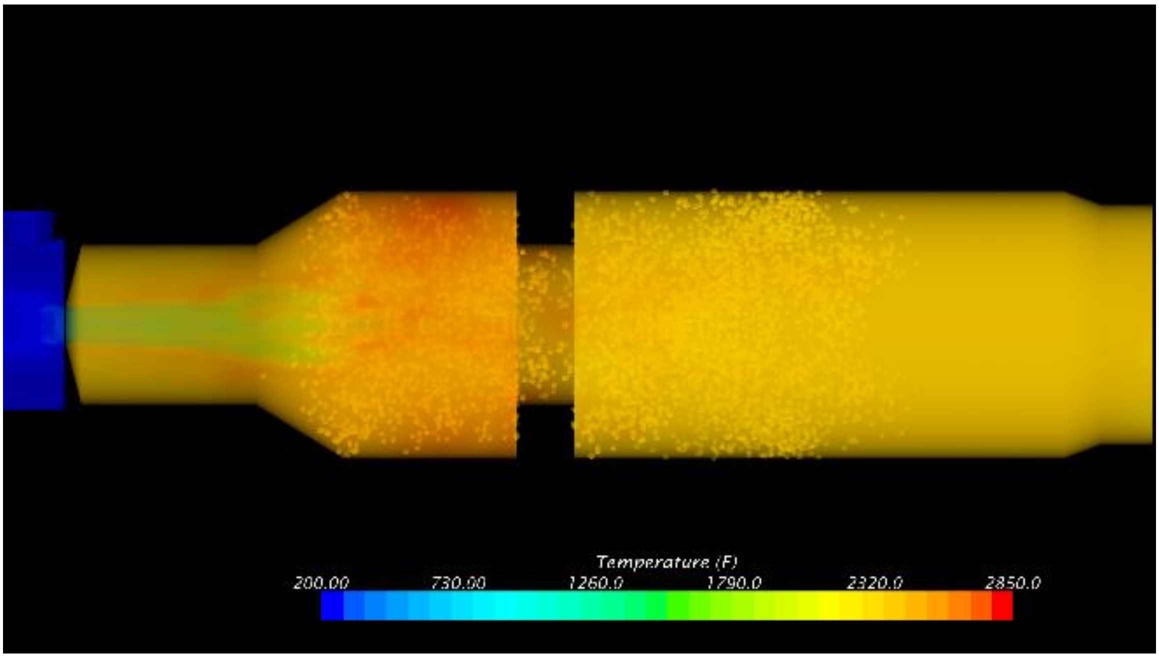

Figure 6 – Sample Tracer Results for Turndown Operation with Choke Ring

2.3.3 High Rate without Choke Ring

Figure 7, below shows the flame shape for the High Rate Operation without Choke Ring case. From the figure and the supplied animation, it can be seen that the flame is centrally located within the TR, as expected.

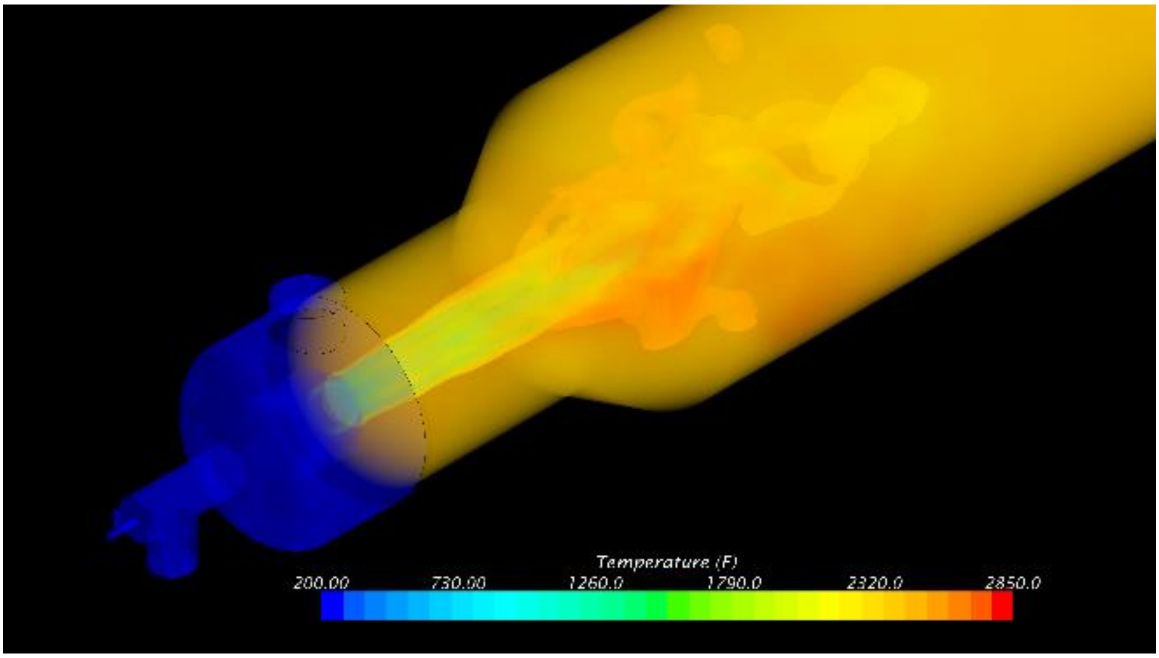

Figure 7: Typical TR Flame Pattern at High-Rate without Choke Ring

2.3.3.1 Summary Acoustic Results for Three Cases

Figure 8 shows the power spectral density (PSD) versus frequency plot of the acoustic pressure computed for the three cases. As can be seen from Figure 8, the High Rate with Choke case displays coherent noise that is an order of magnitude higher in intensity than the other two cases analyzed. Additionally, for the Turndown with Choke Ring case, it is shown that while noise does exist it is spread over a relatively broad range of frequencies. As such, it would be expected that the vibrations evident during the TR's operation would be significantly reduced – as was demonstrated in the field. The High Rate Operation without Choke Ring case shows that the noise levels are reduced by another order of magnitude from the Turndown with Choke Ring case, with no coherent signals evident.

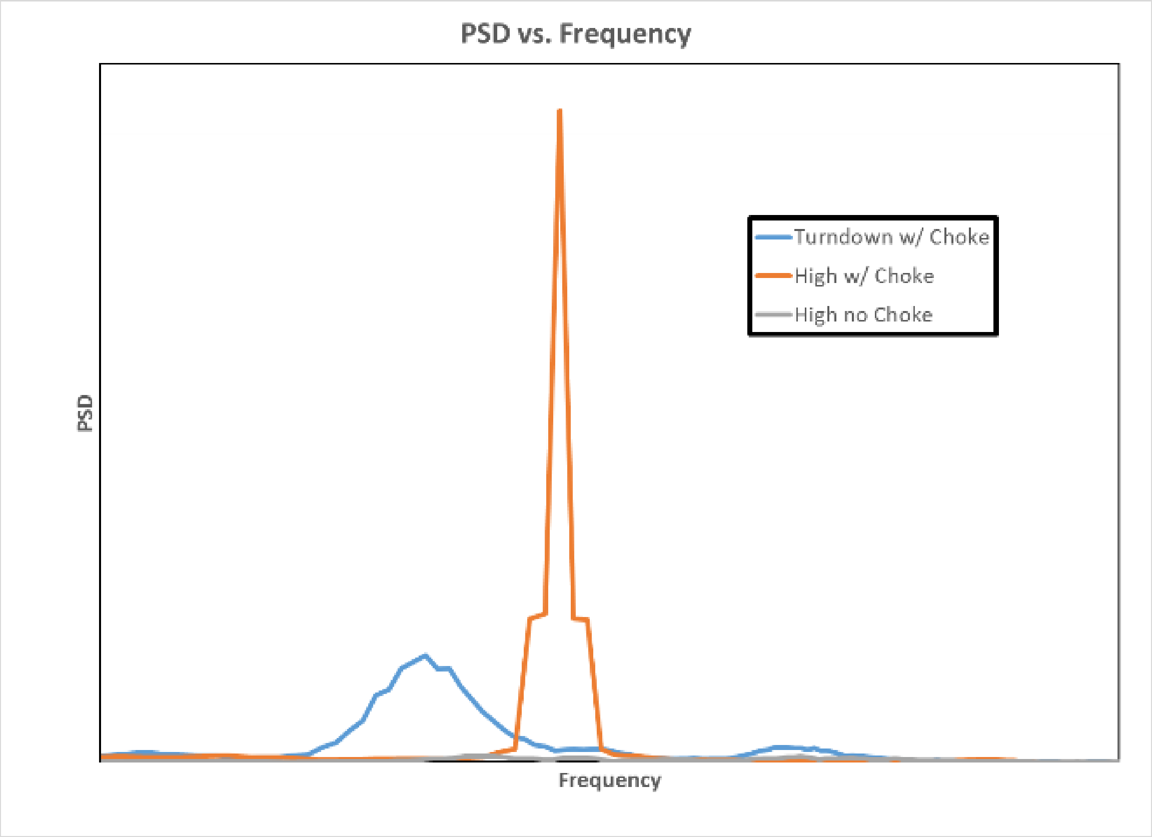

Figure 8 - PSD vs. Frequency – 3 Cases

The strong peak in the acoustic pressure signal at high flow with the choke ring is clear evidence of an acoustic instability in the flame that is caused by an acoustic resonance in the TR. This notion is further supported by the lack of a peak at high flows with the choke ring removed. However, noise (and the associated vibration) is not the only factor dictating the design of the reactor.

2.3.3.2 Summary Residence Time for Three Cases

CDFs are a method of visualizing distribution functions, where the abscissa shows the time recorded and the ordinate shows the cumulative percentage of the measurement. Figure 9 shows the cumulative distribution functions (CDFs) of the retention times for the three cases detailed above evaluated for time above 1,250 °C. To read the CDF - from Figure 9, for the High Rate without Choke Ring case (blue) if one follows 50% (0.5) right from the ordinate to the curve intersection it can be seen that 50% (from the ordinate measure) of the flow has a retention time above 1,250 °C less than 0.6 s. As can be seen from the graph, while there was an increase in slip at high rates for the previous cases, the ~5% maximum slip previously recorded has become 40% slip without a choke ring. In this case it would be expected that ammonia destruction would be significantly affected and that some form of separator should be included in the TR.

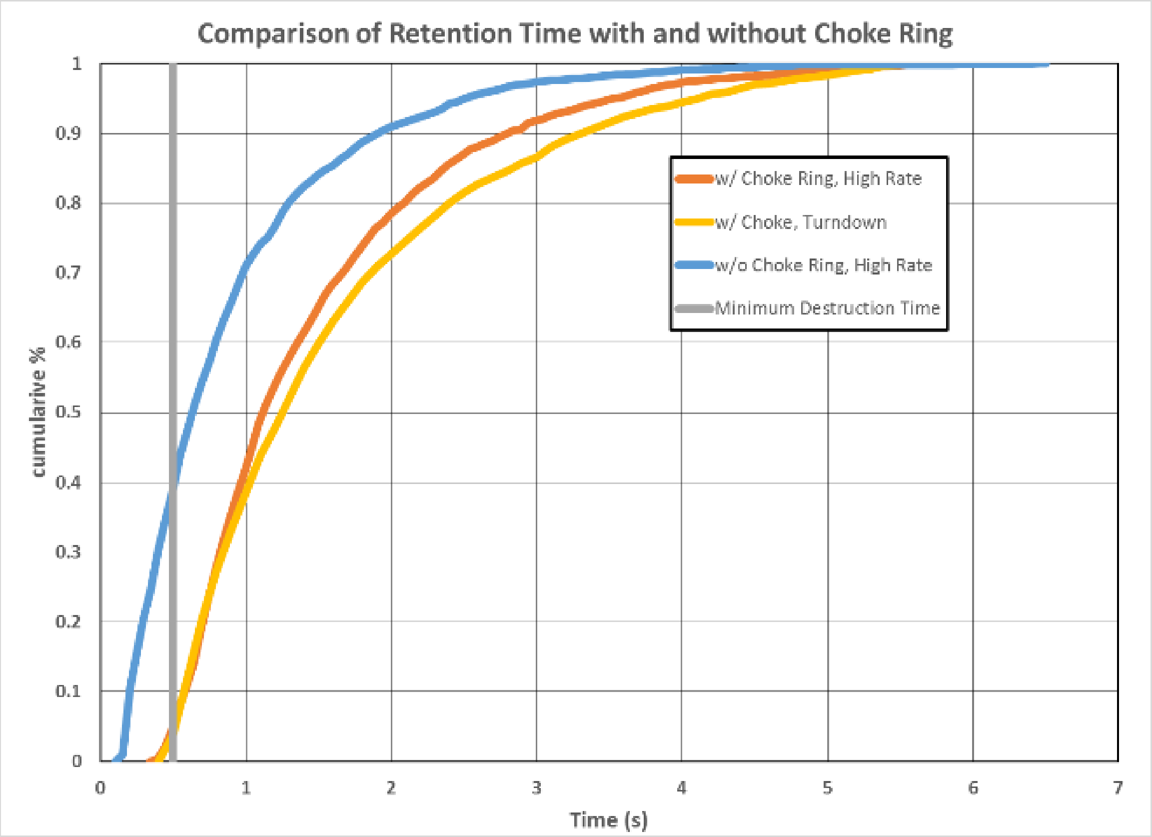

Figure 9 - CDF of Retention Times above 1,250 °C

2.3.4 Choke Ring Position Exploration

The choke ring in the current location causes vibration issues at high rates. However, without the choke ring, the residence time is sub-optimal. Therefore, an analysis was conducted to determine if the choke ring can be moved to a position where for the high rate case that the vibrations are low while at the same time meeting the NH_3 destruction requirements. To address this question, the model was updated by moving the choke ring downstream from its current location (which was determined from the High Rate without Choke Ring analysis) and the previous analysis cycle was performed. This analysis indicated low sound levels; therefore, through a series of analyses (7), the choke ring was moved toward the air nose until flame instability occurred. Figures 10 -12, below show sample results from these analyses. As can be seen from the figures, the choke ring position where the flame shape would be negatively impacted is readily predicted from the CFD analyses.

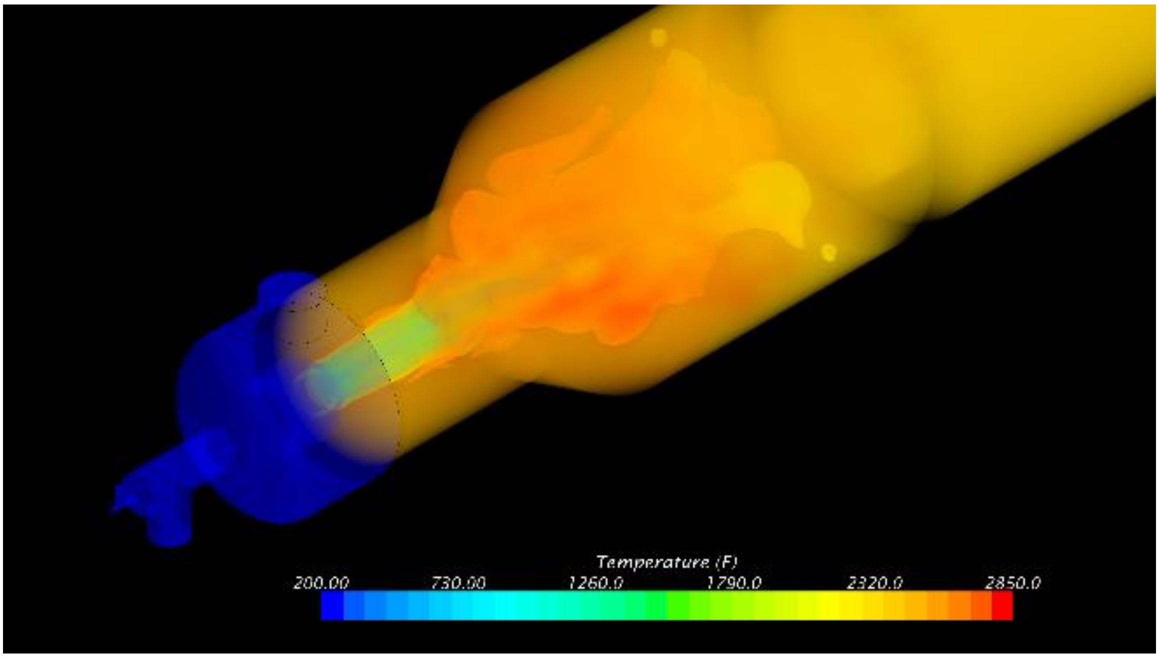

Figure 10 - Choke Ring Position Exploration, Stable Choke Ring Position

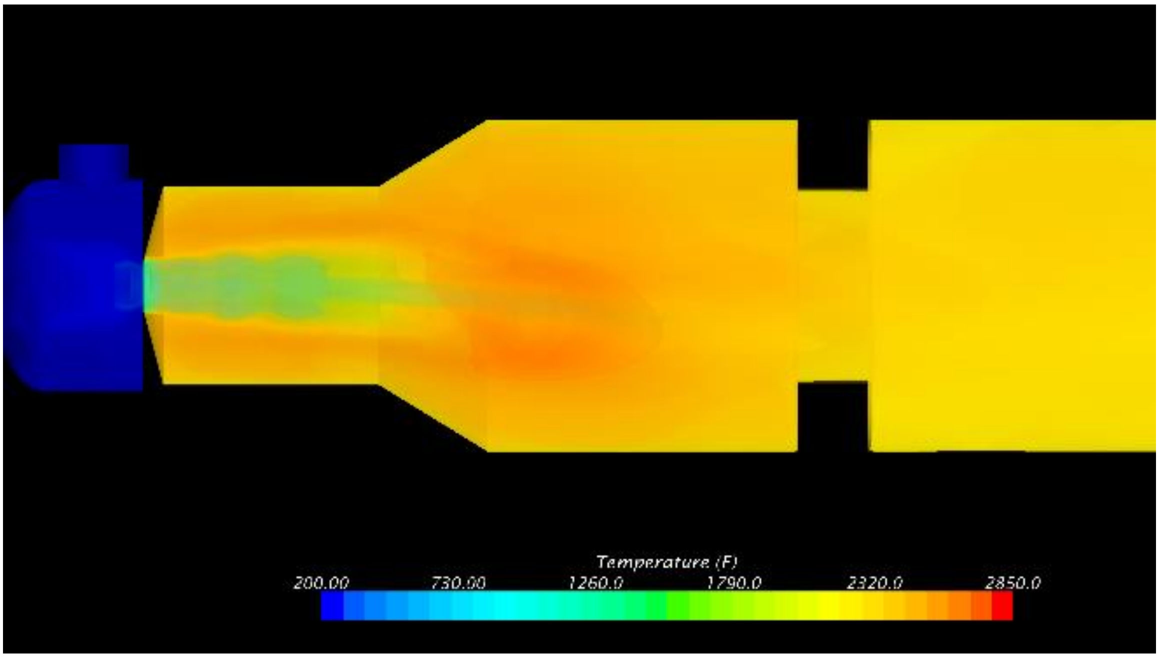

Figure 11 – Choke Ring Position Exploration, Onset of Flame Instability

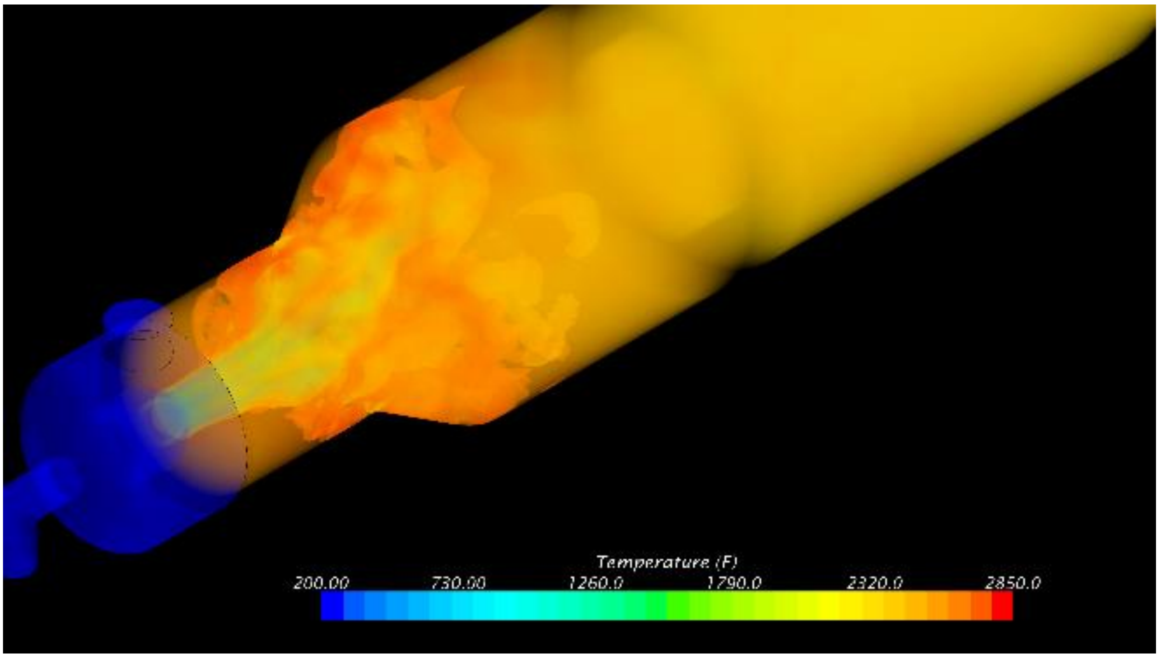

Figure 12 - Choke Ring Position Exploration, Flame Moving into Burner Can

From this sweep, the downstream distance required for a stable flame shape at the high rate conditions was determined. Once this position was established, the tracer test on this configuration was performed. Figure 13 shows the results of this test with the previous results for the high rate tracers (original and moved) with and without a choke ring. As can be seen from the figure, at this choke ring position approximately 35% of the process stream is not exposed to suitable destruction conditions. In fact, with the choke ring in this position, the destruction performance is only slightly better than without a choke ring. From these results, it is likely that the high rates cannot be achieved with minimal vibration, while achieving acceptable NH_3 destruction without further changes to the choke ring geometry used as the separator in this TR.

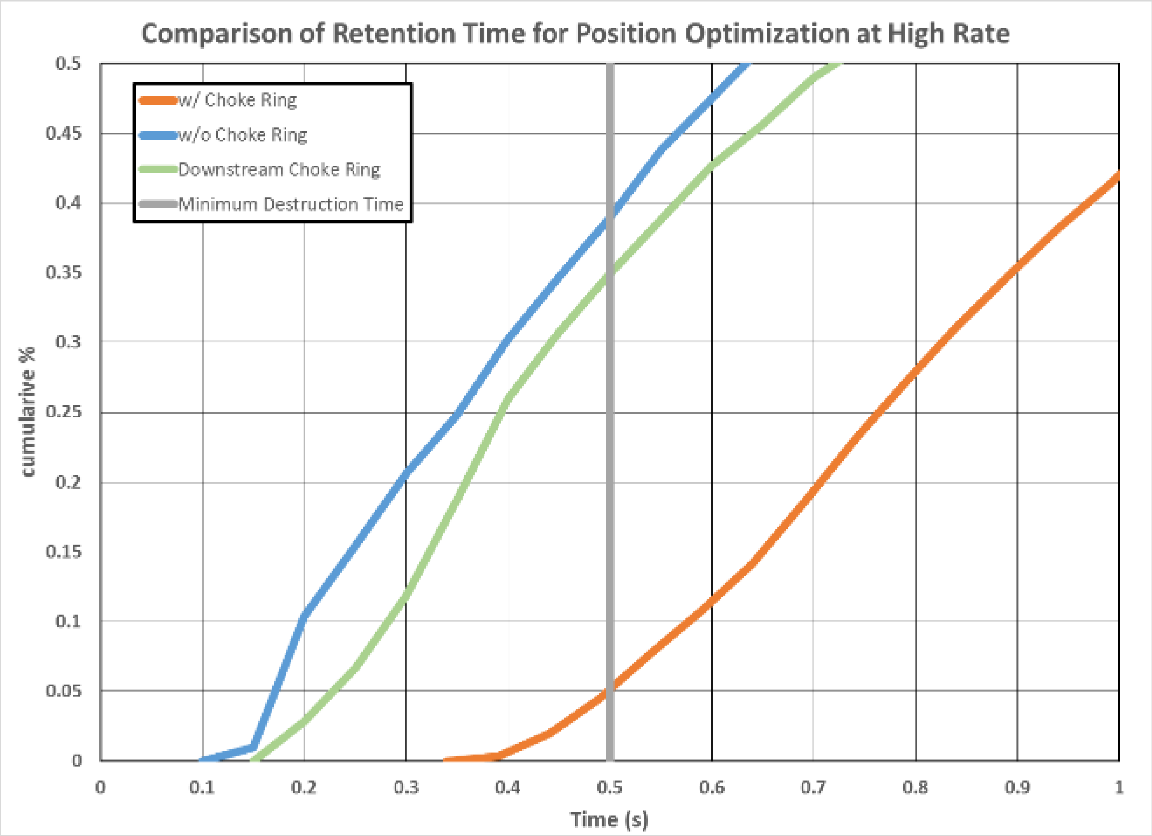

Figure 13 - Tracer Results from Optimization Sweep

It should be apparent to the reader that using the same methodology in further analyses could determine the choke ring position and flow rate that allows acceptable NH_3 destruction while minimizing noise – producing a fully optimized configuration. Additionally, different separator geometries could be considered to determine their impact on the TR's operation.

3.0 DISCUSSION OF RESULTS AND CONCLUSIONS

The methodologies used and validated in this paper demonstrate a new application of CFD technology for the evaluation of TR designs. Where, to this point, the state-of-the-art in TR CFD analysis included steady-state analyses that provide some detail on flame shape and associated refractory temperatures, introduction of this new methodology to the industry also allows for the consideration of acoustic pressures and resonances for given operational conditions. Additionally, the use of hot flow tracer tests for destruction efficiency prediction in TRs has not been demonstrated in public industry literature [10]. As such, it can be stated that by using transient DES CFD methodologies, significantly more information can be extracted about the performance of TRs than has previously been available to the industry.

As shown in this paper, the position of a choke ring or other separator can significantly impact the acoustic and destruction characteristics of a TR. Application of this paper's methodologies allows the consideration of the separator type and position on the TR's performance. Taken to its limit, this methodology allows the user to determine the best separator type and location to maximize the TR's throughput. It should be recognized that changes to the separator are the only viable method to optimize the performance of TRs in the field. The same methodologies can also be used to optimize new "blank-paper" TR designs.

4.0 REFERENCES

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5.0 CFD PROCEDURES - APPENDIX

The following sections document the specific procedures used to analyze the CFD models.

5.1 Selection of Computational Volume

In all sulfur plants, the TR is a component of an overall system that includes the upstream and downstream plant components. On the upstream side are the amine plant and air blowers: on the downstream side are the WHB (shown in Figure 1 as (F)) followed by the condensers, reheaters and catalytic reactors. To minimize model size, these components should not be included in the modeled flow domain, but their influence on the TR's flow dynamics must be included in the model. To reduce the size of the computational domain, the following steps were taken:

- The inlet energies, as described in the Boundary Conditions subsection below, were chosen to include the influence of the upstream components, and
- The WHB and downstream components were included in the model through the use of a porous media [11], defined at the TR outlet location.

Using these steps, the computational domain, shown in Figure 14, below, was reduced to the burner bustle (yellow), the TR interior volume (violet), and the downstream porous media approximation (pink).

Figure 14 – Computational Domains Considered for TR Analysis

5.2 Creation of Computational Grid

The grid constructed for the TR CFD analysis must be able to accurately resolve the eddy energies associated with the acoustic energies (sounds) in the frequencies of interest. This imposes a maximum cell size limit, but for efficiency the model cell count must be minimized. With these factors in mind, the computational grid should be constructed using structured gridding techniques. Additionally, the grid must be refined during the solution process based on the predicted energy distributions during the initial stages of the solution. Figure 15, below, shows the final computational grid constructed for the TR analysis.

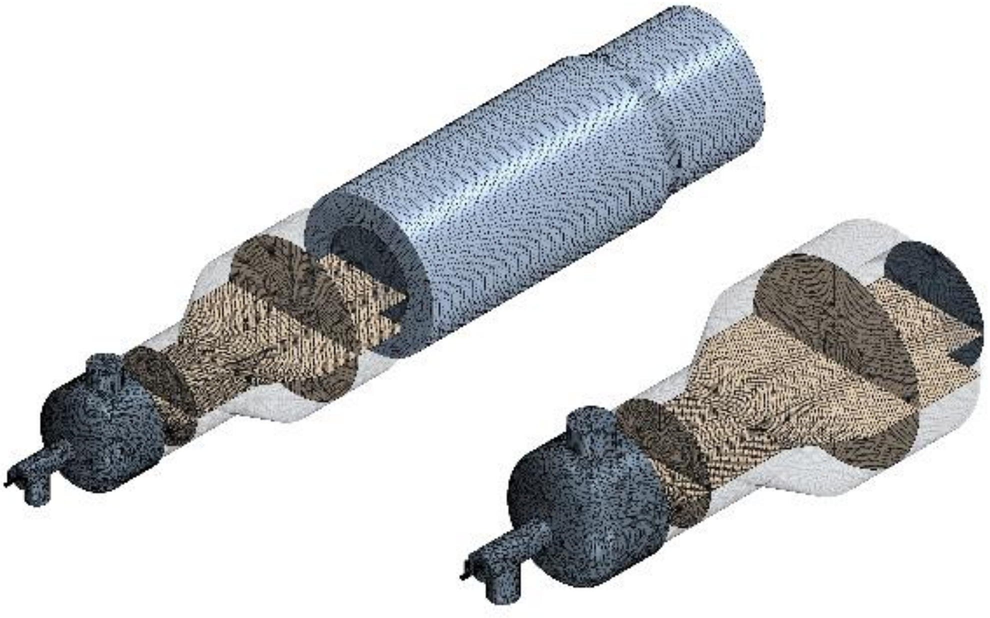

Figure 15 - Computational Grid Developed for TR CFD Analyses

5.3 Physics Models

Three non-standard models must be considered when selecting the physics models for the TR analysis:

- Chemistry
- Turbulence treatment (discussed in the paper's body), and
- Porous media conditions

The following subsections contain a brief discussion of the physics used to address each model's selection.

5.3.1 Physics Models – Chemistry

Solution of the TR problem requires a multi-species physics model with reactions enabled. For all TR analyses, the species that must be considered include:

- O_2
- H_2O
- N_2
- CO_2
- H_2S, and
- SO_2

For TRs in crude service, NH_3 must also be considered.

A kinetics-only reaction model [10], was used to model the thermal step of the Claus reaction. For computational efficiency, no secondary reactions were included. Instead, predicted residence times of selected species at a defined temperature were used to estimate the TR’s chemical destruction performance.

5.3.2 Physics Models – Porous Media Conditions

The inertial and viscous coefficients [11] applied to approximate the WHB were derived from submodel analyses.

5.4 Boundary Conditions

Three flow boundary conditions were applied to the CFD model – the AG and air inlets and the outlet of the porous media.

The model inlets were treated as mass flow boundaries with temperatures, flow rates and gas compositions taken from the TR’s HMB. Since a goal of the analyses was to predict the acoustic response within the TR, all inputs must contain a noise component. Physically, this component should represent the upstream components, both in frequency content and sound power level (loudness). Figure 16, below, shows a typical input sound power distribution curve for an unconstrained flow with 70 dB of background noise – not used in this analysis.

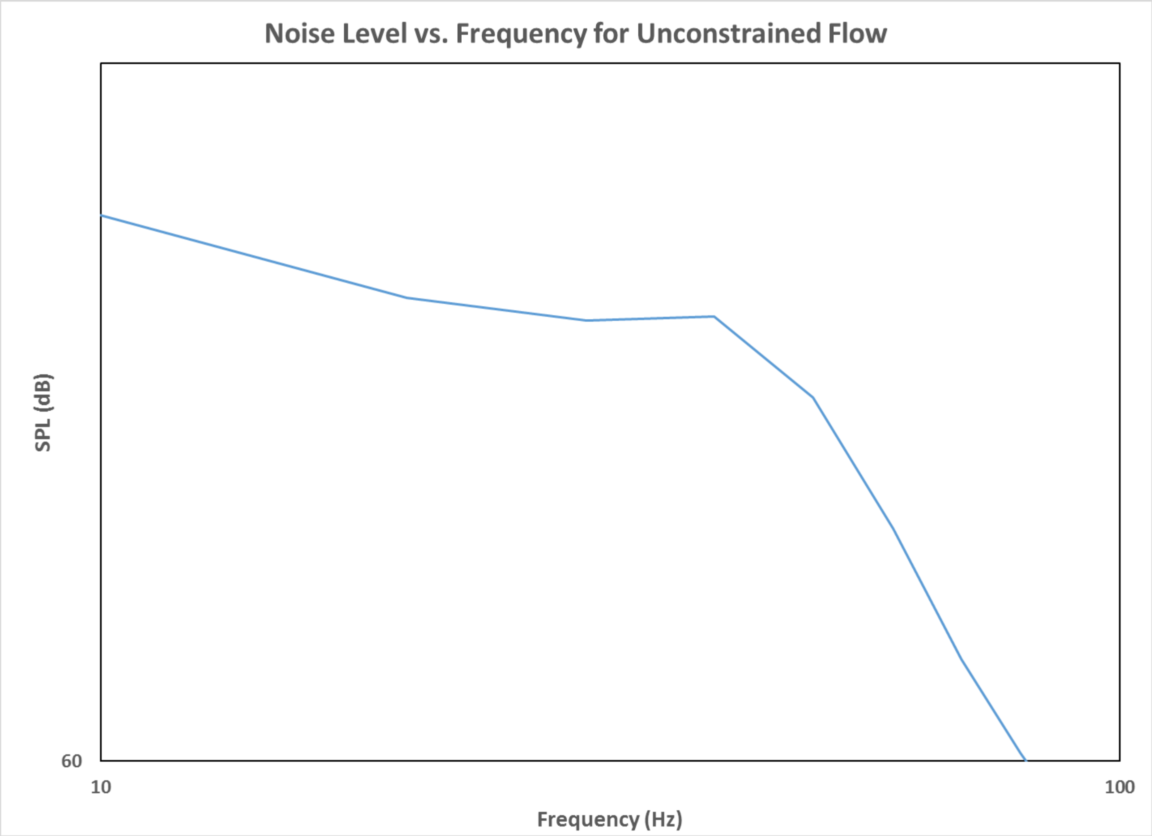

Figure 16 – 70 dB SPL Curve for Unconstrained Flow

The outlet was defined as a constant pressure outlet, with the pressure taken from the WHB's equipment datasheet.

5.5 Solution

The CFD analyses were performed as transient analyses in Star-CCM+ v. 10.04. The time-step for the solution was chosen to allow monotonic convergence for each cycle. The analyses were allowed to proceed for a long enough period of time that the power content of low-frequency (< 10Hz) noise could be verified in the model.