Phase I Final Scientific Report

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Abstract

This Final Scientific Report addresses the accomplishments achieved during Phase I of DE- FE0023985, Coal Syngas Combustor Development for Supercritical CO_2 Power Cycles. The primary objective of the project was to develop a coal syngas-fueled combustor design for use with high-pressure, high-temperature, oxy-fuel, supercritical CO_2 power cycles, with particular focus given to the conditions required by the Allam Cycle. The primary goals, from the Statement of Project Objectives, were to develop: (1) a conceptual design of a syngas-fueled combustor-turbine block for a 300MWe high-pressure, oxy-fuel, sCO2 power plant; (2) the preliminary design of a 5MWt test combustor; and (3) the definition of a combustor test program. Accomplishments for each of these goals are discussed in this report.

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Executive Summary

The primary objective of this project was to develop a coal syngas-fueled combustor design to be utilized with high-pressure, high-temperature, oxy-fuel, supercritical carbon dioxide (sCO_2) power cycles, with particular focus given to the conditions required by the Allam Cycle, in order to lower the cost of coal-based power production with near-100% carbon capture below that of current state-of-the-art coal-based power systems without carbon capture.

The baseline cycle utilized to guide the development of this supercritical CO_2 combustor is the Allam Cycle, an advanced electric power generation cycle that provides a direct path to surpassing the Clean Coal Research Program's (CCRP) goal of a 20% reduction in COE compared to 1st Generation technologies. The Allam Cycle coal power system has the potential to produce electricity at a lower cost than existing coal and natural gas systems without carbon capture, and yet the system includes full carbon capture and eliminates all other air emissions such as SO_2, SO_3, NO_X and mercury.

The combustor required for cycle has not yet been developed for coal-syngas or fuel-flexible (e.g. low-Btu) applications, and thus the turbomachinery component demonstration proposed in this program is necessary to the continued development of these important power cycles. In particular, much of the Allam Cycle used for system-wide modeling in this program is already the subject of large R&D efforts or in commercial operation. For instance, the coal gasification and syngas cleanup steps utilized in this design are based on existing, commercial systems. Additionally, the core Allam Cycle is currently being demonstrated using natural gas as part of a 50MWth plant development effort. The combustor acts as a critical bridge between these two aspects of the overall syngas-fueled supercritical CO_2 cycle, and its demonstration acts as a gating step to move forward with further commercializing this cycle.

In Phase I of this project, (1) the conceptual design for a combustor to be utilized with a nominally 300MWe coal syngas-fueled Allam Cycle plant was developed, (2) a sub-scale 5MWth test combustor was designed and analyzed to confirm its feasibility and potential benefits, and (3) a test rig design and test plan to demonstrate the capability of the design were developed. Specific accomplishments in each focus-area include:

(1) The system designed in this project utilized the sCO_2 Allam Cycle as a baseline cycle to be coupled with coal gasification and syngas cleanup processes. A key technical rationale for this effort was to rigorously define expected combustor inputs from complete power cycle model. Four distinct operational configurations of the syngas Allam Cycle were developed, each utilizing a variety of gasifier configurations and post- or pre-combustion sulfur removal processes. In so doing, a variety of syngas compositions were obtained, the combustor-turbine environment was characterized, and specific combustor test parameters were developed. This data was then scaled to compositions, flowrates, and pressures appropriate for a 5MWt syngas test combustor.

(2) Based on the input streams determined by the system modelling in (1), full-scale and test articles were able to be conceptually and preliminarily designed utilizing sound engineering principles and best practices employed when designing similar components for industry-leading turbine OEMs. The combustor design involved four primary stages: (1) preliminary one-dimensional sizing, (2) multidimensional conceptual design, (3) preliminary mechanical design and analysis of combustor

components and (4) design validation using analytical models. A major focus of this project was to confirm the feasibility of this proposed combustor design, and this objective was achieved. The CFD analysis achieved the test combustor design goals and suggest a highly feasible design has been developed. Analysis demonstrates uniformity in the combustor Primary Zone. Due to this, combustor stability looks promising, but dynamic analysis and actual empirical test data will be required to verify transient state flame stability. CFD analysis also suggests a stable, efficient, well-mixed combustion environment by indicating a Primary Zone that achieves the targeted flame temperature, as well as a highly uniform temperature profile at the desired temperature (~2100 ^{o}F) at the combustor exit. Models also indicate the liner metal temperature will remain below the design limit (~1800 ^{o}F) and is uniformly distributed. FEA and thermal analysis showed that the test rig would be able to withstand 1,000 cycles before failure, and that the TBC coated liner is robust enough to handle the high gas temperatures during testing.

(3) A suitable and executable test plan was developed that includes key tasks, a proposed test site, key test personnel, a budget and time. Additionally, a test auxiliary rig was conceptually designed.

Experimental Methods

The overall approach of the project was to: (1) present a commercial-scale coal syngas-fueled supercritical cycle model; (2) use that model to determine combustor-turbine conditions and inputs and to develop a conceptual understanding of the commercial-scale combustor-turbine block; and (3) design a subscale test combustor, auxiliary test rig, and test program. This process was designed to ensure that the article to be ultimately built and tested is grounded in commercial system requirements. The methods and approach used in each of these aspects of the project is discussed in detail below.

300MWe System Conceptual Design

In order to define a commercially relevant combustor, combustor-turbine conditions and input streams (flowrates, pressures, temperatures, and composition) were derived from the development and process modelling of a complete commercial-scale, nominally 300MWe syngas-fueled sCO_2 power system. Process modeling was conducted in Aspen Plus version 8.8 with an Illinois No. 6 feedstock. All models reflect an Allam Cycle base configuration with full capture of $C0_2$. In addition, the models developed do not reflect fully optimized Allam Cycle coal system configurations. The rationale for this decision is that high-fidelity syngas compositions are critical to this combustor design and modeling effort. Further optimization might alter syngas composition in unintended or unknown ways, and thus models were developed that would provide known commercial syngas compositions, which required leaving the gasification island largely customized to the Allam Cycle.

An objective of this program is that the combustor for this system demonstrate the capability of utilizing a range of fuel compositions while maintain the desired combustion characteristics without requiring any alteration to the physical combustor. In order to evaluate this capability, the combustor design was analyzed across a range of fuel compositions reflecting both dry-feed and slurry-feed entrained-flow gasifiers, first with a pre-combustion sulfur removal system and second with a post-combustion sulfur removal process. The four test cases were as follows: (1) a dry-fed gasifier with pre-combustion sulfur removal; (2) a dry-fed gasifier with post-combustion sulfur removal; (3) a slurry-fed gasifier with pre-combustion sulfur removal; and (4) a slurry-fed gasifier with post-combustion sulfur removal. The cases are shown below in Table 1.

TABLE 1: FOUR PROCESS MODEL CONFIGURATIONS USED

Case	Gasifier Type	Clean-up	CO/H2 Ratio
1	Entrained flow dry-fed	Pre-combustion (AGR)	~2.4
2	Entrained flow dry-fed	Post-combustion (DeSNOx)	~2.4
3	Entrained flow slurry-fed	Pre-combustion (AGR)	~0.9
4	Entrained flow slurry-fed	Post-combustion (DeSNOx)	~0.9

The thermodynamic process modeling results provided input flowrates, temperatures, pressures and compositions for the combustor which were applied to the conceptual design of a nominally 300MWe engine. This combustor was preliminarily sized to accommodate the required heat release rate, flow rates, and residence time for the specified inlet and outlet conditions. A conceptual understanding of its integration with a turbine meeting the required conditions was also developed.

Coal Syngas Allam Cycle System Components and Modelling Approach

The Allam Cycle is a highly recuperated oxy-fuel Brayton cycle utilizing a recirculating, trans-critical carbon dioxide working fluid. A pressurized gaseous fuel is combusted in the presence of nominally pure oxygen prepared by a cryogenic air separation unit and a CO_2 diluent recycle stream at approximately 300 bar. The mix of combustion products and hot recycled CO_2 is then sent to a turbine where it expands to a pressure of approximately 30 bar. The expanded gas exiting the turbine is cooled against a recycle stream of sCO_2 within a high temperature recuperative heat exchanger. The exhaust is then cooled and combustion-derived water is condensed and separated at a water separator, leaving substantially pure carbon dioxide at approximately 30 bar and ambient temperature. The CO_2 stream is recompressed and pumped back to the recuperative heat exchanger to be heated and returned to the combustor at temperatures exceeding 649°C (1200°F). In order to maintain mass balance within the semi-closed cycle, a portion of the high purity carbon dioxide process gas is exported to a high pressure sCO_2 pipeline for transport to sequestration or utilization.

The syngas Allam Cycle requires several additional ancillary operations. The steps include: (1) solid fuel preparation and feed; (2) coal gasification; (3) syngas cooling and cleanup; (4) sulfur removal. The design and modeling approach for each is described below.

1. *Coal preparation and feeding system*

The parasitic load of coal grinding and milling is accounted in net system efficiency calculations in all four cases. For the dry feed gasifier cases (Case 1, 2), pure, ASU-produced nitrogen is pre-heated to dry the coal to 8% moisture using low-grade heat available from the gasifier. Moisture removal requires a heat consumption (per unit mass of water in the feedstock) of approximately 4260 kJ/kg (1830 Btu/lb). A lock-hopper system is used to transport the dry fine coal particles into the gasifier using CO_2 as the feeding gas. For the slurry feed system (Case 3, 4), a rod mill grinds the coal and wets it with treated slurry water. The dry solids concentration of the final slurry is 63%. A slurry pump is used to transport the coal slurry into the gasifier.

2. *Coal gasifier*

While nitrogen conventionally is used as a coal feeding gas in dry feed gasifiers, the Allam Cycle dry feed gasifier cases (Case 1, 2) employ CO_2 as the feeding gas in the lock hopper system, supplied from recycled CO_2 in the base cycle. Steam is used as a moderator gas in all four cases, as required. In the dry feed system (Case 1, 2), the syngas exiting the gasifier attains temperatures of approximately 3000F. For the slurry feed system (Case 3, 4), the syngas exits the gasifier at approximately 1900F.

3. Syngas cooling and cleaning

Dry and slurry feed systems utilize different syngas cooling and cleaning procedures. For the dry feed systems (Case 1, 2), a full water quench design is applied as the primary syngas cooling device, followed by a syngas scrubber to remove fine particulates and soluble impurities. The temperature of the syngas exiting the syngas scrubber is around 400F. For the slurry feed systems (Case 3, 4), a convective cooler is applied as a high-grade heat recuperation device. High temperature steam is generated in the convective cooler to transfer heat from the syngas to a stream of high-pressure CO_2. Following the convective cooler, syngas enters a particulate removal device, followed by a syngas scrubber to remove soluble impurities. The syngas temperature leaving the scrubber is about 340F. A secondary heat exchanger is applied for low grade heat recuperation in all four cases. Within the secondary exchanger, syngas is cooled to near-ambient temperature and condensed water removed in a steam knockout drum. In all cases a mercury removal unit is employed to remove heavy metal from the syngas following water separation. In the post-combustion sulfur removal cases (Case 2, 4), the syngas leaving the mercury removal unit is directed into a syngas compressor (exiting at ~300 bar) then sent to the syngas combustor for power generation. For the pre-combustion sulfur removal cases (Case 1, 3), the syngas leaving the mercury removal unit enters an AGR process before syngas compression and combustion.

4. Sulfur removal processes

Both pre-combustion AGR sulfur removal (Case 1, 3) and post-combustion DeSNOx sulfur removal (Case 2, 4) are modeled in this study. For cases employing AGR, a COS hydrolysis unit is added between the syngas scrubber and the secondary heat exchanger to convert COS to H2S with a conversion rate of 99.9%. The H_2S content in the syngas exiting AGR is ~0.1ppm. The H_2S removed by the AGR system is converted to elemental sulfur in the oxygen-blown Claus Process involving the partial oxidation of H_2S to form elementary sulfur as by-product. In the DeSNOx cases, both the COS hydrolysis and AGR processes are eliminated. In these cases, the downstream post-combustion water separator doubles as a special post-combustion reactive mass transfer device, simultaneously removing SO_X and NO_X formed in combustion, condensing combustion derived water from the CO_2 process gas, and cooling the process gas stream prior to recycle compression and pumping. Rigorous models and ongoing demonstration efforts predict a SO_X removal efficiency of ~99%, and a NO_X removal efficiency of ~90%.

Preliminary Design of a 5MW$_{th}$ Test Combustor

The 5MWth test combustor is a scaled unit meant to test the key operational parameters of the full-scale, 300MWe design. The following design goals were set for the 5MWth test combustor: (1) develop good mixing of fuel and oxidizer in the primary zone; (2) achieve the required exhaust gas temperature of 2100 °F with a uniform exit temperature profile; (3) meet an acceptable combustion liner temperature; and (4) observe uniform performance characteristics across the specific fuel combinations.

The design of a 5MWth test combustor utilized input data from the 300MWe system model, scaled to meet a 5MWth design. The combustor design incorporates the capability of using the range of inputs specified by each of the four syngas cases, as well as using natural gas (methane) for start-up and fuel-alternative purposes. As a result, all mechanical specifications were held constant across fuel combinations.

The combustor design involved four primary stages: (1) Preliminary One-dimensional Sizing, (2) Multidimensional Conceptual Design, (3) Preliminary Mechanical Design and Analysis of Combustor Components and (4) Design Validation using Analytical Models. Stage 1 utilized full cycle thermodynamic modeling data developed in Aspen Plus version 8.8 to specify key conditions of the combustor. Stage 2 involved preliminary sizing of the combustor to accommodate the required heat release rate, flow rates, and residence time to achieve the inlet and outlet conditions from the Aspen model. Stage 3 encompassed designing and modeling the individual combustor components and evaluating their functionality and integration into a package assembly. This process included identifying combustor elements such as the combustor liner, casing, injection pipes and nozzles, interfaces, etc. The last design stage was a computationally extensive step, requiring a Computational Fluid Dynamics (CFD) study to numerically analyze the design principle of the test rig combustor and predict the interior flow field behavior. The commercial code ANSYS FLUENT version 16.2, as well as ANSYS Design Modeler for 3D meshing and Pointwise for 2D meshing, were used to carry out the simulations. The purpose of the numerical analysis was to verify that the aforementioned design goals were being met.

Axisymmetric Model

The following sections describe the methodology behind the two-dimensional (2D) modeling approach and the associated results.

Modeling Approach

The axisymmetric model adopts geometrically simple assumptions which are expected to impact the combustor internal flow behavior. This simplification was necessary to inspect modeling methods and perform parametric studies in a computationally efficient manner. The 2D model was primarily used as an initial step in the CFD analysis and the results were essential in determining the final combustor design.

Geometry and Mesh

The geometry of the combustor was simplified by replacing the holes around the combustor can with slots of equivalent surface area. A structured mesh was created for the 2D model with 175K elements, consisting of mostly hexahedral elements. The commercial meshing tool Pointwise was used to generate the 2D geometry and mesh shown in Figure 1: 2D Axi-Symmetric MeshFigure 1.

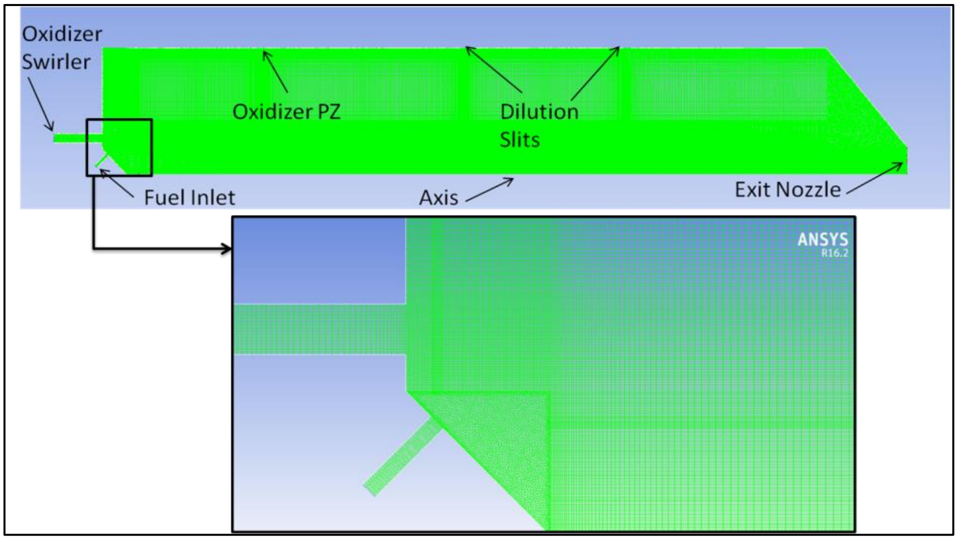


FIGURE 1: 2D AXI-SYMMETRIC MESH

Chemical Mechanism

Several mechanisms for the oxidation of CO-H2 exist in published literature. Temperature, species concentrations and flame structure are highly influenced by the accuracy of the detailed mechanism used, as Hilbert et al. emphasizes in a review on detailed mechanisms. To simulate the chemical reaction kinetics for this specific combustion system, an optimized kinetic model with 38 reactions and 14 species for the oxidation of CO-H2 was employed. The mechanism will be referred to as the USC mechanism in this report. The employed mechanism was validated against a wide range of experimental conditions and was found to perform well over an extended pressure range of up to 87 atm. In particular, CO oxidation rates were found to be accurately predicted by the model up to 10 atm. The mechanism, however, is not validated for the conditions of this combustion system and thus it is necessary to validate the simulation results with experimental data as they become available.

Reactor Network Model

A reactor network model was used for a more accurate estimation of exhaust gas (exit) CO emissions. The model automatically divides the flow domain into a network of perfectly stirred reactors. Cells with similar temperature and mixture fractions are grouped together forming clusters. The clusters with the smallest number of cells are combined with their closest neighbors until the specified number of reactors is obtained.

Simulations employing the reactor network model require a detailed chemical mechanism for estimating species mass fractions. The USC mechanism was used for fuel containing CO, H2, and CO2 and the skeletal mechanism proposed by Smooke was used for the fuel blends containing methane. The model also predicts temperature in each reactor based off the equation of state. Density is assumed constant as the volume and mass in each reactor are fixed.

Turbulence–Chemistry Interaction Models

In order to account for turbulent-chemistry interactions, the Eddy Dissipation Concept (EDC) model was employed for majority of the cases reported in this study. The EDC model has been widely used in a number of applications, and results have agreed well with experiments over relatively low pressure ranges. Moreover, validation studies are not available for combustion models at 300 bar. The Probability Density Function (PDF) model was also used to compare results and for cases containing methane in the fuel stream. The EDC model is computationally expensive, therefore, to substantially reduce run times, the In-situ Adaptive Tabulation (ISAT) algorithm was employed.

Radiation Approach

To analyze the radiation from the combustion flame, the radiative transfer equation (RTE) was solved using the P1 radiation model which is adequate for the optically thick medium being investigated. This model is an efficient estimate of radiation heat transfer; final design cases may use the Discrete Ordinates (DO) model. The gas-phase absorption coefficient was estimated using a weighted sum of gray gases model (WSGG); this model was compared to absorption coefficients at 300 bar at the applicable temperature range, and compared well. The flow is convection-dominated and thus the impact of the gas-phase radiation model on the overall result is small, so only a reasonable estimate of radiation is required.

Solution Method

The elevated pressures at which this combustor operates, necessitates the use of appropriate models and discretization schemes to adequately estimate the flow and fluid properties. There is limited understanding of combustion in such high pressure systems and a lack of experimental data to validate numerical models.

For that reason, the models were carefully chosen to achieve accurate CFD predictions that were not computationally intensive. FLUENT version 16.2 was used to model the combustion cans. A Reynolds Averaged Navier-Stokes (RANS) steady state-solver was used to perform the calculations. The realizable k-epsilon model was used to model turbulence. This two equation model is computationally advantageous and was validated for highly swirling flows. The coupled pressure-velocity numerical method was used for solving the governing integral equations. The PRESTO scheme was used for pressure interpolation which is known to perform better under swirling flows (10). The final solution for all the cases reported in this study was obtained using the second order upwind discretization scheme. Convergence for all cases was reached by using the following criteria

- Overall mass and energy balances are achieved
- The solution no longer changes with subsequent iterations
- Scaled residuals have all decreased by at least three orders of magnitude and scaled-energy residuals have dropped to 10^{-6}
- Exit CO levels are invariable with further iterations

3D Rotationally Periodic Model

Modeling Approach

The approach taken for setting up the 3D model geometry was to replicate the flow behavior as seen in the 2D axi-symmetric model.

Geometry and Mesh

Taking advantage of the symmetry in the geometry of the combustor, a 60 degree section of the combustor was modeled using Space Claim. An unstructured mesh was generated using ANSYS DM comprising of 967K tetrahedral cells. The unstructured mesh was converted entirely into a polyhedral mesh in ANSYS FLUENT reducing the mesh size by a factor of 5.3 resulting in 182k discrete cells. Polyhedral meshes are advantageous in that they offer 2 to 3 times faster solution with similar or improved accuracy compared to tetrahedral meshes. A grid sensitivity study was performed and confirmed that the results in this report are mesh-independent.

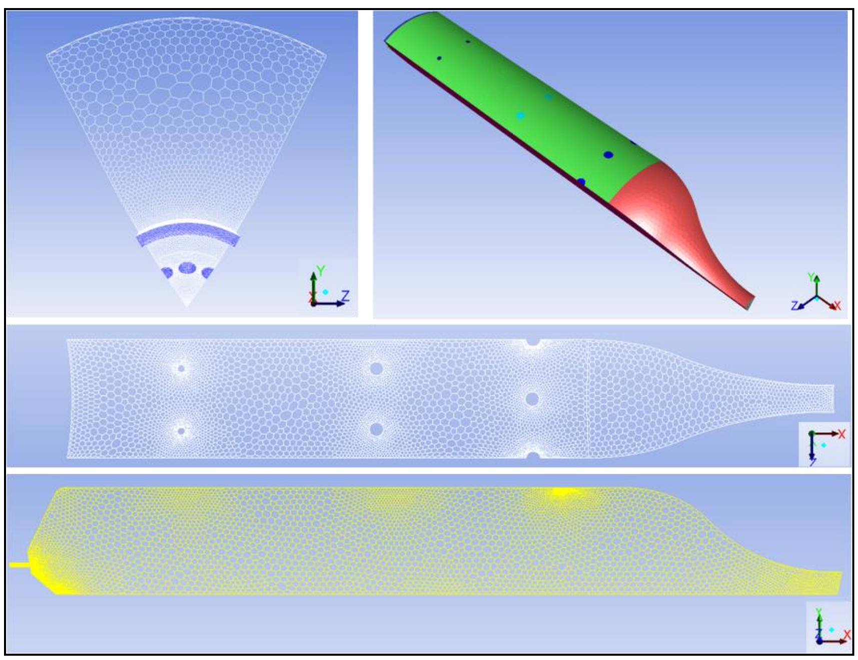


FIGURE 2: ROTATIONALLY PERIODIC GEOMETRY AND MESH

Full 3D Model

A solution from a full 3D model was computed to compare with the rotationally periodic model. The main reason for this investigation was to ensure the rotationally periodic model was set-up correctly. Several variables were compared and revealed that the overall flow pattern inside the combustor remained unchanged with the full 3D model. Thus, the rotationally periodic model was determined to be a valid representation of the full model, which allowed for a more efficient computational time.

Chemical Kinetics

The same chemical kinetics mechanism (USC mechanism) described in the 2D axisymmetric model was used on the 3D Periodic Model.

Turbulence–Chemistry Interaction Models

The EDC model was used for describing the chemistry-turbulence interactions.

Radiation Approach

The RTE was solved using P1 radiation model.

Solution Method

The same solution method was followed as described in the 2D axisymmetric model.

Alternative Fuel Blends

Two of the cases investigated here contain methane which necessitated the use of a different reaction mechanism. Most chemical reaction mechanisms are designated for a specific fuel type and would not be accurate enough if used for a mixture of fuels. For this reason, the non-adiabatic extension of the equilibrium Probability Density Function (PDF) model was used to carry out the simulations reported in this section. In this model, the chemistry-turbulence interactions are described using the PDF table where the average value of the scalars is related to their instantaneous fluctuating values. The model is referred to as PDF herein and is based on the mixture fraction assumption. Under the assumption of chemical equilibrium, species fractions, density and temperature are all uniquely related to the mixture fraction. The mixture fraction and enthalpy data points are calculated prior to performing the simulations and saved in a 3D PDF table and are used in the calculations to describe the instantaneous thermochemical state of a fluid. The benefit of this model is that the species concentrations are determined by solving only one conservation equation for the mixture fraction. The assumption of equal mass diffusivities reduces the mixture fraction into a "source-less" conservation equation due to elemental conservation. The combustion system in this study has three inlet streams which required the use of two mixture fractions. The primary mixture fraction describes the fuel stream, and the secondary mixture fraction is used to describe the dilution CO_2 stream. Twenty chemical species were considered in the equilibrium calculations and a beta function was used to describe the shape of the PDF.

Test Program Definition

The test program was advanced through the development of: a testing plan, schedule, and budget; the preliminary design of the auxiliary rig system required to conduct the test; and the selection of a suitable test site. A schedule was developed in Microsoft Project that includes all required activities to move from the end of Phase I through the successful completion of testing. A budget was developed by designing the overall test rig, plan and schedule, and then working with vendors to develop quotes and estimates for the necessary equipment and work required. A site was selected through the issuance of a Request for Proposal (RFP) and then the completion of an analysis using fifteen weighted criteria to compare and rank each test facility, which are outlined in Table 2.

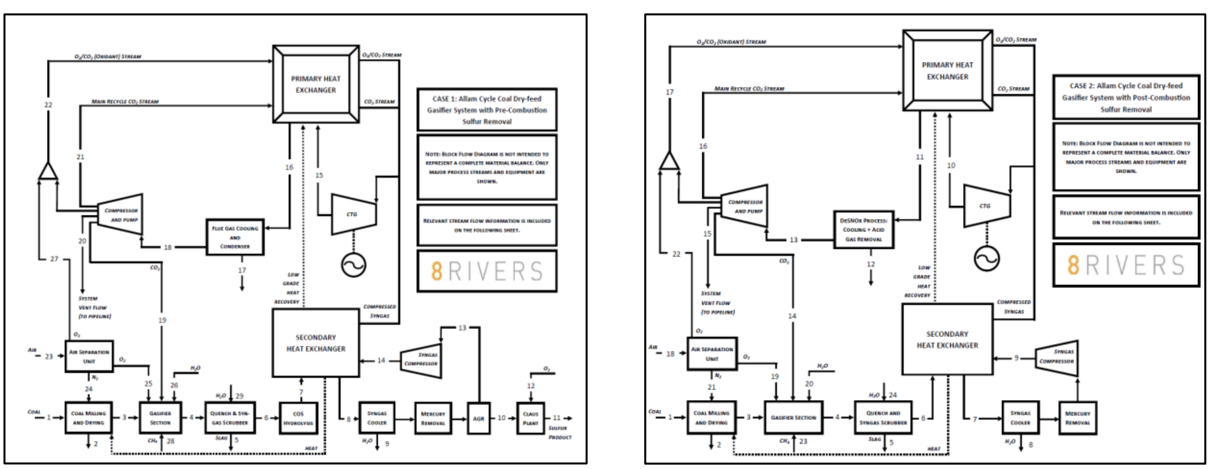
TABLE 2: TEST SITE SELECTION CRITERIA AND WEIGHTING

Selection Criteria	Prioritized Weighting
Customer Desirability	15
Cost Analysis	14
Availability	13
Control/Data Acquisition Systems	12
Cost-Share (External funding)	11
Existing Equipment/Infrastructure	10
Experience/Qualifications	9
Safety	8
Staffing/Technicians	7
Building Structure/Space Constraints	6
Planning Availability	5
Physical Location	4
Noise Constraints (120~140 dB)	3
On-Site Shop	2
Loop Facility (CO2 Recycle)	1

Results and Discussion

300MWe Conceptual Design

Four 300MWe cycle cases were successfully designed and modeled, providing the necessary input streams to size and design the full-scale and test combustor. Net electric efficiencies ranged between 39.8% (HHV) and 44% (HHV). <u>**These cases are non-optimized, but of higher fidelity than more optimized cases. Much higher efficiencies, approaching 50%, have been demonstrated by 8 Rivers and others as achievable with this sCO_2 cycle; however, these cases require further modification of the gasifier island. For the purpose of developing combustor input streams, though, gasifier island optimization was minimized in order to ensure the highest-possible-fidelity syngas compositions were produced.**</u> As predicted, the dry feed cases provided the highest CO/H_2 ratio, while the slurry feed cases provided the lowest. Flow sheets can be seen in Figure 3 below. Performance results are shown in Table 3.



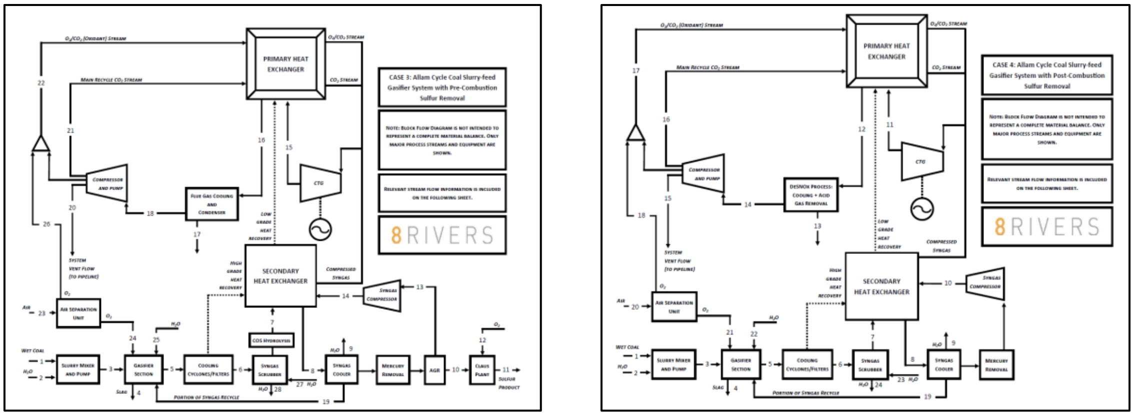


FIGURE 3: BLOCK FLOW DIAGRAMS FOR FOUR CASES

TABLE 3: FOUR NON-OPTIMIZED PROCESS MODEL CONFIGURATIONS USED IN PHASE 1

Energy Components	Case 1 Dry/Pre	Case 2 Dry/Post	Case 3 Slurry/Pre.	Case 4 Slurry/Post.
Thermal input (MW)	670	645.5	699.5	672.9
Cold Gas Efficiency (%HHV)	81.7%	81.7%	78.8%	78.8%
CO/H2 ratio	2.4	2.4	0.9	0.9
Gross Turbine Output	63.9%	66.3%	61.9%	64.3%
Compressor and Pump Parasitic Power	-13.1%	-12.8%	-13.2%	-12.2%
Plant Parasitic Auxiliary Power	-9.7%	-9.5%	-8.9%	-9.3%
Non-Optimized Net Elec. Eff. (HHV)	41.1%	44%	39.8%	42.8%

Based on combustor inputs from these models, a conceptual design for a 300MWe combustor was defined. Taking the turbine inlet conditions and maintenance requirements for a commercial unit into consideration, this led to a can-annular configuration with six film-cooled cans.

Preliminary Design of a 5MW$_{th}$ Test Combustor

Results Overview

The baseline fuel case employing the EDC turbulence-chemistry interaction model was used first for analyzing internal flow field of the combustor. Figure 4 shows temperature contours for the middle-plane and for a plane oriented 15 degrees from the middle plane. The temperature contour of the exit plane shows a uniformly distributed temperature with an average of 2,116 °F.

Figure 5 shows contours of density, pressure and velocity for the baseline case. No significant pressure variations are observed in the combustor as can be seen from the pressure contour plot. The velocity contour shows the nozzle flow is choked with velocity close to 2000 ft/s. The average velocity inside the combustor volume is close to 55 ft/s. For a better visualization of cross-section planes, the full 3D contour plots are shown in Figure 9 by applying the periodicity factor 6 times. The tangential velocity at multiple cross sections is shown in (a). The flow from the swirler creates a strong recirculation zone which can be observed in (c) through the annulus with negative axial velocity in the primary zone plan.

Figure 6 shows temperature contour plots for the four variations in fuel types employing the PDF model. The flame temperature predicted was slightly higher than 3600°F for all cases. No significant variations in the predictions were observed.

Figure 7 shows the temperature plot along the centerline of the combustor. The four plots converge and follow the same trend in the dilution zone which is expected due to the dilution jets penetrating the center. The 2.45 CO/H2 Syngas mixture produces a temperature plot that is almost identical to the Syngas mixture with 0.94 CO/H2 ratios. The fuel mixtures containing methane are injected at a 400 °F as opposed to 158°F (syngas inlet temperature) which explains the difference in the temperature plots near the front end of the combustor.

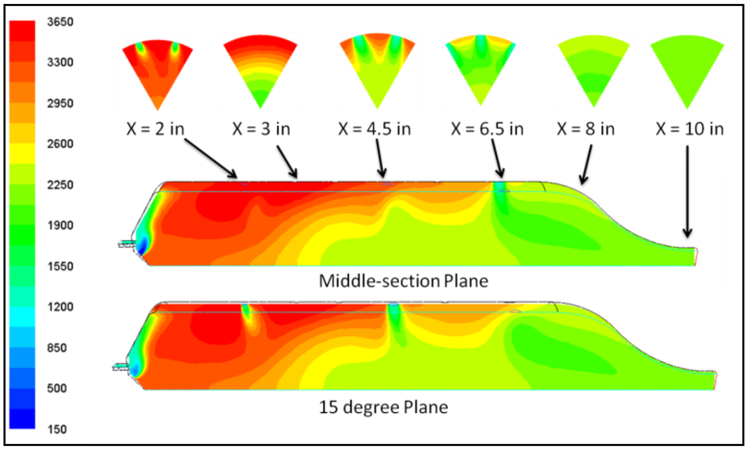


FIGURE 4: TEMPERATURE CONTOURS FOR BASELINE FUEL EMPLOYING EDC MODEL

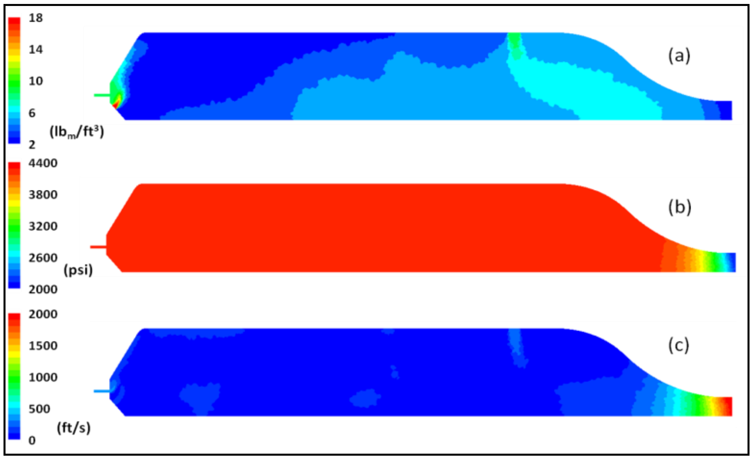


FIGURE 5: DENSITY (A), PRESSURE (B), AND VELOCITY CONTOURS ALONG CENTERLINE FOR BASELINE FUEL

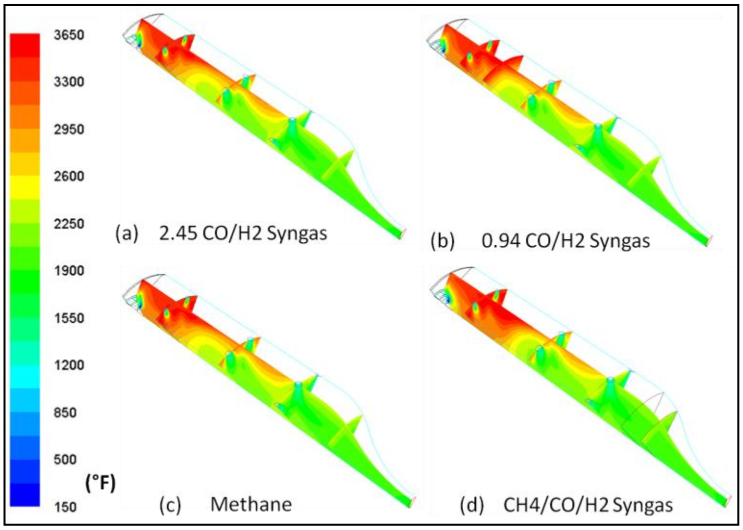


FIGURE 6: TEMPERATURE CONTOURS FOR FOUR FUEL VARIANTS USING THE PDF-EQUILIBRIUM MODEL

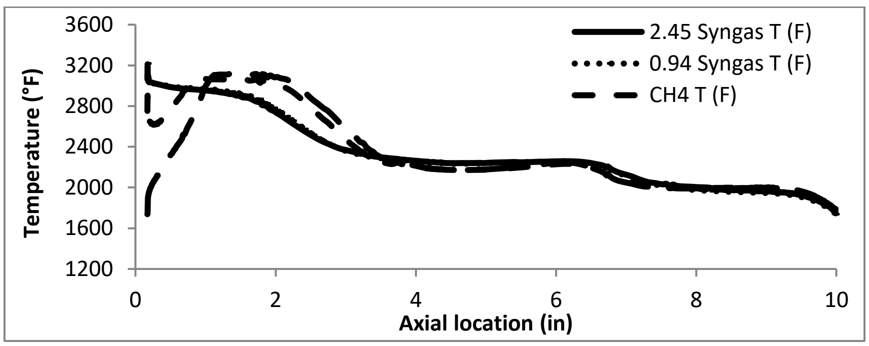


FIGURE 7: CENTERLINE TEMPERATURE PLOTS FOR FOUR FUEL BLENDS

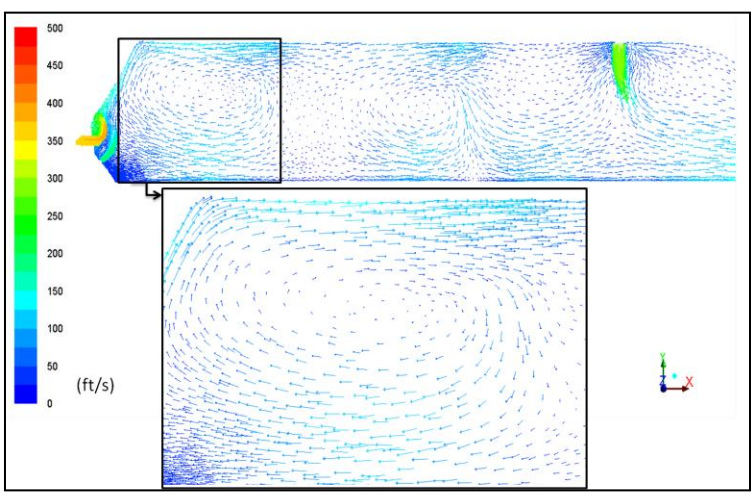


FIGURE 8: VELOCITY VECTORS SHOWING RECIRCULATION ZONE ALONG CENTER PLANE

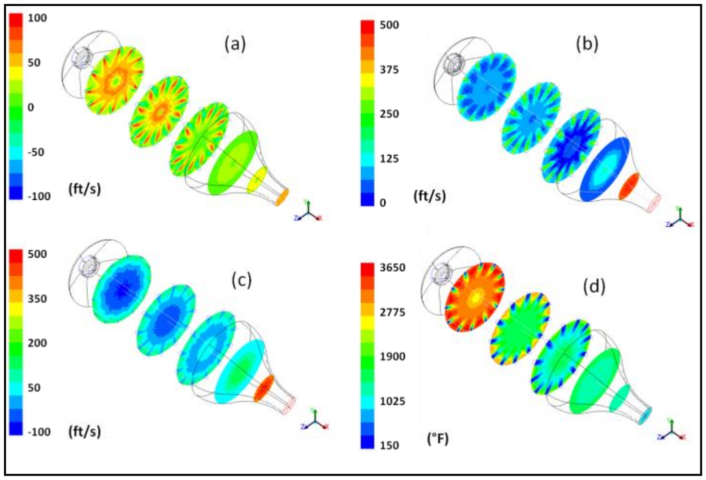


FIGURE 9: TANGENTIAL VELOCITY (A), VELOCITY MAGNITUDE (B), AXIAL VELOCITY (C) AND TEMPERATURE (D) CONTOURS OF SEVERAL CROSS SECTIONS

Fuel and oxidizer were very well-mixed in the primary zone.

2D and 3D CFD model predictions indicate well-mixing of fuel and oxidizer. No significant temperature or pressure variations in the primary zone are characteristics that support high combustor stability. In order to avoid excessive pressure and temperature fluctuations when H2 and O2 are burned, the gaseous fuel and the oxidizer are both diluted with CO2 to limit adiabatic flame temperatures to 3600 °F at the equivalence ratio of 0.99. The combustor primary zone (PZ) at the front half of the combustor is where the combustion reactions take place in a near uniform 3600 °F.

The desired exhaust temp. was met with a highly uniform temperature profile.

The last half of the combustor is the dilution zone (DZ) where CO_2 is injected to lower combustion gas temperatures to 2100 °F with a very uniform profile, indicating that damaging hot streaks, which are a major concern with combustor development for gas turbines, will not occur.

The liner experienced an acceptable temperature.

Carbon dioxide has a high heat capacity, which means it is a suitable fluid medium for heat transfer. This thermophysical property makes it ideal to cool the combustor liner walls. However, there are limitations on the amount of heat that the CO_2 can remove from the liner. To satisfy liner material limitations, a ceramic thermal barrier coating (TBC) will be plasma sprayed to the hot side walls (inside) of the combustion liner. Analysis showed that liner metal temperature is below the limit and uniformly distributed. The near-wall heat transfer model shows TBC running with a high surface temperature. Minor design modifications will be tested to achieve a lower TBC surface temperature. Given expected short test durations, TBC temperatures are not considered to be an issue.

Analysis across fuel types showed highly consistent combustor characteristics.

The combustor appears capable of using a range of fuels without any hardware changes. By adjusting the fuel mix to dilution CO_2 ratios for each fuel, adiabatic flame temperatures were maintained at the desired 3600 °F and combustor exit temperatures remained 2100 °F.

Other promising characteristics were also observed.

The design allows for the use of a very stable diffusion flame injector. The swirl-stabilized diffusion flame permits a wide range of stable operating conditions from ambient start-up to 300 bar at design point pressures and temperatures. Additionally, the inlet temperature of the oxidizer and diluent is above fuel auto-ignition levels, which contributes to flame stabilization. The flame zone is near the fuel injector and combustion occurs as oxidizer and fuel mix near the front of burner. Additionally, at stoichiometric conditions, CO levels were below 10ppm with less than 1% O2 in the exhaust.

Near-Wall Heat Transfer

Backside convective wall cooling will be applied along the combustor liner in the test-rig. A simplified conjugate heat transfer model was formulated to simulate the heat transfer along the combustor liner. The cooling effects were simulated only on the section of the liner exposed to high temperature. The free stream coolant temperature applied was that of the CO2 at 1343 °F. The convective heat transfer coefficient was estimated taking into account the geometry of the fins, the hydraulic diameter of the liner, and the relevant thermal properties of CO2. A thermal barrier coating (TBC) with a 0.02" layer thickness will be applied on the interior side of the liner. The metal layer thickness is 0.157". Figure 10 shows the gas temperature along the liner, the average TBC temperature and the average metal temperature. Alternatively, Figure 11 shows the hot surface temperature of the TBC and Metal. The plots show that the TBC temperature is high and exceeds the limit of commercial applications of TBC materials, but the temperatures are not viewed as an issue for the limited design life of this test article. Several design considerations could also potentially reduce TBC temperature to even lower levels, if it is deemed necessary.

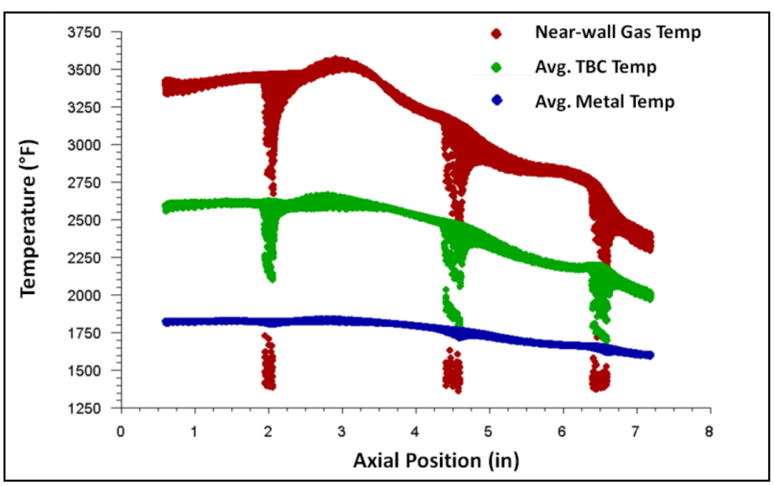


FIGURE 10: TEMPERATURE PLOTS SHOWING THE EFFECT OF WALL COOLING ON METAL AND THERMAL BARRIER COATING TEMPERATURES

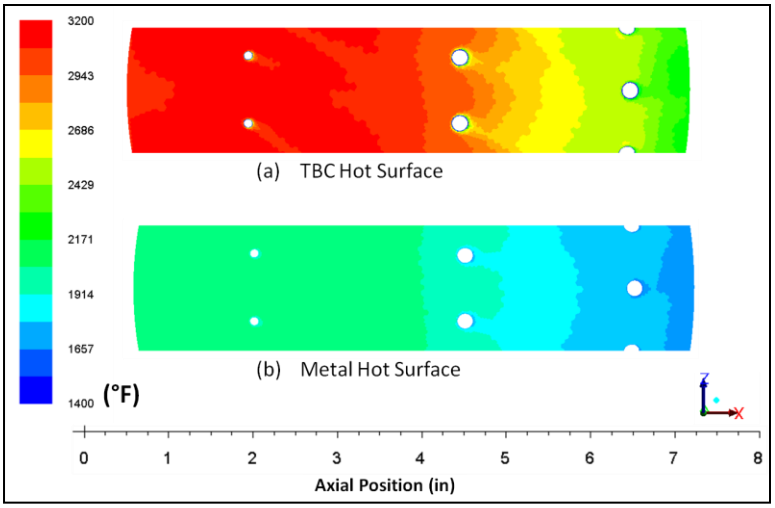


FIGURE 11: TEMPERATURE CONTOUR PLOTS FOR THE HOT SURFACE OF THE TBC (A) AND METAL (B)

Prediction of CO Levels

It is desired to minimize the carbon monoxide (CO) levels in the combustion product stream (exhaust) in order to maximize the efficiency of the combustion cycle. CO levels are very difficult to predict accurately with CFD in conventional gas turbine combustors at low pressures. Due to limited testing, there is a restricted understanding of how to predict CO levels at high pressures, such as the conditions required for the Allam Cycle (300 bar). The best available chemical kinetic model is not validated at 300 bar, but predicts a very fast reaction rate at 300 bar, where syngas fuel is converted very quickly to combustion products.

The Aspen model equilibrium CO levels are very high (~6,000PPM) at near maximum temperatures (3600°F) in the Primary Zone. Therefore, the CO CFD predicted levels are high in that zone as we knew they must be. We also know the equilibrium CO levels are high (~700PPM) at 2900°F which is the normal CO burnout range for ultralow emissions combustors. This is due to the high CO2 makeup of the combustion products. We also know that equilibrium CO levels at 2100°F for this mixture at 300 bar is near zero (~3 PPM).

The CFD code has predicted high levels of CO (>100PPM) at 2100°F burner exit conditions. Table 4 summarizes the combustion product species concentrations as well as temperature at the exit nozzle. The concentrations reported are obtained using the reactor network modeling option in FLUENT which has been used successfully to replicate experimental trends for CO emissions. The analysis yielded lower CO prediction levels by running a case with a 0.9 equivalence ratio. One of the unknowns for this combustion process is the time to reach equilibrium CO values at 300 bar pressure. The ASPEN model and CFD models agree on what the equilibrium CO values are, so the remaining issue is determining how quickly equilibrium is achieved. It should be noted that the full size engine combustor will have approximately four times as much residence time to reach equilibrium CO levels.

TABLE 4: TEMPERATURE CONCENTRATIONS AND EXHAUST TEMPERATURE RESULTS FOR ALL NINE CASES

Case	Type of Fuel	Dilution CO_2 Temp (°F)	Chemistry model	Exhaust Gas Temp(°F)	CO ($*10^{-6}$) mass fraction	O_2 ($*10^{-6}$) mass fraction	H_2O (% mass)	CO_2 (% mass)
1	2.45 Syngas	950	EDC	2,130	486	468	1.68	98.2
2	0.94 Syngas	950	EDC	2,137	350	380	3.14	96.8
3	2.45 Syngas	1343	EDC	2,116	385	397	1.29	98.6
4	0.94 Syngas	1343	EDC	2,123	233	307	2.39	97.6
5	CH4	1343	PDF	2,040	468	446	2.79	97.1
6	CH4/CO/H2	1343	PDF	2,029	85	644	2.88	97.0
7	2.45 Syngas	1343	PDF	2,020	199	255	1.30	98.7
8	0.94 Syngas	1343	PDF	2,020	106	281	2.37	97.6
9	2.45 Syngas (Phi = 0.9)	1343	EDC	2,134	9	3,920	1.27	98.3

Combustor Mechanical Design Results

A full mechanical design for the full test combustor was completed. The design included the creation of a 3D solid model and engineered drawings using ANSYS Spaceclaim. Figure 12 depicts a conceptual view of that combustor. Design elements included: primary liner; cooling liner; ribs along liner for cooling; primary oxidizer flange interface; support flange at aft end; primary oxidizer swirler; dilution hole supplies; exit nozzle; pressure vessel; clamping ring and bolts for liner; isolation ring; clamp connectors; supply line interfaces.

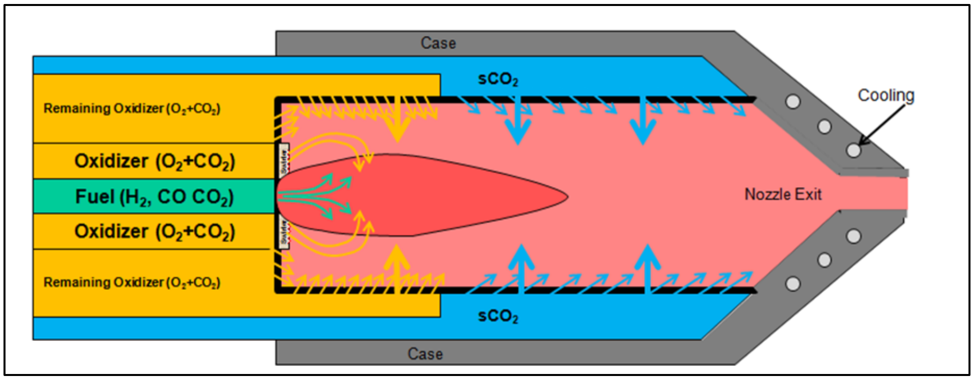


FIGURE 12: CONCEPTUAL VIEW OF THE COMBUSTOR DESIGN

Geometric parameters and materials were analyzed for individual components. A thermal-mechanical analysis was employed on a simplified geometry of the combustor to explore the current life cycle capabilities of the liner. The design of the combustor incorporates instrumentation to capture static and dynamic measurements including combustor pressures, temperatures, dynamics, and chemistry at numerous points throughout the test article. Turbomachinery manufacturers were contacted and confirmed manufacturing feasibility.

Hardware Lifetime Requirements

The mechanical integrity and survivability of the combustor for the commercial application is a primary focus to ensure reliable, safe operation and commercialization. Key components that are subject to severe loading are the combustor casing (pressure containment) and the liner, which can be likened to a pressure vessel. Stress and heat transfer analyses were conducted in order to design the overall combustor assembly.

For the test article, developing a combustor liner that will survive through the test campaign has been established. Survivability of the liner through extended life is not a target of the test campaign but will be a primary target for the commercial combustor. The information gathered from the liner after the test campaign will aid in calibrating the scaled model for commercial combustor development.

Finite Element Analysis (FEA)

A thermal-mechanical analysis was employed on a simplified geometry of the combustor to explore the current life cycle capabilities of the liner. A 2D cross section was taken of the liner at an upstream location less than 2 inches from the dome. Using ANSYS Mechanical, boundary conditions were applied.

As found in the analysis from Figure 13 and Table 5, the stresses observed in the liner are above the target limits for 1000 hour lifecycles in Haynes 230 at the reviewed operating temperatures. However, exploring the results further, the high notch stresses at the fillets are mainly driven by the temperature gradient and are therefore to be treated as secondary stresses. Their main impact on the life of the liner is Low Cycle Fatigue (LCF) damage. Secondary stresses are self-equilibrating stresses and should not be compared against the Ultimate Tensile Stress or Yield Stress, since they do not cause structural collapse or rupture. An estimation of the LCF life for 77.6 ksi at 1520 ^{o}F was completed and found that neglecting the secondary stresses, the liner should be able to undergo 1,000 cycles before crack initiation. Therefore, it is our assessment that the fillet stress concentrations are not critical to the life of the combustor liner for the purposes of this test article, and thus they are allowable.

The creep life should be assessed based on the pressure stresses (primary stresses) only. A 1-D simplified estimation was completed with assumptions about the radial temperature gradient and the fins. It is found that 1000 hours creep life is feasible with the pressure stresses found through FEA. A more thorough analysis is planned for future work.

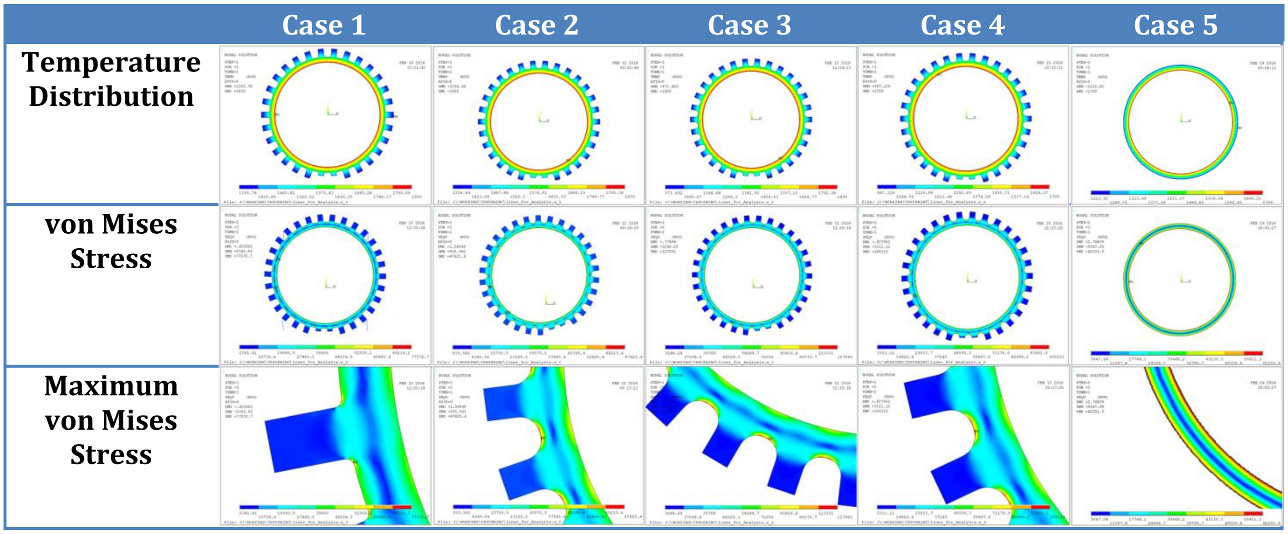


FIGURE 13: THERMAL-STRESS ANALYSIS

TABLE 5: BOUNDARY CONDITIONS AND RESULTS

Description	Case 1	Case 2	Case 3	Case 4	Case 5
Inner Liner Temp [°F]	1850	1850	1850	1700	1700
Cool Side Bulk Temp [°F]	1300	1300	950	950	950
Liner Material	HA230	HA230	HA230	HA230	HA230
Rib Fillet [in]	0.025	0.095	0.095	0.095	None
Cool Side Temp [°F]	1356	1358	971	967	1216
Max vonMisis Stress [ksi]	77.6	67.6	127	105	62.2
Temp at Max Stress [°F]	1520	1560	1300	1230	1700
Ultimate Tensile Strength [ksi]	60	55	88	88	35
Yield Strength [ksi]	40	38	45	45	26
Time to Rupture [hr]	<10	<10	<10	<10	<10
Target Stress for 1000hr with 1% Creep [ksi]	9	8	13	11	4

Thermal Analysis

The CFD simulations show near-wall gas temperatures slightly above 3000°F in the combustor primary zone. To cool the combustor liner, back side convection cooling is employed through use of the dilution CO2. The rig combustor cooling will be more aggressive than the larger commercial unit because CO2 injected into the system will be at a lower temperature of 950°F and the CO2 temperature for the commercial engine from the recuperator will be approximately 1350°F. An yttria-stabilized zirconia (YSZ) thermal barrier coating (TBC) is commonly used on combustion systems to help reduce metal wall temperatures and prolong life of the hardware.

A wide range of TBC and liner wall metal temperatures can be obtained by varying the TBC coating and backside coolant temperature for estimated heat transfer coefficients on hot and cold side of combustor walls (2020 Btu/Hr/ft^2/°F hot side (with CFD confirmed small flame radiation term included) and 5950 Btu/Hr/ft^2/°F). As shown below, for the rig with a 0.020 inch thick YSZ TBC, the metal temperature varies from 1730°F at the base coat interface, 1070°F on cold side of metal, and maximum TBC surface temperature of 3140°F.

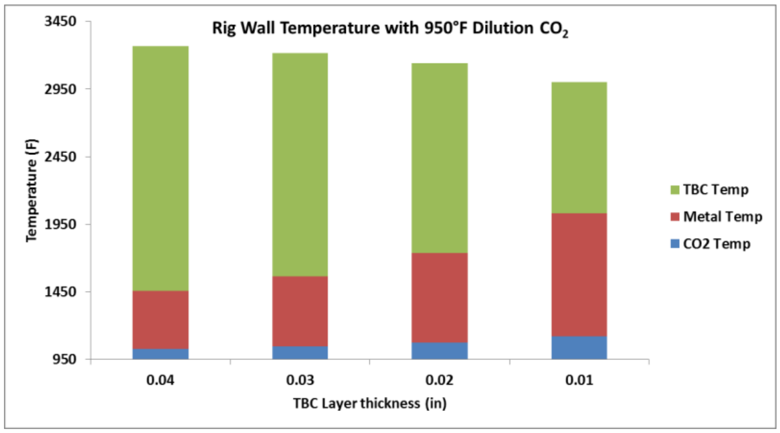


FIGURE 14: RIG WALL TEMPERATURE WITH 950°F DILUTION CO_2

For engine conditions with a warmer diluent CO2 of 1350°F, a thicker TBC is needed to achieve reduced metal temperatures. As shown below for a 0.040" TBC, the metal basecoat interface is 1775°F, the liner metal cold side is 1420°F and the TBC surface temperature is 3300°F. Combustor durability is impacted by large thermal gradients between the hot and cold sides of the TBC and liner metal walls.

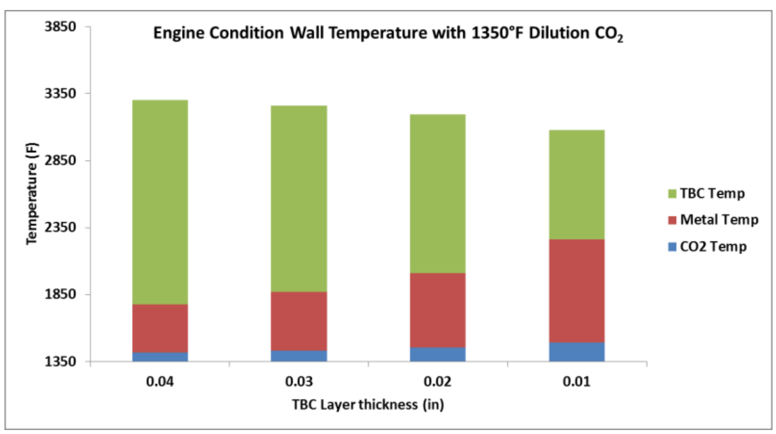


FIGURE 15: ENGINE CONDITION WALL TEMPERATURE WITH 1350°F DILUTION CO_2

The YSZ TBC hot surface is running at very high temperatures (>3000°F) for both rig and engine CO2 coolant levels which is well above typical levels.

The YSZ melting point is 4900 °F; however, the lattice structure changes from tetragonal to cubic for the TBC at temperature levels above 2500 °F, and porosity is reduced with time. The coating becomes more brittle after exposure for approximately 100 hours for fully stabilized with 7.5% yttrium oxide (Y2O3). From the material phase diagram, the lattice structure doesn't change to cubic until 3300°F for 5% Y2O3. As shown in the above plots, roughly half of the TBC layer will be above 2500°F while none of the TBC will exceed 3300°F. This could suggest using partially stabilized 5% Y2O3 to reduce sintering issues associated with a structural change.

While the conditions exceed typical temperature levels, the rig testing can be accomplished with the YSZ TBC for short term proof-of-concept testing at max power; the extended lifetime requirements for the commercial scale combustor will require greater heat transfer at the combustor liner walls, which can be achieved through changes in the flow field. In addition to the anticipated changes associated with a larger volume, the effects of swirler and fuel injector changes and a modified pressure drop will be investigated to center the flame zone closer to the combustor centerline to reduce near wall temperatures and velocities. Film cooling can be introduced as a method to extend the combustor and TBC life on the large scale combustor and test rig.

Film cooling was studied as a potential cooling mechanism. The existing back side convection cooling with the addition of a CO2 film cooling flow produced the TBC temperatures seen in Figure 15. The film effectiveness was conservatively estimated, as it depends strongly on the hot gas flow conditions. Further analysis will be conducted in in future programs through more comprehensive CFD modeling. Considering a maximum TBC surface temperature of approximately 2300 °F, the film is good for approximately 2.3 inches running length. A second film slot should then be needed to maintain life requirements.

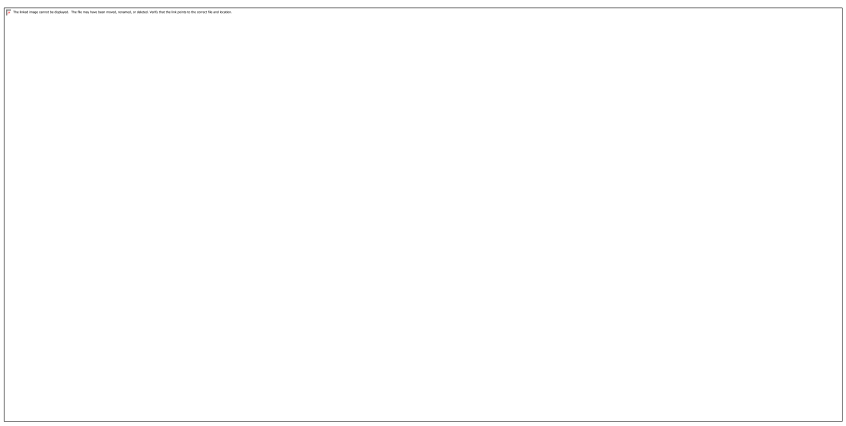


FIGURE 16: FILM COOLING STUDY

Test Program Definition

Test Plan, Schedule, Budget

The test program definition resulted in the successful development of a test plan, schedule, and budget. The test program is expected to take approximately 2 years. The preliminary Test Case Matrix can be seen in Table 6.

TABLE 6: TEST CASE MATRIX

Test Case	Goal of Test	Methods	Success Criteria
Ignition Test	Determine Ignition Characteristics	Attempt ignition at various values of fuel/oxidizer ratios. Repeat procedure for range of mass flows until an ignition loop can be characterized.	Successful ignition indicated by continued burning after ignition source is switched off.
Start-Up Test	Observe combustor performance during start-up conditions.	1.Purge combustor with CO2 2. Light Off 3. Ramp Up (increase flow rates, proportionally, to increase burner pressure).	Control is maintained over range of conditions. Stable Combustion at atmospheric pressures Stable Combustion is Achieved
Performance Test	Achieve 2100°F in exhaust gas stream	Hold Steady State Combustion at pressure	Can be a list/table-i.e. exhaust temperature readings w/t.c., time-temperature curves, durations, etc
Blow-Out Test	Observe the equivalence ratio of oxidizer to fuel at which the flame disappears (blows out)	Increase Fuel to Oxidizer ratio until Flame is lost	Measure temperature at exhaust (flame blows out, exhaust temp will be lower). Record fuel flow and fuel to oxidizer ratio at the blowout condition, exhaust temperature, and gas flows.
Transition Rig Pressure 1	Verify the blowout fuel/oxidizer ratio at 50 PSI rig pressure and at 100 PSI rig pressure by reducing fuel flow until blowout occurs. The rig will tend to be more stable at higher pressure and also at higher inlet temperatures.	After a light off at the low pressure condition maintain fuel/oxidizer ratio at a level above blowout. These ratios are expected to be lower than the values for blowout at near ambient pressure.	Measure temperature at exhaust (flame blows out, exhaust temp will be lower). Record fuel flow and fuel to oxidizer ratio at the blowout condition, exhaust temperature, and gas flows.
Transition Rig Pressure 2	Repeat above with inlet temperatures heated by 200F to verify the expected rig stability improvement at the increased pressure and temperature.	Same as above but heating inlet temperatures by 200 degF to verify rig stability improvement at increased pressure and temperature	Measure temperature at exhaust (flame blows out, exhaust temp will be lower). Record fuel flow and fuel to oxidizer ratio at the blowout condition, exhaust temperature, and gas flows.
Syngas Fuel Mixture A (2.4 Case)	Observe combustor performance with particular fuel type.	Same as performance test	Measure for complete/incomplete combustion, CO levels, flame

			temperature, exhaust temperature
Syngas Fuel Mixture B (0.9 Case)	Observe combustor performance with particular fuel type.	Same as performance test	Measure for complete/incomplete combustion, CO levels, flame temperature, exhaust temperature
Methane Mixture A (Pure Methane)	Observe combustor performance with particular fuel type.	Same as performance test	Measure for complete/incomplete combustion, CO levels, flame temperature, exhaust temperature
Methane Mixture B (Methane with Residuals)	Observe combustor performance with particular fuel type.	Same as performance test	Measure for complete/incomplete combustion, CO levels, flame temperature, exhaust temperature

Test Site Selection

Based on an initial screen with potential test venues, four sites were selected for participation in an RFP process. See Table 7. NASA White Sands Test Facility (WSTF) was selected for testing teaming based on their response to the RFP, which received the highest score in the analysis performed. Key conclusions included: cost, where WSTF scored among the highest and was perceived to have the lowest cost risk; safety, where WSTF scored the highest as the staff is experienced with the gases and conditions required, and the facility is designed for similar testing; and facility, where WSTF also scored the highest due to having high-quality systems in place with significant usable infrastructure.

Table 7: Test Site RFP Respondents

Test Facility	Location	Primary Focus/Area of Expertise
Energy and Environmental Research Center (EERC) at University of North Dakota	Grand Forks, ND	Coal Gasification, Renewable Energy, National Center for Hydrogen Technology
Energy and Environmental Research Center (EERC) at Dakota Gasification Company	Beulah, ND	Same as above including commercial scale gasification plant and CO2 capture and storage systems
Colorado Engineering Experiment Station, Inc. (CEESI)	Nunn, CO	Flow Meter Calibrations, Wet Gas/Multiphase Testing
NASA White Sands Tests Facility (WSTF) with WHA	Las Cruces, NM	Propulsion Testing, Materials and Component Testing, Oxygen Systems, Propellant Systems

Test Site Overview

WSTF has proposed utilizing their “250 Area” for the test campaign to make use of existing systems. The 250 Area is an oxidizer and fuel high flow test area originally constructed to test Space Shuttle components such as the oxygen and hydrogen flow control valves. This area is uniquely qualified to support the combustor test due to the existing infrastructure, although there will be some modifications to accommodate safety and operational requirements.

The 250 Area high flow test facility includes 450,000 SCF tube banks for gaseous oxygen (GOX) storage at up to 6,000 psi supplied from a 9,000-gallon liquid oxygen (LOX) storage tank, pump, and vaporizer system. The existing oxygen storage capacities and pressures provide enough GOX to support more than eight (8), 30-minute duration tests of the combustor at 4,500 psi before having to recharge the tube banks. The LOX cryogenic storage tank has sufficient capacity to support more than 70 combustor tests of 30-minute duration. Similarly, several gaseous hydrogen (or other gaseous fuel) high pressure tube trailers are available in the 250 Area, with a combined storage volume of 300,000 SCF at 6,000 psi is supplied from a 15,000 gallon liquid hydrogen (LH2) tank, pump, and vaporizer system.

The fuel tube trailers have sufficient pressure and capacity to support greater than 10 combustor tests before having to recharge the tubes The LH2 cryogenic storage has sufficient capacity to support the hydrogen requirements for more than 200 combustor tests.

In addition to the high pressure oxygen and fuel storage and supply capabilities, the 250 Area high flow test facility includes piping and flow control to supply a test article with GOX (or other oxidizer) at up to 8 lbm/s at a supply pressure of 5,000 psi. For reference, the combined combustor oxidizer flow stream (O2 and CO2) is approximately 4 lbm/s. Furthermore, the oxidizer flow system includes an 8 MBTU/hr high pressure gas-fired heat exchanger, which can provide the above pressures and flows at temperatures up to approximately 1,000 °F, counting as a first-stage heat exchanger for heating the process oxidizer gas for testing.

The test area includes large set-back distances of equipment, roadways, and inhabited structures to accommodate potentially energetic test articles. **Error! Reference source not found.** shows a general o verhead view of the test area.

Additional infrastructure in the 250 Area includes a control room currently configured with 72 data acquisition channels and 32 control channels, as well as two remote video surveillance systems. Furthermore, the site is a self-contained facility with existing processes and procedures for quality, safety, and environmental aspects related to testing.

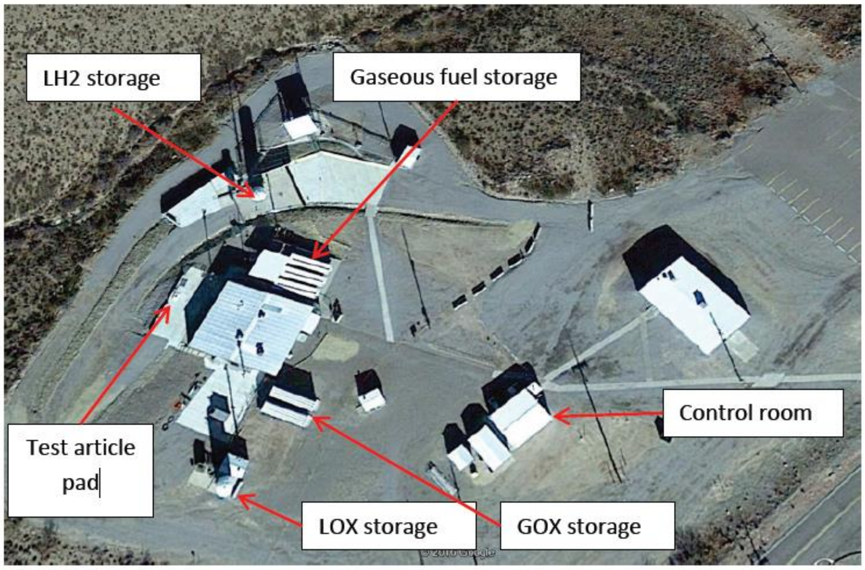


FIGURE 17: ARIAL VIEW OF 250 AREA AT WSTF

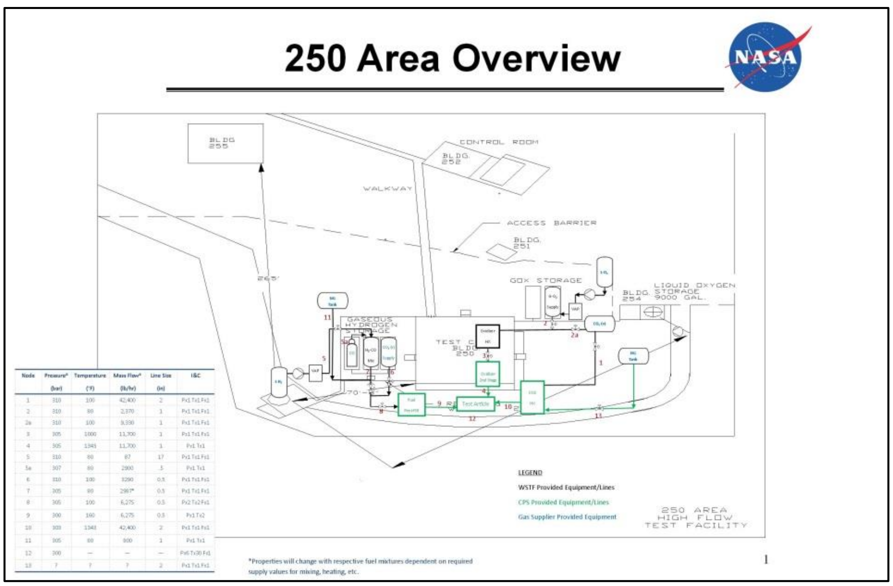


FIGURE 18: LAYOUT OF TEST SITE AND AUX SYSTEMS

Auxiliary Rig Design

A blow-down type rig configuration will be integrated with the WSTF facility. The proposed rig design includes using existing GOX and LOX storage, vaporizers, and intermediate gaseous storage to deliver constituents to the test article and provide sufficient capacity for multiple runs. CO and CO2 will be brought in by an industrial gas supplier on stand-alone skids as cryogenic liquids and then pumped up to test pressure. All required gas streams will be heated to operating conditions by trim heaters, natural gas fired heaters, or cryogenic vaporizers, some of which are already on site. The immediate systems surrounding the rig combustor, including the fuel heater, the CO2 heater, and a second stage of oxidant heating, will be built skid-mounted off-site and brought to the stand for testing. WSTF has a data acquisition system controls, and a control room, which will be integrated with the auxiliary systems to enable smooth operation of the overall rig.

General System(s) Description

The auxiliary systems for the oxy-fuel syngas combustor on the test rig will consist of three primary systems, fuel, oxidizer, and supercritical carbon dioxide, which will be injected into the combustion chamber. There are additional secondary support systems such as electrical, instrument air, exhaust management and controls systems that will also be incorporated into the test rig design. The consumable gases for the primary systems will be pressurized and heated prior to injection in the combustor. The following sections describe the general functionality of each of these systems, along with the respective components.

Syngas/Fuel System

The fuel skid on the test rig includes all components that are involved with the storage, control, and transport of the fuel to the combustor inlet nozzle. This includes, but is not limited to: tanks, pressure vessels, cylinders or tube trailers, control manifolds, pumps, valves, and/or filters.

Due to limited availability and the complexities involved with sourcing and using commercial syngas, a blending station will be utilized to synthesize the properties of the syngas composition as designated in the ASPEN cycles. Table 8 shows the approximate mole fraction percentage of each of the constituent gases for the baseline syngas mixtures where the mole fraction ratio between CO and H2 is adjusted to create a high-CO and low CO mixture. The blending station will use commercial quality gases (CO, CO2, H2) supplied from gas vendors. Each constituent flow rate will be controlled by a pressure or flow control valve.

TABLE 8: 2.45 CO:H_2 SYNGAS COMPOSITION

Gas	Mole Fraction
CO_2	0.337
CO	0.467
H_2	0.195

Oxidizer

The oxidizer will be pure O2 supplied via a liquid oxygen (LOX) tank, and diluted with CO2. The oxidizer system includes any components that are involved with the storage, control, regulating/mixing and transport of the oxidizer from the supply tanks to the combustor nozzle. This includes, but is not limited to, any tanks, cylinders or tube trailers, control manifolds, pumps, valves, vaporizers or filters.

Carbon Dioxide

Carbon dioxide will be supplied as a stand-alone supply as a liquid in a cryogenic tank. The CO2 system includes all components that are involved with the storage, control, regulating/mixing and transport of the carbon dioxide to the combustor nozzle. This includes, but is not limited to, tanks, cylinders or tube trailers, control manifolds, pumps, valves, vaporizers or filters.

Primary Components

Preliminary work was completed to identify requirements for the test rig primary components. This involved calculating volumetric requirements for the constituent gases based on presumed test durations and number of test runs, calculating pumping, compression and heat loads to condition the fluids, and sizing control valves. After these basic calculations were performed, vendors were consulted to develop preliminary technical specifications and budgetary estimates for the major components, including the gas supply and conditioning systems, and heat exchangers.

Storage/Supply and Conditioning Systems

Gas storage and systems have been sized to support the requirements in Table 9 below, and can include tube trailers or high pressure gaseous or liquid storage tanks.

TABLE 9: MASS AND VOLUME REQUIREMENTS FOR EACH GAS STREAM FOR BLOW-DOWN STORAGE CONDITIONS FOR A 30 MINUTE TEST RUN

		Fuel	Oxidizer	Dilution
Required Mass (lb)	O_2	-	1,184	-
	CO_2	1,645	4,665	21,199
	CO	1,448	-	-
	H_2	43	-	-
Required Volume (ft^3)	O_2	-	12,168	-
	CO_2	181	512	2,327
	CO	278	-	-
	H_2	92	-	-

Gas Supply

During Phase I, several gas suppliers were contacted to determine the conditions and storage mediums at which the constituent gases could be provided. Table 10 outlines the conditions at which it was indicated the required gases could be supplied. The supply and flow rates were based off of a thirty minute run time for each test run. While the operating time to achieve steady-state is on the order of milliseconds, thirty minutes allows for buffer time for pre-heating upstream equipment and achieving thermal equilibrium on the rig components to ensure their survivability throughout testing, minimizing thermal stresses.

TABLE 10: AVAILABLE GAS SUPPLY CONDITIONS

	H_2	CO	CO_2	O_2
Pressure (psig)	4,455	4,455	4,500	4,300
Temperature (°F)	Ambient (~70°F)	Ambient (~70°F)	Ambient (~70°F)	Ambient (~70°F)
Flow Rate (SCFH)	17,000	36,000	480,000 SCFH	28,500

Supply Equipment	Tube Trailer, Pressure Control Manifold, Support Equipment	Tube Trailer, Compressor, Pressure Control Manifold	Liquid CO2 Tank, Cryogenic Pump, Control Panel, Support Equipment	Liquid O2 Tank, Cryogenic Pump, Vaporizer, Pressure Control Manifold, Support Equipment

Heat Exchangers

Most of the constituent gases will be supplied at roughly ambient conditions, but the operating requirements for the test rig require the fuel supply to be heated to approximately 160 °F, the oxidizer to be heated to 1350 °F, and the carbon dioxide to be heated to 950 °F. For the fuel supply, a standard trim heater can be used since the heating requirements are marginally low, however, the oxidizer and carbon dioxide systems will require a heat exchanger with a much higher heating capacity.

The heating stage for these two streams is by far the most energy intensive step in any of the previously discussed design configurations. Preliminary calculations show that to heat the volume of carbon dioxide required for the test would require approximately 5 MWe of power. The Allam Cycle requirements for the carbon dioxide process gas require the combustor inlet temperature to be 1350 °F. At 300 bar, this temperature requires the equipment material specifications to go from standard stainless to expensive high-temperature alloys, such as Haynes 230 or Inconel 617. The cost increase associated with high-temperature alloys is almost tenfold (based on a budgetary estimate received from a commercial heat exchanger vendor). For this reason, the decision was made to limit the CO2 temperature on the test rig to 950 °F, affording several heat exchanger options that can be selected in the detailed design phase.

Secondary Components

A first-pass at sizing secondary components, such as sizing control valves for compressible fluids using FluidFlow®, was conducted. A detailed process and instrumentation diagram will be developed in future work. Secondary components include piping and in-line components, instrumentation and controls.

Conclusion

Phase I of the "Coal Syngas Combustor Development for High-Pressure, Oxy-Fuel Supercritical CO_2 Cycle Applications" project achieved the following objectives:

1. A nominally 300MWe high-pressure, oxy-fuel, sCO_2 power plant was developed and utilized to produce combustor inputs, and an associated combustor-turbine block was conceptualized. The modeled cycle demonstrates non-optimized efficiencies with full carbon capture that exceed the efficiencies of each of even the most efficient IGCC case, without capture, in NETL Cost and Performance Baseline for Fossil Energy Plants Volume 1.
2. A 5MWt test combustor was preliminarily designed. CFD analyses and mechanical design studies indicate the design met its goals, will be capable of design and test requirements, and has highly promising characteristics for commercial applications.
3. A test program was developed that has a high likelihood of success.

Appendix

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