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A validated analysis framework for thermal reactors: An industry first

Using Simcenter STAR-CCM+ CFD simulation for design and operating space exploration

Executive summary

The advanced physics models in Simcenter™ STAR-CCM+™ software have significantly increased the amount of insight that computational fluid dynamics (CFD) simulations can provide in the analysis of thermal reactors. As a result, users can understand otherwise opaque processes and enhance the performance of thermal reactors far beyond the limitations of steady-state analyses. This highlights the value of using multiphysics CFD as part of a comprehensive approach that combines observation, measurement, experiment and simulation to solve previously intractable real-life multidisciplinary problems.

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Executive summary

Large, unexpected vibrations. Cracks forming around instrument ports. It's never a good sign when a piece of equipment exhibits these unsafe behaviors, especially when it's in the thermal reactor of a sulfur plant, where high-temperature gaseous streams chemically react as part of the process that produces elemental sulfur. Most of the world's sulfur supply is produced this way, through the processing of natural gas and the by-products of crude oil refining operations. So it was particularly vexing when a thermal reactor began exhibiting precisely these worrisome symptoms; and it was precisely the situation that engineers at Porter McGuffie, Inc., a Lawrence, Kansas-based computational analysis and engineering measurement services company, were tasked with remedying.

The solutions Porter McGuffie came up with were based on a novel application of CFD using Simcenter STAR-CCM+ software from Siemens Digital Industries Software; solutions that not only addressed its client's problems, but also resulted in the development of a first-of-its-kind framework for analyzing the thermo-acoustic and chemical processing performance of any combustion-fired unit. The framework combines observation, measurement and multiphysics CFD simulations to provide detailed insights into the complex interactions occurring within the reactors; interactions that simply would not be revealed without multiphysics simulation as part of the comprehensive approach. The result is a powerful toolset for troubleshooting problems in existing reactors, as well as designing new, higher performing ones.

Anatomy of a thermal reactor

The process of producing (or recovering) elemental sulfur from gases containing hydrogen sulfide is based on the modified Claus process, a multi-step series of chemical reactions that begin in the thermal reactor, where two process streams are mixed and reacted: one containing an acid gas mixture, and another with an oxidizer stream consisting of air, or oxygen-enriched air. As the first step in the process, the thermal reactor's performance directly impacts the sulfur plant's throughput, and affects the performance of components further down the line (such as waste heat boilers).

A typical reactor consists of two primary zones: the combustion zone and the reactor zone (marked C and E, respectively, in figure 1), which are usually separated by a choke ring or perforated wall/separator (D). The two incoming process streams are combined in the reactor's burner bustle (A), which imparts a high spin to the flows before injection into the burner can (B) to promote vigorous mixing for the sub-stoichiometric first

(thermal) step of the Claus reaction. The reactor zone is designed to provide sufficient residence time for the completion of the destruction and reformation reactions, the chemical reactions that promote the destruction of ammonia (which must be entirely completed to prevent salt formation on the downstream catalyst beds), and the conversion of hydrogen sulfide into multiple species. The extent to which a reactor can provide the conditions suitable for these reactions to be completed is therefore a key metric in assessing a reactor's performance from a chemical efficiency standpoint.

The purpose of any separator (choke ring, checker wall, or vector wall) is to break up and disperse the jet flow from the burner, so the reactor zone more closely mimics the behavior of a plug flow reactor, a configuration which avoids back mixing (mixing in the lengthwise direction, which dilutes the reactants and reduces the rate of reaction, reducing the efficiency of the furnace).

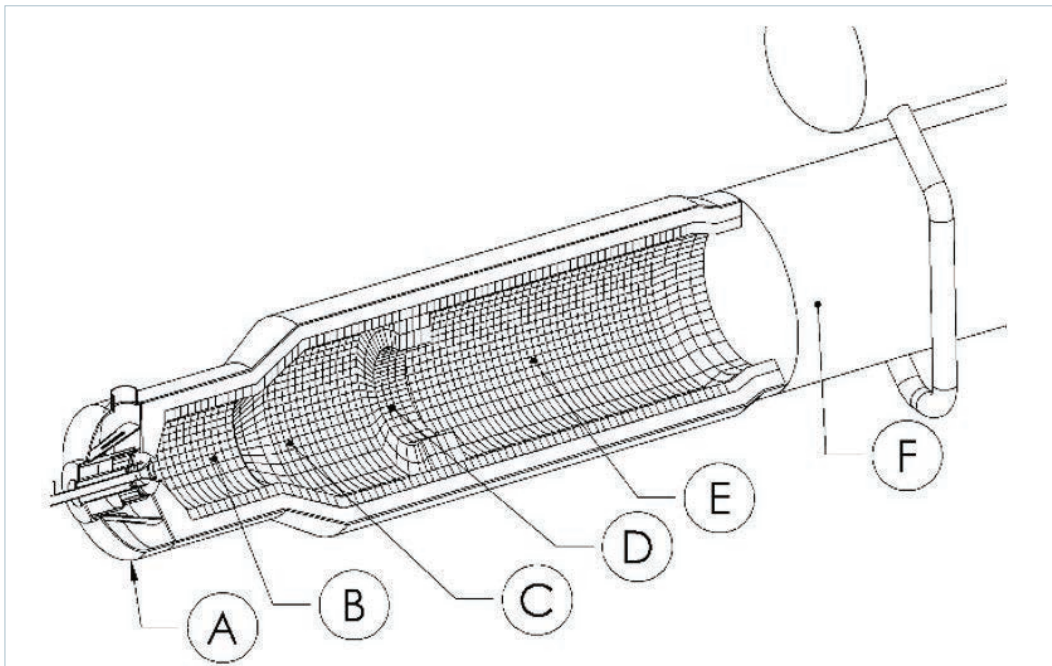


Figure 1: General layout of a thermal reactor.

Expanding the role of CFD

The performance of thermal reactors is affected by the flame shape, flame stability, high-temperature durability of the refractory material, combustion-induced vibrations/burner noise and the extent of reactions.

Steady-state CFD simulations have been used to address problems related to some of these (flame shape and refractory reliability), but the fundamentally time-dependent nature of other important phenomena – such as vibrations, noise and chemical performance – require the use of transient methods. Having used CFD to address a wide variety of chemical process industry problems over the years, the engineers at Porter McGuffie knew that the ability to simulate the time history of the chemical and fluid interactions within a reactor would provide a far more complete characterization of reactor performance. In particular, it would provide the ability to explore the factors affecting two important reactor performance metrics:

- Thermo-acoustic performance: Determining whether the frequency and magnitude of burner noise is concentrated at a single frequency, and if its magnitude is high enough to cause undue equipment damage
- Chemical performance: Determining the degree to which a reactor provides sufficient residence time to allow for the completion of the destruction and reformation reactions and the reactions' relationship to the vibrations and flame instability

The ability to assess reactor performance on the basis of these metrics represents a significant increase in the amount of insight that can be derived from CFD simulations, further amplifying its value as part of a comprehensive approach (including measurement, observation and experiments) to problem solving and design. Indeed, multiphysics CFD-based simulation is the only way you can gain insight into the multidisciplinary and typically opaque interactions occurring in the equipment without the constraints and cost of experiments. The approach allows older, traditional reactor designs to be examined more comprehensively, but perhaps more importantly, it can also guide the design of entirely new, higher performing ones. For example, the CFD simulations can be used to guide the selection of the type, geometry and placement of the choke ring or perforated wall based on exploring the design space to find the characteristics that best meet multiple objectives (such as minimum vibration and maximum chemical performance) for any given operational rate.

This is a far cry from current design processes that rely primarily on experience for guidance. It should be noted that assessing the effects of choke ring geometry and placement is particularly significant because the choke ring (which is part of the reactor's brickwork, and is periodically replaced) is the only component that can reasonably be changed in order to address problems once a reactor's steel has been fabricated.

The right model for the job

The engineers at Porter McGuffie use CFD-derived data to support engineering decisions that need to be made within the constraints of production time lines. In the case of the thermal reactor simulations, this led them to select the detached eddy simulation (DES) model in Simcenter STAR-CCM+. DES is a hybrid modeling approach that combines features of Reynolds-Averaged Navier-Stokes (RANS) simulation in some parts of the flow (such as in the boundary layers) and large eddy simulation (LES) in the unsteady separated regions. This method strikes a good balance between providing the fidelity required to capture acoustic characteristics while still requiring reasonable computational time and resources. By comparison, LES, which is typically used for the analysis of acoustic phenomena, requires much finer computational grids, leading to prohibitively large amounts of memory and computing time.

Since the thermal reactor is part of a larger chemical process, the effects of upstream air blowers and downstream waste heat boilers were taken into account by the judicious application of the appropriate boundary conditions, rather than including the devices in the model domain. This allowed the domain of the simulation to be reduced to the components shown in figure 2, beginning with the burner bustle (in yellow), the interior volume of the reactor (in violet) and a downstream portion (in pink) meant to model the effects of all downstream components using a porous medium approximation. Temperatures, flow rates and gas compositions taken from the reactor's heat and material balance (HMB) were applied at the model inlets (treated as mass-flow boundaries). It should be noted that all the inputs also contained a realistic noise component since a goal of the simulation was to predict the acoustic response within the reactor¹. From a chemistry standpoint, the simulation employed a multi-species physics model with reactions enabled.

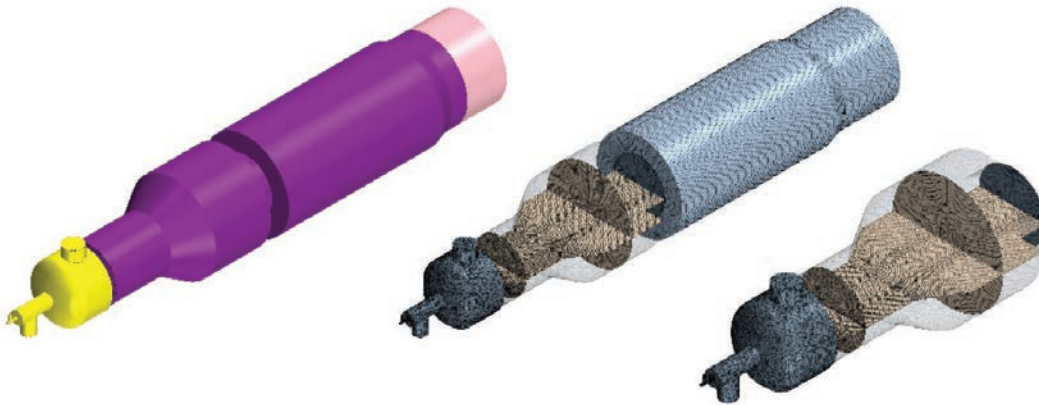


Figure 2: Domain (left) and two views of the computational grid (two images on right) developed for the CFD simulations.

CFD plus measurement equals confidence

The simulation method was used to successfully identify the cause of vibrations in a reactor that was experiencing vibration levels high enough to cause damage². The Porter McGuffie engineers used another of their core skills – instrumentation and measurement – to validate their computational results, showing their predicted vibrations from the CFD models were within 5 percent of those measured on the problematic reactor.

To further illustrate its utility without publicizing proprietary burner information, the same simulation method was applied to three scenarios using geometry and process flow conditions that were similar to (but not exactly the same as) those of a reactor with known vibration issues. In each scenario, the performance of the reactor was evaluated based on the two metrics described earlier.

Figure 3 shows the flame patterns from the CFD simulation of the reactor at a high-rate operation, which was known to have caused problems. Two modes were observed in this case – one in which the flame was long and lazy due to delayed mixing, with the flame extending beyond the choke ring (left image in figure 3), and another in which the acoustic pressures force the flame to flash back into the burner can (usually caused by slower reaction), where it can cause significant damage to the high-temperature refractory materials (right image in figure 3).

Figure 4 shows the flame patterns from the CFD simulation of the reactor at turndown (left image in figure 4), and at high-rate operation without a choke ring. No vibrations were observed in the turndown operation scenario, although the flame pattern shows that the flame extends near the choke ring. Without a choke ring, the flame remains centrally located within the reactor.

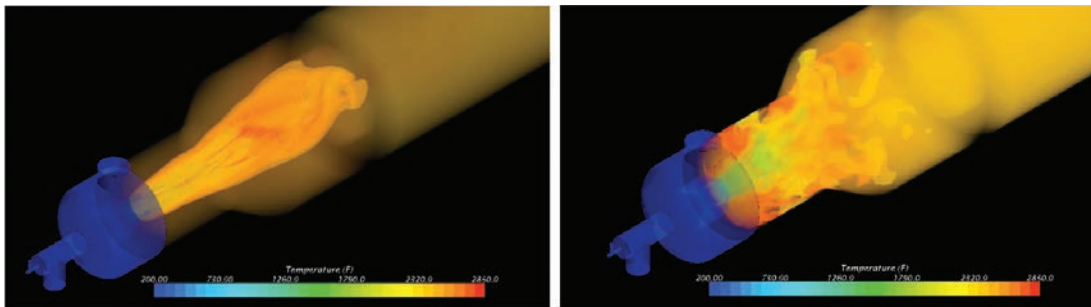


Figure 3: CFD simulations showing flame patterns in a thermal reactor at high-rate operation and two quasi-stable modes of operation: flame near choke ring (left) and in burner can (right).

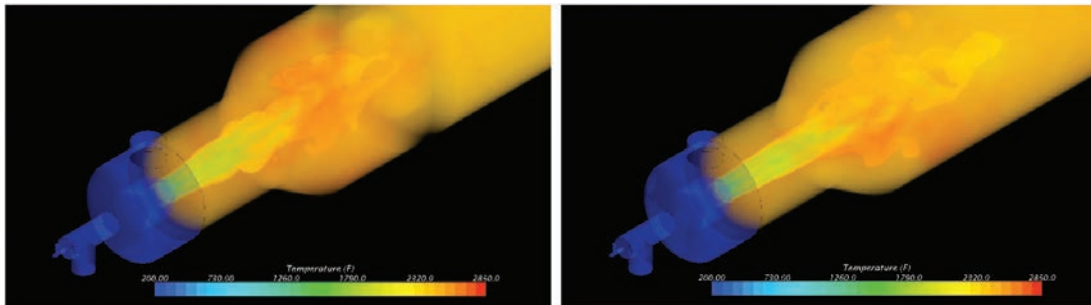


Figure 4: CFD simulations showing flame patterns in a thermal reactor at turndown operation (left) and at high-rate operation without choke ring (right).

The reactor’s predicted acoustic performance is shown in figure 5, a plot of the power spectral density (PSD) of the acoustic pressures computed in each scenario (high rate, turndown, no choke ring) versus frequency. The markedly higher intensity of the noise in the high-rate case (with choke ring) correlated extremely well with field measurements; there was less than 5 percent difference between the predicted frequencies and measured vibrations.

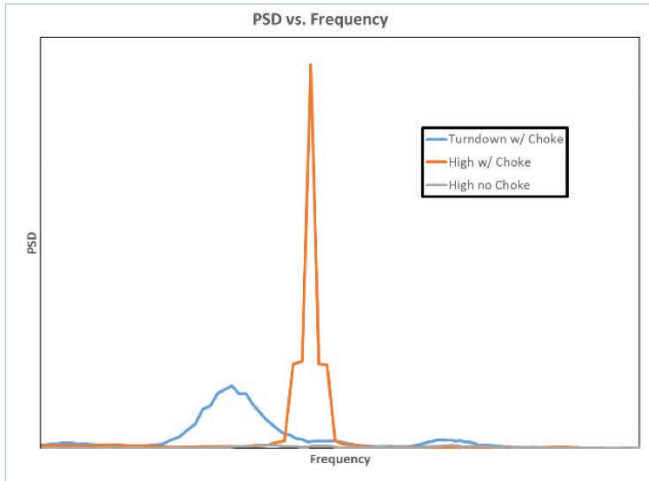


Figure 5: Power spectral density versus frequency for three scenarios.

In each scenario, the reactor’s chemical performance was quantified by the combined effect of the predicted residence times of selected species at a defined temperature. Chemical performance is important because the conversion rate (the overall throughput/generation of sulfur) depends on minimizing/eliminating the amount of incoming pollutant species in the process stream that do not meet the destruction residence time requirements established for specific compounds. Recent unpublished work by Porter McGuffie has explicitly modeled the chemical kinetics of ammonia destruction in thermal reactors, whereas the currently considered simulation uses hot-flow tracers to track the amount of time that chemical species are exposed to a particular temperature range. In the case of the reactor used in these scenarios, the tracers were queried to see if they were exposed to temperatures greater than 1,250 Celsius (°C) for at least .5 seconds, a criteria commonly used to quantify acceptable ammonia (NH₃) destruction. Visualizations of these tracers are shown in figure 6 for the high rate and turndown operations. In the high rate (with choke ring) case, it was found that 5.1 percent of the incoming acid gas flow did not meet the requirement.

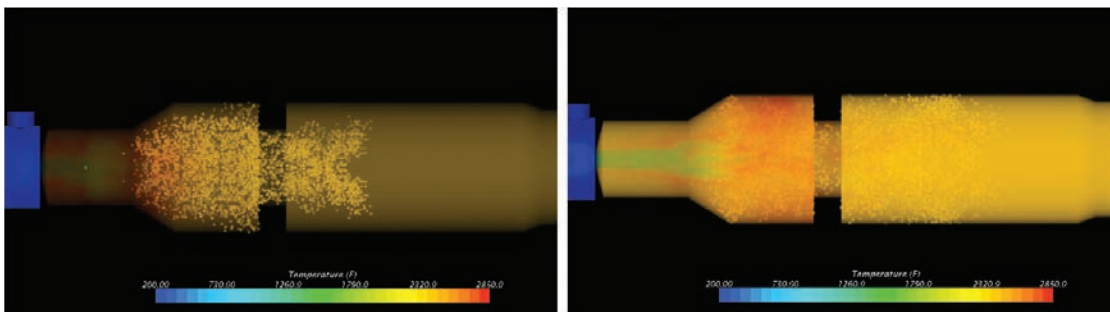


Figure 6: Sample tracer results from CFD simulations of high-rate operation (left) and turndown operation (right).

Cumulative distribution functions are a useful way to summarize and compare the residence time results for different flow rate cases: Figure 7 shows the results for the three scenarios discussed earlier. Each point on each curve represents the percentage of the tracers that were exposed to greater than 1,250 °C for that amount of time during the simulation. As such, the intersection of each curve with the minimum required residence time value (.5 seconds, shown as the prominent vertical gray line) represents the percentage of process stream that did not meet the residence time requirement. In figure 7, it is clear that a significantly larger portion of the incoming stream in the high rate/no choke ring scenario (blue curve) did not meet the requirement, although it exhibited good acoustic behavior (as shown in figure 5).

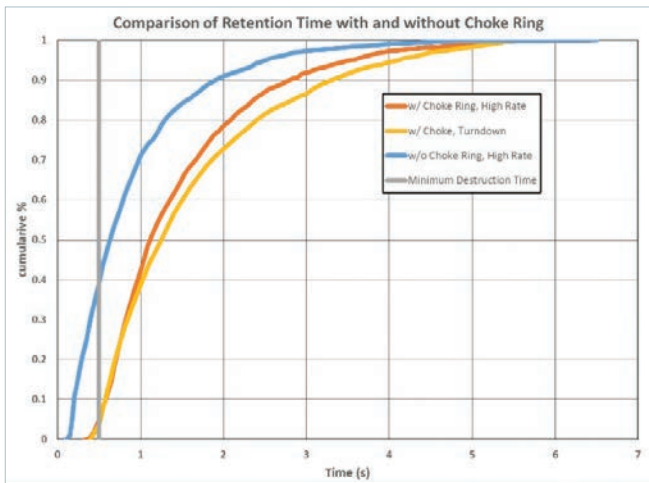


Figure 7: Cumulative distribution function of residence times above 1,250 °C, predicted by CFD, for scenarios with and without the choke ring.

The simulation results showed that keeping the choke ring in the current location precludes running at high-operation rates because of vibration issues, but without the choke ring, the residence time does not meet the process requirements. This prompted the Porter McGuffie engineers to perform a preliminary design exploration to determine if a choke ring position could be found that would allow high-rate operation (with low vibration levels) while simultaneously meeting the residence time (process) requirements for NH₃ destruction. They began by updating the computational model so the choke ring was downstream of its current location, since the no-choke ring simulation had indicated low sound levels (as shown in figure 5). A series of analyses was then performed with the choke ring position moving upstream toward the air nose until flame instability was observed in the simulation (and beyond which the flame entered the burner can). Results from these simulations are shown in figure 8. Once the position corresponding to a stable flame shape was established, the tracer test on this configuration was performed to determine the percentage of process stream that did not meet the residence time requirements. In the case shown, approximately 35 percent of the stream did not meet the requirements, only slightly better than without a choke ring, indicating that it is unlikely that high rates can be achieved with minimal vibration while still achieving acceptable NH₃ destruction, with the current choke ring geometry. Still, the exercise hints at the tantalizing possibility that the analysis framework allows, for instance, exploring the design and operating conditions space with the geometry of the separator as a design parameter. The analysis framework also reveals the interplay of these parameters and their sensitivities to the engineering objectives.

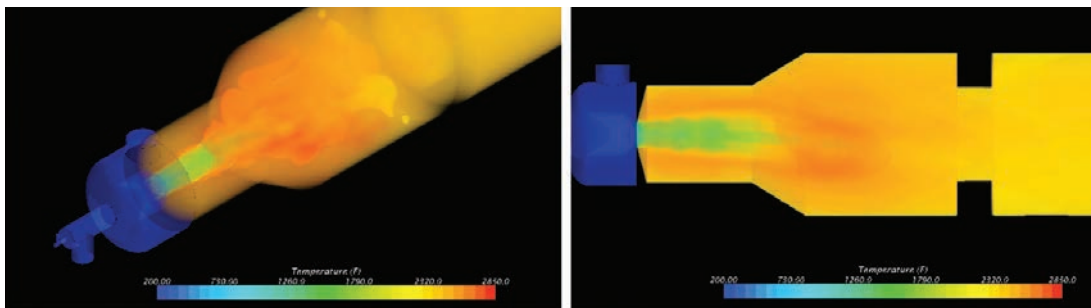


Figure 8: CFD simulations showing stable flame pattern (left) and pattern at onset of flame instability.

Conclusion

Porter McGuffie's novel application of advanced physics models in Simcenter STAR-CCM+ has significantly increased the amount of insight that simulations can provide in order to understand otherwise opaque processes and improve the performance of thermal reactors far beyond the limitations of steady-state analyses. Indeed, it resulted in the development of an industry first: a validated analysis framework capable of comprehensively assessing problematic reactors, as well as conducting explorations of the design and operating space to come up with entirely new regimes of operation.

Their work highlights the value of multiphysics CFD as part of a comprehensive approach combining observation, measurement, experiment and simulation to solve previously intractable real-life multidisciplinary problems. Consistent with their stated goal to "always find a practical and economically feasible solution to a problem, not simply analyze," Porter McGuffie's continuing work further demonstrates the practical use of complex 3D multiphysics CFD simulations; not just as an afterthought for troubleshooting problems in existing devices, but as part of a proactive, predictive approach to engineering design and analysis in the chemical process and refining industries.

References

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