SIMULATION OF THE THERMAL-ACOUSTIC COUPLING INSIDE AN INDUSTRIAL HAZARDOUS WASTE INCINERATOR

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ABSTRACT

To analyze the coupling between combustion reactions and the natural acoustic behavior of a reactor, a transient LES based CFD code has been used. Previous transient analysis of ignition inside large process heaters, of multi-tipped elevated gas flares and waste incinerators has shown the ability of the LES based CFD code called C3d. Initially, this code was used to model pool fires [1] but more recently has been used to study wind effects on ignition of multi-point ground flares (MPGF) [2]. The LES based CFD code has also been used to investigate transient operation of incinerators and process burners [3]. The work reported in this paper extends previous work to explore the transient behavior of process equipment including burners, flares, and incinerators to consider the more complex coupling between turbulent combustion inside an incinerator with the natural acoustic behavior of the combustion chamber itself. The code used is fully compressible and capable of predicting the propagation and amplification of pressure waves in confined spaces. Results from this work show a pressure wave inside an incinerator (see Figure 1). This problem can be remedied by changing the burner location with respect to the chamber or by adding flow resistance at the exit. The left-hand plot shows gas pressures at 3 locations along the burner/furnace center line with an approximate amplitude of 1,000 Pa. The plot also shows an oscillating exit pressure with a 100 Pa magnitude.



Figure 1 – Combustion generated sound measured as pressure fluctuations in transient analysis

The pressure fluctuation reduction was accomplished by adding flow resistance at the reactor exit. If not addressed, the thermal-acoustic behavior can damage a system over time. This work

discusses the effects of incinerator size, reflective boundary conditions and damping mechanisms to minimize and possibly eliminate the destructive nature of these complex phenomena.

INTRODUCTION

Coupled transport processes, such as mixing + reaction or heat transfer + reaction, are common in combustion equipment used in the chemical process industry. For example, poor fuel/air mixing can reduce combustion efficiency leading to excessive emissions from an incinerator. Coupling between turbulent mixing and chemical reactions may lead to combustion instabilities that may result in unsafe operation due to flashback and explosions inside combustion equipment. In some cases, combustion instabilities may also result in pressure oscillations that amplify the natural acoustics of a combustion chamber. This thermo-acoustic coupling between flame heat release and the acoustic modes of a combustion chamber can lead to serious damage of the combustor itself.

Early work related to thermo-acoustic coupling was observed by glass blowers when they heated a blub of gas joined to a cooler tube [4] and more recently related to gas turbines [5], [6], [7]. This same phenomenon has been observed in the Chemical Process Industry where Ultra-Low NOx burners rely on lean premixed flames to reduce NOx emissions. In both cases, thermo-acoustic coupling affects flame stability and reactor performance.

Over the years, different tools have been used to analyze unstable thermo-acoustic coupling inside combustion equipment including:

- *"Lumped parameter"* models which describe unstable oscillations in very rough fashion without considering spatial relation of acoustic modes and the flame front [8],
- *"Acoustic Element Network"* models which simulate flow with dynamic loses to obtain frequencies and growth rates of acoustic modes with the flame effects on pressure and velocity fields modelled with a flame transfer function [9] and more recently
- *"Transient CFD simulation of turbulent reacting flow"* with using grid refinement and complex physical models for turbulence and chemical kinetics to capture thermos-acoustic coupling inside the reactor [10].

Of these approaches, the most successful has been use of transient CFD models which approximate the chemical time scales and the turbulent mixing time scales and their impact on flame heat release and acoustic modes. In the present work, we have taken this approach using the "Large-Eddy Simulation" (LES) based CFD code called C3d. [1] This code has been previous used to analyze other transient phenomena such as flare ignition and unsteady burner operation. [3] [11] [12]

In this paper, C3d is used to assess acoustic performance of an incinerator used to convert hydrogen sulfide into elemental sulfur. Results illustrate the potential coupling between the reaction chemistry occurring inside the reaction furnace with the natural acoustic modes of the furnace.

This work illustrates the capabilities of using advanced CFD tools to predict expected noise frequency and power level inside a waste incinerator. This work also illustrates the ability to assess reactor performance that can help optimize the reactor design and/or modify operating conditions to minimize safety issues associated with excessive noise generated during standard operation.

TRANSIENT CFD COMBUSTION MODELING

The CFD tool used to simulate turbulent reaction chemistry coupled with radiative transport between buoyancy driven fires (i.e., pool fires, gas flares, etc.) and surrounding objects (i.e., wind fence, process equipment, etc.). The code provides "reasonably" accurate estimates of various risk scenarios for flare operations including wind speed and direction, % flame coverage, and thermal fatigue for a given geometry. CFD analysis of flares generally can be completed on the order of hours to a few days using a "basic" desktop workstation. For transient combustion analysis, Large Eddy Simulation (LES) is used to describe turbulent reacting flows. The code used in this work was derived from an earlier CFD tool referred to as ISIS-3D [13]. ISIS-3D was initially validated for simulating pool fires [14]. ISIS-3D was commercialized into a new CFD tool called C3d for use to analyze large gas flares. C3d has previously been applied to MPGFs, elevated air-assisted flares, and utility flares with detailed kinetics to describe general hydrocarbon combustion [15], [11]. C3d predicts flame size and shape, smoking potential and radiation flux from flames [16]. C3d simulations of flame height and flame-to-ground radiation have been validated by direct comparison to measured flame size, shape, and radiation measurements taken during single-burner and multi-burner tests conducted under no-wind and low-wind ambient conditions [12].

MODELING METHODOLOGY

To analyze transient operation of large combustion equipment (i.e., process burners, gas flares, waste incinerators) the transient, LES based CFD model described above was used. Initially, this code was developed to simulate the combustion process occurring in large pool fires [14] but more recently it has also been applied to study wind effects on multi-point ground flares [15], transient ignition of elevated multi-point flares [12], and safety issues related to radiation from adjacent ground flares [17]. This code has also recently been applied to investigate safety issues related to transient operation of process burners. Current Low NOx lean premixed burners often exhibit long lazy (unsteady) flames. Ignition delays of these burners poses a significant safety risk to plant operators. In addition, flame flicker related to operating these lazy flames inside a process heater can also alter radiation transfer to process tubes, which impacts plant efficiency.

LES based CFD codes are well suited to investigate transient coupling of turbulent combustion and acoustic phenomena inside combustion equipment such as a process heater or incinerator. This CFD describes the turbulent mixing of fuel and oxidizer coupled to transient chemical reactions occurring inside the combustion chamber. The C3d code has been successfully validated for application to transient combustion using simplified global chemical reaction kinetics. The following simplified global reaction mechanism has been used to simulate transient ignition of an elevated multi-point flare [11]:

$$1 \text{kg } F + (2.87 - 2.6S_1) \text{ kg } O_2 \rightarrow S_1 \text{ kg } C + (3.87 - 3.6S_1) \text{ kg } PC + (50 - 32S_1) \text{ MJ}$$
(1)

$$1 \text{kg} \boldsymbol{F} + 0.3 \text{ MJ} \rightarrow \text{S}_2 \text{ kg} \boldsymbol{C} + (1 \text{-} \text{S}_2) \text{ kg} \boldsymbol{IS}$$
(2)

$$1 \text{kg } C + 2.6 \text{ kg } O_2 \to 3.6 \text{ kg } \text{CO}_2 + 32 \text{ MJ}$$
(3)

$$\frac{1 \text{kg } IS + (2.87 - 2.6\text{S}_2)/(1-\text{S}_2) \text{ kg } \mathbf{O}_2 \rightarrow}{(3.87 - 3.6\text{S}_2)/(1-\text{S}_2) \text{ kg } \mathbf{PC} + (50-32\text{S}_2)/(1-\text{S}_2) \text{ MJ}}$$
(4)

In this case, the first reaction (Eq. 1) describes the incomplete combustion of hydrocarbon fuel (F) with oxygen to produce products of combustion (PC) and black carbon (C). This reaction produces S_I kilograms of black carbon per kilogram of fuel consumed. In this case, S_I depends on the fuel; 0.005 shown to be appropriate by Gao et al. [18] for light hydrocarbons. Reaction 2 (Eq. 2) approximates endothermic fuel pyrolysis cracking which produces S_2 kilograms of black carbon; 0.15 shown appropriate for light hydrocarbons. Reaction 3 (Eq. 3) consumes black carbon and oxygen to produce carbon dioxide and some energy. Reaction 4 (Eq. 4) consumes the Intermediate Species (IS) formed in the second reaction with additional oxygen to form more combustion bi-products and energy. These reactions are approximated using the Eddy-Dissipation Concept method originally developed by Magnussen and Hjertager [19] and elsewhere by Smith, et al., [15]. This simplified combustion model that has only 6 species is adequate for many combustion simulations.

MODIFIED COMBUSTION MODEL

If greater detail is needed and more complex hydrocarbons are included an improved combustion model is recommended that includes a wide variety of fuel types and intermediate species [13], [20]. The combustion is separated into two mechanisms, primary fuel breakdown into a group of intermediate species followed by combustion of those intermediate species.

Primary Fuel Breakdown reactions shown in the list below have been used successfully for a wide range of combustion simulations. These reactions can be used individually or combined into a single fuel breakdown reaction by applying mole weighting and adding the mole fraction weighted reactions together to form a mixed fuel type:

$1.5C_2H_4+1.5O_2 \rightarrow CO+C_2H_2+2H_2O$	Ethylene breakdown	(5)
$C_3H_8+1.5O_2 \rightarrow C_2H_2+2H_2O+CO+H_2$	Propane breakdown	(6)
$C_2H_6+0.5O_2 \rightarrow 0.5C_2H_2+CO+H_2$	Ethane breakdown	(7)
$C_3H_4+O_2 \rightarrow C_2H_2+H_2O+CO$	Propadiene breakdown	(8)
$C_5H_{12}+4O_2 \rightarrow C_2H_2+5H_2O+3CO$	N-Pentane breakdown	(9)
$C_4H_6+4O_2 \rightarrow 2C_2H_2+H_2O$	1,2, Butadiene breakdown	(10)
$C_3H_6+1.5O_2 \rightarrow C_2H_2+2\ H_2O+CO$	Propylene breakdown	(11)

 $C_{12}H_{26} + 6.5O_2 \rightarrow 7H_2O + 2CH_4 + 2C_2H_2 + 6CO \text{ Dodecane breakdown}$ (12)

Other hydrocarbons not in the list can be added by breaking down the hydrocarbon into CO, C_2H_2 , H_2 and H_2O . The various coefficients of breakdown products can be estimated following a few simple rules: 1) Heavy sooting hydrocarbons produce more C_2H_2 and possibly a small amount of soot, 2) The heat release for primary fuel breakdown can be adjusted by producing more H_2O for higher heat release vs. more H_2 for less heat release, 3) The balance of oxygen consumption, and CO production are determined by the elemental balance. It turns out that this combustion model has mild sensitivity to the primary breakdown reactions, which gives the user a lot of flexibility in modeling combustion of various fuels, while the secondary reactions mostly determine the flame temperature and soot production.

The secondary reactions used in all simulations reported here have been calibrated against test data (where available) and do not change from simulation to simulation and are grid independent.

 $H_2 + 0.5O_2 \rightarrow H_2O$ Hydrogen Combustion $C_2H_2 + 0.9O_2 \rightarrow 1.8CO + H_2 + 0.01C_{20}$ (soot) Acetylene Combustion + Soot Nucleation $C_2H_2 + 0.01C_{20} \rightarrow H_2 + 0.11C_{20}$ Soot Growth $CO + 0.5O_2 \rightarrow CO_2$ CO Combustion $C_{20} + 10O_2 \rightarrow 20CO$ Soot Combustion $CH_4 + 0.5O_2 \rightarrow 2H_2 + CO$ Methane Combustion $C_2H_2 + 3H_2 \rightarrow 2CH_4$ Acetylene-Hydrogen-Methane Equilibrium $(+)^3$ $2CH_4 \rightarrow C_2H_2 + 3H_2$ Acetylene to Hydrogen/Methane Equilibrium (-)

In conditions of low oxygen and high temperature, hydrocarbon and soot reforming reactions occur. The reforming reactions are especially important in the central rows of a large ground flare where there is low oxygen within the flame zone because the outer rows have consumed most of it. The primary fuel breakdown reactions produce H^+ and OH^- radicals which are modeled as water vapor (H₂O) – similar to the approach used by Westbrook and Dryer. The reason that water vapor is used as the oxidizing agent is because measurements indicate that actual mole fractions of OH^- and H^+ radicals are on the order of 1% or less, so they are present as trace quantities even though they are the primary reactive species. The water vapor can react both with primary fuel to produce C₂H₂, CO, and H₂. It can also oxidize soot to produce CO and H₂. Thus, typical reforming reactions for ethylene would be:

 $C_2H_4 + H_2O \rightarrow CO + 0.5C_2H_2 + 0.5H_2$ Ethylene – Water Reforming $C_{20} + 20H_2O \rightarrow 20CO + 20H_2$ Soot – Water Reforming

A global Arrhenius rate model is used for all reactions. The primary reactants f_1 and f_2 , the effective activation temperature T_A , the pre-exponential coefficient C, global exponent p, and the

temperature exponent *B* for each reaction are given in Table 1. The values in the table were derived from published values in some cases and by comparisons with experiment in others.

The reactions listed above all obey the normal Arrhenius or global reaction kinetics equation. CO oxidation includes a square root of water mole fraction weighting factor from Westbrook and Dryer. It turns out that the kinetics coefficients for soot oxidation are such that at high enough temperatures where soot oxidation occurs, the reaction rate quickly becomes boundary layer diffusion limited. This is because soot is a particle with a boundary layer, not a gas mixture. The temperature dependence for soot oxidation is due to the variation in mass diffusion coefficient with temperature. Soot oxidation due to water reforming reactions is of higher reactivity than that due to oxygen. Thus, the soot oxidation due to oxygen is less than that for water reforming reactions and furthermore is combined with an eddy breakup time delay because oxygen must diffuse into the flame zone from outside.

Reaction	f 1	f2	Т А (К)	C (1/s)	В
Primary Fuel Breakdown (ethylene)	[C ₂ H ₄] ^{0.1}	[O ₂] ^{1.65}	0 K	1	2
Hydrogen Combustion	[H ₂] ^{0.33}	O ₂	10000 K	1e8	0
Acetylene combustion & soot nucleation	$[C_2H_2]^{0.33}$	O ₂	15110 K	2e8	2
Acetylene + soot growth	[C ₂₀] ^{0.33}	C_2H_2	15110 K	1e7	0
CO – Oxygen combustion	со	[O ₂] ^{0.25} [H ₂ O] ^{0.5}	20142 K	1e18	0
Soot combustion	[C ₂₀] ^{0.33}	O ₂	0 K	0.5	0.75
Methane combustion	CH₄	O2	15000 K	1e12	0
Forward Acetylene – Hydrogen – Methane	C ₂ H ₂	H ₂	15110 K	5e7	0
Reverse Acetylene – Hydrogen - Methane	CH4	CH ₄	23500 K	4e9	0
Ethylene - Water Reforming	C ₂ H ₄	H ₂ O	15000 K	5e6	0
Soot – Water Reforming	$[C_{20}]^{0.1}$	[H ₂ O] ^{1.7}	0 K	1.0	0.75

Table 1 - Arrhenius Reaction Coefficients for a Typical Hydrocarbon Fuel Fire

THERMOACOUSTIC VALIDATION – SONDHAUSS TUBE SIMULATION

A Sondhauss tube is a thermo acoustic device wherein a long tube is heated (quite hot) on one end and cold on the other. The hot end is sealed and the cold end is open. An acoustic oscillation will occur in such conditions. A simple schematic of a Sondhauss tube is shown in Figure 2.



Figure 2 - Simple schematic of a Sondhauss tube outlining the basic components

The phenomenon was first observed by glassblowers and was first described in 1850 by the German physicist Karl Friedrich Julius Sondhauss (1815–1886). The frequency of the oscillation is described by a ¼ wave oscillating within the tube. A demonstration/validation calculation was performed by C3D wherein a 10 m long tube filled with air, has a 1 m long heated section with thermal radiator fins at 3000K. The cold end is a 9m long empty tube filled with room temperature air at 300K with the end open to the atmosphere. The calculation was run as a transient starting with still air and heat transfer was allowed to occur between the radiator fins and the air. A sound wave formed naturally with the tube and continued to oscillate as shown in Figure 3.



Figure 3 - The predicted pressure history at two locations within the Sondhauss tube. An initial transient develops which eventually evolves to a steady oscillation

Figure 3 shows that an initial transient is followed by steady oscillations that continue indefinitely, so long at heat is supplied to the system. The magnitude of the pressure oscillations is quite large, which is consistent with complaints by neighbors of those who have successfully constructed such devices. The frequency of the oscillations cannot be determined from Figure 3 because of the time scale. Figure 4 has an expanded time scale so that the frequency can be determined.



Figure 4 - An expanded time scale of the steady pressure waves so that frequency can be determined

Examining the peaks of Figure 4, the frequency is somewhere between 8 and 9 Hz. The theoretical frequency is given by the formula for the resonant frequency of a tube with one end open and the other closed (¹/₄ wave will fit into the tube length):

$$f = c/(4L) \tag{1}$$

where *f* is the frequency, *c* is the speed of sound (~345m/s at room temp), and *L* is the length of the tube (~10m). Substituting 10 m as the tube length (*L*) and 345 m/s as the speed of sound (*c*) results in a frequency of 8.6 Hz.

The ability to create and sustain a thermos-acoustic oscillation in a Sondhauss tube where the heat source is a hot structure has been properly simulated using a transient LES based CFD code. The predicted frequency agrees with theory demonstrating that this prediction is not a spurious numerical effect but instead an accurate representation of a naturally occurring phenomenon also observed in industrial equipment. The next section discusses some other examples of transient

phenomena the C3d code has been used to simulate before the thermal-acoustic behavior of a generic incinerator is examined.

TRANSIENT ANALYSIS OF INDUSTRIAL COMBUSTION EQUIPMENT

The transient operation of fired equipment has been studied using CFD to assess the safety and environmental issues associated with industrial operation [3]. This paper discusses another transient phenomenon which occurs in large industrial combustion devices such as the reaction furnace used in a Sulfur Recovery Unit (SRU). The results of several previous studies are presented to illustrate this work.

Ignition and the accompanying overpressure effects in flaring systems are highly transient in nature. The transient ignition process is often accompanied by pressure spikes and temperature oscillations, as well as fluctuations in mass flow. Four phenomenological periods have been observed following ignition initiation, namely – pilot ignition, flame propagation, fireball formation and finally steady flame development.

- Heat flux color contours shown W/m²
- Flux to ECU furnace ranges from 1000 1500 W/m² (300 -500 BTU/hroft²)
- Ground directly below stacks reaches 2000 W/m² (600 $BTU/hr^{\circ}ft^{2})$
- Plume tilted slightly due to 5m/s (11 mph) wind
- Note: full overhead summer sun gives heat flux of 1000 W/m^2 (300 BTU/hroft²)



Figure 5 - Ignition and Radiation for enclosed flare using Transient LES based CFD Analysis [3]

C3d was used to analyze an enclosed ground flare system as shown in Figure 5. The tilt of the plume observed is due to a wind velocity of 5m/s (11mph) with the direction shown. The resultant radiation heat flux on the ground and surrounding equipment was also analyzed. In the analysis of the relative location of the flares to surrounding process equipment showed that radiation flux to the ECU furnace ranged between 1000 - 1500 W/m2 (300 - 500 BTU/hr°ft2). It was also shown that radiation levels reached 2000 W/m2 (600 BTU/hr°ft2) on the ground below the stacks. By comparison, direct overhead summer sun gives a heat flux on the order of 1000 W/m2 (300 BTU/hr°ft2). In addition, this work also examined the transient ignition process which occurs when the enclosed flare is lit with a single pilot. As shown in Figure 6, a pressure wave of approximately 2,500 Pa (0.363 psi) is created inside the flare chamber during the

ignition process. This pressure wave represents a potential safety issue which may also impact equipment performance and lifetime.



Figure 6 – Gas pressure generated during the ignition process inside an enclosed ground flare predicted by LES based CFD Analysis [12]

A second example of transient behavior in process equipment used in the petro-chemical industry involves Multi-Point Ground Flares (MPGFs). These devices use hundreds of gas burners, operated in stages according to gas flow rate. MPGFs burn large amounts of flammable gases produced in the refining process. A surrounding fence protects the large flare fire from ambient wind to ensure high combustion efficiency. During MPGF ignition, a key safety concern is related to the potential igniting a large flammable vapor cloud created by gas flow through the burner tips together with ignition delay. A previous CFD analysis of an elevated multi-point flare, C3d simulations showed the potential to generate a 5 psi pressure wave when ignition was delayed by 150 ms [11]. Prior testing of this flare had confirmed a pressure wave was created during routine flare ignition. Based on this analysis, the initial ignition methodology used by the company was modified to reduce the potential for any ignition delay.

Another example of MPGF transient ignition analysis using C3d considered several operating scenarios of the flare field under various wind conditions relative to flare gas flows and various stage operation. This work was conducted to minimize potential safety risks associated with burner cross-lighting. The flare field analyzed (see Figure 7) was approximately 131m (430ft) long by 85m (280ft) wide with 19 stages containing 756 tips capable of processing more than 4 million pounds per hour (lb/hr) of light hydrocarbon gases mixed with hydrogen and inerts (average flare gas MW= 22-25). Results shown here (see Figure 8) correspond to a scenario where the cross wind was blowing perpendicular to the row of flare burners included in a single operating stage. shown results shown here safety risk considered in this analysis was the potential impact the pressure wave created by ignition delay of this flare might have on surrounding structures and personnel.



Figure 7 – Multi-point Ground Flare transient ignition with 10 mph wind blowing perpendicular to two rows of burners included in the first stage of this flare



Figure 8 – Multi-point Ground Flare ignition: a) 360 Pa (0.052 psi) pressure wave created during ignition, b) unignited burners in an adjacent row of burners ignited by neighboring row with 20 mph wind blowing perpendicular to ignited burner row

In the process burner industry, particularly in the study of heat transfer, mass transfer, temperature and species distributions within industrial furnaces an LES combustion tool such as C3d is invaluable in assessing transient burner operation. One particular interest is the development of pressure oscillations and thermo-acoustic coupling. Of particularly concern is when the thermal and pressure oscillations in a burner system are in phase with each other, in

other words, with a relative phase angle of less than 90°. As an example, a generic cabin-type burner/furnace system was studied using C3d as illustrated in Figure 9.

The cabin-type process heater included 8 burners shown in the above figure at time t = 0 seconds, the air was reduced to 10% of the normal flow rate, and at t = 2.5 seconds, the air flow was increased to 500% of the normal rate. The accompanying flow, thermal and pressure transients were studied using C3d.

In the chemical and petro-chemical process industry, particularly when heat transfer, mass transfer, temperature and species distributions inside of large process heaters are of interest, an LES based combustion tool such as C3d is invaluable in studying transient phenomena. A phenomenon of particular interest is the development of pressure and temperature oscillations associated with thermo-acoustic coupling. This is of particular importance when the temperature and pressure oscillations in a burner system are in phase with each other, in other words, with a relative phase angle of less than 90°. A generic system involving 8 round flame burners included in two rows along the length of a cabin-style process heater has been used to analyze transient behavior using C3d (see Figure 9).



Figure 9 – Transient Burner Operation in a Cabin-Style Process Heater

As shown in Figure 12, at time t = 0 seconds (Figure 9a), with burners operating in steady condition, combustion air is reduced to 10% of the normal flow rate resulting in the burner flame "going out" as shown in Figure 9b. After 2.5 seconds, combustion air flow is increased to 500% the normal rate resulting in the "long" flame as shown in Figure 9c. This transient event results in a pressure fluctuation inside the furnace which can affect adjacent flames and burners thus creating a pressure oscillation inside the process heater. If the process heater experiences unanticipated transients, NOx emissions can increase due to uncontrolled mixing. In addition, heat transfer from the flames to the process tubes can also be negatively affected by the

"flickering" flame which will reduce heater efficiency and downstream distillation columns as well.

Given these examples showing the ability of C3d to simulate transient combustion phenomena, a detailed analysis of thermo-acoustic coupling will be presented. This work involves the generic design of reaction furnace included in a Sulfur Recovery Unit. Thermoacoustic coupling is a common problem in incineration systems like the reaction furnace. Because this transient phenomena is related to turbulent reacting flows and the acoustic behavior of a heated enclosed device, similar to a Sondhauss tube discussed earlier, the potential for this non-design operation exists. Having a tool like C3d gives process engineers a way to check for this phenomena before building and installing a unit in the field.

THERMAL-ACOUSTIC COUPLING INSIDE AN INDUSTRIAL INCINERATOR

A typical industrial sulfur recovery reaction furnace was simulated to illustrate the acoustic effects that can arise in such industrial equipment. The assumptions and method of analysis is depicted in figure x below.

Table 1 - Assumptions and methodology used in the analysis of a typical industrial reaction furnace

- The LES code C3d is used to simulate reaction furnace
- · Generic geometry, size, gases, and flow rates found in industry
- Simulation run to quasi steady state
- Transient Analysis of typical Reaction Furnace Performed
- Analysis includes sulfur and nh3 chemical reactions
- Pressure waves observed in result, consistent with combustion zone dimensions
- Outlet flows observed to have Fundamental Frequency (1/4 Wave)

The geometry chosen for this simulation is shown in Figure 10. On the left-hand side are two coaxial annulus' which inject combustion air and acid gas (primarily $NH_3 + H_2S$ + other waste gases). The outer annulus injects combustion air while the inner annulus is the acid gas injector. Just upstream of the burner are axial spin vanes which add a swirl to the incoming feed gases. The feed gases burn within the small cylindrical throat just before the conical expansion. The large cylindrical chamber downstream of the burner includes a refractory choke ring which separates a primary combustion zone from a secondary combustion zone. Acoustically this geometry includes several reflection points that can resonate with combustion noise generated by the burner. The throat section is approximately 2.5 m long while the reaction furnace is approximately 12 m long not including the cone. The temperature within the furnace varies from the cold inlet flow to the hot reaction temperatures, thus a simple sound speed calculation does not completely characterize the furnace acoustics as a whole. In addition to temperature variations, the chemical species vary significantly from the inlet of the reaction furnace to the exit of the furnace. To predict acoustic effects, a variable sound speed and all acoustic reflection modes must be accounted for. A fully compressible CFD code, such as C3d, which takes into account all phenomena mentioned here is an excellent option for this analysis.



Figure 10 – Typical sulfur recovery reaction furnace



Figure 11 – Combustion performance of generic reaction furnace: a) Iso-surface for H_2S , b) Iso-surface for NH_3 , and c) Centerline gas temperature profile inside the SRU reaction furnace

The C3d simulation of the generic reaction furnace produced satisfactory results for chemistry and temperature profiles (see Figure 11). Acoustically is also produced pressure waves that are observed either directly, as pressure oscillations, or indirectly as oscillatory motion of

combustion gases. The time accurate pressure history inside the combustion throat provides an estimate of the oscillation frequency. Examining this shows the simulation is consistent with the 2.5m length of the combustion throat. The magnitude of the pressure oscillations is about 800 Pa (0.12 psi) peak to peak. A lower frequency modulation of the pressure waves was also observed.



Figure 12 - Gas Pressure History In Combustion Zone, Resonant with Local Burner Geometry



Figure 13 – Average Gas Temperature at Exit of Furnace

Pressure oscillations (see Figure 12) and associated gas temperature oscillations (see Figure 13) propagated throughout the furnace where hot gases from the furnace mix with cooler gases coming from other parts of the SRU. Examining the exit flow rate of sulfur, the high frequency pressure waves are smoothed some and the fundamental oscillation mode can be seen as

approximately 8 Hz (see Figure 14). The fundamental mode is that associated with the two large reaction zones in the reaction furnace with the approximate length of 12m not including the expansion cone. The imprint of the burner pressure oscillation is observed in the ammonia flow rate at the exit of the burner throat (see Figure 15). The pressure oscillations cause a back and forth motion of the gases that shows up as a species flow oscillation due to species gradient at the throat exit.



Figure 14 - Sulfur Mass Flow Rate at furnace exit (Fundamental Frequency, Observed, 8Hz, modulated with higher frequencies in combustion zone)



Figure 15- NH₃ flow rate at burner throat

SUMMARY AND CONCLUSIONS

The present work has focused on conducting transient analysis of a generic incinerator used to convert H₂S mixed with NH₃ to elemental sulfur. The LES based CFD code called C3d has been used. Several transient analyses examples conducted with C3d have been included to illustrate the capabilities of this software. In this application, transient pressure waves were predicted inside both a Sondhauss tube for verification of the ability to accurately predict the expected sound frequency (pressure fluctuations) inside a heated enclosed tube (Sondhauss tube). The code was then used to predict pressure waves inside a generic reaction furnace with the expected sound frequency and power level from the operating conditions considered. The impact this has on the exit temperature and composition are shown. Based on other experience with waste incinerators, thermal-acoustic coupling has been observed to have a serious impact on equipment performance and expected service life. It is recommended that the CFD analysis, such as shown in this work, be used whenever possible to address questions about potential thermal-acoustic coupling. The benefit of such an analysis is to eliminate the coupling and improve process efficiency and performance. It is also recommended that this code be used when transient behavior might lead to unsafe operation such as shown in the examples included in this paper.

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