

## Computational Modeling of a Direct Fired Oxy-Fuel Combustor for sCO<sub>2</sub> Power Cycles

**Jacob Delimont, Ph.D.**  
Southwest Research Institute  
San Antonio, Texas, USA  
[Jacob.Delimont@swri.org](mailto:Jacob.Delimont@swri.org)

**Nathan Andrews**  
Southwest Research Institute  
San Antonio, Texas, USA  
[Nathan.Andrews@swri.org](mailto:Nathan.Andrews@swri.org)

**Lalit Chordia, Ph.D.**  
Thar Energy  
Pittsburg, PA, USA  
[Lalit.Chordia@thartech.com](mailto:Lalit.Chordia@thartech.com)

### Abstract

*Significant interest has developed over the past several years in direct fired oxy-fuel combustion as a heat source for supercritical carbon dioxide (sCO<sub>2</sub>) power cycles. This is a promising and innovative method for providing the needed thermal energy input for highly efficient power generation, while integrating carbon capture directly into a sCO<sub>2</sub> power cycle, thus maintaining extremely environmentally friendly emissions. sCO<sub>2</sub> power cycles rely on a very high degree of recuperation when compared to traditional Rankine or open Brayton cycles. This large amount of recuperation results a high combustor inlet temperature. This high inlet temperature makes design of the combustor challenging for a variety of reasons. Additionally since the amount of oxygen is precisely controlled, proportions of CO<sub>2</sub>, O<sub>2</sub>, and fuel in the primary burning zone can all be controlled independently. This adds considerable flexibility to the design process not typically found in a combustion system using air as the oxidizer. Another major challenge and difference between this combustion system and more typical gas turbine combustion systems is the vast variation in density of the inflowing CO<sub>2</sub> that occurs between the startup state and the design point condition.*

*The current work focuses on the design of a 1MW thermal sized combustor. This work lays out some of the basic design sizing and cases studied as part of the design effort. This design will need to be capable of startup, part load, and full load operation. The maximum exit temperature of this design will approach ~1200°C. Past cycle analysis has shown this temperature to be the maximum temperature the current state of the art recuperators will permit a closed sCO<sub>2</sub> cycle to operate. Simplified combustor geometry is described in detail so that other researchers interested in simulating oxy-fuel combustion for sCO<sub>2</sub> environments will have a starting point on which to base their work. The results of this work will be useful for others considering some of the design challenges of a direct fired oxy-fuel combustor for sCO<sub>2</sub> application.*

### INTRODUCTION

Supercritical carbon dioxide (sCO<sub>2</sub>) power cycles offer a potential pathway to increase the efficiency and decrease the costs of power generation. A great deal of interest in sCO<sub>2</sub> power cycles has developed over the past decade. These power cycles offer higher efficiencies than achievable in Rankine power cycles. At the same time many of the components, especially the turbomachinery, are considerably smaller in size when compared to those used in a steam Rankine cycle with comparable power output.

The method of heat addition into a direct fired sCO<sub>2</sub> power cycle also has a number of advantages. Direct fired sCO<sub>2</sub> cycles utilize a combustor which burns fuel and pure oxidizer with the CO<sub>2</sub> acting as a diluent and temperature moderator. The first major advantage is that all of the energy released from the combustion process is captured within the CO<sub>2</sub> stream. This removes the losses associated with heat exchangers of less than 100% effectiveness. In addition, fuel and oxidizer are both mixed and reacted entirely within a closed loop stream of CO<sub>2</sub>. Thus, the CO<sub>2</sub> produced as part of the combustion process is easily managed and the excess CO<sub>2</sub> can be bled off at the low temperature portion of the cycle. Typically the low side pressure and temperature of a sCO<sub>2</sub> power cycle is comparable to the pressure of CO<sub>2</sub>

pipelines which makes carbon capture and sequestration very simple and not a major parasitic power loss, as might be in a conventional combined cycle power plant.

This relative ease with which 100% carbon capture can be implemented on a direct fired oxy-fuel combustor power version of these cycles makes this technology extremely attractive for future base load power generation. Many of the supercritical CO<sub>2</sub> cycles being considered for use in power generation require a high degree of recuperation. This large amount of recuperation relative to the small amount of thermal input leads to a high temperature stream of CO<sub>2</sub> entering the combustor. For a sCO<sub>2</sub> power cycle with a turbine inlet temperature of 1200°C, combustor inlet temperature of between 750-900°C can be experienced [1]. The exact combustor inlet temperature depends on the type of cycle which is chosen. These elevated combustor inlet temperatures are a significant difference between an oxy-fuel combustor for direct fired sCO<sub>2</sub> application and typical gas turbine combustor designs.

In addition to the challenges posed by high inlet temperatures, the high pressure and high CO<sub>2</sub> concentration lead to other difficulties. Many chemical kinetic mechanisms available in the literature are not appropriate for such high levels of CO<sub>2</sub> at pressure in the 150 to 300 bar range [2]. Recent work conducted by several investigators is beginning to shed light on the ignition delay time [3] [4]. These investigations are expected to continue to provide useful information at higher pressures and conditions at which oxy-combustors for supercritical CO<sub>2</sub> are expected to operate. Further investigations are needed into other aspects of the combustion process, specifically CO oxidation and flame speeds in supercritical CO<sub>2</sub> conditions. Recently there has been some publication of continuous flow combustion testing. Some limited results have been presented for continuous flow oxy-fuel combustion testing showing some details of oxy-combustor design for sCO<sub>2</sub> combustors [5] [6] [7]. These works are expected to result in a demonstration of oxy-fuel combustion in a semi closed cycle within the next couple of years.

A team of Southwest Research Institute, Thar Energy, and others is currently working to design and build a 1MW(thermal) scale direct fired oxy-fuel combustor for sCO<sub>2</sub> applications. Presently, the initial primary objective addressed in this work is the study of the behavior of a sCO<sub>2</sub> swirl-style injector in a combustor. Specifically studied are the thermal performance, flow behavior and combustion processes under the effects of various design variables, including: the combustion chamber geometry, mainstream flow swirl angle, fuel injection scheme, and cooling strategy. To-date various configurations of each of these design variables have been studied in a myriad of computational simulations. The purpose of the discussion in this paper is not to give a detailed accounting of the observations and sensitivities of each of these, but rather to provide a detailed description of the computational setup and modeling details sufficient for other groups to perform their own simulations. Still, a small sampling of simulation results will accompany the problem setup. This approach will hopefully establish a more-common baseline and promote collaboration and accelerated progress in achieving viable solutions to the direct fired oxy-fuel sCO<sub>2</sub> combustor.

## **GEOMETRY**

The initial geometry for the oxy-fuel combustor is very similar to a traditional style gas turbine combustor. The envelope of the combustor is cylindrical in form with three main sections comprising the domain considered in this work, namely, the swirler, the combustion chamber, and the bypass flow. The swirler is the most upstream portion of the combustor and initially contains a portion of the pure CO<sub>2</sub> coming into the combustor. Here, the oxidizer will be mixed with the CO<sub>2</sub>. Once oxidizer has been introduced into the CO<sub>2</sub>, the swirler will then impart rotational swirl into the mixed flow by swirling veins, channels, or some other means. Then the flow is directed into the main combustion chamber.

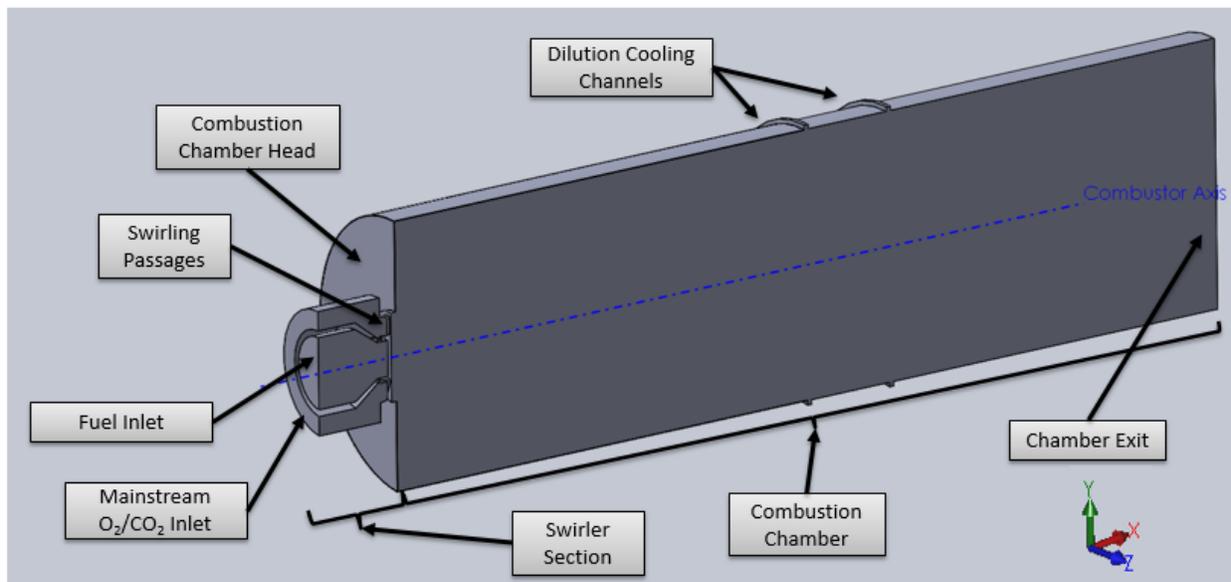
The remainder of the pure CO<sub>2</sub> is diverted into a bypass stream, to be introduced into the combustion chamber as cooling and dilution flow. Typically this bypass stream flows in the annulus between the combustion chamber and the outer combustor annulus and flows parallel to the main CO<sub>2</sub> stream. There

are multiple methods by which the flow is introduced into the main chamber. Typically flow enters via slots or holes in the combustion chamber liner. Depending on the size, orientation, and flow rate of the entrance zone, these orifices are used as film and/or effusion cooling for protection on the chamber walls, and as stream dilution and quenching of the hot reaction gases to achieve a suitable final temperature for equipment downstream.

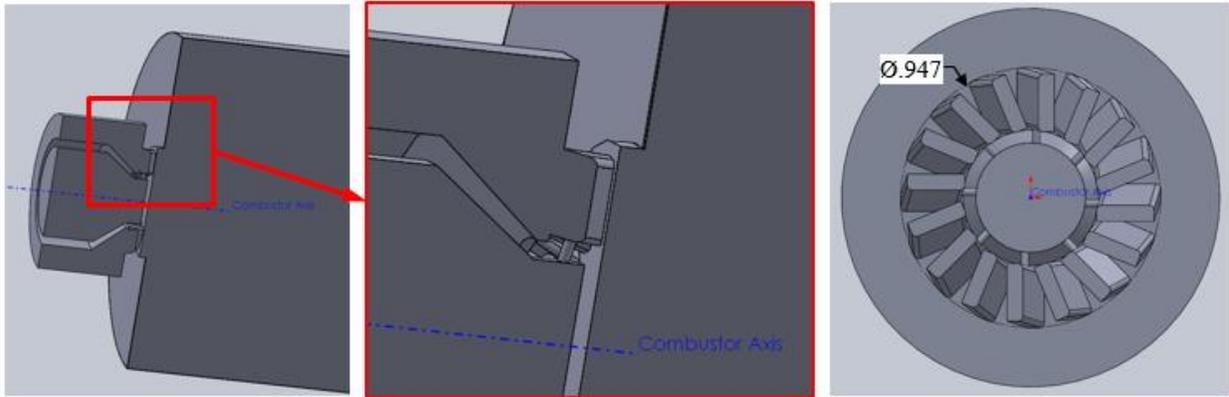
Fuel is introduced into the system through strategically placed injectors, either during the swirl process or shortly after leaving the swirler. The authors have already considered two examples of fuel injection schemes. The first, termed the partial-premix scheme, injects fuel into the oxidizer/ $\text{CO}_2$  within the swirling veins, before exiting into the main combustion chamber. The second scheme injects fuel streams directly into the combustion chamber, from fuel injectors which impart unique swirl characteristics to the fuel streams in attempt to promote good mixing and control location of the combustion process.

The geometry used to generate the sample results of this work is depicted in Figure 1 and Figure 2. These figures only show the fluid domain for the computational simulations. The outer diameter of the combustion chamber is 3.0-inches and is 10.0-inches from chamber head to exit. Two 0.05-inch wide dilution cooling slots were used, the most upstream slot located 5.0-inches from the head of the combustor, with a spacing of 1.0-inch between them. The remainder of the bypass  $\text{CO}_2$  was introduced as effusion cooling sources at the 5.0-inch long outer chamber wall upstream of the dilution slots and the chamber head. This is explained in more detail in the following section.

The swirler contains two inlet flow streams. The first is for the mainstream  $\text{CO}_2$  and  $\text{O}_2$  and has an outer diameter of 1.38-inches and inner diameter of .95-inches. The second inlet is to serve as the plenum for the fuel injectors. As depicted in Figure 2, 16 swirling channels were used to impart swirl of  $40^\circ$  degrees onto the main  $\text{CO}_2/\text{O}_2$  inlet stream. Swirl angle is defined here as measured from the combustor centerline axis; thus, a higher swirl angle results in a greater radial component (lesser axial component) of the incoming flow streams. In addition, the passages were tilted with a  $10^\circ$  down angle, toward the combustor centerline axis, *i.e.*, as measured from the top (short-edge) plane of each channel. The swirl channels begin with an exterior diameter of 0.947-inches, as shown in Figure 2. Swirl channels had a cross section of 0.506-inches by 0.207-inches and extend 0.135-inches in the x-direction. Fuel was injected with a partial-premix scheme. Eight fuel ports of diameter 0.0049-inches were located in half of the 16 swirling passages, alternating in every other passage.



**Figure 1. Cross-section of the Simulated Fluid Domain within the Combustor Geometry.**

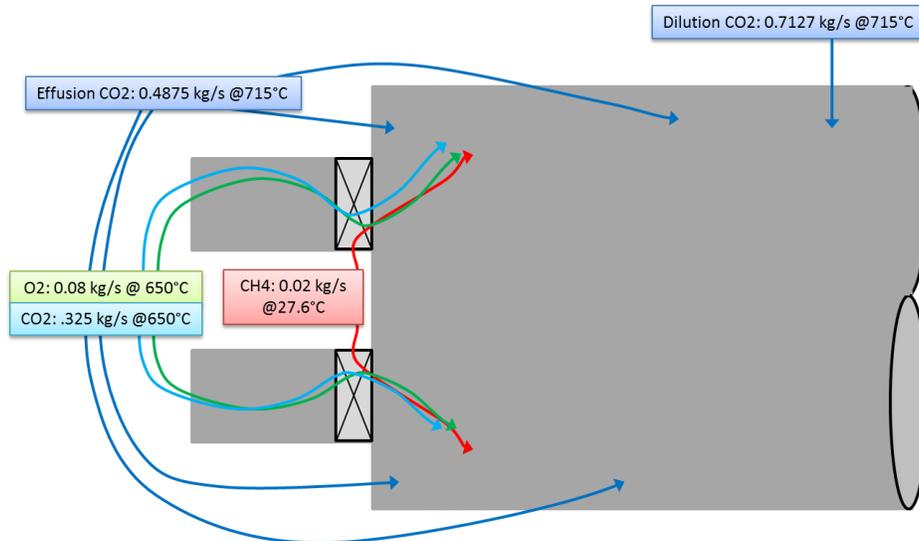


**Figure 2. Details of the swirler section of the combustor: Left and center: Cross-section of the swirler. Right: View of the swirler from combustor exit.**

## BOUNDARY CONDITIONS

Boundary conditions used for the modeling of an oxy-fuel combustor design can vary substantially with the combustor design. The ability of the designer to select the oxidizer to diluent ratio, as opposed to being confined to the ratio found in air, offers a significant additional degree of design freedom not found in traditional gas turbine combustors. Apart from that significant difference modeling of a direct fired oxy-fuel combustor proceeds in a similar manner to what would be expected from a typical gas turbine combustor. Design, part load, cold start, and other cases need to be considered. Presented herein are the design point boundary conditions, startup conditions, and another condition particular to closed loop operation, termed the “fast start” condition.

The design point boundary conditions for the combustor geometry described in the preceding section are as follows. The downstream fluid boundary was set as a pressure outlet equal to the operating pressure of 200 bar. Mass flow inlet boundary conditions were set for the primary  $\text{CO}_2/\text{O}_2$  mixed inlet and  $\text{CH}_4$  fuel plenum. A diagram of the inlet mass flow split is provided in Figure 3.  $\text{CO}_2$  enters the primary inlet at 0.325 kg/s. This is equal to 20% of the total combustor flow ( $\text{CO}_2$  plus fuel and oxidizer). The remainder of the inlet  $\text{CO}_2$  is split between the cooling flow to the head and walls of the combustion chamber and the dilution flow. The split used in this model is 0.4875 kg/s or 30% of the total flow for cooling, with 0.7127 kg/s (43.9%) utilized as dilution flow to cool the temperature of the combustor outlet flow. Incoming  $\text{CO}_2$  streams were prescribed as 700°C while  $\text{O}_2$  and  $\text{CH}_4$  as 26.7°C. The mixture temperature of the  $\text{CO}_2/\text{O}_2$  stream was 650°C.



**Figure 3. Schematic of combustor with design mass flow splits.**

In this case neither the cooling flow nor the dilution flow contains any oxidizer. This lack of oxygen in either of these streams is a significant difference from a traditional gas turbine design, and makes the distinction between a primary and secondary burning zones largely irrelevant for this design. Other cases could be considered where portions of the cooling or other flows contain oxygen, but since a large amount of excess oxygen are undesirable, care should be taken in assuming unreacted oxygen leaves the combustion chamber. Any unreacted oxygen imposes a negative penalty on the system by increasing the demands on the air separation unit. Complete oxidation of carbon monoxide may call for a mixture which is slightly oxygen rich. Mixtures presented in this paper have 1% excess  $O_2$  by mole fraction to account for this factor.

Apart from the design cases two other extreme types of cases should be considered for modeling of an oxy-fuel combustor for direct  $sCO_2$  applications. Examples of these two cases for the mass flow rates needed for a  $1MW_{th}$  scale combustor are shown below in Table 1. The operating conditions represented by these cases occur in actual plant operation during the startup of a  $sCO_2$  plant. During startup, both the mass flow and pressure ratio of the cycle will be at some fraction of the design operating point. For these cases  $2/3$ 's of the design pressure ratio and mass flow were selected as a representative startup point. The actual startup pressure and mass flow for a given combustor will be dependent on the cycle type, off-design turbomachinery performance, and depending on heat rejection scheme, ambient conditions. Each combustor designer will need to select conditions appropriate for the cycle for which their combustor is being designed, however the conditions presented here represent a plausible startup condition for the current application.

In considering the startup case it is helpful to remember that  $CO_2$  is chosen as a working fluid because of its very large density difference, which allows for efficient cycle design point operation. This same large density difference can potentially cause problems for a combustor during start up. As can be seen in Table 1 the density of the  $sCO_2$  entering the combustor during startup varies dramatically from the design point case. During cold start the fluid entering the combustor is roughly 6 times as dense as at design point operation. This will significantly alter combustor residence times. Simultaneously designing a combustor to handle both of these conditions requires careful consideration. The cold start case mass flow rates are specified in Table 1 with  $1MW_{th}$  input.

In addition to the cold start case, another case, termed the "fast start" case is also worth considering. This case arises from the need to bring the cycle to thermal equilibrium and thus design point as rapidly

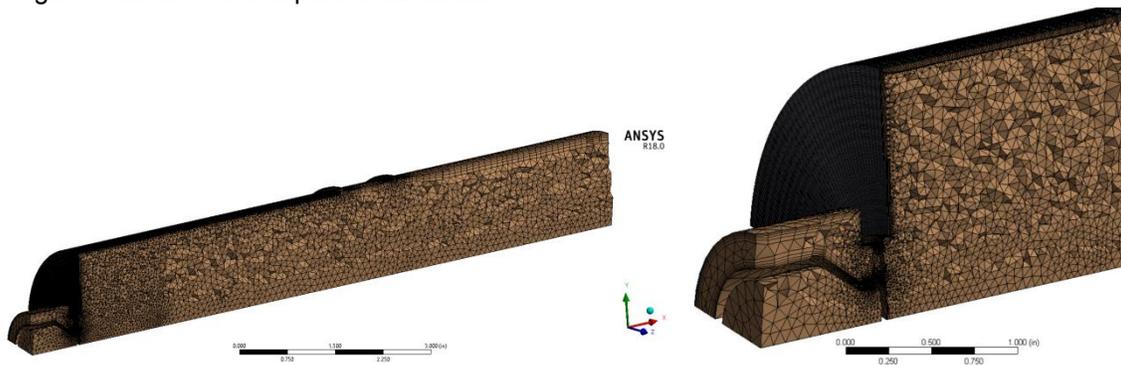
as possible in order to minimize the inefficient startup operation. As shown in Table 1 this case uses significantly more fuel than the design point in order to rapidly increase the cycle temperature. This case shown here assumes some amount of time has been spent at start up condition, sufficient to elevate the combustor inlet temperature of the CO<sub>2</sub> to 150°C prior to the “fast start.” In the example case the fuel and oxidizer flow rate is 68% higher than at design point. This percentage was selected by adding enough fuel and oxygen to the system to increase the outlet temperature to that of the design point combustor outlet condition, with a combustor inlet temperature near startup. As with startup the level of combustor thermal duty required will depend on cycle design considerations. Combustor thermal duty during this start up process primarily depend on, the desired cycle temperature ramp rate, which may be dependent on component thermal stresses. In addition, practical considerations, like, the air separation unit and fuel system’s ability to supply oxygen and fuel in excess of design point demands, and the extra cost of these larger systems or potential storage systems need to be accounted for. While termed a “fast start,” in reality the combustor may be required to operate in this condition for an extended period of time, perhaps as long as several hours, depending on the cycle’s thermal mass.

**Table 1. Mass Flows for Several Cases to be Considered for Combustor Modeling**

	Design Point	Cold Start	Fast Start
CO <sub>2</sub> Mass Flow (kg/s)	1.53	1.02	1.02
Pressure (bar)	200.00	133.33	133.33
CO <sub>2</sub> Inlet Temp (°C)	700	50	150
CO <sub>2</sub> Density (kg/m <sup>3</sup> )	104.2	649.4	203.5
O <sub>2</sub> Mass Flow (kg/s)	0.0806	0.0806	0.1360
CH <sub>4</sub> Mass Flow (kg/s)	0.0200	0.0200	0.0338

## MODELING

Once a solid model was created for the fluid domain, a computational mesh was generated using mainly tetrahedron elements, with 5-6 hexahedron elements used for boundary layer inflation along wall boundaries. A quarter section of the domain, with periodic boundary conditions was used to reduce computational load. For the results presented in this document, a mesh of 1.125 million elements was used. Figure 4 shows the computational mesh.



**Figure 4. Computational mesh for the Fluent simulations.**

The simulation was performed in ANSYS Fluent 18.0. The simulation was completed with a pseudo steady-state RANS model using the realizable k-epsilon turbulence model. Standard wall functions and compressibility effects with the default set of turbulent Prandtl and Schmidt numbers were prescribed.

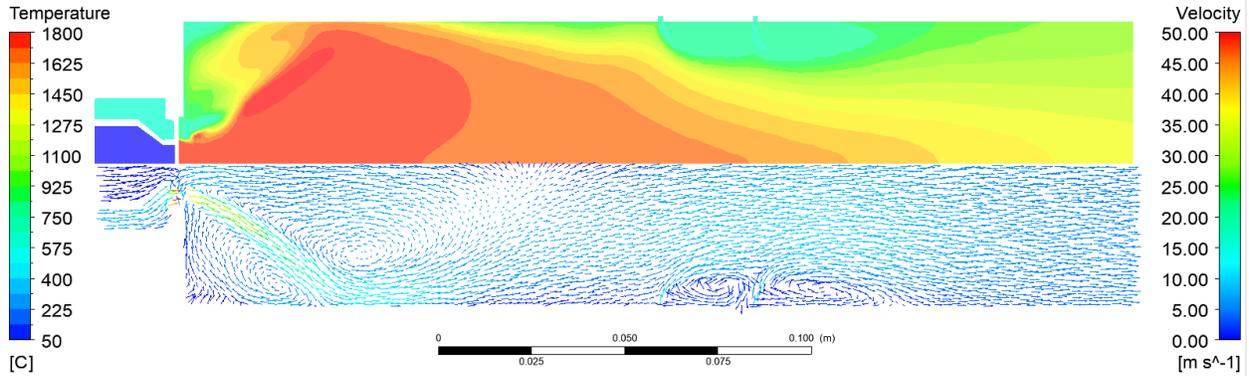
The downstream fluid boundary was set at a pressure of 196 bar, which equates to a total of a 2% total pressure drop from the operating pressure of 200 bar. A mass flow inlet boundary condition was set for the mainstream CO<sub>2</sub>/O<sub>2</sub> flow inlet. A perfectly mixed fluid composition was prescribed, assuming that O<sub>2</sub> was introduced into the system far enough upstream to become well-mixed with the CO<sub>2</sub>. A mass flow boundary was also used for the CH<sub>4</sub> fuel plenum. Dilution CO<sub>2</sub> from the bypass flow was injected into the domain with mass flow boundaries at the two dilution slots. These slots are used to simplify the computational domain, actual dilution ports will most likely be circular holes. The remainder of the cooling CO<sub>2</sub> enters the domain as effusion cooling along the 5.0-inches of the combustor liner upstream of the dilution ports and in the combustor head. The effusion cooling was implemented as CO<sub>2</sub> mass and energy sources at cells nearest the outermost walls. This was accomplished in Fluent by creating thin volumes of fluid directly adjacent to the outer wall in the geometry CAD. These thin volumes were then meshed individually as unique zones in the CFD domain setup. Mass and energy sources were then assigned to the volumes, such that the total integrated mass of the volumes was equal to the balance of the prescribed total flow minus the primary inlet. Mass entering the flow uniformly distributed in each cell and was assigned zero initial velocity. The total energy flux of the source was set by determining the energy necessary to achieve the desired incoming temperatures within the volume under flowing, but non-reacting conditions. This technique of modeling effusion cooling is one method to achieve both mass and energy sources with no-slip wall conditions in Fluent, which is not achievable by simply prescribing the combustor liner walls as mass flow inlets.

Fluid properties were calculated using the ideal gas equation of state, kinetic-theory for mass diffusivity, polynomial regressions for specific heat and other transport properties, and mixing rules for mixture properties. The ideal gas assumption is expected to yield errors of 10% for density and specific heat, as independently estimated and as reported by Manikantachari *et al.* [8] as compared to NIST REFPROP and other cubic equations of state. Chemical kinetics were modeled using a custom reaction mechanism with 12 species and 25 reactions [9]. Calculating fluid properties with these assumptions were considered adequate for these initial studies, and future works will likely include better estimations. The mechanism was created leveraging the USC Mech II kinetic mechanism. USC Mech II was first reduced, then optimized by an in-house code at Georgia Institute of Technology and finally validated against auto-ignition calculations using detailed USC Mech II. The stiff chemistry solver in Fluent was used for CFD simulations.

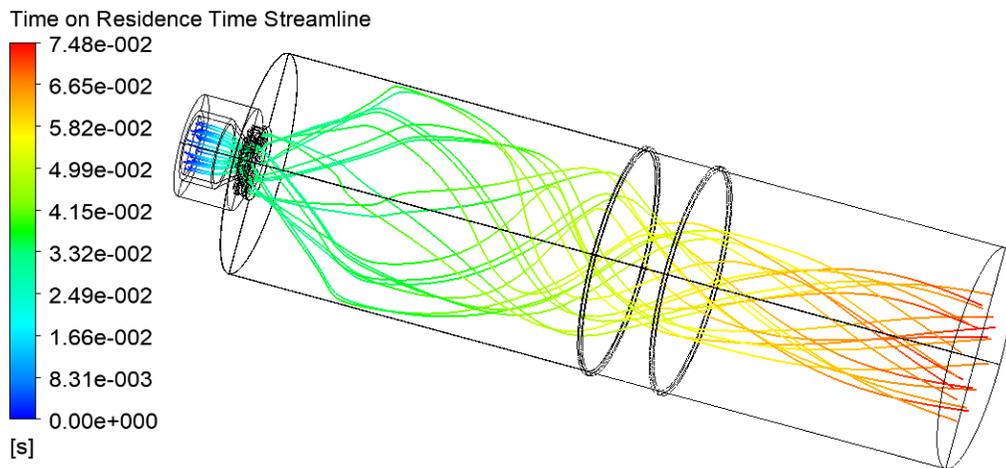
## **SAMPLE RESULTS AND DISCUSSION**

Presented in this section are selected sample RANS results from the previously described geometry, at design point boundary conditions. It should be remembered that these results are generated from the sample geometry, which has several potential issues which would need to be corrected before attempting to use the geometry for an actual combustion experiment.

Figure 5 shows a contour of the temperature field in addition to a velocity vector plot in the lower half of the figure. The velocity vectors clearly show the strong recirculation zone which forms in the center of the combustor. The temperature contour shows that this recirculation zone contains very high temperature gas. The mixing of this high temperature gas with the fresh unburned fuel and oxidizer stabilizes the flame. In addition to the flame stabilization several other features are worth mention from this figure. The recirculation zone in the corner of the combustion chamber is much colder and does not contribute to the flame stabilization and primarily contains CO<sub>2</sub> from the combustor head cooling. When looking at the temperature contour it is apparent that there are a couple of concerning areas in which very high temperature gas is in close proximity to the combustor walls. Although the walls are set to adiabatic, so the hot spots magnitude may be lessened when heat transfer effects are included, temperature of this level would likely pose a problem in an actual hardware test.



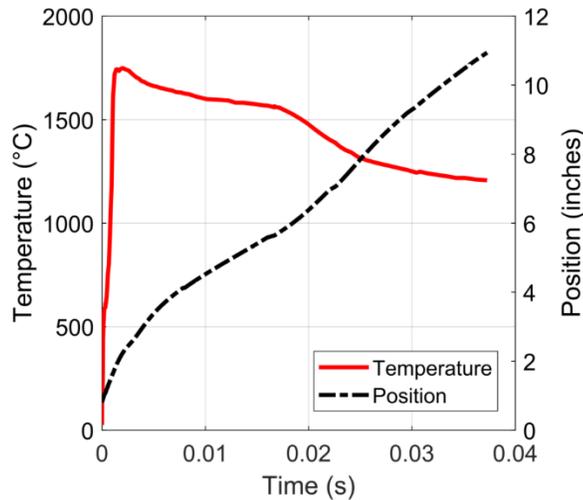
**Figure 5. Temperature contour (top) and velocity vector plot (bottom)**



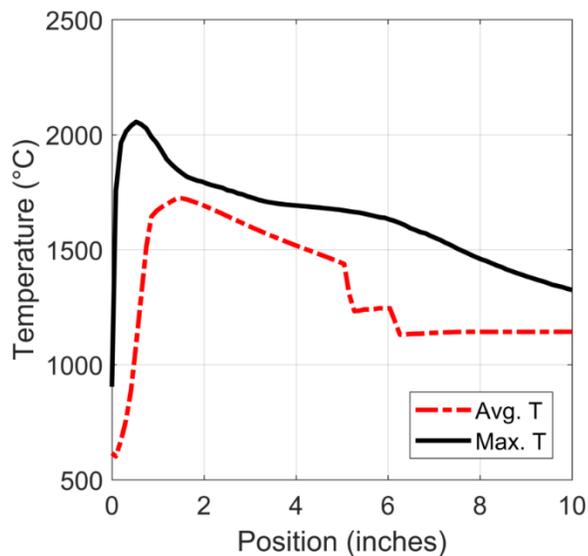
**Figure 6. Streamlines originating in the fuel plenum, colored by residence time**

Figure 6 shows the streamlines which originate in the fuel manifold. None of these streamlines enter the recirculation zone. A significant portion of the residence time shown in this figure occurs within the fuel manifold. Figure 7 shows the position and temperature of streamline trace as a function of residence time. This figure shows that the total residence time in the combustor is just under 0.04 seconds. At approximately 0.02 seconds of residence time the dilution flow is injected. As this mixes with the hot combustion gasses, the reactions in the flow will rapidly stop.

Figure 8 shows the temperature maximum and average of the combustion gases along the length of the combustor. This temperature plot indicates that the temperatures in the zones of maximum heat release are extremely hot. These temperatures are extremely localized burning over high concentrations of oxygen and fuel. It is important to realize that this is a RANS simulation and does not fully capture the unstable nature of the structures formed in the shear layer, which will affect the local maximum temperatures substantially. Average temperatures exceed 1700°C at approximately 1.75in from the injector plane. This temperature corresponds to the axial location at which the very little cooling boundary layer is present, as seen in Figure 5. The sharp changes in the average temperature profile seen at 5 and 6 inches are caused by the dilution flow injection.

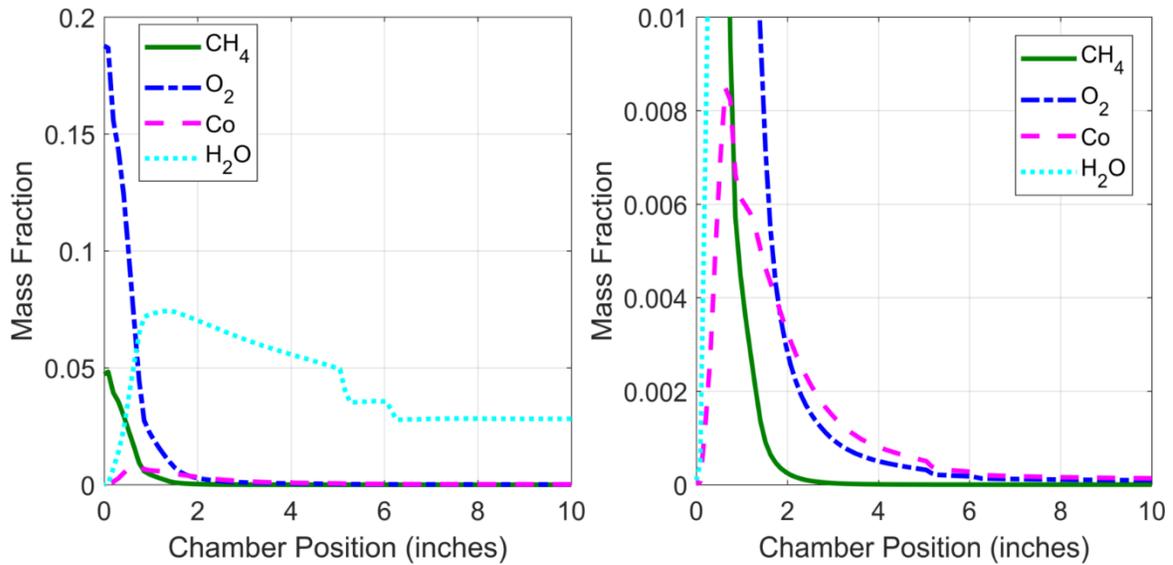


**Figure 7. Temperature and axial position as function of time**



**Figure 8. Average temperature and maximum temperature through the combustor**

Figure 9 contains the species mass fractions of some important species as function of axial distance from the injector face. In studying these graphs it is important to recall the amount of  $\text{CO}_2$  which is entering the combustor chamber through effusion and dilution. This means that the total mass flow in the combustor is increasing as the combustion progresses axially. Given the fairly long residence time of this combustor compared to the required chemical kinetics residence times it is unsurprising that most of the reactions and heat release occur within the first two inches of the combustion chamber. Carbon monoxide oxidation is the major exception to this. It is expected that CO oxidation is likely to be the governing factor determining the sizing of an oxy-fuel combustor for direct fired applications. Several different approaches can be taken to minimize the time taken to completely oxidize the CO. This may include operating with excess oxygen, insuring longer residence times, or higher temperatures.



**Figure 9. Species mass fractions as a function of axial distance. Right graph contains smaller mass fraction range**

## CONCLUSIONS

The rapid pace at which sCO<sub>2</sub> power cycles have advanced over the last several years is very promising in terms of near term commercialization potential. One of the most promising technologies associated with sCO<sub>2</sub> power cycles is the direct fired power cycle configuration. This configuration requires a unique combustor configuration capable of operating in a wide range of conditions. Demonstration of continuously operating direct fired oxy-fuel combustors for sCO<sub>2</sub> cycles is very limited in literature. A team of SwRI, Thar Energy, Georgia Tech, UCF, and GE is working to develop a 1MW thermal demonstration combustor.

This paper has provided a discussion of some of the requirements for such a combustor. A geometry example of such a combustor has been laid out in a high level of detail. This geometry discussion should be sufficient for the interested researcher to reconstruct the combustor geometry. This geometry is not the combustor geometry which will be built and tested at the 1MWth scale, due to its lack of detail in cooling, dilution hole patterns, combustor head contouring, among other areas, but is an example of a similar geometry which allows interesting conclusions to be drawn. In addition, three boundary condition cases which are considered important for study of sCO<sub>2</sub> oxy-fuel combustors are presented. The large differences in inlet density between the startup case and design point operation of this type of combustor pose a unique design challenge. It is hoped that this paper will encourage the further study of methods and novel techniques to allow for successful operation at these varied conditions. Limited modelling results from RANs simulations were presented. These results may allow investigators interested in chemical kinetics, and other areas of combustion research some context into which to place their studies.

This study provides a much needed description of the geometry and boundary conditions likely to be seen in a direct-fired oxy-fuel combustor for sCO<sub>2</sub>. While these boundary conditions and cases described are specifically for a 1MW thermal combustor, they can be scaled to larger or smaller scales as desired by interested researchers. It is hoped that this description will provide the basis from which many simulations can be performed and improvements to collaboration and progress in this exciting field can be achieved. It is hoped that others will utilize high fidelity simulation techniques to study the combustion process within this combustor design and benefit all those researching this field.

## ACKNOWLEDGEMENTS

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