Fuel-Flexible Combustion System for Co-production Plant Applications

Final Report

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Abstract

Future high-efficiency, low-emission generation plants that produce electric power, transportation fuels, and/or chemicals from fossil fuel feed stocks require a new class of fuel-flexible combustors. In this program, a validated combustor approach was developed which enables single-digit NO_x operation for a future generation plants with low-Btu off gas and allows the flexibility of process-independent backup with natural gas. This combustion technology overcomes the limitations of current syngas gas turbine combustion systems, which are designed on a site-by-site basis, and enable improved future co-generation plant designs. In this capacity, the fuel-flexible combustor enhances the efficiency and productivity of future co-production plants.

In task 2, a summary of market requested fuel gas compositions was created and the syngas fuel space was characterized. Additionally, a technology matrix and chemical kinetic models were used to evaluate various combustion technologies and to select two combustor concepts. In task 4 systems analysis of a co-production plant in conjunction with chemical kinetic analysis was performed to determine the desired combustor operating conditions for the burner concepts.

Task 5 discusses the experimental evaluation of three syngas capable combustor designs. The hybrid combustor, Prototype-1 utilized a diffusion flame approach for syngas fuels with a lean premixed swirl concept for natural gas fuels for both syngas and natural gas fuels at FA+e gas turbine conditions. The hybrid nozzle was sized to accommodate syngas fuels ranging from ~100 to 280 btu/scf and with a diffusion tip geometry optimized for Early Entry Co-generation Plant (EECP) fuel compositions. The swizzle concept utilized existing GE DLN design methodologies to eliminate flow separation and enhance fuel-air mixing. With changing business priorities, a fully premixed natural gas & syngas nozzle, Prototype-1N, was also developed later in the program. It did not have the diluent requirements of Prototype-1 and was demonstrated at targeted gas turbine conditions. The TVC combustor, Prototype-2, premixes the syngas with air for low emission performance. The combustor was designed for operation with syngas and no additional diluents. The combustor was successfully operated at targeted gas turbine conditions.

Another goal of the program was to advance the status of development tools for syngas systems. In Task 3 a syngas flame evaluation facility was developed. Fundamental data on syngas flame speeds and flame strain were obtained at pressure for a wide range of syngas fuels with preheated air. Several promising reduced order kinetic mechanisms were compared with the results from the evaluation facility. The mechanism with the best agreement was selected for application to syngas combustor modeling studies in Task 6. Prototype-1 was modeled using an advanced LES combustion code.

The tools and combustor technology development culminate in a full-scale demonstration of the most promising technology in Task 8. The combustor was operated at engine conditions and evaluated against the various engine performance requirements.

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3 Introduction

3.1 Task 2 (Fuel Flexible Combustor Design Approaches)

The purpose of this task is to develop a technology scorecard to select two conceptual configurations for a low emissions fuel flexible combustor that burns natural gas and syngas fuels. Two combustor prototypes: a hybrid of a diffusion burner for syngas and premixed swirl burner for natural gas and a trapped vortex combustor for both syngas and natural gas were selected for further consideration. The methods and processes used in developing the technology scorecard along with preliminary modeling results from evaluating technologies for a fuel flexible combustor in Task 2 are discussed. Details of the chemical kinetics calculations employed in Task 2 and the results thereof are published in the 2005 ASME Turbo-Expo (Iyer et al., 2005).

3.2 Task 3 (Syngas Flame characterization)

Combustor design tools for synthetic gas fuels will require simplified models for predicting combustor stability performance based on reduced order (e.g., time-averaged) quantities. Specifically, appropriate methodologies are needed to predict the effects of variable fuel composition upon combustor stability limits.

Our approach is to obtain experimental measurements of flame speed for ranges of synthetic gas compositions, and under ranges of temperature, pressure and strain. Laminar flame speed (S_L) is defined as the velocity of steady, one-dimensional propagation of a planar, adiabatic, unstrained laminar flame into a uniform premixed fuel-air mixture at rest. Laminar flame speed is an important parameter, because it contains fundamental information regarding reactivity, diffusivity, and exothermicity of a combustible mixture.

In order to address the feasibility of synthetic gas for fuel-flexible gas turbine combustion, one must be able to accurately predict flame behavior under preheating and high-pressure conditions. Preheating increases reaction rates and diffusivity. Pressure not only influences molecular collision frequencies, but also the relative efficiencies of the two-body branching reactions versus the three-body termination reactions. Pressure changes the chemical kinetics and the flame speed; hence, data of S_L at high pressures is important and the experiments described below include plans for high-pressure studies.

Syngas fuels also have a large variability in diluents content, e.g., the composition of CO_2 can range from 1.6-30% (Zhu *et al.*, 1988). The presence of CO_2 in the fuel will impact the flame in at least four ways, through changes in: 1) mixture specific heat, 2) adiabatic flame temperature, 3) chemical kinetic rates, and 4) radiative heat transfer. First, the molar specific heat of CO_2 is larger than that for the fuels it displaces (CO and H_2). Therefore the addition of CO_2 will lower the reactant temperatures in the preheat region of the flame. Second, addition of any diluent reduces the adiabatic flame temperature, and thus the laminar flame speed. Since CO_2 has a

higher molar specific heat than air, it reduces the adiabatic flame temperature and flame speed more than an equal amount of air dilution. Thus the flammability limits and extinction strain rates of the CO₂ mixtures are correspondingly narrower.

Third, CO₂ does not act as a passive diluent in the fuel, but interacts kinetically. The kinetic effects of CO₂ dilution are manifested primarily in the main CO oxidation reaction, $\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$. Higher CO₂ levels lead to enhanced back reaction rates and, hence, reduced CO oxidation and enhanced consumption of H atoms. In lean H₂/CO flames, the H atoms are extremely important as they control the main branching ($\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$) and termination ($\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$) reactions. Since CO₂ dilution alters the H atom concentration, and consequently the chain branching and termination reactions, CO₂ can have profound effects on flame propagation and flame speeds of H₂/CO flames. This effect is further pronounced at higher pressures, as the three-body termination reaction dominates, resulting in lower flammability limits on the lean side. Chemical kinetic studies have emphasized this point by comparing the flame speeds of mixtures with CO₂ dilution, and a fictitious chemically inert species with the same specific heat as CO₂, showing that the CO₂ diluted flame speed had lower flame speeds (Zhu *et al.*, 1988).

The fourth effect of CO₂ dilution is through enhanced levels of radiation, as CO₂ is an effective absorber and radiator. CO₂ dilution can result in lower flame temperatures and lower laminar flame speeds (compared to air dilution) due to radiative losses from the flame (Qin *et al.*, 2001). Numerical studies in methane flames (Ruan *et al.*, 2001) have shown that the optically thin model loses effectiveness for large CO₂ dilution ratios and low equivalence ratios. Thus, CO₂ can also reabsorb the flame radiation and provide a means for heat transfer across greater regions of the flame.

Despite its importance, there is substantial scatter in the data of laminar burning velocities (see review by Andrews and Bradley, 1972; Egolfopoulos *et al.*, 1989) due to the difficulty in experimentally achieving planar, adiabatic, steady, unstrained laminar flames. Various methods have been adopted to determine laminar flame speed. One easily implemented approach is denoted the Bunsen burner method, i.e., a laminar, premixed jet flame. Another approach that has been reasonably successful for accurate S_L measurements is the counterflow technique (Wu and Law, 1984; Law, 1988) where a planar flame is established between two opposed jets. Using this technique, flame stretch effects can be systematically subtracted out to obtain unstretched laminar flame speeds.

In addition to the experiments, computational chemical kinetic studies are being used to identify appropriate chemical mechanisms to model synthetic gas mixtures under these conditions. With the experimental data and kinetic mechanisms, reduced chemistry and appropriate correlations can be used to capture flame propagation and premixed extinction limits as functions of fuel composition, strain rate, pressure and temperature. Four kinetic mechanisms were tested. The first is mechanism is GRI Mech 3.0, a well-tested mechanism that has been validated extensively for methane chemistry, and therefore also includes oxyhydrogen and carbon monoxide mechanisms. The second mechanism that we chose is a mechanism developed recently for H₂/CO combustion. This mechanism (Davis *et al.*, 2004) is built on the kinetic model of Mueller *et al.* (1999) with rate parameters and efficiencies that have been revised over the last few years.

This “full” mechanism involves 11 chemically reactive species (as well as various diluents) and 30 kinetic steps. The other two mechanisms were for this program by J. Y. Chen. They are reduced mechanism: one uses 14 species, the other tracks only 9 species (which has significant advantages for CFD implementations).

3.3 Task 4 (Systems Plant Performance Modeling)

This task identifies critical plant level requirements by reviewing the DOE Co-generation plant program plan and EECF Phase 1 report. A Quality Flow Down (QFD) method is utilized to establish combustor level requirements flowing down from plant level requirements. This task provides combined cycle performance evaluations of various conceptual combustor designs to help downselect the combustor technologies for further development of a low emissions fuel flexible combustor. Results from the performance analysis are also used determine the fuel flexible combustor operating conditions for operation in existing conventional gas turbine power systems.

3.4 Task 5 (Fuel Flexible Combustor Prototype Design)

The purposes of this task are to design and fabricate two prototypes of a fuel flexible combustor and operate them in a single nozzle combustion test rig under heavy-duty gas turbine operating conditions. The prototypes were designed from the down selected technologies in Task-2 with operating conditions estimated from Task 4 results and current industrial gas turbine cycle conditions. This report discusses the performance of all prototypes. Prototype-1 is a hybrid of a lean premixed DLN burner for natural gas and a diffusion burner with diluents injection for syngas. Prototype-2 is based on the Trapped Vortex Combustion technology adapted to syngas applications. The performance of the TVC combustor was measured at advanced gas turbine conditions. Prototype-1N is a premixed DLN burner for both natural gas and syngas. It was substituted for Prototype-1 later in the program based on revised program goals.

Based on changing goals of the program and the needs of the DOE High IGCC/H₂ Gas Turbine Program (DOE Cooperative Agreement DE-FC26-05NT42643), the DOE approved revising this program. Instead of testing Prototype-1, experiments were performed on high hydrogen fuels on modified swirl based nozzles, Prototype-1N (new). Based on the results of these experiments, additional modifications were made to the nozzle design and the design was promoted to a can combustor test as part of Task 8.

3.5 Task 6 (Syngas Methodology for Advanced CFD tools)

It is also important to develop the capability to apply the syngas information and kinetic mechanisms to complex combustor flows. Therefore, we have been developing CFD methodologies to explore extinction limit issues in practical combustors. Current studies include DNS and LES studies. The former is intended to examine the application of the reduced order

mechanisms required for LES studies. The second study is intended to develop and explore capabilities to predict extinction phenomena in practical combustor geometries.

Flow features occurring inside industrial gas turbine combustors have been studied in details with many research groups especially for the combustion of natural gas fuels (Kempf, *et al.*, 2006; Eggenspieler and Menon, 2004; Selle, *et al.*, 2004). However combustion characteristics of synthetic gaseous fuels, especially flame stabilization and local extinction processes are not well known and have to be studied further. Typically, flow inside a combustor is regulated as to be turbulent in order to reach an optimum level of mixing between fuel and oxidizer to enhance the combustion. In turbulence mixing is controlled to a great extent by vortex motion and specifically by the large scale vortices developing in the highly sheared regions of the flow (Trounev, 1991). More specifically, turbulence may be described as organized motion in which the largest scale superposed on a fine grain random background of fluctuations in the small scales, so that, the combustion process is dominated by the continuous distortion, extension, production and dissipation of the flame surface by vortices of different kinds (Renard, *et al.*, 2000). Thus, study of a turbulent reactive flow application deals with the interaction of a flame front by all of these ranges of scales.

Normally, the different regimes of turbulent premixed combustion are identified based on the ratio of root-mean-square velocity fluctuations to the laminar flame velocity and the ratio of the turbulence integral length scale to the laminar flame front thickness. According to this classical approach, eddies at a size of smaller than the laminar flame thickness can penetrate into the reaction zone and would be able to locally extinct the flame as they induce the maximum amount of strain. Actually such a formulation is not always correct as it lacks the following points as stated by Poinso *et al.* (1991) (i) Kolmogorov scales may be too small to induce any significant amount of strain, (ii) these scales may be already dissipated by viscosity before they can induce any strain, (iii) if they can survive, then they will cause curvature type of effects which may counteract with the effect of strain, and (iv) the interaction process is unsteady and flame response will depend on the eddy lifetime. Thus, based on these effects, a turbulent flow field which is expected to wrinkle the flame front may drastically alter the whole combustion process leading to a failure of the energy production process.

Based on this physical picture, within the first part of the study, DNS and LES computations for simplified configurations have been conducted with special emphasis on the determination of combustion characteristics of synthetic gaseous fuels based on different fuel compositions and turbulence levels and the test cases that are selected are: (i) flame vortex interaction (FVI) and (ii) flame turbulence interaction (FTI) problems.

The second part of the study deals with investigation of the flow features inside a gas turbine combustor using LES. In LES, scales larger than the grid size are computed directly and smaller scales are modeled (Menon and Calhoun, 1996; Kim *et al.*, 1999). LES has been studied extensively for different combustion regimes in realistic (Sankaran and Menon, 2004; Pitsch, 2005; Mahesh *et al.* 2000), and simplified geometries (Kempf *et al.*, 2006), for which it is possible to get experimental data (Weigand *et al.*, 2006; Meier *et al.*, 2006; Meyer *et al.*, 2005) for validation purposes. The configuration and test conditions were provided by GE for this study. Mixing characteristics of the fuel and air together with the diluent streams injected

through holes and the accurate representation of the chemical state space by reduced reaction mechanisms have been the important investigation parameters. LES computations are started on the exit plane of the diffuser cap and the injection of fuel and diluents from the holes are handled with special care. Results show that the effective mixing of fuel and oxidizer occur due to the existence of a diluent stream and flame starts at this location. A recirculation zone exists on the inner section of the combustor which carries the hot products upstream, causes pre heating and also perhaps, flame holding.

As oversimplified (e.g., single-step) global reaction models are not expected to be reliable to predict the flame dynamics over a wide range of operating conditions, our work also involves evaluation of multi-step, but reduced kinetic mechanisms designed especially for CO-H₂ combustion. Two reduced but multi-step mechanisms: a 5-step, 9-species and 10-step, 14-species mechanism were evaluated. Based on comparison with data, we have chosen the latter mechanism for all the LES simulations since it appears to be accurate enough for the current effort.

3.6 Task 8 (Combustor Design and Validation)

From the two combustor prototypes one was selected for further development and evaluation. Based on the changing goals of the program and the needs of the DOE High IGCC/H₂ Gas Turbine Program (DOE Cooperative Agreement DE-FC26-05NT42643), the DOE approved revising this program. Prototype-1N was selected for further evaluation in a can combustor test in support of the high H₂ program. The design from the prototype evaluation was improved upon to integrate it into a can combustor, preparing it for more practical implementation.

Executive Summary

Current commercially available combustion systems cannot meet the fuel flexible requirements targeted by this program: sub-9 ppm NO_x & CO with either natural gas or syngas operation and fuel flexibility to operate over a range of syngas compositions. The goal of this program was to evaluate and improve upon current leading combustor designs that can partially meet these requirements and to develop new technologies as appropriate to meet performance requirements and expand operability limits. The targeted syngas fuel was fuel for a co-production plant and the fuel-flexibility goals were to address other market representative fuels. The program focused on summarizing the market relevant syngas compositions. Furthermore, research was conducted to characterize syngas flame fundamentals and further develop the kinetic and CFD models needed to advance syngas flame modeling for advanced combustors.

The most promising combustor technology for syngas and natural gas operation was selected using performance models and representative syngas compositions. A database was compiled for market relevant syngas fuels. The syngas data falls into 10 representative fuel groups, which can be used to focus fuel-flexible combustor development. Eight different combustor technologies were evaluated with respect to emissions, cost of electricity, and Reliability/ Availability/ Maintenance (RAM). GE Energy combustion technology priorities were applied to these criteria and the analysis resulted in the selection of a premixing-diffusion hybrid combustor and TVC combustor. The modeling tools and selection process are recommended for future development efforts in the ever-changing syngas market landscape.

Combustor technologies were further developed by this program to enable operation with either syngas or natural gas while maintaining low emissions. A multi-circuit fuel injection strategy was developed for the hybrid burner to operate with syngas fuels with heating values from 100 to 280 Btu/scf. The broad range was accomplished through a fuel injection strategy implemented with three syngas fuel circuits. With shifting business priorities, the prototype was replaced with a fully premixed swirl stabilized design, Prototype-1N. The nozzle demonstrated good operability with both natural gas and syngas at engine operating conditions as well as acceptable emissions. Four syngas compositions in the range of 190 to 450 Btu/scf were evaluated representing H₂ compositions of 45% to 80%. The TVC combustor design was further developed to support low emission syngas combustion. The TVC combustor demonstrated 3 ppm NO_x emissions with 170 Btu/scf syngas at full load engine conditions. In a previous program a 60% reduction in NO_x from current technology has been reported for advanced cycle TVC combustors with natural gas. Prototype-1N was selected for further improvements and incorporation into a full-can premixed syngas demonstration. The nozzle successfully met the F-class performance requirements using both natural gas and syngas. The work represents a GE milestone - the first-ever full head end (multi-nozzle) test with 100% syngas fuel in a full premixed (DLN) mode.

Another goal of this program was to advance the status of development tools for syngas systems. A syngas flame evaluation facility was developed. Fundamental data on syngas flame speeds and flame strain were obtained at pressure for a wide range of syngas fuels with preheated

air. This data was used to select the most promising reduced order kinetic mechanisms for modeling syngas combustion over these conditions. The 14 species Chen mechanism was selected from the four candidate mechanisms.

The validated reduced order mechanism was applied to design modeling efforts for Prototype-1. LES modeling techniques were used to incorporate the 14 species Chen mechanism. The time resolved flame position, fuel-mixing and turbulent quantities were characterized. The hybrid nozzle flow field and temperature field were described by this method as well as the fuel burnout profiles.

This program has advanced the state of the art in both industrial syngas combustor design as well as syngas combustion-modeling tools. A comprehensive landscape of the syngas fuel space has been described, and the relevance to co-production plant integration in particular has been demonstrated. The advances in syngas combustor designs offer opportunities for ultra-low emissions or alternatively broad operability. The result is a promising array to combustion technologies and tools for future low emission

4 Experimental

4.1 Task 2 (Design Approaches)

4.1.1 Fuel Space Classification

The database of low heating value syn-gas fuels created in task 1 consists of over 500 fuels from different sources. The four main sources of fuel are:

- O₂ blown gasifier: Includes air separation unit (ASU). LHV = 132 – 365 btu/scf
- Air blown gasifier: No ASU. LHV = 93 – 170 btu/scf.
- Steel mill: Off-gas from steel mill. LHV = 95 – 285 btu/scf.
- Co-production: Utilizes off-gas from Fischer Tropsch reactor to produce electricity/steam and liquid fuel. LHV = 166 – 348 btu/scf.

To simplify the combustor evaluation in this task, it was decided to parameterize the fuel space and reduce it to a tractable number of fuels. The fuel space is classified in this task according to five independent parameters:

1. Percentage of combustibles (H₂, CO and HC's) in the fuel.
2. Percentage of H₂ in the combustibles.
3. Percentage of HC in the combustibles.
4. Percentage of N₂ in the inerts.
5. Percentage of H₂O in the inerts.

The above parameters are conjured based on the fact that the fuels composition can be broadly split into combustibles and inerts, the combustibles primarily being H₂, CO and CH₄. There are small amounts of higher hydrocarbons that are combined under the parameter HC. The inerts in the fuel are mainly composed of N₂, H₂O and CO₂. The fuel space is categorized into different boxes based on these five parameters.

Figure 4.1 shows the space for fuels obtained from O₂ blown gasifiers from three different parameter combinations. Figure 4.1(a) shows the fuel space in co-ordinates of combustibles and H₂ in combustibles. Figure 4.1(b) and (c) show the fuel space in co-ordinates of H₂ in combustibles and HC in combustibles and N₂ in inerts and H₂O in inerts respectively. Four distinct boxes of fuel space are obtained by this parameterization as represented in the figure. Similarly boxes of fuel composition are obtained for low heating value fuels from the other sources. Table 4-1 shows the fuel categories obtained for all the sources of fuel. A total of 11 fuel categories are obtained. EECF stands for early entrance co-production fuel that is a blend of synthetic-gas from O₂ blown gasification and off-gas from Fischer Tropsche reactor. NG stands for natural gas, which is treated as pure methane for this evaluation. Representative fuels from each category are chosen based on a fraction factorial design spanning the range of the variable parameters. The number of representative fuels for each category depends on the range of variation of the parameters. Three levels of the percentage combustibles, H₂ in combustibles and HC in combustibles are considered if the respective parameter varies by more than 20%, otherwise only two levels are considered in the fractional factorial design. For the

percentage N_2 and H_2O in combustibles two levels are considered irrespective of the range of variation. If a parameter varies by less than 5% only one level at the average value is considered.

Figure 4.1 Fuel space categorization for O₂ blown IGCC fuels

	% comb	% H ₂ in comb	%HC in comb	%N ₂ in inerts	%H ₂ O in inerts
O ₂ blown 1	52 – 95	28 – 55	1.5	2 – 63	0 – 8
O ₂ blown 2	97	25 – 49	56 – 85	100	0
O ₂ blown 3	58 – 73	89	0.03	2 – 74	1.07
O ₂ blown 4	39 – 94	31 – 53	0 – 9	0 – 20	26 – 97
Air blown 1	33 – 47	99	1	72 – 44	26 – 54
Air blown 2	28 – 40	37 – 50	11 – 27	50 – 77	3 – 22
Steel mill 1	28 – 52	2 – 13	20 – 73	69	1
Steel mill 2	30 – 44	5 – 56	0 – 12	0 – 94	0 – 17
Co-production	95 – 96	45 – 48	2 – 5	28 – 52	0.9 – 1.1
EECP	53 – 57	44	0.6	51 – 60	0.4
NG	100	0	100	0	0

Table 4-1 Fuel categories and parameter ranges

4.1.2 Scorecard Structure

The technology scorecard consists of three axes: fuels, combustor CTQ's and the technologies. The details of fuel classification are listed in Figure 4.1. The first 9 categories in the table are IGCC fuels and have been grouped into one fuel class for the purpose of the scorecard. Thus there are three fuels for the scorecard: IGCC, EECP and natural gas. Since this project is specifically building a combustor for the early entrance co-production plant, the primary focus is the EECP fuel with natural gas as a back-up fuel. IGCC fuels have also been considered to account for the variability in fuel composition. The weights assigned to the fuels in the scorecard reflect these priorities. The EECP fuel is given the maximum weight of 0.6 followed by NG with a weight of 0.3 and IGCC with a weight of 0.1. The sum of all weights adds to one. The sub-categories within IGCC are weighted according to their sample size in the field as shown in Figure 4.2.

Category	Sub-category	Category weight	Sub-category weight
EECP		0.6	
Natural gas		0.3	
IGCC		0.1	
	O2 Blown 1		0.42
	O2 Blown 2		0.02
	O2 Blown 3		0.02
	O2 Blown 4		0.27
	Air Blown 1		0.03
	Air Blown 2		0.01
	Steel Mill 1		0.07
	Steel Mill 2		0.13
	Co-production		0.03

Figure 4.2 Fuel categories weightings

The combustor CTQ's are classified into three main categories: emissions, cost of electricity (COE) and reliability, availability and maintainability (RAM). There are different sub-categories within each category and they are weighted with respect to their relevance to the main category. For example, the plant spends 75% of its time at full load, so the emissions at full load get a total weight of 0.75 that is equally divided into NO_x and CO emissions; so each one of them gets a weight of 0.375. The CTQ's and their weights are shown in Figure 4.3. The sum of all sub-category weights within a main category adds up to one and so does the sum of all the main category weights.

The following technologies are evaluated for a fuel flexible combustor:

1. Diffusion flame combustor with diluent (N₂ or steam) injection.
2. Lean premixed flame combustor without diluent (Dry low NO_x, DLN).
3. Rich-catalyst lean-burn (RCLTM) combustor.
4. Rich-burn quick-quench lean-burn (RQL) combustor.
5. DLN with O₂ enrichment.
6. Trapped vortex combustor (TVC).

Category	Sub-category	Category weight	Sub-category weight
Emissions	NOx 100% load	0.5	0.375
	CO 100% load		0.375
	NOx 75% load		0.125
	CO 75% load		0.125
	NOx 50% load		0.1
	CO 50% load		0.025
COE	Power Output	0.25	0.3
	Cost of diluent		0.15
	Cost of combustor hardware		0.15
	Cycle efficiency		0.4
RAM	Dynamics	0.25	0.25
	Flame holding		0.25
	CI Interval		0.15
	Impact of diluent on life		0.15
	Profiles (Nozzle/Bucket)		0.075
	Cost of Scheduled Maintenance		0.075
	Proven Technology		0.05

Figure 4.3 Combustor CTQ weightings

The scorecard is constructed by combining the fuels and the combustor CTQ's on one axis and laying out the technologies on the other axis. The structure of the scorecard is illustrated in Figure 4.4. Every combination of fuel and CTQ category gets an effective weight that is the product of the weights of the fuel category, CTQ category and CTQ sub-category. The product is then multiplied by 100 so that the sum of all the weights adds up to 100. For example the combination of EECF fuel and full load NOx emissions gets a weight of $100 \times 0.6 \times 0.5 \times 0.375 = 11.25$. Therefore if a technology gets full score for full load NOx emissions for EECF fuel then it gets 11.25 points for this combination. The scorecard is populated with both quantitative and qualitative scores. Quantitative values are obtained for NOx and CO emissions using chemical reactor models that is discussed in the following sub-section. Targets and upper specification limits (USL) are specified for full load and part-load emissions in the scorecard. NOx USL is 9 ppm dry corrected to 15%O₂ and the target is set at 7.2 ppm dry at 15%O₂. The target is set at a value 20% less than the USL to account for variability in the field according to standard practice. The USL for full load CO emissions is set at 10 ppm dry at 15%O₂ and the target is 8 ppm. A Z-score is calculated for each emissions category for each fuel category based on the values predicted by the reactor model. The Z-score is defined as

$$Z = \frac{USL - \mu}{\sigma} \quad (3.1)$$

where μ is the mean value for all the fuels in the category and σ is the standard deviation due to variation in fuel composition and field variability defined as $(USL - \text{target})/3$. The Z score can be negative if the mean value is greater than the USL.

							DLN				DLN with O2 enrichment						
							Qualitative	mean	stdev	Z	SCORE	Qualitative	mean	stdev	Z	SCORE	
FUEL	Level 1 CTQs	Level 2 CTQs	LSL	Target	USL	Wt factor											
EECP	Emissions	NOx 100% load		7.2	9	11.25		1.00	3.35	0.32	-0.93	-1.74	1	3.12	0.30	-0.34	-0.64
EECP	Emissions	CO 100% load		8	10	11.25		1.00	3.39	0.50	7.93	11.25	1	2.90	0.39	9.16	11.25
EECP	Emissions	NOx 75% load		7.2	9	3			3.35	0.32	-0.93	-0.46	0	3.12	0.30	-0.34	-0.17
EECP	Emissions	CO 75% load		8	10	3			3.39	0.50	7.93	3.00	0	2.90	0.39	9.16	3.00
EECP	Emissions	NOx 50% load		7.2	9	0.75			3.83	0.39	-1.88	-0.24	0	3.64	0.39	-1.46	-0.18
EECP	Emissions	CO 50% load		12	15	0.75			5.47	0.91	7.05	0.75	0	4.83	0.82	7.85	0.75
EECP	RAM	Operability (Dynamics)			2	3.75		-0.50				-1.88	-0.5				-1.88
EECP	RAM	Flame holding			20%	3.75		-0.25				-0.94	-0.5				-1.88
EECP	RAM	CI Interval (Availability)	12000			2.25		1.00				2.25	0				0.00
EECP	RAM	Impact of diluent on life		0	1000	2.25		1.00				2.25	1				2.25
EECP	RAM	Profiles (Nozzle/Bucket)				1.125		0.75				0.84	0.8				0.90
EECP	RAM	Cost of Scheduled Maintenance				1.125		0.00				0.00	-0.5				-0.56
EECP	RAM	Proven Technology				0.75		-0.25				-0.19	-1				-0.75
EECP	COE (ST VC)	Power Output		?		4.5		1.00				4.50	1				4.50
EECP	COE (ST VC)	Cost of diluent (lb dil/lb F)		0	1	2.25		0.00				0.00	0				0.00
EECP	COE (ST VC)	Cost of combustor hardware				2.25		0.00				0.00	-0.25				-0.56
EECP	COE (ST VC)	Cycle efficiency	40%	41%		6		0.00				0.00	-0.25				-1.50
NG	Emissions	NOx 100% load		7.2	9	5.625		1.00	2.08	0.06	4.42	4.14	1	1.91	0.08	5.09	4.78
NG	Emissions	CO 100% load		8	10	5.625		1.00	2.43	0.02	11.35	5.63	1	2.10	0.05	11.83	5.63
NG	Emissions	NOx 75% load		7.2	9	1.5		0.00	2.08	0.06	4.42	1.10	0	1.91	0.08	5.09	1.27
NG	Emissions	CO 75% load		8	10	1.5		0.00	2.43	0.02	11.35	1.50	0	2.10	0.05	11.83	1.50
NG	Emissions	NOx 50% load		7.2	9	0.375		0.00	2.03	0.26	2.93	0.18	0	1.61	0.20	4.96	0.31
NG	Emissions	CO 50% load		12	15	0.375		0.00	2.08	0.08	12.88	0.38	0	1.84	0.09	13.10	0.38
NG	RAM	Operability (Dynamics)			5	1.875		-0.50				-0.94	-0.5				-0.94
NG	RAM	Flame holding				1.875		0.25				0.47	0				0.00
NG	RAM	CI Interval (Availability)	24000			1.125		1.00				1.13	0				0.00
NG	RAM	Impact of diluent on life		0	1000	1.125		1.00				1.13	1				1.13
NG	RAM	Profiles (Nozzle/Bucket)				0.5625		1.00				0.56	1				0.56
NG	RAM	Cost of Scheduled Maintenance				0.5625		0.00				0.00	-0.5				-0.28
NG	RAM	Proven Technology				0.375		1.00				0.38	-1				-0.38
NG	COE (ST VC)	Power Output	2350	2350		2.25		0.00				0.00	0				0.00
NG	COE (ST VC)	Cost of diluent (lb dil/lb F)		0	1	1.125		0.00				0.00	0				0.00
NG	COE (ST VC)	Cost of combustor hardware				1.125		0.00				0.00	-0.25				-0.28
NG	COE (ST VC)	Cycle efficiency		5%	6%	3		0.40				1.20	0.15				0.45
IGCC	Emissions	NOx 100% load		7.2	9	1.875		0.00	3.48	1.04	-0.46	-0.14	0	2.84	1.52	0.10	0.03
IGCC	Emissions	CO 100% load		8	10	1.875		0.00	3.34	1.17	4.93	1.54	0	2.81	0.93	6.30	1.88

Figure 4.4 Scorecard structure

For COE and RAM CTQ's, a qualitative score is assigned for each technology based on existing knowledge from laboratory and field experience. For example lean premixed combustors are known to be susceptible to flame-holding in the burner tube especially with H2 containing fuels (EECP and IGCC fuels) whereas diffusion flame combustors does not suffer from this drawback. So lean premixed combustors are given a negative score for flame-holding compared to diffusion combustors that receive a positive score. The qualitative score can range from -1 to $+1$ for each CTQ category. Sometimes the qualitative score is based on quantitative predictions, for example the score for the cost of diluent is scaled according to the amount of diluent required to meet the target NOx level for diffusion combustors.

The final score for each combination of fuel and CTQ category for a given technology is calculated either from the Z-score if quantitative data is available or from the qualitative score for categories that cannot be quantified at this stage. For quantitative data, the final score for category i is given by

$$S = (Z / 6) \times W_i \quad (3.2)$$

where W_i is the weight of the category. A Z-score of 6 is assumed as a perfect score of W_i . The score is limited to the range $[-W_i, +W_i]$ in the event $S > W_i$ or $S < -W_i$. For qualitative data, the final score S is the product of the weight and the qualitative score.

4.1.3 Apparatus (Reactor models)

Reactor network models are developed to evaluate the NO_x and CO emissions with fuel flexible operation for diffusion flame, lean premixed (DLN), rich catalytic lean premixed (RCLTM), rich-burn quick-quench lean-burn (RQL) and trapped vortex (TVC) combustors. The models consist of a network of well-stirred reactors that are solved using Chemkin software package.

4.1.3.1 Diffusion flame combustor

The diffusion flame combustor can be schematically represented as shown in Figure 4.5. The mixture of fuel and any added diluent entrains the amount of air required for stoichiometric combustion at the maximum flame temperature for the fuel/diluent mixture. The products of stoichiometric combustion then entrain the remaining amount of air required to achieve the desired combustor exit temperature. This process is represented by the network of three well-stirred reactors shown in Figure 4.6.

Figure 4.5 Schematic of diffusion flame

Figure 4.6 Reactor network model for diffusion flame combustor

The residence time in reactor 1, τ_1 , depends on the mixing time scales in the stoichiometric zone where the injected fuel/diluent mixtures entrains the air required for stoichiometric combustion. This residence time is obtained based on the mixing length model for turbulent axis-symmetric jets. τ_1 is defined as the average mixing time in the stoichiometric zone over the entire length of the flame:

$$\tau_1 = \frac{1}{L_f} \int_0^{L_f} \tau(x) dx \quad (32.3)$$

where L_f is the length of the diffusion flame given by Turns, 1996 for momentum controlled jets as

$$L_f = 23d_j (\rho_{inj} / \rho_{amb})^{1/2} (1 + (A/F)_{st}) \quad (3.4)$$

where d_j is the jet diameter, ρ_{inj} is the density of the injected fluid, ρ_{amb} is the density of the ambient fluid and $(A/F)_{st}$ is the stoichiometric air to fuel mass ratio. $\tau(x)$ is the mixing time at a distance x from the jet exit and is given by

$$\tau(x) = \frac{l_m^2}{\varepsilon} = \frac{\left(2.5 \times 0.08468 \times x \times \left(\frac{\rho_{inj}}{\rho_{amb}} \right)^{1/2} \right)^2}{0.01425 \times U_{inj} \times d_j \times \left(\frac{\rho_{inj}}{\rho_{amb}} \right)^{1/2}} \quad (3.5)$$

where l_m and ε are the mixing length and the eddy diffusivity for the turbulent round jet, the expressions for these are as given by Turns, 1996. U_{inj} is the injection velocity of the jet. Integrating Eq. (3.3) using the expressions in Eqs. (3.4) and (3.5) gives the following equation for the residence time in the stoichiometric zone:

$$\tau_1 = \frac{3.12d_j}{U_{inj}} (1 + (A/F)_{st})^2 \left(\frac{\rho_{inj}}{\rho_{amb}} \right)^{3/2} \quad (3.6)$$

The residence time in reactor 2, τ_2 , is calculated by estimating the volume of the jet between the stoichiometric contour and the contour of full entrainment and dividing by the total volume flow rate of the fuel and the air. The resulting expression is:

$$\tau_2 = \frac{10.98d_j}{U_{inj}} \left(\frac{\rho_{inj}}{\rho_{amb}} \right)^{5/2} \frac{(1 + A/F)^3 - (1 + (A/F)_{st})^3}{\left(1 + \frac{\rho_{inj}}{\rho_{amb}} \frac{A}{F} \right)} \quad (3.7)$$

The residence time of the third reactor is chosen to match the total residence time to the overall combustor residence time.

4.1.3.2 Lean premixed combustor

Figure 4.7 : Reactor network model for lean premixed combustor

Figure 4.7 shows the reactor network model for a lean premixed combustor. Fuel and air are fully or partly premixed in reactor 1. Reactor 1 represents the primary zone of flame stabilization achieved by the recirculation of hot products into the reactant mixture. The value of the residence time in reactor 1 is fixed by validating with experimental data on DLN NO_x and CO emissions data. The effect of variation in this residence time is discussed in the results and discussions section. Reactor 2 represents the zone of secondary burning where the products of the primary reaction burn towards complete combustion. In case of partial premixing, any air that is not mixed in reactor 1 is added in reactor 2. Reactor 3 is added to make up the remainder of the overall combustor residence time. Leakage air due to seals, cross fire tubes and igniters are added in reactor 3 to maintain the required combustor exit temperature. Partial premixing is also allowed. The degree of premixing is defined as the percentage of the head end combustion air that mixes with the fuel in reactor 1. The value of the degree of premixing is fixed by validation with experimental data on DLN premixers. The process of validation is described in the EPACT protected appendix.

4.1.3.3 Rich catalytic combustor

Figure 4.8: Schematic of rich catalytic lean burn combustor

Figure 4.9: Reactor network model for rich catalytic combustor

Rich catalytic combustion is a relatively new method to obtain low emissions and stable combustion. PCI Inc. has recently developed a rich catalytic burner that can be combined with lean premixed combustion to achieve low NO_x emissions (Karim et al., 2002). Figure 4.8 shows

the schematic of a rich catalytic lean burn (RCLTM) combustion system (Smith et al., 2002). Fuel-rich mixture is partially oxidized in a catalytic reactor that is cooled by the remaining combustion air to maintain catalyst surface temperature within material limits. The products of the rich catalytic reaction then mixes with the cooling air that is heated by the heat release of the rich reaction. The resulting lean mixture burns as a lean premixed flame. This system is modeled by adding a rich reaction zone ahead of the lean premixed system as shown in Figure 4.9. The rich catalytic reactor is approximated by an equilibrium calculation where it is assumed that the combustibles in the fuel react with all the available oxygen and gets converted to CO_2 and steam. Since the mixture is fuel-rich, not all the combustibles get converted. The resulting product is composed of CO_2 , steam, unreacted fuel and nitrogen from the air. The products are assumed to be formed at the specified catalyst temperature, T_{cat} . Here, the enthalpy release of the rich reaction is transferred to the remaining combustion air that is used to cool the catalyst surface, thereby increasing the temperature of the air. According to second law of thermodynamics, the temperature of the cooling air cannot be greater than the temperature of the catalyst surface that is heating the air. If the air gets heated to a temperature that is greater than the specified catalyst temperature then T_{cat} is increased such that the T_{cat} is equal to the temperature of the heated air. The rich catalytic reactor is followed by a network of well-stirred reactors representing the lean premixed combustor similar to that described in the previous subsection. Allowance is given for partial premixing whereby only a fraction of the heated air mixed with the products of the rich reaction in the first well-stirred reactor.

Figure 4.10 NO and CO as a function of combustor exit temperature for rich catalytic combustor: Comparison with experiments, natural gas fuel

The RCL model was validated with published measurements. Figure 4.10 shows comparison of predicted emissions with measurements in a rich catalytic combustor reported by Smith et al., 2003. The measurements were performed with natural gas as the fuel and the combustor pressure was 16 atm, the inlet air temperature was 705 K (810 F) and the inlet fuel

temperature was 294 K (70 F). The total combustor residence time was 30 ms. The flow rate of air passing through the rich reaction zone was 15% of the total airflow through the combustor. The remaining air was used to cool the rich catalytic reactor and it mixed with the products of the rich reaction downstream. The calculations were performed with identical conditions. The residence time of the premixed reactor downstream of the rich reactor (refer Figure 4.9) is chosen as 0.15 ms and degree of premixing of the products of the rich reactor with the remaining combustion air is assumed to be 71.25%. For these reactor model parameters, there is reasonable agreement of the predicted NO and CO emissions with the measurements. These validated parameters are used to predict the emissions for RCL combustor for all the required fuels.

4.1.3.4 RQL combustor

Figure 4.11 Schematic of RQL combustor (Feitelberg and Lacey, 1997)

Figure 4.12 Reactor network model for RQL combustor

Figure 4.11 shows the schematic of a rich-burn quick-quench lean-burn (RQL) combustor. Fuel is partially oxidized in a rich stage, the products of the rich combustion are quenched by adding more air and the resulting mixture burns to completion in a downstream lean stage. Figure 4.12 shows the reactor network model for predicting the emissions from the RQL combustor. The rich stage is modeled as a well-stirred reactor with a residence time of 10 ms. 50% of the remaining air is assumed to mix and react with the products in the quench zone. The

lean stage and the downstream portion are modeled by two more well stirred reactors. The total residence time is assumed to be 20 ms. A 30/70 rich/lean air split is assumed for the calculations.

4.1.4 Experimental & Operating Data

4.1.4.1 Fuels and combustor operating conditions

Fuel category	% combustibles	% H ₂ in combustibles	%HC in combustibles	%N ₂ in inerts	%steam in inerts	LHV (btu/scf)	CH ₄ co-fire (lb/lb fuel)
O ₂ -blown standard	64 – 94	28 – 55	0 – 1	1 – 50	0 – 15	193 – 291	0 – 2.5
O ₂ -blown advanced	41 – 95	32 – 53	0 – 9	1 – 30	11 – 95	131 – 305	0 – 0.12
O ₂ -blown with carbon shift/sequestration	58 – 92	87 – 99	0 – 0.06	2 – 100	0 – 4	163 – 259	0 – 11.9
Co-production	63 – 95	45 – 53	2 – 6	2 – 29	1 – 4	205 – 295	0.12 – 0.2
EECP	52 – 57	43 – 46	0 – 2	44 – 61	0 – 1	162 – 176	0
Air-blown standard	27 – 44	33 – 53	3 – 20	49 – 89	3 – 22	106 – 147	0.011 – 0.24
Air-blown with carbon shift/sequestration	33 – 47	98 – 99	1	44 – 73	26 – 54	93 – 132	0
Steel mill	28 – 42	2 – 56	0 – 31	62 – 88	0 – 17	96 – 167	0 – 0.59

Figure 4.13 Fuel categories and parameter ranges

The fuels considered for evaluation are broadly divided into three classes, EECP, natural gas and IGCC. The IGCC fuels are further subdivided into several categories base on the fuel composition and the type of gasifier.

A summary of the IGCC and EECP fuel categories is given in Table 4-1. Three categories of O₂-blown fuels are listed along with two categories of air-blown fuels and fuels from steel mills, co-production and early entrance co-production (EECP) plants. The ranges of the lower heating value (LHV) and the amounts of CH₄ co-fire used in these plants are also listed in the table. . The standard O₂-blown gasified fuels have total combustibles ranging from about 65% to 95% with about 30% to 55% H₂ among the combustibles. The category named advanced O₂-blown gasified fuels includes fuel moisturization and gasification of biomass and wastes. These fuels have a larger range of combustibles from about 40% to 95% with about 30% to 45% H₂ in the combustibles. There is a category of fuels that has high percentage of hydrogen (about 90% to 100%) in the combustibles. These fuels are based on conceptual studies of gasifiers combined with a carbon shift reactor and a CO₂ sequestration plant. Air blown and steel mill fuels have lower percentage of combustibles due to the large fraction of N₂ inherent in the products of gasification. The LHV of these fuels are therefore lower than that of O₂-blown fuels. The EECP fuel consists of a blend of O₂-blown syngas and off-gas from Fischer-Tropsch reactor for producing liquid fuels. The EECP fuel has higher degree of nitrogen compared to standard co-production fuel and hence lower range of LHV. In many cases co-firing with natural gas (CH₄) is employed to meet the requirements of the combustion system. For very low heating value

fuels such as those from steel mills, co-firing with CH₄ increases the heating value so as to meet the required turbine firing temperatures.

4.1.4.2 Mean & StdDev of Emissions Data

The emissions data reduction procedure is illustrated with emissions data for EECP fuel for a diffusion flame combustor with steam diluent to control NO_x. Table 4-2 shows the emissions and operating conditions for the set of EECP fuel compositions considered. The amount of steam diluent is varied to achieve 7.2 ppm NO_x for each case. The mean and standard deviation of NO_x, CO and diluent/fuel ratio are calculated and shown in the table. The standard deviation due to field variability is added to the calculated standard deviation due to fuel variability. For example the total standard deviation of CO emissions for this case is calculated as:

$$\sigma_{CO} = \sqrt{0.3983^2 + ((10 - 8)/3)^2} = 0.7765 \text{ ppm} \quad (3.8)$$

Fuel Composition (percent volume)						T _{fuel}	T _{air}	P	T ₃₉	NO _x	CO	Diluent/Fuel
CH ₄	H ₂	CO	N ₂	CO ₂	H ₂ O	F	F	psia	F	ppm dry @ 15%O ₂		mass ratio
0.34%	23.33%	29.56%	28.08%	18.50%	0.20%	400	762	225	2439	6.92	7.20	0.1389
0.34%	23.33%	29.56%	23.83%	22.74%	0.20%	400	762	238	2439	7.36	7.03	0.1111
0.34%	23.33%	29.56%	23.83%	22.74%	0.20%	400	784	225	2439	7.29	7.29	0.1165
0.34%	23.33%	29.56%	28.08%	18.50%	0.20%	400	784	238	2439	6.97	6.58	0.1423
0.34%	23.33%	29.56%	23.83%	22.74%	0.20%	400	762	225	2537	7.11	7.04	0.1173
0.34%	23.33%	29.56%	28.08%	18.50%	0.20%	400	762	238	2537	7.05	6.28	0.1385
0.34%	23.33%	29.56%	28.08%	18.50%	0.20%	400	784	225	2537	7.04	6.51	0.1432
0.34%	23.33%	29.56%	23.83%	22.74%	0.20%	400	784	238	2537	7.09	6.53	0.1220
0.36%	24.85%	31.49%	22.07%	21.05%	0.19%	400	762	225	2439	7.09	7.03	0.1619
0.36%	24.85%	31.49%	25.99%	17.13%	0.19%	400	762	238	2439	7.14	6.35	0.1816
0.36%	24.85%	31.49%	25.99%	17.13%	0.19%	400	784	225	2439	7.16	6.58	0.1862
0.36%	24.85%	31.49%	22.07%	21.05%	0.19%	400	784	238	2439	7.10	6.43	0.1666
0.36%	24.85%	31.49%	25.99%	17.13%	0.19%	400	762	225	2537	7.16	6.29	0.1835
0.36%	24.85%	31.49%	22.07%	21.05%	0.19%	400	762	238	2537	7.10	6.28	0.1640
0.36%	24.85%	31.49%	22.07%	21.05%	0.19%	400	784	225	2537	7.13	6.51	0.1682
0.36%	24.85%	31.49%	25.99%	17.13%	0.19%	400	784	238	2537	7.16	5.84	0.1885
Mean										7.12	6.61	0.15
Std. Dev										0.1069	0.3983	0.0266

Table 4-2 Predicted emissions for EECP fuel for diffusion flame combustor with steam diluent

The Z-score for emissions is then calculated from Eq. 3.2. This score goes into the scorecard for EECP fuel for diffusion flame with steam injection technology. The diluent requirements shown in Table 4-3 are used to calculate the score for cost of diluent and impact of diluent on life. The scores are calculated as follows:

$$S_{\text{cost of diluent}} = -F(\text{Mean}(D/F) + 2\sigma(D/F)) \quad (3.9)$$

$$S_{\text{impact of diluent on life}} \text{ (only for steam diluent)} = 1 - (\text{Mean}(D/F) + 2\sigma(D/F))$$

The cost factor F is 1 for N₂ diluent and 2 for steam diluent implying that steam is twice as expensive as N₂ in terms of the plant operating cost. According to Eq. (3.9) the addition of diluent penalizes both cost of electricity and hardware life.

Fuel	Full load				50% load			
	Inlet air temperature	Combustor pressure	Combustor exit temperature	Specific Humidity	Inlet air temperature	Combustor pressure	Combustor exit temperature	Specific Humidity
EECP	762 – 784	225 – 238	2439 – 2536	0.00753	672	153	2319 – 2416	0.00753

Natural gas	762 – 784	225 – 238	2630	0.00753	672	153	2510	0.00753
IGCC	754	225	2510	0.00753	672	153	2390	0.00753

Table 4-3 Operating conditions

Similar reduction procedures are applied to natural gas and IGCC fuels and for all the technologies. Technologies that do not require diluent obviously do not suffer from penalty on cost and life. Also N_2 diluent is assumed to have no impact on life and so gets a score of 1 in that category. For IGCC fuels the mean and standard deviations of the emissions are calculated as the weighted sum of the values for the different IGCC sub-categories as given in Table 4-2. For all technologies involving premixed combustion, the NO_x emissions values are multiplied by a factor of three to account for the fact the predicted values are less than what is observed in the field for natural gas DLN combustors. Though the model agrees with single nozzle laboratory data, effects of non-uniform premixing, can-can variations and liner heat transfer increase the NO_x in the real machines by almost a factor of three.

4.1 Task 3 (Syngas Fuel Flame Characterization)

4.1.1 Apparatus

(a) Laminar Flame Speed Measurement

The schematic of the experimental setup for the laminar flame speed (S_L) measurement is shown in Figure 4.14. The desired fuel composition is first prepared using a bank of calibrated rotameters, one for each gas. After mixing thoroughly, the fuel is split into two flows: the desired flow rate of fuel passes through another rotameter (calibrated for the particular fuel composition), while the remainder is flared in a diffusion flame. Finally, the required quantity of air is added, and the mixture goes to the burner. This arrangement allows simple control over the equivalence ratio (ϕ) and the average velocity through the burner. All the rotameters are calibrated with a bubble flow meter to $\pm 1\%$ accuracy, with fuel flows in the range of 0.1 to 5 slpm.

Various burners are employed; each is a straight cylindrical stainless steel tube, with inner diameters (D) ranging from 4.5 to 18 mm. The length of each tube is at least 50D in order to ensure that the flow is laminar and that the exit velocity profile is fully developed. The burner diameter is chosen to ensure that the flow remains laminar (Reynolds number, $Re_D < 2000$) and that the average velocity is at least five times greater than the estimated laminar flame speed for a given fuel composition. Thus the premixed flame is stabilized on the rim of the burner. The reactants are preheated by electrical resistance tape wrapped around the burner. Once the desired reactant temperature is achieved (as determined by a type-K thermocouple, TC2, temporarily placed at the burner exit), the surface temperature of the burner is monitored by a second thermocouple, TC1, and held constant by a temperature controller.

Digital images of the flame emission are recorded by a 12-bit intensified CCD camera (576×384 pixels) and a 105 mm, f/4.5 UV camera lens. The camera system is sensitive in the ultraviolet and visible regions (~ 220 -650 nm), and hence is capable of capturing OH^* , CO_2^* and

CH^* chemiluminescence from the flame reaction zone. Figure 4.15 shows a more detailed view of the imaging system, which includes an unusual feature, a horizontal knife edge placed in front of the lens in order to vary the collection solid angle along the flame height.

Figure 4.14 Schematic of the experimental setup for laminar flame speed measurements

Figure 4.15 Detailed view of the imaging system with a horizontal knife edge.

(b) Strained Laminar Flame Measurements

Strained flame data were acquired in a stagnation flow configuration. This configuration, like the more common opposed flow, allows for stretch corrected S_L measurements of **a one-dimensional flame**. Furthermore, it is advantageous over the opposed flow arrangement for determining laminar flame speeds for the following reasons: (1) the use of a solid wall leads to more stable flames (Egolfopoulos *et al.*, 1997), (2) problems related to heating of the upper burner are eliminated, (3) since only one burner is used, fuel consumption is halved, and (4) ease of operation of a single jet especially at higher pressures.

A general schematic of the stagnation flow burner is shown in Figure 4.16. Fuel (H_2 , CO and CO_2 mixtures) and air flows are monitored with rotameters and the fuel/air mixture is premixed in the mixing section ahead of the burner. The burner is a smoothly contoured nozzle with the exit diameter (D) of either 6.25 or 9 mm and a contraction ratio of either 144 or 72. The purpose of having a contoured nozzle is to get a top hat velocity profile at the burner exit so that the flame stretch will be uniform throughout the flame area. Moreover, the high contraction ratio contoured nozzle ensures laminar flow even at high Reynolds number based on the burner exit

diameter. Flow straighteners have been used before the contoured nozzle to remove any unsteadiness in the incoming flow. Care has been taken to reduce the size of the wake region created due to the finite thickness of the contoured nozzle at the burner exit.

A stainless steel plug was used to induce the stagnation zone. The plug was produced from a stainless steel rod (1.5" diameter), with the end first formed into a hemisphere. Then the end is removed to produce a small flat 0.5" long. The distance (L) between the burner exit and the stagnation plug can be adjusted depending on the burning velocity of the fuel mixture and the desired strain rate. As the burning velocity increases, decreasing the distance between the burner exit and the plug leads to a stable stagnation flame. In the current data, L/D was ~ 0.6 - 0.8 . The burner exhaust is shielded by a quartz tube to prevent entrainment of ambient air, while allowing optical access for laser Doppler velocimetry (LDV) and flame imaging.

The reactants are preheated by electrical resistance tape wrapped around the burner. Once the desired reactant temperature is achieved (as determined by a type-K thermocouple, TC_1 , placed at the center of the burner 1" below the exit), the surface temperature of the burner is monitored by a second thermocouple, TC_2 , and held constant by a temperature controller. The mixture temperature at the exit of the burner has a nearly uniform radial profile ($\Delta T \approx 3$ - 5 K).

Figure 4.16 Schematic of stagnation flame burner.

With this arrangement were able to achieve burner stabilized stagnation flames that remain stable for extremely high flame speed mixtures (~ 4 to 5 m/s) at high preheat levels (~ 600

to 700K). In the literature, these stagnation flames are normally produced in a configuration where the flame is detached (highly lifted) from the tube walls that form the reactant jet. However at high flame speeds, this configuration results in unstable flames due to a strong unsteady shear layer development along the periphery of the jet. But in the burner stabilized stagnation flame configuration, since the flame is stabilized on the lip of the burner, the strong shear layer development could be avoided. This in turn leads to a stable circular flat flame at the center of the nozzle.

Figure 4.17 Pressure vessel for housing the high pressure flame experiments.

(c) High Pressure Measurements

A picture of the high-pressure vessel used to house the jet and stagnation flow experiments at high pressure is shown in Figure 4.17. The high-pressure, cylindrical, stainless steel vessel is 6 inches in diameter and ~18 inches long and designed to withstand pressures of 30 atm and wall temperatures of ~600 °F. The interior walls of the pressure vessel are cooled with a nitrogen co-flow and the temperature is to be monitored at several axial (and radial) locations with thermocouples. The vessel is designed for optical access with three windows at 0°, 90°, and 180°. The 0 and 180° optical ports allow resolved axial velocity measurements with a laser Doppler velocimetry (LDV) system. The 90° port can be used for flame imaging and chemiluminescence measurements.

4.1.2 Experimental and operating data

(a) Laminar Flame Speed Measurement

Figure 4.18 shows a typical image of flame chemiluminescence for the atmospheric pressure, laminar flame speed measurements. The majority of the flame emission comes from the flame edge, i.e., chemiluminescence from the reaction zone. The less intense region in the central portion of the image is due primarily to chemiluminescence from the front and back edges of the flame.

Figure 4.18: Image of flame emission for a fuel mixture $\text{H}_2:\text{CO}=95:5$ at an equivalence ratio $\phi=0.61$. The color scale is black and dark blue for low intensities, and green, yellow and red for higher intensities.

(b) Strained Flame Speed Measurement

Figure 4.19 shows an image of the stagnation flame from a high pressure case. The stagnation flames are flat and stable at the center but slightly curved at the edges. The distance between the flame and stagnation plate varies from about 1 to 3mm, depending on the average inflow velocity. Figure 4.20 shows LDV velocity measurements. Results are shown for one fuel-air mixture and various flow velocities, i.e., different strain rates. The main flame zone occurs in the sharp velocity gradient region between the velocity minimum and the maximum to the left.

Figure 4.19 Image of flame emission from a stagnation flame at $p=5.0$ atm for a fuel mixture $H_2:CO=10:90$ at an equivalence ratio $\phi=0.6$; average inflow velocity $\sim 4SL$; $L/D=0.5$.

Figure 4.20: Velocity measurements along the centerline of a stagnation flame for 90% CO and 10% H_2 fuel mixture, $\phi=0.6$, $p=5.0$ atm at seven flow rates. The flow direction is right to left in this figure, i.e., cold reactants are present at 3.75 mm, while there are hot products at 1.5 mm.

In addition, radial and axial velocities (not shown here) were measured for our unique burner stabilized stagnation flame configuration to make sure the flow remains one dimensional along the stagnation stream line and so that comparison can be made to the Chemkin OPPDIFF flame code predictions. The results indicate excellent agreement with the one-dimensional assumption along the centerline.

4.1.3 Data Reduction

(a) Laminar Flame Speed Measurement

The laminar flame speed is defined as the velocity that a planer flame front travels relative to the unburned gas in a direction normal to the flame surface (Law and Sung, 2000). Though the laminar flame speed is straightforward in definition, in practice it is difficult to measure. Hence some assumptions have to be made in its measurement. A flame stabilized on the rim of a cylindrical burner is conical in shape and not one-dimensional (1-d). This conical flame is affected by strain and curvature; their influence on local flame speed depends on the Markstein length of the mixture. As such, our flame speed measurement is an area weighted average over the entire flame surface. The average flame speed is calculated by dividing the volume flow rate of the mixture with the luminous cone surface area (flame reaction zone area). It is clear from the definition of the *unburned* laminar flame speed that the true flame area should be the unburned flame area, just upstream of the preheat zone of the flame. Though the unburned flame area can be measured with the schlieren technique, this does not address the problem that the conical flame is strongly affected by curvature and stretch. Thus the measured flame speed would still not be the 1-d flame speed. However, as outlined below, use of the reaction zone area to calculate the flame speed can provide a result that more closely matches the unstretched flame speed.

Sun *et al.* (1999) derived the sensitivity of the unburned and reaction zone flame speeds (S_u and S_b respectively) for a curved flame traveling in a non-uniform flow field with a generalized integral analysis that includes thermal expansion in the preheat zone and neglects higher order terms. Generally the flame speed is affected by flame movement ($\dot{R}$), strain (κ) and pure curvature (γ). For a stationary flame, they showed that the burned flame speed at the reaction zone is only affected by strain, while the unburned flame speed is affected by both strain and pure curvature effects. Their analysis produces the following expressions for the unburned (S_u) and reaction zone (S_b) flame speeds relative to their 1-d values (S_u^0 and S_b^0),

$$\frac{S_u}{S_u^0} = 1 + \frac{Ze}{2} \left(\frac{1}{Le} - 1 \right) \frac{\alpha^0 \kappa \delta_T^0}{S_u^0} + \gamma \delta_T^0$$

$$\frac{S_b}{S_b^0} = 1 + \left[\frac{Ze}{2} \left(\frac{1}{Le} - 1 \right) - \frac{1}{Le} \right] \frac{\alpha^0 \kappa \delta_T^0}{S_u^0}$$

where Ze is the Zeldovich number; α is a factor that accounts for thermal expansion; $\gamma = \nabla_t \cdot n$ is the curvature of the flame front; $\kappa = \nabla_t \cdot \left[\frac{u_t}{u} \right]$ is the strain rate; δ_T is the flame thickness.

Since S_b is affected only by flame strain, the effect of strong azimuthal curvature in our conical flame case should not influence the flame speed at the reaction zone. Considering the effect of flame strain on S_b , Choi *et al.* (2001) have shown that the magnitude of the strain rate measured at the reaction zone in the shoulder region of the conical flame is much less compared to that at the tip, and its effect on the reaction zone speed is minimal. All the flames reported here were stabilized with the highest possible velocity, such that the heights of the flames are large compared to the burner diameter. This reduces the ratio of strain affected flame tip area to the flame shoulder area. Hence considering both curvature and strain effects, it can be concluded that the measured flame speeds at the reaction zone for the conical flame should be very close to the 1-d reaction zone flame speed. Hence the mass balance for the conical flame can be shown as,

$$S_b^0 \approx S_b = \frac{\dot{m}}{\rho_b A_b}$$

where ρ_b is the density and A_b is the surface area at the end of the heat release zone. From a 1-d flame mass balance,

$$S_b^0 = \frac{\rho_u}{\rho_b} S_u^0$$

and this expression for S_b^0 can be substituted into the former expression to produce,

$$S_u^0 \approx \frac{\dot{m}}{\rho_u A_b} = \frac{\dot{Q}}{A_b}$$

where $\dot{Q}$ is the volumetric flow rate of the unburned mixture. Since chemiluminescence is primarily produced in the thin heat release zone of the flame, the surface area measured from a chemiluminescence image can approximate A_b . Hence it can be seen that for a conical flame, the flame speed calculated by dividing the volumetric flow rate of the mixture with the luminous cone surface area should closely approximate the unstretched (one-dimensional) *unburned* laminar flame speed.

An edge detection program was developed to determine A_b from the chemiluminescence images. Since these Bunsen flames are essentially axisymmetric, each flame image is split in half along the burner axis. The edge detection program detects the reaction zone edge by locating the maximum derivative of the flame intensity along the radius of the flame. The flame area is then found by revolving the detected edge along the axis of the burner. The same procedure is repeated for the other half of the flame image (the change between these two areas is always below 1%). For each experimental condition, 25 images are typically recorded, and the reported flames speeds are based on the average of the 50 A_b values (25 images $\times$ 2 half-flames).

Figure 4.21: Measured laminar flame speeds for H₂:CO 50:50 and 5:95 compositions, including previous spherical flame experiments (McClean *et al.*)

In order to validate this approach, experiments were conducted for two H₂:CO fuel compositions (50:50 and 5:95 by volume) previously measured with a spherically expanding flame method (McClean *et al.*). The burner diameters used for these two compositions were 4.5 and 13.6 mm, and the equivalence ratio was varied from 0.6 to 1. As seen in Figure 4.21, the measured flame speeds for the 50:50 H₂:CO fuel mixture are in good agreement with values obtained from stretch-corrected spherically expanding flames throughout the lean equivalence ratio range tested. For example, the reported stoichiometric flame speed for the 50:50 mixture is 115 cm/s; the present measurement is 112 cm/s (a 2.6% difference). The 5:95 results are also in close agreement, though with slightly greater differences (<10%) near stoichiometric mixtures. Overall, these comparisons indicate that the errors in flame speed measurement associated with the reaction-zone-area based Bunsen approach are small, and the technique is reasonably accurate for a wide range of lean syngas fuel mixtures.

(b) Strained Flame Speed Measurement

To illustrate this method, the measured axial velocity along the stagnation stream line for a H₂:CO 50:50 fuel mixture with equivalence ratio of 0.58 is shown in Figure 4.22. The axial velocity decreases from the exit of the nozzle and reaches a minimum where the preheat zone starts. After reaching a local minimum, the axial velocity increases sharply inside the flame and then decreases to zero at the wall.

Figure 4.22 Measured axial velocity along the stagnation streamline for $\text{H}_2\text{:CO}$ 50:50 fuel mixture with equivalence ratio $\Phi=0.58$. Figure insert shows layout of nozzle generated wall stagnation flame.

Based on a common approach (Wu and Law, 1984), the minimum velocity before the preheat zone is considered as the reference strained unburned flame speed (S_u), and the maximum gradient of the axial velocity before the minimum velocity location is taken as the imposed strain rate (K) (see Figure 4.22). The imposed strain rate is controlled by changing the nozzle exit velocity. As the nozzle exit velocity increases, the flame moves closer to the stagnation surface. For each fuel mixture, the strain rates and corresponding strained flame speeds are measured for a range of nozzle exit velocities. Effort has been taken to measure the strained flame speeds at low strain rates, limited either by flashback or flame stability (unsteadiness).

Based on these definitions, raw data such as that shown in Figure 4.20 and Figure 4.22 is reduced to a measure of laminar flame speed as a function of strain rate (see Figure 4.23). In this case, the extrapolated zero-strain laminar flame speed is nearly 15 cm/s.

Figure 4.23 Measured flame speeds corresponding to results shown in Figure 4.20

4.2 Task 4 (Systems Modeling)

The combined cycle performance analysis is based upon the EECP combined cycle configuration developed in Phase 1 as shown Figure 4.24:

Figure 4.24: EECP Combined Cycle Schematics

The EECP combined cycle design is a STAG 106 FA+e with two-pressure levels non-reheat HRSG and a non-condensing steam turbine. The combined cycle supplies steam/water for use in a gasification island and refinery, besides producing electrical power. Therefore, steam production will be taken into account for performance comparison. Both commercially available software and GE in-house software packages were utilized in this task. The simulation will be performed on ISO ambient conditions. Twelve different EECP fuels (1 – 9b), which represent different plant operating scenarios and designs, and backup (natural gas) were selected for the simulation. The fuels are shown in Figure 4.25. Case 1 will be the design case for the HRSG and steam turbine. In case 2 – 10, HRSG will run in off-design mode.

Case #	1	2	3	4	5a	5b	7a	7b	8a	8b	9a	9b	10
Description	Design												Backup
Fuel Composition (Mol%)													
H2O	0.19%	0.18%	0.20%	0.19%	0.18%	0.19%	0.20%	0.20%	0.19%	0.20%	0.20%	0.21%	0.00%
H2	23.76%	24.42%	24.47%	24.66%	23.05%	23.72%	24.12%	24.91%	24.02%	24.72%	23.57%	24.41%	0.00%
CO	31.32%	32.23%	29.74%	30.53%	30.37%	28.68%	31.79%	30.27%	31.18%	29.61%	31.08%	29.54%	0.00%
CO2	19.82%	16.85%	21.24%	18.97%	20.87%	22.42%	18.62%	19.85%	19.76%	21.17%	20.61%	21.85%	0.00%
AR	0.21%	0.00%	0.22%	0.00%	0.20%	0.21%	0.21%	0.22%	0.21%	0.22%	0.25%	0.26%	0.00%
N2	24.28%	26.27%	23.74%	25.62%	24.93%	24.42%	24.65%	24.15%	24.16%	23.62%	23.89%	23.36%	0.00%
C1	0.19%	0.04%	0.16%	0.03%	0.22%	0.19%	0.19%	0.16%	0.23%	0.20%	0.23%	0.20%	100.00%
C2	0.07%	0.00%	0.07%	0.00%	0.09%	0.09%	0.08%	0.07%	0.08%	0.08%	0.09%	0.09%	0.00%
C3	0.06%	0.00%	0.05%	0.00%	0.06%	0.06%	0.06%	0.05%	0.06%	0.05%	0.07%	0.07%	0.00%
C4	0.04%	0.00%	0.04%	0.00%	0.04%	0.04%	0.04%	0.04%	0.04%	0.04%	0.05%	0.05%	0.00%
C5	0.02%	0.00%	0.02%	0.00%	0.03%	0.02%	0.02%	0.02%	0.03%	0.02%	0.03%	0.03%	0.00%
C6	0.02%	0.00%	0.02%	0.00%	0.01%	0.01%	0.02%	0.02%	0.02%	0.02%	0.02%	0.02%	0.00%
C7	0.01%	0.00%	0.01%	0.00%	0.00%	0.00%	0.01%	0.01%	0.01%	0.01%	0.01%	0.01%	0.00%
C8	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
C9	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
C10+	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
H2S	0.00%	0.01%	0.01%	0.01%	0.00%	0.01%	0.00%	0.01%	0.00%	0.01%	0.00%	0.01%	0.00%
COS	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
NH3	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MDEA	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
O2	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
LHV (BTU/SCF)	173.11	170.59	169.50	165.67	168.47	164.44	175.71	172.49	174.04	170.42	173.73	170.46	911.58
HHV (BTU/SCF)	185.78	182.95	182.48	178.13	180.82	177.08	188.58	185.70	186.91	183.59	186.47	183.57	1011.50

Figure 4.25: Fuel Matrix

4.3 Task 5 (Prototype Design)

4.3.1 Hybrid DLN Nozzle Design (Prototype-1)

The design of the hybrid burner borrows features from both diffusion and lean premixed DLN based combustion systems. Industry based best practice methods for diffusion based IGCC combustion systems and lean premixed DLN combustion systems are employed for the design of the hybrid burner.

Syngas combustion occurs via diffusion where the fuel is injected through the centerbody of the nozzle. The diffusion mode offers a wider range of dynamic tolerance which helps increase fuel flexibility with the varying composition of most coal gasified fuels. Based on the systems performance analysis, N₂ and steam are used as diluents to increase cycle efficiencies and suppress emissions. The diluents are also injected through the centerbody. The syngas and diluent passages are sized based on the range the range of calorific heating values that can be produced by coal gasification systems, ~90-310 BTU/scf. The diffusion nozzle tip geometry is designed to maximize performance based on the swizzle design that gives best performance for the premixed system, i.e. the tip geometry is optimized for the airflow pattern that the swizzle creates. The design of the diffusion centerbody is performed using a combination of the 1-D flow sizing equations, chemical kinetic calculations for estimation of flow ratios based on performance requirements, and 3-D CFD calculations to optimize geometry.

Natural gas is burned via a conventional lean premixed swirled burner as employed in GE's dry low NO_x combustion systems. The swirl vanes are engineered using aerodynamic principles for airfoil design. Vane shape profiles from existing DLN premixer designs are employed and are scaled according to the required flow conditions. CFD calculations are performed to verify the air-flow field around the vane and to check for the presence of any flow separation. No standard design rule is available to place the holes at optimum locations. However, the injection strategy for the hybrid swizzle is used to maximize fuel jet penetration into each vane section,

and thereby reducing emissions through increased mixing. The design of the hybrid swizzle is an iterative balance of maximizing jet momentum and penetration, fuel hole size, and hole placement. Proper injection hole sizing and placement are critical design parameters and are extremely difficult to quantitatively determine. The mixing strategy is therefore validated using CFD and iteratively optimized until the desired mixing is achieved.

The CFD calculations are performed using the commercially available Fluent software package. A segregated solver is employed where the equations of continuity, momentum, energy and turbulence are solved in an iterative manner until sufficient convergence of the steady state solution is achieved. Turbulence is approximated by the standard realizable k - ϵ model. Changes in gas phase thermo-chemical properties are accounted for in the reacting flow computations. Since the length and time scales of chemical reaction are very small compared to the fluid mechanical scales, it is not practically feasible to directly incorporate the chemical reactions in the conservation equations. For the diffusion flame combustion process, a pdf approach is used whereby the degree of mixing between the fuel, air, and the injected diluents is expressed in terms of two mixture fractions. The primary mixture fraction, f_{fuel} , represents the local mass fraction of all species originating from the fuel stream and the secondary mixture fraction, f_{dil} , represents the local mass fraction of all species originating from the diluents stream. The composition of the reacted mixture and its temperature and density are calculated as a function of the two mixture fractions. These calculations are performed using equilibrium chemistry a-priori to the CFD calculations using the prepdf program supplied by Fluent. Figure 4.26 shows an example of the output of prepdf. The figure shows the temperature of the products as a function of the primary and secondary mixture fractions. During the CFD calculations, transport equations for the mean primary and secondary mixture fractions and their variances are solved. The local averaged properties of the mixture such as temperature, density and species composition are then calculated from the prepdf output. The output is convoluted using a probability density function (pdf) to account for turbulence-chemistry interactions. There are two choices for the convoluting pdf: beta distribution function and the double-delta function. The beta is more accurate, but it is also computationally more expensive. To speed up the computations the double-delta function is employed in this work.

NO_x emissions in the diffusion flame process are calculated using the thermal NO_x model available in Fluent. Thermal NO_x is assumed independent of the NO_x chemistry from the fuel oxidation chemistry and is based on partial equilibrium concentration of O and OH atoms in the post combustion products. Recently Fluent has incorporated the NO_x formation via the N_2O intermediate mechanism. NO_x from both these mechanisms are calculated from the CFD results for the diffusion flame syngas burner.

Parametric CAD models of the important design features are created in Unigraphics (UG). The parametric model allows for easy modification of the dimensions of the design features. The parametric model is used for computational fluid dynamics (CFD) analysis of the combustor flow-field and mixing characteristics. Meshing the computational domain defined by the parametric model is performed with the ICEMCFD mesh generation software. ICEMCFD decomposes the domain into hexahedral and tetrahedral finite control volumes. In this work hexahedral (six-sided) elements are primarily used. A multi-block structured meshing procedure

Figure 4.26: Temperature as a function of mixture fractions

is used. The edges and faces of the blocks are associated to the appropriate curves and surfaces of the parametric CAD model. The hexahedral volume mesh is then created from the multiple blocks. Quadrilateral surface elements are defined so that boundary conditions can be assigned for the CFD analysis.

A hybrid burner was designed with three central circuits for low btu fuel and diluents. The design also has a swirler for natural gas premixing. For syngas operation, no fuel is injected through the swirl vanes. The fuel and the diluents are brought in through the manifolds in the centerbody. The fuel and diluents are issued as jets via holes drilled at the tip of the centerbody. The diffusion nozzle circuitss are designed so that the combustion nozzle can be used with either O₂-enhanced or with traditional air-gasification units, thus providing N₂ and steam or only steam as the diluents, respectively. For this work, EECF fuel produced by an O₂-enhanced gasifier is used for the design calculations. All passages are designed based on the range of calorific heating values that can be produced by coal gasification systems, ~90-310 BTU/scf which consists of all the fuels listed in Table 4-1.

Figure 4.27 Schematic of hybrid burner design

Figure 4.27 shows the schematic of the hybrid burner. The left hand side (LHS) shows a longitudinal section along the axis of the combustor and the right hand side (RHS) shows the tip of the diffusion nozzle with holes for fuel and diluents injection. The swirler in the LHS figure represents the premixed passage. Combustion air is brought in through the swirler where natural gas is injected through holes in the swirl vanes in the premixed mode. For syngas operation, no fuel is injected through the swirl vanes. The fuel and the diluents are brought in through the manifolds in the centerbody shown in the LHS figure. The syngas fuel manifold is sandwiched between two diluents manifolds. The manifolds are sized to accommodate all of the fuels along with their associated steam diluents required to meet 9 ppm NO_x. The fuel and diluents are issued as jets via holes drilled at the tip of the centerbody as shown in the RHS figure. The jets can be imparted axial, radial and tangential velocity components depending on the direction of the hole. There are 16 equally spaced holes in each row of holes. There is one row of holes for syngas and two rows of diluents holes. Steam is used as the diluents. The holes have to be sized depending on the composition and the heating value of the syngas. EECF fuel is used for the design calculations performed in this work. The size of the centerbody is fixed based on the sizes of the manifolds required to flow the syngas and diluents. The area of the annular passage between the centerbody and the burner tube is decided based on the flow rate of combustion air for one burner of the 6FA+e GT and the velocity specification in the burner tube for DLN combustion systems. The velocity is specified according to existing design practice for DLN combustors and it is chosen so that the premixed natural gas-air mixture does not flashback in the burner tube and the lean premixed flame does not blow-out during normal operating conditions for the premixed mode. The diameter of the burner tube is easily calculated from the annulus area. The combustion liner diameter is chosen so that the ratio of the cross-section area of the liner to the cross-section area of the burner tube is maintained the same as in the full can of the 6FA+e GT. Note that we are designing a single burner of an array of burners in the actual machine.

The pressure drops across the fuel and diluent passages are optimized for the EECF fuels, but the diffusion tip geometry is still flexible enough to operate over the entire range of syngas fuels without significant pumping/volumetric flow losses or dynamic effects. The flow requirements for sizing the air, fuel, and diluent holes are determined by calculating the air/fuel and diluent/fuel mass ratios required to meet performance targets and then scaling the results of

the systems performance analysis to 7FA+e GT system operating flow conditions. The volumetric and mass-flow ratios are determined from detailed chemical kinetic analysis, which has been described in Iyer et al., 2005.

Physical sizing limitations are imposed on the design such that the hybrid nozzle can be retrofitted into existing 7F-class and larger gas turbine combustion systems. The size of the centerbody is fixed based on the manifold sizes required to flow the syngas and diluents. The area of the annular passage between the centerbody and the burner tube is decided based on the flow rate of combustion air for one burner of a 7FA+e GT and the velocity specification in the burner tube for DLN combustion systems. The velocity is specified according to existing design practice for DLN combustors and it is chosen so that the premixed natural gas-air mixture does not flashback in the burner tube and the lean premixed flame does not blow-out during normal operating conditions for the premixed mode. The diameter of the burner tube is easily calculated from the annulus area. The combustion liner diameter is chosen so that the hot gas residence time and the ratio of the cross-section area of the liner to the cross-section area of the burner tube is approximately the same as in the full can of the 7FA+e GT. Note that we are designing a single burner of an array of burners in the actual machine.

The CFD optimization experiments are performed on a 1/16th sector model representing one hole in each row of holes. The premixed passage is approximated by specifying axial and tangential velocity components to the air stream. Velocity components are specified according to the air swirl angle in the design of experiments. The inlet mass flow rates are specified for the air, syngas, and diluents inlets. The airflow is fixed according to the 7FA+e airflow for one burner. The fuel and diluents flow rates such that the desired combustor exit temperature and the 9 ppm NO_x emissions target are achieved. The ratios of the flows are estimated from reactor network calculations. The molar composition of the fuel for the CFD calculations is 0.47% CH₄, 23.05% H₂, 30.37% CO, 21.05% CO₂, and 25.13% N₂. The LHV of the fuel is 168 btu/scf.

4.3.2 Trapped Vortex Combustor Design (Prototype-2)

Trapped vortex combustion (TVC) is one of the leading technologies for fuel flexible combustion as determined in Task 2 of this program. Research into the performance of trapped vortex combustors with natural gas was conducted in the Advanced Combustion System for Next Generation Gas Turbines DE-FC26-01NT41020 program. The scale of the combustor evaluated in that program is the same as the scale used here. Some of the components were passed on to this program at the completion of DE-FC26-01NT41020.

Several components of the TVC combustor were redesigned to facilitate operation with syngas. The cavity pre-mixer was redesigned to handle the higher volumetric flow of the syngas. The cavity air flow passage and the cavity fuel injection passages were appropriately resized for the higher volumetric flow associated with syngas. Downstream of this, a new cavity driver supply tube was designed with discrete fueling passages for the forward wall jets. The new tube maintains a higher flow velocity in the pre-mixer for additional flashback protection. The main pre-mixer was modified as well. The main mixer is comprised of a 3.5" schedule 10 pipe with static mixing elements. Additional mixing elements were added, bringing the total number to 7,

to increase the level of mixedness between the air and the large volume of syngas. The additional elements were predicted to enable the mixer to perform at the level of entitlement. The entrance to the main burner ports was also modified to keep the syngas-air mixture moving at a higher velocity to better avoid flashback. The main burner port design was the same as was used in the previous program.

The cavity aft-wall utilized in impingement cooled approach. The wall was continuous and had not cooling slots or holes. The aft-wall shape was welded directly to the outer-wall and combustion liner, and the wall was constructed from 2 sheets welded together. The flat part of the wall was a machined disk; the nose was custom machined. The aft-wall was backside cooled. The shroud cooling hole size and distribution were determined by the local wall heat transfer coefficients. The offset of the shroud was determined by the design analysis.

The outer-wall and transition piece were cooled in the same manner as the aft-wall. The cooling shroud extended from the forward end of the outer wall to the start of the hula seal. The combustion air was directed through cooling holes by designing a seal between the premixers and the reverse flow liner. In this manner air was forced to travel through the cooling shroud before passing into the combustor.

Effective area tests were performed to determine the air splits in the regions of the combustor shown in Figure 4.29. Region A is leakage air between the hula seal on the combustion liner and the downstream combustion liner (not pictured). Region B is cooling air used to cool the metal wall temperatures of the combustion liner. Region C is air that passes through the cavity pre-mixer and cavity slots into the cavity zone of the combustor. Region D, passes through the main premixing section and main slots in the main zone of the combustor. Region E is effusion cooling air used to cool the surface of the combustion injector plate, which is also referred to as the forward wall.

Figure 4.28: Prototype-2 TVC Combustor Design Features

Figure 4.29: Prototype-2 Air Flow Passages

4.3.3 Prototype-2 Experimental Measurements

The TVC (Prototype-2) hardware was evaluated at advanced syngas cycle conditions. The cycle conditions were established by preheating the air, closing the back-pressure valve, and adjusting the mass flow of air and fuel to the combustor to match the targeted cycle conditions. The fuel composition was set to the targeted EECF composition shown in Figure 4.30. The syngas has moderate levels of Hydrogen. In this set of experiments CH₄ concentrations were increased in the absence of CO to obtain the targeted fuel heating value. Evaluation of the prototype-2 hardware was performed in a high-pressure test vessel. The firing temperature was far above current syngas firing temperatures, and represented an advanced syngas machine.

Syngas Fuel	
H ₂	24.6%
CH ₄	11.5%
N ₂	44.6%
CO ₂	19.3%

Figure 4.30: Syngas Composition

Emission data was obtained using traversing sample probes in two locations. By making multi-point measurements of the exhaust profile, and accurate description of the combustor emissions can be obtained. Making these measurements at two different locations allowed the effect of residence time to be studied. Operating conditions were held constant during each traverse.

Emissions are measured using several gas analyzers. The sample is initially kept hot; then it is rapidly quenched and dried. The dry sample is fed to analyzers for O₂, CO₂, NO_x, and CO. The NO_x and CO emission levels are calibrated to a standard 15% O₂ level so that they are insensitive to dilution effects.

Combustion dynamics in the combustor are measured using multiple pizo-electric pressure transducers at three locations. The pressure fluctuations are measured using a semi-infinite boundary condition for the pressure waves. The peak-to-peak amplitude and frequency of the three dominant components in the pressure fluctuations are characterized for each transducer.

Figure 4.31 shows the measured performance results at the targeted operating conditions. The NO_x emission was very low at 3.1 ppmvd at the shorter residence time sampling location. The CO emission was a little above desired values, but a small increase in length would bring this inline with the targeted. Consistent with earlier studies the combustion dynamics were relatively small with the TVC combustor, remaining below 0.5 psi.

NO _x @ 15%O ₂	3.1 ppmvd
CO @ 15%O ₂	18.7 ppmvd
Peak-Peak Dynamics	< 0.5 psi

Figure 4.31: Prototype-2 Performance Data at Advanced Syngas Gas Turbine Cycle Conditions

The turndown performance of the TVC combustor was also evaluated. As shown in Figure 4.32 the combustor maintained ultra-low NO_x and acceptable CO levels at operating points 500 F below the targeted firing temperature. The combustor maintained combustion dynamics below 0.5 psi as well at these ultra-lean conditions.

NO _x @ 15%O ₂	1.2 ppmvd
CO @ 15%O ₂	2.6 ppmvd
Peak-Peak Dynamics	< 0.5 psi

Figure 4.32: Prototype-2 Performance With 500 F Turndown

4.3.4 Prototype-1N Single-Nozzle Testing of Modified Premixers

Aerodynamic modifications to the baseline swirler were made to support the combustion of high hydrogen fuels in support of the goals of DOE IGCC/H₂ Gas Turbine Program (DOE Cooperative Agreement DE-FC26-05NT42643). It was reasoned that the modifications to

accommodate operability with carbon-free syngas would allow less-reactive, “traditional” syngas fuel to be used as well.

Further design modifications were made based on both the results of experiments conducted under this program and the DOE IGCC/H₂ Gas Turbine Program. This final configuration was recently tested in a full combustor with syngas.

4.3.5 Prototype-1N Experimental Setup and Measurements

Fired tests of the baseline and modified swirl-based premixers were conducted in a single nozzle rig at GE’s Global Research Center. Testing was done at engine-realistic air temperature and pressure with natural gas and high-hydrogen fuels. Measurements were obtained for pressure drop through the premixer, NO_x emissions, and combustor temperature based on O₂ concentration. Flame holding was detected by up to six K-type thermocouples embedded in the centerbody and burner tube walls. Figure 4.33 shows the baseline nozzle bolted to an endcover after being removed from the rig.

Figure 4.33 Baseline premixer on endcover after removal from the single-nozzle rig.

4.4 Task 6 (Advanced CFD tools)

4.4.1 Syngas Methodology for Advanced CFD tools

The LES equations are obtained by applying a top hat spatial filtering operation on the Navier Stokes equations. The LES equations for continuity, momentum, total energy and species conservation are:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0 \quad [1]$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i} [\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij} - \bar{\tau}_{ij} + \tau_{ij}^{sgs}] = 0 \quad [2]$$

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial}{\partial x_i} [(\bar{\rho} \tilde{E} + \bar{p}) \tilde{u}_i + \bar{q}_i - \tilde{u}_j \bar{\tau}_{ji} + H_i^{sgs} + \sigma_{ij}^{sgs}] = 0 \quad [3]$$

$$\frac{\partial \bar{\rho} \tilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_j} \left[\bar{\rho} \tilde{Y}_m \tilde{u}_j + \bar{\rho} \tilde{D}_m \frac{\partial \tilde{Y}_m}{\partial x_j} + \Phi_{jm}^{sgs} + \Theta_{jm}^{sgs} \right] = \bar{\rho} \tilde{\omega}_m \quad [4]$$

Here, $\sim$ represents Favre averaging operator and is calculated for a given quantity $\tilde{f}$ as $\overline{\rho f} / \bar{\rho}$, where the over bar stands for volume averaging. Filtering operation introduced new terms into the set of governing equations and they represent the effect of the scales smaller than the grid size, on the resolved variables. These terms are denoted with the sgs superscript and are;

the sub-grid shear stress tensor $\tau_{ij}^{sgs} = \bar{\rho} [u_i u_j - \tilde{u}_i \tilde{u}_j]$, sub-grid heat

flux $H_i^{sgs} = \bar{\rho} [E u_i - \tilde{E} \tilde{u}_i] + [\overline{p u_i} - \bar{p} \tilde{u}_i]$, sub-grid viscous stress $\sigma_i^{sgs} = u_j \tau_{ji} - \tilde{u}_j \bar{\tau}_{ji}$, sub-grid mass flux $\Phi_{jm}^{sgs} = \bar{\rho} [Y_m u_j - \tilde{Y}_m \tilde{u}_j]$, and sub-grid diffuse mass flux $\Theta_{jm}^{sgs} = \bar{\rho} [Y_m V_{jm} - \tilde{Y}_m \tilde{V}_{jm}]$, respectively.

Total energy is given as $\tilde{E} = \tilde{e} + \frac{1}{2}(\tilde{u}_k \tilde{u}_k) + k^{sgs}$ and the filtered pressure is calculated by the

filtered equation of state by neglecting the effect of the sub-grid scale temperature as $\bar{p} = \bar{\rho} R \tilde{T}$, where $\tilde{e}$ is the filtered internal energy, k^{sgs} the sub-grid scale kinetic energy and R gas constant.

4.4.2 Subgrid Momentum Closure

Since the major effect of the small scales is to provide dissipation for the energy cascade from large scales through the inertial range, an eddy viscosity type sub-grid model appears to be suitable for the calculation of sub-grid stresses, heat flux and species flux. Based on this formulation spatial and temporal evolution of the sub-grid kinetic energy k^{sgs} is required in order to evaluate the eddy viscosity coefficient and the unclosed sub-grid scale terms. For this purpose an additional transport equation for k^{sgs} have been solved which is in the form of;

$$\frac{\partial \bar{\rho} k^{sgs}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i k^{sgs}) = P^{sgs} - D^{sgs} + \frac{\partial}{\partial x_i} \left(\frac{\bar{\rho} v_t}{Pr_t} \frac{\partial k^{sgs}}{\partial x_i} \right) \quad [5]$$

Here, P^{sgs} represents the production term and D^{sgs} is the dissipation term, and are given

as; $P^{sgs} = -\tau_{ij}^{sgs} \frac{\partial \tilde{u}_i}{\partial x_j}$ and $D^{sgs} = c_\epsilon \bar{\rho} \frac{(k^{sgs})^{3/2}}{\Delta}$, respectively. Based on these theoretical

assumptions, sub-grid scale terms are closed as;

$$\tau_{ij}^{sgs} = -2\bar{\rho}\nu_T \left(\tilde{S}_{ij} - \frac{1}{3} S_{kk} \delta_{ij} \right) + \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij} \quad [6]$$

$$H_i^{sgs} = -\bar{\rho} \frac{\nu_T}{Pr_t} \frac{\partial \tilde{H}}{\partial x_i} \quad [7]$$

The sub-grid eddy viscosity is then obtained as $\nu_t = c_v (k^{sgs})^{1/2} \bar{\Delta}$. Within this formulation there are two coefficients, c_ϵ, c_v , whose values are computed on the test filter and used for closing the subgrid scale momentum transport in a dynamical way (Kim, *et al.*, 1999; Kim, *et al.*, 1999). LES governing equations are solved using a finite-volume scheme that is nominally second-order accurate in space and time. A fourth-order accurate scheme is also available and is typically used during the later stage of the simulation for data acquisition. All simulations are conducted in parallel using MPI on Intel PC cluster.

4.4.3 Subgrid Combustion Closure

LES is capable of providing accurate information on the unsteady flow features by resolving the large scales in both space and time. This feature of LES makes it a powerful tool for combustor simulations since most important processes like local extinction, lift off are unsteady processes. However, combustion, heat release, volumetric expansion and turbulent stirring occur at the small scales, and are directly related with the flame dynamics. These small-scale processes are not resolved in a conventional LES approach and thus, any model used for combustion closure can lead to gross errors. Thus, a subgrid scale modeling of combustion is needed that explicitly accounts for the small-scale reaction-diffusion processes in the combustor. In this study, a subgrid Linear Eddy Mixing (LEM) (Kerstein, 1988) model is used within the LES approach (call LEMLES, hereafter) to capture explicitly the small-scale processes.

The key advantage of the LEMLES approach is that both the large-scale processes and small-scale processes are resolved at their respective space and time-scales. The large-scale structures in the flow are resolved using a conventional LES closure but the small-scales are resolved using a finer-grid embedded within each LES cell. The resolution for the subgrid can be chosen to resolve all scales down to the Kolmogorov scale and therefore, reaction kinetics and molecular diffusion (including differential diffusion) effects are closed in an exact manner. Further, the effect of subgrid stirring by eddies smaller than the LES grid size is also explicitly included as well. The general ability of the LEMLES has been demonstrated in the past by application to many types of flames: premixed, non-premixed and spray flames without requiring any model adjustment or changes. Since there are no ad hoc model parameters to adjust in LEMLES it can be used to evaluate new combustion systems for which limited data is available. Basically LEM model is based on the fact that for combustion, large scales are responsible only for convection of the subgrid scalar fields, whereas reactions, diffusion and turbulent stirring occur at the small scales. This is numerically implemented as a two-step process. Consider the following transport equation for a scalar ψ :

$$\frac{\partial \psi}{\partial t} = -\tilde{u}_k \frac{\partial \psi}{\partial x_k} - u'_k \frac{\partial \psi}{\partial x_k} + \frac{\partial}{\partial x_m} \left[D_\psi \frac{\partial \psi}{\partial x_m} \right] + \omega_\psi \quad (8)$$

This transport equation is solved in a two-step procedure: a large scale advection process that is computed at the LES grid (supergrid) level:

$$\frac{\psi^* - \psi^n}{\Delta t_{LES}} = -\tilde{u}_k \frac{\partial \psi}{\partial x_k} - (u'_k)^{face} \frac{\partial \psi}{\partial x_k} \quad (9)$$

and a subgrid process that solves for reaction, diffusion and turbulent stirring within the small-scales:

$$\psi^{n+1} - \psi^n = \int_t^{t+\Delta t_{LES}} \left[u'_k \frac{\partial \psi}{\partial x_k} + \frac{\partial}{\partial x_m} \left(D_\psi \frac{\partial \psi}{\partial x_m} \right) + \omega_\psi \right] \quad (10)$$

The large scale advection is carried out using a 3D Lagrangian transport model that advects subgrid scalar fields across LES cell faces. The reaction-diffusion equations are solved within the subgrid on 1D lines embedded inside LES cells. The 1D line is not a physical Cartesian line, rather it is oriented in the direction of the flame normal (for premixed) or in the direction of the scalar gradient (for non-premixed).

More specifically, following reaction-diffusion equations are solved on a 1D LEM line: for species mass fraction

$$\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho} \frac{\partial \rho Y_k V_k}{\partial s} + \frac{\dot{\omega}_k W_k}{\rho} + F_{kstir} \quad (11)$$

and for temperature:

$$\frac{\partial T}{\partial t} = -\frac{1}{C_p} \sum_{k=1}^N C_{p,k} Y_k V_k \frac{\partial T}{\partial x} + \frac{1}{\rho C_p} \frac{\partial T}{\partial x} \left(\kappa \frac{\partial T}{\partial x} \right) - \frac{1}{\rho C_p} \sum_{k=1}^N h_k \dot{\omega}_k W_k + F_{Tstir} \quad (12)$$

Effect of turbulent stirring is represented by F_{kstir} and F_{Tstir} . The location of the stirring event is chosen from a uniform distribution, and the frequency of stirring is derived from 3D inertial range scaling laws derived from Kolmogorov's hypothesis as:

$$\lambda = \frac{\nu \text{Re} \left[\frac{\Delta}{\eta} \right]^{\frac{5}{3}} - 1}{C_\lambda \Delta^3 \left[\frac{\eta}{\Delta} \right]^{\frac{4}{3}}} \quad (13)$$

C_λ represent the scalar turbulent diffusivity and is determined as 0.06719 (Chakravarthy and Menon, 2001). The eddy size (l) is chosen from the following PDF:

$$f(l) = \left(\frac{5}{3}\right) \frac{l^{-8/3}}{\eta^{5/3} - \Delta^{5/3}} \quad (14)$$

where $\eta = N_\eta \Delta \text{Re}^{-4/3}$. The empirical constant N_η reduces the effective range of scale between the integral scale and η but does not change the turbulent diffusivity. This parameter is chosen as 11 based on an earlier study. Once these constants are defined they are held fixed for LEMLES studies.

4.5 Task 8 (Combustor Design and Validation)

4.5.1 Prototype-1N Full Head End Testing of a Combustor with Syngas

Testing of the new Prototype-1 premixer in an existing combustion head end was conducted in the Gas Turbine Technology Lab at GE Energy in Greenville, South Carolina. The premixer design retained the features of the prototype hardware tested in the single-nozzle rig. It should be noted that the hardware was procured with funds from the DOE IGCC/H₂ Gas Turbine Program (DOE Cooperative Agreement DE-FC26-05NT42643), which also funded testing on high-hydrogen fuels. The present program funded the validation testing on syngas, which resulted in a milestone at GE Energy- the first-ever full head end (multi-nozzle) test with 100% syngas fuel in a full premixed (DLN) mode.

4.5.2 Prototype-1N Experimental Setup and Measurements

Testing was conducted with a high-reactivity syngas fuel, which consisted of H₂ and CO. During subsequent testing of the same hardware for the DOE IGCC/H₂ Gas Turbine Program, a high-hydrogen (in natural gas) fuel was used. Because of restrictions with the hardware and test stand, combustor inlet conditions were limited to E-class levels.

During testing, combustion dynamics were measured via PCB probes. A total of six K-type thermocouples were placed on the backside of the burner tube to detect flame holding. Additionally, a camera was fitted to look through the endcover and the center premixer to view the flame in the combustion chamber or inside the premixer during a flame holding event.

5 Results and Discussion

5.1 Task 2 (Design Approaches)

5.1.1 Emissions predictions for different technologies

Fuel compositions representing categories of standard O₂-blown and air-blown are chosen for illustration of the combustor emissions prediction. The representative O₂-blown fuel composition is selected as 95% combustibles, 45% H₂ in combustibles, 1.5% CH₄ in combustibles, 2% N₂ in the inert and 0% steam in the inert. The LHV of this fuel is 289 btu/scf. The O₂-blown fuel is introduced in to the combustor at a temperature of 450 K. The representative air-blown fuel composition is 45% combustibles, 30% H₂ in combustibles, 0% CH₄ in the combustibles, 90% N₂ in the inert and 10% steam in the inert. The LHV of this fuel is 136 btu/scf. The air-blown fuel is introduced in the combustor at a higher temperature of 633 K.

Figure 5.1 NO and CO emissions as a function of diluents/fuel: combustor exit temperature = 1900 K

Figure 5.1 shows the predicted NO and CO emissions for the representative oxygen and air-blown fuels as a function of the ratio of mass of diluents to the mass of the fuel. The calculations are performed for a combustor exit temperature of 1900 K. The emissions are reported as parts per million by dry volume (ppmv) normalized to 15% O₂ in the products. The NO emissions decrease exponentially with the addition of diluents (note the logarithmic scale for the NO axis). The adiabatic stoichiometric flame temperature decreases from 2581 K to 1952 K with the addition of 3.6 kg of N₂ per kg of fuel. Also, the residence time of the stoichiometric-burning zone as given by Eq. (4) decreases from 1.12 ms to 0.23 ms with the addition of N₂. The combined effect of the decrease in stoichiometric flame temperature and the flame residence time leads to the reduction in NO emissions. The CO emissions on the other hand increase with addition of diluents because of the decrease in excess O₂ concentration and the flame residence

time. The mass of steam required to reduce NO to a certain level is almost $1/3^{\text{rd}}$ of the mass of

N_2 required as seen in the figure for the O_2 -blown fuel. About 3.6 kg of N_2 kg lb of fuel is required to reduce NO to 10 ppm whereas only about 1.2 kg of steam per kg of fuel is required to achieve the same effect. The amount of steam required to reduce NO from the air-blown fuel is much less than that required for O_2 -blown fuel. The air-blown fuel has a large amount of N_2 present in the fuel mixture that acts as in-built diluents. Also as shown in the figure, the trade-off between NO and CO becomes important when adding diluents to reduce NO emissions.

Figure 5.2 NO and CO as a function of combustor exit temperature: lean premixed combustor, O_2 blown fuel, effect of degree of premixing.

Figure 5.2 shows NO and CO emissions for the representative O_2 blown fuel for a lean premixed combustor for different degrees of premixing. The degree of premixing is expressed as the percentage of the combustion air that reacts with the fuel in the primary zone, the remaining air mixes with the products in a downstream reactor as shown in Fig. 7. The degree of premixing has a strong effect on the NO emissions. According to Fig. 15 at an exit temperature of 1800 K, the NO increases by 20% when the premixing decreases from 100% to 90%, but increases by a factor of 1.8 when the premixing decreases to 80% and by a factor of 2.5 when the premixing further decreases to 70%. The increase in NO is evidently because of the increase in the primary zone temperature with decrease in the degree of premixing. Thus it is extremely critical to have good premixing at the head end to maintain low NO emissions with a lean premixed combustor. The flame stability is however improved with lower degree of premixing as shown by the CO at low temperatures. The temperature of rapid CO rise decreases by about 50 K when the degree of premixing reduces to 90% from fully premixed. However the predictions do not show a further decrease in the lean blowout temperature as the degree of premixing is decreased below 90%.

We have submitted an article for the 2005 ASME Turbo Expo that contains details of our kinetic analysis and results for diffusion, lean premixed and rich catalytic combustion systems (Iyer et al., 2005).

5.1.2 Scorecard

Figure 5.3: Technology matrix for fuel flexible combustion system

Figure 5.3 shows the hybrid technology matrix based on the model predictions for emissions and the qualitative scores for COE and RAM. The hybrid technology matrix is built based on the scores for emissions, COE and RAM for the individual technologies. The cells in green highlight the promising technologies or combination of technologies. The circled cells represent the technologies that we have chosen for building prototypes of the fuel flexible combustion system. Based on the scores shown in the matrix, we have chosen three concepts:

1. Diffusion with steam as a diluent for syngas and DLN for natural gas.
2. Diffusion with steam as a diluent for syngas and TVC for natural gas.
3. TVC for both natural gas and syngas.

Two prototypes will be built to accommodate the above-mentioned three concepts:

Prototype 1: A hybrid diffusion/DLN burner allowing syngas and diluents to flow through the diffusion nozzle and natural gas through the swirled premixed passage.

Prototype 2: A trapped vortex combustor allowing for both syngas and natural gas. A diffusion passage with diluents injection will also be incorporated.

The selection of the technologies for fuel flexible combustor was made on the basis of the scores projected by the technology matrix. The scores are relative to the CTQ's of emissions, COE and RAM as set for FA+e cycle conditions for natural gas, EECP and IGCC fuels. The scores for syngas are weighted between EECP and IGCC fuels with EECP getting most of the weight because it is the focus of this study. The most important emissions CTQ was the requirement of meeting 9 ppm NO_x with single digit CO emissions at baseload conditions. According to the matrix, for natural gas, DLN, Rich catalytic and TVC get promising scores because of their ability to meet the emissions CTQ's without the need for diluents addition. Diffusion with N₂ diluents is not an option with natural gas because the ASU is shut down when

running on natural gas. Diffusion with steam diluents does not meet the NO_x emissions requirement because of the limitation on the amount of steam that can be added. So these technologies do not get good scores with natural gas as fuel. On the other hand for syngas, diffusion with steam diluents gets a promising score because the NO_x requirements can be met with minimal quantities of steam addition, thereby keeping CO emissions under control. Other technologies like DLN and rich catalytic can also meet the NO_x requirements, however they get a lower score on reliability because of risks with dynamics and flameholding. TVC also showed potential for low NO_x emissions with syngas and it does not have as much reliability concerns as DLN and rich catalytic because of simplicity of design. The diagonals of the matrix represent single technology solutions for both the fuels. The only single technology that shows a green on the matrix is the TVC and so it was selected as one of the concepts for the prototype. Among the cross diagonal combinations the diffusion with steam for syngas combined with DLN for natural gas was selected. This is an extension of two proven technologies and has a good chance of a successful implementation. A third concept was also selected: a combination of diffusion with steam for syngas and TVC for natural gas. This concept in fact got the highest numerical score in the matrix.

5.2 Task 3 (Syngas Fuel Flame Characterization)

5.2.1 Model Comparisons: Effect of Preheating and CO₂ Dilution

One of the prime objectives of the present work is to measure the flame speed for syngas compositions with varying levels of CO₂ dilution and preheating under lean conditions. The effect of CO₂ dilution and unburned temperature are examined for three different H₂: CO compositions: 95:5, 50:50 and 5:95 ratios by volume. These compositions were chosen in order to cover a broad range of syngas mixture variations, and to aid in validation (or improvement) of syngas flame speed models for use in the CFD simulations.

Four kinetic mechanisms (GRI Mech 3.0, the H₂/CO mechanism of Davis *et al.* and two reduced order mechanisms of J Y Chen: a 14 species and a 9 species model) were studied. The laminar stagnation flame was simulated using the Chemkin OPPDIF flame code with appropriate detailed transport properties. It is important to note that in all our flame modeling *multi-component diffusion and thermal diffusion (Soret) effects are included*. These effects have a significant influence on the predicted flame properties especially at high preheat temperatures.

In the OPPDIF flame simulation, there are two premixed flames on either side of the stagnation plane and hence the stagnation surface is truly adiabatic. Moreover at the stagnation plane, the radial velocity gradient is normally considered finite. In our experiments, which use a solid wall at the stagnation plane, potential issues arise. First, it imposes a zero radial velocity gradient. Second, there is some amount of heat loss to the plug. Hence the effect of downstream heat loss and zero radial gradient at the stagnation surface have been studied and the results (not shown here) indicate that the unburned strained flame speed is not affected if the flame is located at least two flame thickness away from the stagnation surface. Thus in all our experiments care has been taken to stabilize the flame sufficiently away from the wall.

Effect of CO₂ Dilution

The equally weighted, 50:50 H₂:CO, fuel mixture was tested with 0 and 20% CO₂ dilution. The burner diameter used for these mixtures was 4.5 mm. For very lean mixtures with 20% dilution, the tip of the flame becomes less intense, and hence, the knife edge was used to make the tip more visible. Figure 5.4 shows the measured flame speeds of these two mixtures, with horizontal error bars indicating the uncertainty in the measured equivalence ratios associated with the flow metering uncertainties. The flame speed increases with equivalence ratio, and decreases with CO₂ dilution. This is not surprising, as dilution with excess air or CO₂ decreases the flame temperature, which reduces the rate of CO and H₂ oxidation reactions and hence flame speed. Figure 5.4 also shows the flame speeds for these mixtures computed with the two reaction mechanisms. Generally the GRI predictions are lower than the measurements for both diluted and undiluted mixtures. The calculated speeds are in good agreement (~5%) with the measured values over the whole equivalence ratio range tested for the undiluted fuel mixture. For 20% CO₂ dilution, however, the discrepancies between the measurements and the GRI results increase, especially for leaner equivalence ratios (0.6-0.8), where the model under predicts the measurements by 10 to 15%.

Figure 5.4 . Laminar flame speeds for fuels with 50:50 H₂:CO composition, and 0 and 20% CO₂ dilution of the fuel; experimental data (symbols) and PREMIX predictions (lines).

On the other hand, the Davis *et al.* H₂/CO mechanism is able to more accurately predict the data, within ~5% for the undiluted mixture and ~7% for 20% CO₂ dilution (see Figure 5.4). The Davis *et al.* H₂/CO mechanism shows better agreement with the diluted data at lean conditions, compared to GRI, while it matches the GRI simulations closer to stoichiometric mixtures. Like the GRI results, the H₂/CO mechanism values consistently under predict the experimental data for 20% CO₂ dilution. At a minimum, the predicted flames speeds can be characterized as being in reasonable agreement with the data for atmospheric pressure, ambient temperature conditions.

Figure 5.5 Strained flame speeds for lean mixtures with 50:50 H₂:CO fuel with 20% CO₂ dilution (i.e., 40:40:20 H₂:CO:CO₂); data (symbols and linear fit) and OPPDIF predictions (lines).

Since the model predictions systematically under predict the diluted data using both chemical mechanisms, with greater fractional differences for the leanest mixtures, this fuel composition was also studied in the stagnation flame configuration. The burner nozzle diameter D was 12.5 mm with $L/D=1$. Figure 5.5 shows the variation of measured flame speed with strain rate at three equivalence ratios ranging from 0.6 to 0.8. Also shown are the corresponding strained flame speeds predicted with the two kinetic mechanisms. As in the Bunsen flame results, the leanest mixtures still show the greatest fractional difference between experiments and predictions, however the models now tend to over predict the flame speeds (except at high Φ and low strain).

Both the measurements and predictions show the flame speeds linearly increasing with strain rate. The mixture Markstein length (L_M), a measure of the sensitivity of the flame speed to strain, can be found from the slope of these lines, i.e.,

$$S_u = S_u^0 - L_M \kappa$$

While the measurements indicate similar values of L_M for $\Phi=0.68$ and 0.78 , the strain sensitivity for the leanest mixture ($\Phi=0.59$) is nearly twice as large. There is also a significant difference between the observed and predicted Markstein lengths. Table 5-1 Measured and predicted unburned Markstein lengths L_M for a 40:40:20 H₂:CO:CO₂ fuel mixture at three lean equivalence ratios. lists the measured and predicted L_M values for this medium H₂ level fuel composition at the three equivalence ratios. The predicted strain sensitivity by the two

mechanisms are very similar at all Φ , but roughly twice the measured strain sensitivity at $\Phi=0.68$ and 0.78 and 1.5 times the value for $\Phi=0.59$.

Φ	L_M (cm) Experiment	L_M (cm) GRI Mech 3.0	L_M (cm) Davis <i>et al.</i> Mech
0.78	-0.0131	-0.0247	-0.0240
0.68	-0.0128	-0.0311	-0.0294
0.59	-0.0250	-0.0399	-0.0371

Table 5-1 Measured and predicted unburned Markstein lengths L_M for a 40:40:20 H₂:CO:CO₂ fuel mixture at three lean equivalence ratios.

Φ	Experiment			GRI Mech 3.0			Davis <i>et al.</i> Mech		
	Bunsen flame	Stag-nation flame	% Δ	PRE-MIX	OPP-DIFF	% Δ	PRE-MIX	OPP-DIFF	% Δ
0.78	57.4	59.1	3.0	52.5	54.4	3.6	53.5	55.7	4.1
0.68	43.9	45.1	2.7	39.7	42.0	5.8	42.0	43.8	4.3
0.59	31.7	31.0	-2.2	28.6	31.0	8.4	30.9	33.1	7.1

Table 5-2 Measured and OPPDIFF predicted unstrained flame speed by linearly extrapolating to zero strain and their comparison with Bunsen flame measurements and PREMIX predictions for 40:40:20 H₂:CO:CO₂ mixture at three different equivalence ratios.

Unstrained flame speeds are commonly determined from strained flame measurements by extrapolating the measured flame speeds to zero strain rate. Table 5-2 compares the Bunsen flame measurement and the linearly extrapolated strained flame speeds for this fuel composition at all three equivalence ratios. There is remarkably good agreement between the two distinct measurement approaches; for the experimental data, the difference is less than 3%.

At this point it should be considered that there is some uncertainty in the way the unstrained flame speed is calculated in the stagnation flame technique. Ideally the strained flame speeds (from OPPDIFF) extrapolated to zero strain rate should equal the unstrained flame speeds predicted in the PREMIX simulation. However significant differences, as much as 8.4%, are seen between these two predictions. For both mechanisms, the differences increase with a reduction in Φ , and the linearly extrapolated strained speeds always over predict the PREMIX results. This disagreement between the unstrained model (PREMIX) and the strained extrapolation may simply be a result of the somewhat arbitrary definition of the unburned strained flame speed as the minimum velocity point in the approaching velocity profile. In addition, the increasing discrepancy between the models for leaner mixtures may be attributable to the corresponding increase in flame thickness. Although large L/D values were employed (in the experiment and computations) finite domain effects may be influencing the strained flame

results at the leanest equivalence ratios. Due to this significant uncertainty in extrapolating the stagnation flame experiment technique, this technique is used to verify the measured flame speeds only at conditions where there is a large discrepancy between the PREMIX and Bunsen flame data. Moreover, because of this finite domain effect, all the remaining strained flame speed measurements are only compared with the corresponding strained flame speed prediction in the same strain rate range.

Overall for this 50:50 H_2 :CO fuel mixture, the measured and predicted flame speeds are in good agreement for both diluted and undiluted cases but there is a significant difference between the measured and predicted strain sensitivity by both models. Moreover, results for the two distinct measurement approaches are in very good agreement within the measurement uncertainties, further supporting the accuracy of the current conical Bunsen flame approach (using the reaction zone area).

The high CO content fuel mixture, 5:95 H_2 :CO, was tested with 0 and 10% CO_2 dilution. The burner diameter used for these mixtures was 13.6 mm. Figure 5.6 shows the flame speeds for these mixtures over a range of lean equivalence ratios. Again, the flame speed increases with equivalence ratio and decreases with CO_2 dilution. For this low H_2 mixture, with and without CO_2 dilution, both mechanisms prediction are essentially the same for all lean conditions, and they are in reasonable agreement with the measurements (within 5-7% over most of the range).

Figure 5.6 Laminar flame speed for fuels with 5:95 H_2 :CO composition, and 0 and 10% CO_2 dilution; experimental data (symbols) and PREMIX predictions (lines).

The high H_2 content fuel composition, 95:5 H_2 :CO, was evaluated for 0 and 20% CO_2 dilution. Due to the very high flame speeds of these mixtures, the burner diameter was reduced to 4.5 mm. For lean conditions with this high H_2 content fuel, the tip of the flame becomes less

intense, and hence the knife edge was used to make the tip more visible for accurate flame area calculations.

Figure 5.7 Laminar flame speed for fuels with 95:5 H₂:CO composition, and 0 and 20% CO₂ dilution; experimental data (symbols) and PREMIX predictions (lines). shows the measured and computed flame speeds for a range of lean equivalence ratios. The GRI Mech 3.0 predictions are consistently lower than the measured flame speeds. For the undiluted mixture, the discrepancy between the GRI predictions and measurements is about 15% near stoichiometric conditions and increases to 20% as the equivalence ratio decreases to 0.6. The Davis *et al.* H₂/CO mechanism predictions are similar to those with the GRI mechanism near stoichiometric conditions, but unlike GRI, the deviation from the measurements decreases as the equivalence ratio is reduced. At the leanest conditions studied ($\Phi=0.6-0.75$), the agreement between the H₂/CO mechanism predictions and measurements is within 3-4% for the undiluted mixture.

Figure 5.7 Laminar flame speed for fuels with 95:5 H₂:CO composition, and 0 and 20% CO₂ dilution; experimental data (symbols) and PREMIX predictions (lines).

Similar behavior is observed for 20 % CO₂ dilution. However as the dilution increases, the agreement between GRIMech 3.0 and the measurement improves near stoichiometric conditions, but worsens at lean conditions. For 20% CO₂ dilution, GRI under predicts the measurements by as much as 25-30% at very lean equivalence ratios. On the other hand, the Davis *et al.* H₂/CO mechanism predicts the measured flame speed within 5% at the very lean equivalence ratio for 20% dilution. Moreover the H₂/CO mechanism predictions are much better for the diluted mixtures near stoichiometric conditions compared to that of the undiluted mixture. Overall, the laminar flame speed predictions with the H₂/CO mechanism are considerably more accurate than with GRIMech 3.0 for this high H₂ content fuel mixture, especially at lean equivalence ratios. Since the Davis *et al.* H₂/CO mechanism, which was nominally optimized for hydrogen mixtures, shows good agreement with measurements for both diluted and undiluted cases, stagnation flame experiments were not conducted for this mixture.

Effect of Preheating

Experiments were carried out for lean mixtures with the same three $\text{H}_2:\text{CO}$ ratios over a range of reactant preheat temperatures from 300 to 700 K. As the unburned reactant temperature increases, the flame speed should increase due to increased chemical rates, and thermal and mass diffusivities. This increase in flame speed requires the burners to be operated at higher average flow velocities (compared to the room temperature case). Fortunately, the increase in the unburned reactant temperature also increases the viscosity of the unburned mixture, which allows the flow to remain laminar even at the higher operating velocities. Hence, the same diameter burners used for the room temperature cases were used for the preheated cases. Figure 5.8 reveals the influence of preheat temperature on flame speed for the low hydrogen content fuel (5:95 $\text{H}_2:\text{CO}$). As was the case for the no preheat case, the predictions from the GRI and Davis *et al.* H_2/CO mechanisms are essentially the same at each preheat temperature, and the measured flame speeds are higher than the predictions. The agreement between the measurements and predictions improves as the equivalence ratio drops. For example, the discrepancies are within 5% for the leanest mixtures ($\Phi=0.6-0.7$) for preheat temperature up to 400 K. Beyond 500 K, the discrepancy between the measurements and predictions increases to 10-15% in this lean equivalence ratio range. Because preheating improves flame stability, measurements were possible for even leaner mixtures at high reactant temperatures (for the same burner diameter). Measurements at these very lean conditions are in good agreement with the prediction by both the mechanisms.

Figure 5.8 Laminar flame speed for fuels with 5:95 $\text{H}_2:\text{CO}$ composition for various preheat temperatures; experimental data (symbols) and PREMIX predictions (lines).

Similar results for the high hydrogen content fuel (95:5 $\text{H}_2:\text{CO}$) are shown in Figure 5.9. As the flame speeds are extremely high (>8 m/s) for this mixture with preheating, the velocities needed to stabilize the flames are also high. To reduce the exit velocities and maintain laminar

conditions, the fuel stream was diluted with 20% CO₂, thereby reducing the flame speeds. Hence the results include the effects of both dilution and reactant temperature.

The computed flame speeds from the two mechanisms are nearly the same at near stoichiometric conditions for all the preheat temperatures. However for lean conditions, the GRI Mech predictions are lower than those from the Davis *et al.* H₂/CO mechanism, by as much as 30% at very lean equivalence ratios. As in the room temperature case, the predictions with the H₂/CO mechanism are in good agreement with the experiments (within 10%) up to 500 K throughout the tested equivalence ratio range. For the 600 K preheat case, the H₂/CO mechanism over predicts the measurements across the complete Φ range, while the GRI results now better reproduce the measurements. Given the poorer prediction with the GRI mechanism at lower temperatures, the improved agreement at high preheat temperatures may simply be fortuitous.

Figure 5.9 Laminar flame speed for fuels with 95:5 H₂:CO composition with 20% CO₂ dilution for various preheat temperatures; experimental data (symbols) and PREMIX predictions (lines).

The influence of preheat temperature for the 50:50 H₂:CO composition is shown in Figure 4.20. The measured flame speeds increase rapidly with the unburned temperature for any given equivalence ratio and are in good agreement (within ~5%) with the GRI Mech 3.0 predictions, up to a preheat temperature of about 500 K. For further increases in preheat temperature, the discrepancy between the measured and GRI Mech 3.0 predictions increases. For the 600 K preheat temperature, the GRI predictions are higher than the measured flame speeds by roughly 10% throughout the equivalence ratio range. For the highest preheat case (700 K), the simulations with GRI Mech 3.0 over predict the measured flame speeds by as much as 15% near stoichiometric and 30% at the leanest conditions tested. The flame speeds predicted with the Davis *et al.* H₂/CO mechanism are also shown in Figure 4.20. The H₂/CO mechanism predictions are very similar to those found with GRI Mech 3.0 except at the leanest Φ , where the H₂/CO mechanism predictions are higher than the GRI predictions by 5%. Thus the H₂/CO mechanism

has an even larger over prediction for the undiluted, 50:50 H₂:CO mixture at 700 K preheat temperature.

Figure 5.10 Laminar flame speed for fuels with 50:50 H₂:CO composition for various preheat temperatures; experimental data (symbols) and PREMIX predictions (lines).

The wall stagnation flame method was used to measure the strained flame speed for the 50:50 H₂:CO fuel mixture at high preheat temperatures (600 K and 700 K) and lean equivalence ratios (0.6 and 0.8) where larger discrepancies were found between the Bunsen flame measurements and the PREMIX flame model predictions. Due to the high flame speeds of these mixtures and the need for significant hydrodynamic strain rate to achieve a stable flame, a nozzle diameter 6.25 mm with a nozzle-wall separation distance of 5 mm was used. Figure 4.21 shows the measured strained flame speeds for this composition at 600 K preheat temperature for 0.8 equivalence ratio. The measured flame speed increases with increasing strain rate, which indicate the negative Markstein length for the unburned flame speed. It should be noted that though the calculated strained flame speed increases linearly with the imposed strain rate, the unstrained flame speed found by linearly extrapolated to zero strain rate does not converge to the one dimensional laminar flame speed predicted by the Chemkin PREMIX code. A difference of as much as 10% has been observed for these conditions. Hence it is more appropriate to compare the measured strained flame speed with that predicted with the OPPDIF code. Figure 5.11 also shows the OPPDIF predictions for 0.6 and 0.8 equivalence ratios in the same strain rate range as that of experiments for all four mechanisms. As observed with the Bunsen flame measurements, both detailed mechanisms (GRI Mech 3.0 and the H₂/CO mechanism of Davis *et al.*) slightly over predict the measurements. The reduced 14 species mechanism is in good agreement with the measurements while the 9 species mechanism over predicts the measurements by 10%.

Figure 5.11 Flame speeds for a 50:50 H₂:CO composition at 600 K preheat temperature for 0.6 equivalence ratios. (vertical bars on measurements indicate a 10% deviation band - not uncertainties in the measurements.)

Figure 5.12 shows the measured strained flame speeds for the same 50:50 H₂:CO composition at 700 K preheat temperature for 0.6 and 0.8 equivalence ratios. The measured strained flame speed increases with the imposed strain rate linearly for both equivalence ratios. It is important to note that the flame at 0.6 equivalence ratio (ϕ) is more strain sensitive than at $\phi=0.8$. Figure 5.12 also shows the OPPDIF predictions for $\phi=0.6$ and 0.8 in the same strain rate range as that of experiments for all four mechanisms. It can be observed from the Figure 5.12 that again the model results with all four mechanisms overpredict the measurements. The Chen 14 species mechanism is again closest to the measurements, while the 9 species mechanism overpredicts the measurements by more than 10%. As the equivalence ratio is reduced to 0.6, the difference between the measurements and the model predictions increases, which is qualitatively similar to our Bunsen flame measurement results. Predictions with GRI Mech 3.0 and the Chen 14 species mechanism is very similar, and they overpredict the measurements by 10%. However the H₂/CO mechanism of Davis *et al.* and the Chen 9 species mechanism overpredict the data by 15% and 20% respectively. These trends are similar to that found for the conical flame results (Figure 5.10).

Figure 5.12 Flame speeds for a 50:50 H₂:CO composition at 700 K preheat temperature for two equivalence ratios. (vertical bar on measurements indicate 10% deviation from the data. It is not the error in measurement).

Combined Effect of Preheating and Dilution

The effect of CO₂ dilution at 700 K preheat temperature was studied for the 50:50 H₂:CO mixture with 40% CO₂ dilution, which also resembles the syngas composition of interest to the full-scale plant. The appropriate nozzle diameter and the nozzle wall separation distance used for these measurements are 9 mm and 6 mm respectively. Figure 5.13 shows the measured strained flame speeds for this composition at 700 K preheat temperature for 0.6 and 0.8 equivalence ratios. At $\phi=0.8$, both GRI Mech 3.0 and the Chen 14 species mechanism overpredict the measurements by 10% while the H₂/CO mechanism of Davis *et al.* and the reduced Chen 9 species mechanism overpredict the measurements by 15%. For the lower equivalence ratio to 0.6, the trends remain the same for the GRI Mech 3.0 and 14 species Chen mechanisms. However, the 9 species Chen mechanism overpredicts the measurements by as much as 18%. Comparing the undiluted 50:50 H₂:CO mixture measurements with the diluted case indicates that the spectral radiation reabsorption of CO₂ dilution does not make significant changes, in the agreement between the models and experiments.

Figure 5.13 Flame speeds for a 30:30:40 H₂:CO:CO₂ composition at 700 K preheat temperature for two equivalence ratios. (vertical bar on measurements indicate 10% deviation from the data. It is not the error in measurement)

Effect of Pressure

The effect of higher operating pressure was studied for three H₂:CO compositions: 5:95, 10:90 and 20:80 at 5 atm and $\Phi=0.6$ using the stagnation flame technique (Figure 5.14). As in the earlier measurements, the flame speed increases linearly with strain rate, indicating a negative (unburned) Markstein length. As the amount of H₂ increases in the mixture, the strain sensitivity increases. For the 5:95 H₂:CO fuel, predictions produced by both mechanisms are in excellent agreement (less than 5% discrepancy) with the measurements; this is similar to the finding from the atmospheric pressure tests. Similar agreement between the measurements and predictions is observed for the 10:90 fuel mixture with the Davis *et al.* H₂/CO mechanism, while the GRI mechanism results slightly under predict the measurements. For both these low H₂ content fuels, the predicted strain sensitivities also are in good agreement with the measurements. Thus the good agreement observed at atmospheric pressure between the model predictions and measurements is maintained at this higher operating pressure.

Figure 5.14 Strained laminar flame speeds for different H₂/CO fuel compositions at 5 atm and F=0.6; data (symbols and linear fits) and OPPDIF predictions (lines).

As the amount of H₂ is raised to 20%, the discrepancy between the measurements and predictions increase. The GRI mechanism now under predicts the measurements by about 10%. More importantly both mechanisms fail to predict the higher strain sensitivity for this mixture. Recall that the model predictions also failed to accurately capture the strain sensitivities for the atmospheric pressure cases with intermediate H₂ levels (Figure 5.5).

5.3 Task 4 (Systems Modeling)

The plant level requirements from the DOE Co-generation program plan and EECF phase 1 report are stated below:

- **Fuel Flexible** – *“it could use one or more of several different feedstock for example, coal, natural gas, or petroleum coke. Any of these could be mixed with biomass. Biomass-only plants are excluded.”*
- **Process Flexible** – *“A 21st Century Energy Plant is not a single configuration, instead it will be a group of plants with different configurations that would be tailored to meet specific market needs.”*
- **Output Flexible** and **Economical** - *“Produce one or more of a number of high-value products such as electric power, clean fuels, chemicals, or hydrogen. Clean, affordable transportation-quality fuels at costs equivalent to \$20 per barrel or less (1998 \$).”*

- **Output Flexible** and **High Efficiency** - **“Secondary products such as heat/steam for industrial use could also be produced. Combined Heat/Power: Overall thermal efficiencies of 85-90%.”*
- **Low Air Pollutant Emissions** – **“Eliminating environmental issues associated with the utilization of fossil fuels – Emissions of air pollutants such as sulfur dioxide, nitrogen oxides, and mercury would be reduced to essentially zero levels.”*
- **High Efficiency, Process Flexible** and **Fuel Flexible** - **“Emissions of carbon dioxide, a greenhouse gas, would be dramatically reduced because of the higher efficiency. The plant design would also include the option for capturing and sequestering carbon dioxide. Carbon dioxide emissions reduced by 40-50% by efficiency improvements; reduced to zero [net] if coupled with carbon sequestration.”*
- **High Efficiency** - **“The plants would be designed to use as much of the energy in the fuel as possible. Power Generating efficiencies greater than 60% using coal and greater than 75% using natural gas.”*
- **Economical** - *“Costs of electricity competitive with market clearing prices at the time of deployment.”*

* Quotes from DOE Co-generation Program Plan.

The critical combustor level requirements are established as the following:

- **Fuel Flexible** – exceed current +/- 10% Wobbie Index variation without hardware modification.
- **Co-Firing capability** – capable of operation on syngas and NG simultaneously over a wide range of load.
- **Low NO_x emission** – less than 9 ppmvd @ 15% O₂, comparable to standard DLN combustor.
- **Diluent reduction** – uses less diluent than diffusion type combustor for NO_x abatement.
- **Air extraction capability** – supply air to ASU.
- **Hardware life** – exceed 24000 hrs, which is same as standard DLN combustor.

A Quality Flow Down analysis was performed to rank the importance of the combustor level requirements and there effects on critical plant performance. The importance of the combustor requirements is indicated by the order in which they are listed.

Task 4 was completed by incorporating each of the combustor models into the system model. In these validation runs, the EECF diffusion combustor cases included steam and nitrogen as diluents. The important finding in this plant analysis is that the 9 ppm NO_x requirement is only is satisfied by using both steam and nitrogen as diluents. The DLN & TVC systems do not include diluent augmentation as none is required to meet the NO_x emissions limit. The co-generation efficiency for a TVC system is lower than that for the diffusion combustor, due to the additional steam injection in the diffusion combustor. However, the advantage of the TVC system is that NO_x emissions are lower even without diluent injection (for natural gas and EECF fuels).

Additional diffusion and TVC combustor system analysis were performed to verify the previous analysis and for use in optimizing the performance of the prototype designs. The outputs of the performance analysis are used to estimate the optimal combustor operating conditions. Additionally, the analysis helps establish the appropriate full-scale scaling requirements for the design of both combustion systems.

5.3.1 Integration of Combustor Concepts into EECF Plant Model

Three hybrid combustor concepts were chosen for system level evaluations in Task 2:

- Concept #1- Diffusion Syngas & DLN CH₄ combustor.
- Concept #2 - Trapped Vortex (TVC) Syngas & CH₄ combustor.
- Concept #3 - Diffusion Syngas & TVC CH₄ combustor.

Results of the EECF fuels diffusion combustor cases (concept #1 and #3) are summarized in Figure 5.15 & Figure 5.16. The EECF diffusion combustor cases include steam and nitrogen as diluents. By using both steam and nitrogen as diluents, 9 ppm NO_x requirement is satisfied as shown in Figure 5.21.

Results of the EECF fuels TVC combustor cases (concept #2) are summarized in Figure 5.17 & Figure 5.18. Results of the Backup fuel (Natural Gas) cases are summarized in Figure 5.19 & Figure 5.20.

Case #	1	2	3	4	5a	5b	7a	7b	8a	8b	9a	9b
Combustor Description	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm
GT Output (kW)	90000	90000	90000	90000	90000	90000	90000	90000	90000	90000	90000	90000
ST Output (kW)	3014	2968	3013	2982	3024	2661	3010	2999	2824	3026	3032	3032
CC Net Output (kW)	92649	92607	92647	92618	92657	92315	92646	92635	92471	92660	92666	92666
GT HC LHV (MMBtu/hr)	815	812	814	813	816	817	814	814	808	815	815	816
CC Cogen Net Eff HHV (%)	79.3%	78.6%	79.9%	79.5%	80.0%	78.5%	78.8%	79.1%	79.0%	79.6%	79.5%	79.8%
NOx ppmvd @ 15% O2	9.0	9.0	9.0	9.0	9.0	8.5	9.0	9.0	9.0	9.0	9.0	9.0
Syngas - 10046												
Flow (lb/hr)	306135	299911	312019	312775	31486	327046	297090	302540	300252	309835	306451	312603
Pressure (psia)	315	315	315	315	315	315	315	315	315	315	315	315
Temperature (F)	400	400	400	400	400	400	400	400	400	400	400	400
Diluent - 115												
Flow (lb/hr)	133655	137070	131129	134274	132915	133059	134812	132417	132609	131351	133073	130938
Pressure (psia)	300	300	300	300	300	300	300	300	300	300	300	300
Temperature (F)	550	550	550	550	550	550	550	550	550	550	550	550
Air to GT - 1201												
Flow (lb/hr)	1493254	1481294	1487075	1483397	1494954	1495222	1491333	1492533	1503405	1493351	1493718	1494296
Pressure (psia)	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67
Temperature (F)	59	59	59	59	59	59	59	59	59	59	59	59
Air Extraction - 1200												
Flow (lb/hr)	105709	106203	105150	111164	112118	120026	102084	102578	86734	106264	104651	106817
Pressure (psia)	226	225	226	225	227	227	226	226	228	226	227	227
Temperature (F)	773	770	771	770	773	773	772	773	775	773	773	773
GT Exhaust												
Flow (lb/hr)	1848827	1833384	1846542	1840684	1854800	1856890	1842566	1846373	1871291	1849776	1850098	1852556
Pressure (psia)	14.87	14.88	14.87	14.88	14.87	14.87	14.87	14.87	14.87	14.87	14.87	14.87
Temperature (F)	1084	1084	1084	1084	1083	1084	1084	1083	1084	1084	1084	1084
Stack - 1202												
Flow (lb/hr)	1848827	1833384	1846542	1840684	1854800	1856890	1842566	1846373	1871291	1849776	1850098	1852556
Pressure (psia)	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70
Temperature (F)	296	296	295	295	295	294	296	296	298	296	296	295
BFW - 1254												
Flow (lb/hr)	472779	468186	475698	475577	479448	475756	467620	470206	464653	474958	473424	476701
Pressure (psia)	25	25	25	25	25	25	25	25	25	25	25	25
Temperature (F)	240	240	240	240	240	240	240	240	240	240	240	240

Figure 5.15 Syngas Combined Cycle Performance Summary (Diffusion Combustor)

Case #	1	2	3	4	5a	5b	7a	7b	8a	8b	9a	9b
Combustor Description	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm	Diffusion N2 + Stm
LP BFW to Gasification- 1203												
Flow (lb/hr)	169665	166214	172926	173345	175956	181254	164652	167672	166404	171716	169840	173249
Pressure (psia)	185	185	185	185	185	185	185	185	185	185	185	185
Temperature (F)	330	330	330	330	330	328	331	331	332	330	330	330
LP Steam from 185psia Header - 1252												
Flow (lb/hr)	196941	192936	200726	201213	204243	210393	191122	194628	193156	199321	197144	201102
Pressure (psia)	185	185	185	185	185	185	185	185	185	185	185	185
Temperature (F)	375	375	375	375	375	375	375	375	375	375	375	375
LP Superheated Steam to Refinery - 1204												
Flow (lb/hr)	201947	197913	205619	206053	209146	215457	196235	199714	198852	204284	202164	206059
Pressure (psia)	185	185	185	185	185	185	185	185	185	185	185	185
Temperature (F)	460	461	459	458	458	451	462	461	463	459	460	459
HP Saturated Steam to SRU - 1205												
Flow (lb/hr)	4036	3954	4114	4124	4198	4312	3917	3989	3958	4085	4040	4121
Pressure (psia)	1005	1000	1004	1001	1005	970	1004	1003	988	1006	1006	1006
Temperature (F)	545	545	545	545	545	541	545	545	543	545	545	545
HP Saturated Steam to Gasifier - 1206												
Flow (lb/hr)	21507	21069	21920	21973	22304	22976	20871	21254	21093	21766	21529	21961
Pressure (psia)	1005	1000	1004	1001	1005	970	1004	1003	988	1006	1006	1006
Temperature (F)	545	545	545	545	545	541	545	545	543	545	545	545
HP Saturated Steam from SRU - 1253												
Flow (lb/hr)	15406	15092	15702	15740	15977	16458	14950	15225	15109	15592	15421	15731
Pressure (psia)	620	620	620	620	620	620	620	620	620	620	620	620
Temperature (F)	490	490	490	490	490	490	490	490	490	490	490	490
HP Superheated Steam to Refinery - 1207												
Flow (lb/hr)	278867	272010	283364	280013	284330	278608	274077	278099	272159	282673	280022	284384
Pressure (psia)	620	620	620	620	620	620	620	620	620	620	620	620
Temperature (F)	720	720	720	720	720	720	720	720	720	720	720	720
Steam Injection to GT												
Flow (lb/hr)	9104	15052	4183	7022	3746	0	13940	9332	10451	10451	8394	3760
Pressure (psia)	300	300	300	300	300	0	300	300	300	300	300	300
Temperature (F)	467	467	467	467	467	0	467	467	467	467	467	467

Figure 5.16: Syngas Combined Cycle Performance Summary Cont' (Diffusion Combustor)

Case #	1	2	3	4	5a	5b	7a	7b	8a	8b	9a	9b
Combustor	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC
GT Output (kW)	90000	90000	90000	90000	90000	90000	90000	90000	90000	90000	90000	90000
ST Output (kW)	2344	2299	2323	2314	2346	2353	2330	2331	2341	2346	2350	2354
CC Net Output (kW)	91826	91781	91805	91796	91828	91835	91812	91813	91823	91828	91832	91836
GT HC LHV (MMBtu/hr)	817	814	816	817	820	822	815	817	817	819	818	820
CC Cogen Net Eff HHV (%)	79.0%	79.2%	78.7%	78.7%	78.8%	78.1%	79.0%	78.6%	78.8%	78.4%	78.8%	78.4%
NOx ppmvd @ 15% O2	4.2	4.2	3.5	3.7	4.0	3.4	4.3	3.7	4.1	3.5	4.1	3.6
Syngas - 10046												
Flow (lb/hr)	307022	300488	312804	314211	318906	328913	297482	303549	303464	311163	307413	314090
Pressure (psia)	375	375	375	375	375	375	375	375	375	375	375	375
Temperature (F)	400	400	400	400	400	400	400	400	400	400	400	400
Diluent - 115												
Flow (lb/hr)	124912	122254	127264	127837	129747	133819	121030	123499	123464	126597	125070	127788
Pressure (psia)	300	300	300	300	300	300	300	300	300	300	300	300
Temperature (F)	550	550	550	550	550	550	550	550	550	550	550	550
Air to GT -1201												
Flow (lb/hr)	1517870	1511927	1501876	1510682	1517204	1515723	1518080	1516640	1517839	1516457	1518074	1516660
Pressure (psia)	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67	14.67
Temperature (F)	59	59	59	59	59	59	59	59	59	59	59	59
Air Extraction - 1200												
Flow (lb/hr)	96642	88756	102052	107141	111988	126256	84956	94173	92491	103717	96782	106827
Pressure (psia)	230	230	234	229	230	230	230	230	230	230	230	230
Temperature (F)	780	778	776	778	780	779	780	780	780	780	780	780
Stack - 1202												
Flow (lb/hr)	1874949	1867614	1861530	1867287	1875665	1873976	1873402	1871256	1874050	1872255	1875568	1873480
Pressure (psia)	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70	14.70
Temperature (F)	296	297	295	295	295	294	297	296	296	296	296	295

Figure 5.17: Syngas Combined Cycle Performance Summary (Trapped Vortex Combustor)

Case #	1	2	3	4	5a	5b	7a	7b	8a	8b	9a	9b
Combustor	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC	TVC
BFW - 1254												
Flow (lb/hr)	464799	459270	467468	468156	472208	478465	458480	462253	462535	467409	465277	469465
Pressure (psia)	25	25	25	25	25	25	25	25	25	25	25	25
Temperature (F)	240	240	240	240	240	240	240	240	240	240	240	240
LP BFW to Gasification- 1203												
Flow (lb/hr)	170156	166535	173361	174140	176743	182289	164869	168231	168184	172451	170373	174074
Pressure (psia)	185	185	185	185	185	185	185	185	185	185	185	185
Temperature (F)	330	330	329	329	329	328	330	330	330	329	330	329
LP Steam from 185psia Header - 1252												
Flow (lb/hr)	197512	193308	201231	202136	205157	211594	191374	195277	195222	200176	197763	202059
Pressure (psia)	185	185	185	185	185	185	185	185	185	185	185	185
Temperature (F)	375	375	375	375	375	375	375	375	375	375	375	375
LP Superheated Steam to Refinery - 1204												
Flow (lb/hr)	203261	199141	206710	207712	210692	216863	197292	201058	201018	205823	203500	207664
Pressure (psia)	185	185	185	185	185	185	185	185	185	185	185	185
Temperature (F)	455	456	453	453	453	451	457	455	455	454	455	453
HP Saturated Steam to SRU - 1205												
Flow (lb/hr)	4048	3962	4124	4142	4204	4336	3922	4002	4001	4102	4053	4141
Pressure (psia)	973	968	971	970	973	974	971	971	972	973	973	974
Temperature (F)	541	541	541	541	541	541	541	541	541	541	541	541
HP Saturated Steam to Gasifier - 1206												
Flow (lb/hr)	21569	21110	21975	22074	22404	23107	20899	21325	21319	21860	21596	22065
Pressure (psia)	973	968	971	970	973	974	971	971	972	973	973	974
Temperature (F)	541	541	541	541	541	541	541	541	541	541	541	541
HP Saturated Steam from SRU - 1253												
Flow (lb/hr)	15450	15121	15741	15812	16048	16552	14970	15275	15271	15659	15470	15806
Pressure (psia)	620	620	620	620	620	620	620	620	620	620	620	620
Temperature (F)	490	490	490	490	490	490	490	490	490	490	490	490
HP Superheated Steam to Refinery - 1207												
Flow (lb/hr)	278726	276955	278270	278034	279368	280016	277843	278191	278505	279006	278986	279385
Pressure (psia)	620	620	620	620	620	620	620	620	620	620	620	620
Temperature (F)	720	720	720	720	720	720	720	720	720	720	720	720

Figure 5.18: Syngas Combined Cycle Performance Summary Cont'd (Trapped Vortex Combustor)

Case #	10	10	10
Combustor	Diffusion	DLN	TVC
GT Output (kW)	83352	69082	69091
ST Output (kW)	2454	1995	1995
CC Net Output (kW)	85289	70559	70568
GT HC LHV (MMBtu/hr)	791	712	712
CC Cogen Net Eff HHV (%)	77.7%	77.1%	77.1%
NOx ppmvd @ 15% O2	25	4	3.9
Syngas - 10046			
Flow (lb/hr)	36748	33075	33077
Pressure (psia)	315	315	315
Temperature (F)	80	80	400
Diluent - 115			
Flow (lb/hr)	0	0	0
Pressure (psia)	300	300	300
Temperature (F)	550	550	550
Air to GT -1201			
Flow (lb/hr)	1610464	1610298	1610298
Pressure (psia)	14.67	14.67	14.67
Temperature (F)	59	59	59
Air Extraction - 1200			
Flow (lb/hr)	0	0	0
Pressure (psia)	224	208	207
Temperature (F)	771	749	749
Stack - 1202			
Flow (lb/hr)	1756236	1662653	1662655
Pressure (psia)	14.70	14.70	14.70
Temperature (F)	317	316	316

Figure 5.19: Natural Gas Combined Cycle Performance Summary

Case #	10	10	10
Combustor	Diffusion	DLN	TVC
Description	Steam Inj	NG Dry	NG Dry
BFW - 1254			
Flow (lb/hr)	286839	269687	269689
Pressure (psia)	25	25	25
Temperature (F)	240	240	240
LP BFW to Gasification- 1203			
Flow (lb/hr)	0	0	0
Pressure (psia)	185	185	185
Temperature (F)	375	375	375
LP Steam from 185psia Header - 1252			
Flow (lb/hr)	0	0	0
Pressure (psia)	185	185	185
Temperature (F)	375	375	375
LP Superheated Steam to Refinery - 1204			
Flow (lb/hr)	17892	16626	16627
Pressure (psia)	185	185	185
Temperature (F)	514	511	511
HP Saturated Steam to SRU - 1205			
Flow (lb/hr)	0	0	0
Pressure (psia)	981	934	934
Temperature (F)	542	536	536
HP Saturated Steam to Gasifier - 1206			
Flow (lb/hr)	0	0	0
Pressure (psia)	981	934	934
Temperature (F)	542	536	536
HP Saturated Steam from SRU - 1253			
Flow (lb/hr)	0	0	0
Pressure (psia)	620	620	620
Temperature (F)	490	490	490
HP Superheated Steam to Refinery - 1207			
Flow (lb/hr)	180272	253063	253064
Pressure (psia)	638	638	638
Temperature (F)	720	720	720

Figure 5.20: Natural Gas Combined Cycle Performance Summary Cont'd

Figure 5.21: Hybrid Concepts Performance Comparison

Figure 5.21 shows the comparison of the hybrid concepts with respect to co-generation efficiency, gas turbine air extraction, high-pressure steam production and NOx emissions for the 12 syngas cases (cases 1 – 9b) and the natural gas case (case # 10). The co-generation efficiency for TVC is lower than that for the diffusion combustor. This is primarily due to the additional steam injection in the diffusion combustor. The NOx however is lower for the TVC even without any steam injection. The diffusion combustor is able to meet the 9-ppm NOx with adequate steam injection.

5.4 Task 5 (Prototype Design)

5.4.1 Hybrid DLN-Diffusion Nozzle (Prototype-1)

Preliminary CFD calculations have been performed to investigate mixing and the flow-field phenomenon. The results show a flowfield comprised of recirculation zones due to the swirling air and fuel flows. Mixing of the fuel, air, and diluent streams are studied by looking at the diluents/fuel/air mass ratio distributions along different cross-sections at downstream axial locations in the combustor. The generated iso-surfaces of stoichiometric fuel-air distribution represent the flame zone. The shape and the length of the flame zone provide us with information of the rate of mixing between the fuel and the air streams. The calculations showed drastically different flame shapes implying a strong correlation of the diffusion flame zone to the

geometric parameters being studied. The changes in the flame shape also influence the exit temperature profile and the thermal NO_x emissions at the combustor exit.

Drawing from these previous investigations, a design of experiments was conducted as described in section 2.4.2. The influencing geometry variables were examined, resulting in an 8 experiment DOE to examine the combustion characteristics of the hybrid nozzle design. CFD calculations of the combustor flowfield are performed for the eight different combinations of geometric parameters for the hybrid burner operated on syngas. Geometric parameters include the orientation of the fuel and the diluents jets in terms of swirl and radial angles. The degree of swirl in the air stream is also included as a parameter. The response of the hybrid nozzle combustion characteristics for each of the 8 geometry sets are estimated and used to generate perturbation plots for each of the geometry variables. The final combustor geometry is selected by analyzing the perturbation plots to obtain the optimized variable settings that meet the critical combustor design criteria. The final configuration is selected based on an optimum compromise between the requirements for lower NO_x , flame length, pattern factor, and gas temperature impinging on the diffusion tip. The optimized design of the diffusion tip geometry is then validated using CFD.

5.4.1.1 Flame Shape and Exit Profile

Analysis of the three dimensional flame surfaces defined by the fuel/air stoichiometric contour as functions of static temperature for the 8 geometry cases show significant differences in the flame structure. The flame shape and flame length depend on the orientation of the fuel and diluents jets and the swirl imparted on the combustion are by the swizzle assembly. An optimized flame shape and length determine the combustor exit temperature distribution which is critical for combustor performance in terms of hardware life, emissions levels, combustion efficiency, and pattern factor (hot-gas uniformity) for entry of the hot gas into the turbine. A pareto/perturbation analysis was used to determine the geometry parameters that most effectively influence flame length and shape. In the pareto/perturbation analysis, the results of the design variables are analyzed as a function of their minimum and maximum values in DOE to investigate their corresponding effects on flame structure. The angles of the syngas and diluent jets are significant parameters affecting the flame length. These effects are expected since increasing or decreasing the angles of the jets helps the fuel/diluents mix slower or faster with the combustion air. The diluent splits and the air swirl angle are also other significant parameters that affect the flame length.

A uniform pattern factor, or exit plane temperature profile, is desirable to reduce the heat load on the turbine. From the analysis, the angles of the syngas jet have a large impact on pattern factor. This is because the syngas jet angles also significantly affects the flame length. Under ideal cases the flame should be as short as possible to allow for more post-combustion mixing of the hot gases to create a more uniform temperature distribution. Air swirl angles also affect the pattern factor. In general, the geometry influence on pattern factor is similar to the responses for flame shape and length. The geometry that produces a smaller flame length generates a lower pattern factor. Typically these are the observed trends for diffusion flame

combustion in gas turbine systems since the process is mixing rate limited, i.e. the mixing length determines the flame characteristics.

5.4.1.2 Temperature Profiles

The swirling flow induces a flow recirculation in the dump zone of the combustor. The recirculating gas is comprised of the hot gas combustion products. The hot gases impinge on the diffusion tip, which can impose large thermal loads and potentially lead to failure of the diffusion tip. Therefore it is necessary to minimize the temperature of the recirculating gases. Axial temperature distribution plots of the CFD results were examined. The figures show the presence of a central recirculation zone and hot gases impinging on the diffusion tip. Temperature at the diffusion tip varied as a function of the geometry with longer flame length geometry resulting in lower tip temperatures, but greater pattern factors (as indicated by the flame shape analysis). Thus in terms of obtaining lower recirculation zone temperatures for lower tip temperature and increased hardware reliability, the optimal tip configuration conflicts with the optimal design settings for shorter flame lengths and pattern factor. It appears that variables that lead to shorter flame lengths and lower pattern factors tend to increase the gas temperatures impinging on the diffusion tip.

5.4.1.3 Emissions

Profiles of thermal NO_x , which is the pathway for NO_x formation since diffusion flames burn at stoichiometric conditions, at the exit plane of the diffusion combustor system indicate a maximum at the centerline and decrease radially outward. This trend is expected as thermal NO_x is a strong function of temperature and the pattern factor at the exit plane. This is also indicated in the 8 geometry cases tested, since the shortest flame lengths and correspondingly lowest pattern factors produced the lowest thermal NO_x and the longest flame lengths and highest pattern factors produced the highest NO_x levels. Cross-sectional mass averaged emissions profiles along the axial length of the combustion chamber are used to provide insight into the history of NO_x formation. For the short flame length cases the averaged NO_x levels increase with axial distance upto the corresponding axial location of peak flame temperature and then reach either a steady state level based on the hot-product gas temperature or slightly lower level as the hot-products cool downstream near the combustor exit plane. The geometries that result in longer flame lengths produce NO_x at a linear rate as a function of axial distance, all the way upto the axial location of peak flame temperature and even to the combustor exit plane. These results are consistent with thermal NO_x theory and experimental observations, which state that flames with higher peak flame temperatures tend to produce more NO_x since the thermal NO_x pathway depends on the maximum temperatures and the corresponding flow residence times. Thus for the diffusion combustor the NO_x emissions are directly related to flame length and pattern factor, with flames of shorter length and lower pattern factor being more desirable. However, these factors lead to higher temperatures at the diffusion tip and pose hardware life risks due to the high thermal loads.

The temperature history, and therefore NO_x formation, in the combustion chamber is a function of the mixing between the fuel, air and diluents streams. Faster mixing leads to faster decrease of the maximum temperatures in the combustion chamber. The mixing in the diffusion nozzle design is investigated by examining the maximum fuel mixture fraction as a function of the axial distance in the combustion chamber. The fuel mixture fraction is the mass fraction of all species originating from the fuel stream. Maximum fuel mixture fraction is 1 at axial distance of zero, which is close to the point of fuel injection. The mixture fraction decreases as the fuel stream mixes with the combustion air and the diluents streams. The geometries with shorter flames show rapid decreases in mixture fraction immediately downstream of the injection tip. This implies a very short axial extent of the flame and hence faster combustion, which reduces the residence times for NO_x formation. Correspondingly, the longer flame length geometries show the slowest fuel/air mixing rate.

The mixing between the diluents and the fuel and air streams is another important parameter the effects NO_x formation. In a similar manner, mixing rate effects on NO_x formation are examined by comparing the minimum ratios of the mass of the diluents to the fuel stream as a function axial distance. Results indicate that fast diluent-fuel mixing is critical to mitigate NO_x formation. This is the desired and expected trend based off of diluent augmentation theory. Faster diluent mixing lowers the peak flame temperature and thus lowers emissions. For the 8 cases studied, the maximum temperatures and thermal NO_x characteristics depend on the combination of the mixing between the fuel and air streams and the diluents and fuel streams. Note: the shortest flame length did not always produce the most rapid diluent-fuel mixing. In short, NO_x formation is a direct function of the temperature history in the combustor, which is determined by the fuel, air, and diluent mixing rates. These rates are controlled by the diffusion tip geometry.

The analysis of the optimal configuration shows a reasonable flame length and exit temperature profile. The maximum gas temperatures near the diffusion tip are also lower than some of the extreme cases examined in the design of experiments. The NO_x values appear to be higher than 10 ppm, but the values are sensitive to the turbulence-chemistry interaction model. Also the NO_x values can be lowered by increasing the diluents during the experimental testing phase of this program. Overall we feel that we have a diffusion combustor design that can be tested for syngas performance.

Just say that we have optimized the design according to the DOE results to get the lowest tip to, best emissions, pattern factor, best mixing.

5.4.1.4 Prototype-1 Premixed Swozzle

CFD calculations for the airflow around the swirl vanes have been performed to examine the characteristics of the swirling flowfield at the burner tube exit. We also examined the capability of the swirling flow to induce a recirculation zone. The premixed natural gas injection strategy is also examined using CFD calculations. Through a parametric design of experiments and in conjunction with the detailed computations, we have been able to determine the optimum

jet momentum and penetration, fuel hole size, and hole placement to ensure effective premixing of the fuel and combustion air at the exit plane of the burner tube.

5.4.2 Trapped Vortex Combustor (Prototype-2) Experimental Results

The trapped vortex combustor was operated with EECF syngas fuel. The combustor components described previously were needed to prevent flashback into the premixers. During the evaluation no flashback events were encountered, and the premixers performed in accordance with the design intent despite the presence of Hydrogen. The syngas fuel was composed of 24.6% Hydrogen, 44.6% Nitrogen, 11.5% methane, and 19.3% CO₂. The hydrogen content was representative of the levels seen in the EECF fuels, and methane was added to the mixture to keep the overall heating value of the fuel in line with the EECF fuel spec.

The combustor was lit in a natural gas mode, and then operation was changed to a syngas-only mode of operation. The syngas was premixed in both the cavity and main portions of the combustor, and flow rates were controlled independently.

Wall temperatures were monitored at critical locations throughout the combustor. The combustor wall surface temperatures remained within acceptable limits throughout the experiment. Cavity combustion temperatures were adjusted to reach the low NO_x performance conditions.

The NO_x emission results from the combustor exceeded expectations. The ultra-low NO_x emissions demonstrated the value of the TVC approach. The CO emissions were above the targeted levels, but experiments showed a strong sensitivity to combustor length. It is believed that the combustor could be lengthened to bring the CO to the targeted levels. Combustion dynamics were extremely low throughout the experiments. The design has good stability at both high and low firing temperatures. The CO levels were acceptable and well within the limits at the low firing temperature condition. The strong turn-down performance of the TVC allows for a simpler design and control scheme.

5.4.3 Prototype-1N Experimental Results: Modified Premixers

Flame holding results for the modified premixer were superior to the baseline hardware, but not as good as the reduced-scale premixers tested in Phase I of the DOE IGCC/H₂ Gas Turbine Program. NO_x emissions for syngas fuel were slightly below the levels for natural gas.

Additional modifications to the burner tube and centerbody profiles were made in an attempt to further improve operability. These changes proved successful, as tests demonstrated the new design's capability to now operate to engine-realistic flame temperatures on a variety of high-hydrogen fuels. The operability came at the expense of slightly higher NO_x emissions, which are plotted over the successful operating range in Figure 5.22 and compared to entitlement (perfectly-premixed) data obtained as part of the DOE IGCC/H₂ Gas Turbine Program.

Figure 5.22 NOx emissions on hydrogen fuel for the modified premixer with the best operability

5.5 Task 6 (Syngas Methodology for Advanced CFD Tools)

5.5.1 Chemical Mechanism Validation

As noted in a previous section, two reduced mechanisms (the 14 species-10 step mechanism compared to the experiments above, and a 9 species-5 step mechanism, also provided by J. Y. Chen) were investigated for the LES computations. The 10-step mechanism's accuracy for flame speed prediction was addressed in the previous section. As the 5-step mechanism is computationally less expensive, it may be preferable for the LES calculations. To be sure it predicts the chemical state-space reasonably well under the actual flow configurations inside the combustor, we examine its predictive accuracy for detailed flame parameters. The accuracy of this simpler mechanism is validated by comparing results obtained with more detailed reaction mechanisms.

First, we compare the 5-step mechanism to a detailed mechanism with laminar flame (PREMIX) and perfectly stirred reactor (PSR) models. Figure 3.5-1 shows results for flame speed that indicate the 5-step (9-species) mechanism provides results reasonably close to the more detailed mechanism for two common syngas compositions. Similarly, Figure 3.5-2 presents output of a PSR as a function of residence time for H mole fraction and temperature for two other syngas compositions. In general, the predictions match quite well with the detailed results.

Next, we compare the detailed predictions obtained with the 5-step and 10-step mechanisms for two test cases: a PREMIX flame calculation and DNS of a flame vortex interaction. The one-dimensional laminar flame (PREMIX) calculations are shown in Figure 3.5-3 for a 50:50 H₂:CO fuel composition under atmospheric pressure and for an equivalence ratio of

0.6. The CO mole fraction and temperature profiles are identical for both reduced mechanisms. The intermediate species profiles are slightly different. For example, the peak H mole fraction is ~10% higher for the 5-step (9 species) mechanism, while the peak OH level is about 20% higher. Given the reduced number of intermediate species in the smaller mechanism, it is not surprising that it over-predicts the concentrations of those intermediates that it does track. The DNS comparisons for the same fuel composition are shown in Figure 3.5-4. This is the same DNS code that was validated in the previous phase of the project. The velocity profiles are nearly identical in the unburned (left) and vortex (middle) region of the flame. There is a small difference for the velocities obtained in the post flame region (right).

The relatively similar predictions with the 5-step, 10-step and detailed mechanisms demonstrated to date indicate that both reduced mechanisms provide cost-effective chemical models for LES of full-scale combustors. This is because in LES with finite-rate kinetics, chemistry evaluation can be over 90% of the total computational cost. We are exploring further modifications to these mechanism (perhaps by adding additional reaction steps), but the current mechanisms are employed in the LES studies reported below.

Figure 5.23: Flame speed calculation with PREMIX for two syngas compositions:
a) ILVA (H₂:CO:CO₂:N₂=8.6:26.6:14.3:51) and b) TAMPA
(H₂:CO:CO₂:N₂:H₂O= 37.2:46.6:13.3:2.6:0.3).

Figure 5.24: PSR comparisons for two syngas compositions: a) mole fraction of H for PSI ($\text{H}_2:\text{CO}:\text{CO}_2:\text{N}_2:\text{H}_2\text{O}=24:40:9:4:23$) and b) temperature for PUMPE ($\text{H}_2:\text{CO}:\text{CO}_2:\text{N}_2=61.9:26.2:2.8:8.7$).

Figure 5.25: Comparison of laminar flame (PREMIX) predictions obtained with the 5-step and 10-step mechanisms for a 50:50 $\text{H}_2:\text{CO}$ mixture with $\phi=0.6$.

Figure 5.26: Comparison of the axial (u) velocity profiles obtained by DNS of a vortex interacting with an atmospheric-pressure, laminar flame of 50:50 H₂:CO fuel composition with an equivalence ratio of 0.6. Results are shown for two times during the interaction: a) at t=200 and b) t=1000 time step iterations ($\Delta t = 0.317 \cdot 10^{-7}$ sec).

5.5.2 Flame Dynamics

Effect of the syngas fuel composition on the flame dynamics is investigated by a flame vortex interaction (FVI) problem. An initial vortex is generated within a rectangular domain and two cases with different fuel compositions are simulated. Case 1 corresponds to a fuel with a volumetric ratio of 95:5 CO and H₂ together with a 20% CO₂ dilution, whereas for Case 2 fuel mixture is composed of 5:95 CO:H₂. In general, both H₂ and CO exhibit different diffusivities and thus, these two limiting cases allows an investigation of extreme conditions of this type of fuel mixture. The equivalence ratio is selected to be 0.6 for both cases. Symmetry (Slip wall) and periodic conditions are employed on the lower and upper boundaries in *y* direction. The velocity and pressure field inside the domain is altered by the superposition of a counter rotating vortex pair, and as the flow is symmetrical with respect to the *x* axis, only the upper part is calculated. Since the laminar flame velocity and the flame thickness of each fuel mixture is different, in order to achieve a same kind of vortex interacting with the flame front regardless of the type of the fuel, the ratio of maximum velocity induced by the vortex to the laminar flame velocity and the ratio of vortex diameter to the laminar flame thickness are kept constant at 10.1 and 3.1, respectively. These values were identified as a strong vortex case in an earlier experimental FVI investigation study (Mueller, *et al.*, 1998). In the current computational the flame thickness is resolved with 9 grid points for both cases.

The simulations yielded pocket formation process in both cases. The variation of CO and H₂ reaction rate contour plots superimposed onto mass fraction surface plot right after pocket formation are given in Figure 5.27. What is common for both simulations is that the size of the initial vortex is reduced as it is passing through the flame and the flame front is highly wrinkled by this process. H₂, being a relatively light and reactive species, diffuses more rapidly than CO. Thus, although the picture for H₂ suggests that the flame is already torn off and burning within a pocket the situation is quite different for CO. As it is seen in Figure 5.27 (b) and (c), there is

actually a neck region which still connects the wrinkled flame front with a pocket of unburned fresh gases. Since the CO content within the fuel mixture is significantly lower for Case 2 compared to Case 1, the neck region is not as strong as that is seen in Figure 5.27 (b).

Figure 5.27: Evolution of CO (a, b) and H₂ (c, d) mass fraction for Case 1 (a, c) and Case 2 (b, d). Vorticity contour plot superimposed onto dilatation term for Case 1 (e) and Case 2 (f).

Both CO and H₂ contour plots for Case 2 shows that the reaction rate iso-surfaces are not continuous at the negatively curved regions indicating local extinction. This can be seen better by Figure 5.27 (e) and (f) where the z component of vorticity contour plot is superimposed on to the surface plot of dilatation term of the vorticity equation. The plots correspond to a time right before flame front is torn by the initial vortex. The picture, as given in (f), indicates that Case 2 flame exhibits flame generated vorticity (FGV) at the negatively curved regions of the flame. Although the level of dissipation is higher compared to the Case 1 flame, it is not prominent through the flame and is not sufficient enough to limit the vorticity generation. Thus, the flame front is broken in these regions.

The flame dynamics is then investigated in a turbulent flow field using LEMLES. Vortex shedding from the dump plane can create coherent structures that can interact with the existing flame and change its dynamics. The impact of large scale structures in turbulent flow on the flame physics can be simulated using a simplified canonical test case of flame-turbulence interaction. We therefore, consider a flame front interacting with a pair of vortices superimposed on top of an isotropic turbulent field. LES approach is needed since full resolution using DNS is computationally prohibitive. Furthermore, LEMLES is needed to capture both the large-scale effects and the small-scale subgrid reaction-diffusion processes.

The fuel composition and the size of the coherent structure are held constant, whereas two different background turbulence levels corresponding to a length scale ratio of $D_c / l_f = 5$ and a velocity ratio of $u' / S_L = 10$ (Case 3) and 5 (Case 4) are simulated. The fuel composition is selected similar to that of referred as PSI by GE: 0.0678:0.113:0.0254:0.0650:0.1507:0.5781 H₂:CO:CO₂:H₂O:O₂:N₂/Air mixture with an equivalence ratio of 0.6, which corresponds to a laminar flame speed and laminar flame thickness of 0.2105 m/s, 0.0008755 m, respectively. A 64³ grid is used for both cases and the size of the computational domain is selected to yield a minimum spacing of approximately 3 times larger than the Kolmogorov length scale. Twelve LEM cells are used in each LES grid.

Figure 5.28 Evolution of H₂ reaction rate contour plot superimposed onto vorticity surface plot for Case 3 (a, b) and Case 4 (c, d) at t=(a)&(c) 0.69, (b)&(d) 0.90 ms.

The evolution of the flame surface, which is identified by H₂ reaction rate contours for two different instants together with the vorticity surface plot for Case 3 and Case 4 are shown in Figure 5.28. Similar to the laminar case the flame is stretched and curved by the vortex sheet, but the strength of these vortices decrease significantly before they could locally extinct the flame. Since there is no driving mechanism for the production of vorticity on either side of the flame front, the amount of vorticity decays, especially faster in the products side due to the increased viscosity (due to the elevated temperature field in this region). The vortex sheet is also affected by this process but as the flame front acts as a source for production of vorticity via Baroclinic torque (due to density and pressure gradient misalignment) term, it does not vanish rapidly. The strength of the vortex sheet decreases as it stretches the flame front but the effect of this interaction is not similar to the earlier laminar case, where the initial vortex strength decreased completely. Significant amount of vorticity is present around the flame front suggesting perhaps that there is some flame-induced vorticity production via baroclinic torque effect.

Compared to Case 3 the background turbulence is not very intense for Case 4 and the amount of vorticity induced by the vortex pair is more prominent on the overall flame dynamics. The interaction between the flame front and the coherent vortex pair for Case 4 as it is given in (c) and (d) resembles the laminar case, and the duration of the interaction is longer even though

characteristic eddy turnover time calculated based on the characteristics of the vortex sheet is the same. Also, the amount of vorticity generated by the flame seem to be larger than for Case 3.

5.5.3 LES Computations

5.5.3.1 Instantaneous and Time Averaged Data

LES computations have been performed for a combustor geometry with the synthesis gas fuel composition that was provided by GE. Schematics of the combustor and a close-up view of the flow field are given in Figure 5.29. The fuel composition corresponds to 0.23:0.31:0.21:0.25 $H_2:CO:CO_2:N_2:H_2O$.

Figure 5.29 Schematics of the (a) side view of the combustor and (b) front view of the diffuser cap.

In this combustor configuration, air is injected through an annular gap without any swirl, whereas fuel and diluents (N_2 and H_2O) are injected by a diffuser cap. The diffuser provides swirl for an outer diluent (N_2) and fuel. The inner diluent (H_2O) is injected in such a way as to avoid the diffusion of fuel into the inner section of combustor, so that an effective level of mixing between air and fuel is achieved. Finally, there is another air stream that is used for cooling the walls of the combustion chamber. Except for the main air stream, all other species are injected through set of holes with different diameters and orientations which enhances the mixing. The final version of the computational grid uses $210 \times 110 \times 145$ (cylindrical) and $210 \times 37 \times 37$ (Cartesian), with a total of 3,332,496 grid points, and is shown in Figure 5.30. A convergence section is added to the end of the computational domain to avoid any flow reversal in this region.

Figure 5.30 (a) Isometric, (b) front and (c) side view of the computational domain

For LES computations, the location of the cut-off between resolved and unresolved scales is very important and this is dictated by the grid that is employed. The quality of the final version of the grid that is used for our computations is checked by analyzing the spectra of the instantaneous u and v velocity time trace data, which is measured at $x=0.0211$, $y=0.0402$ m. The spectra are given in Figure 5.31 along with the $-5/3$ Kolmogorov scaling of the inertial range. It can be seen that some portion of the inertial range is properly resolved in high turbulence region and therefore, this grid is considered acceptable for the LES.

Figure 5.31 Spectra obtained from instantaneous U and V velocity data, probed at $(x,y) = (0.0211, 0.0402)$ m.

Figure 5.32 Time trace of (a) u velocity, (b) w velocity, and (c) v velocity at two different locations; and (d) location of the points from which data are taken.

Time traces of the velocity components at two different locations, $(x, y) =$ (a) $(0.0211, 0.0402)$ and (b) $(0.0211, 0.055)$ m are shown in Figure 5.32. Both traces are obtained at the same x and z locations but different y . First location is a point which is in-between the diluent and the air stream, whereas the second one is located downstream of the air stream. Hence, v and w components of the data obtained from second point fluctuates around approximately a zero mean since the air stream is not swirling. On the other hand, time trace of the v and w data obtained from first point shows highly swirling flow at this location. A frequency of around 3 kHz is seen in the time trace and in the movies that appear to correspond to the flapping of the fuel and outer diluent jets, which can be seen in the following figures.

Figure 5.33. (a) Side and (b) front view of the instantaneous temperature field. (c, e) Instantaneous and (d, f) time averaged variation of CO mass fraction. Here, (c, d) are side and (e, f) are front views.

Instantaneous profiles of temperature, velocity vectors, N_2 mass fraction, CO mass fraction and its reaction are given in Figure 5.33. The temperature field shown in Figure 5.33 (a) suggests that the flame is anchored in the shear layer and then spreads downstream and in the circumferential direction as the effect of the air inlet vanishes, and is eventually convected as far as the walls of the combustor. After this region the downstream temperature is greater than 1300

K at all points up to the exit plane. Maximum temperature occurs in the shear layer. The region between the shear layers contains hot gases that are convected upstream due to recirculation zone (e). The recirculation zone acts as a pre-heater for the incoming fuel jet.

The effect of outer diluent, N_2 , is predominant very close to the diffuser cap and acts as a dilution region between fuel and air streams and prevents early ignition. A careful investigation of the temperature plot reveals that close to the diffuser cap the maximum values are not between the fuel and the air streams but actually between the center region and the fuel stream, which supports the above interpretation. This phenomenon is also seen in the time averaged profiles of CO mass fraction and its reaction rate, which are shown in (d). Here, the mass fraction surface plot shows that the fuel is injected towards the air stream initially but then is deflected by the diluent stream and is redirected to the center region. Later, the fuel stream interacts with the inner diluent and turns this time towards the air stream. The reaction rate iso-lines starts at this location and follow the fuel stream, which is aligned to the air stream. Thus, the ignition of the fuel occurs first by the recirculating hot gases and then the flame spreads along with the fuel-air mixing stream as the effect of the outer diluent vanishes.

Temperature surface plot obtained at a cross section 0.0182 m away from the diffuser cap is given in (b) the profiles follows the same trend discussed above. There is a core region where the hot gases exist compactly due to the recirculation zone. This inner section is surrounded by a region which is broken since the injection occurs from discrete holes. Above this broken region there are several locations where there are hot gases but they do not correspond to a whole flame since the diluent in this region inhibits combustion.

Instantaneous profiles of CO mass fraction and vorticity contours are shown in (c). The movies of this simulation clearly show a rotating flapping of the fuel streams. This is also evident in the figure as the lower fuel stream is deflected towards the center region whereas the upper fuel stream is directed to the air stream by the outer diluent. Maximum vorticity occurs along the highly wrinkled region of the fuel stream, which results in breaking of the fuel into pockets that are convected downstream. Comparison of the variations in the time averaged and the instantaneous data for the fuel mass fraction suggests that combustion occurs on small pockets which are formed after the fuel stream has broken up. Although it is not shown here, the vorticity values on a given plane increases when the leading section of the swirling flow passes through the plane. In such a case, contrary to the picture given here, not only the region close to the diffuser cap but all the reaction zones becomes full of with high vortical structures. Also, this swirling nature of the flow field is a major cause for the flapping of the fuel stream.

The instantaneous and time-averaged variation of CO mass fraction in a cross sectional plane located at 0.01239 m away from the diffuser cap is given in (e) and (f), respectively. Both instantaneous and average variations, although not plotted on the same scale, shows clearly the effect of injecting the fuel through holes. The instantaneous picture is slightly asymmetric indicating a precessing vortex core and it is not possible to identify the core of the fuel jets in the region that are farthest from the centerline. On the other hand, the time averaged data is symmetric and it is possible to see each of the fuel jets. The time averaged data shows that the center region of the combustor is nearly full of CO. The vector field clearly show the swirling feature of the fuel jets.

Figure 5.34 Time averaged variation of (a) U velocity, (b) Temperature, (c) H_2 mass fraction and (d) N_2 mass fraction.

Time averaged surface plots of u velocity component and temperature are shown in Figure 5.34. Recirculation region in the center is clearly observable in the time averaged u velocity profiles shown in Figure 5.34 (a). There is another recirculation zone formed by the dump plane on upper and lower regions of the plot. The cooling air stream emerging onto this region is not very powerful to affect the size of the region, and it vanishes as soon it is injected. The flame resides on either side of the center is apparent in Figure 5.34 (b). Along the centerline, close to the diffuser cap a low temperature region can be observed that is due to the inner diluent stream (H_2O). The velocity of this stream is so low that it cannot penetrate further.

The mass fraction and reaction rate surface plot of H_2 is given in Figure 5.34 (c). The variation is very similar to the CO case except for the fact that H_2 is consumed earlier than CO and the reaction rate iso-lines start close to the diffuser cap. This property may be associated with the higher reactivity of the H_2 compared with CO. As it was suggested by the FVI and FTI studies, H_2 is consumed very early leaving CO to sustain the flame. This feature here is extended by the fact that H_2 is consumed whereas CO may build up in the center region and can even burn there eventually, which is not desired.

Finally the time averaged mass fraction variation of N_2 , the outer diluent is given in Figure 28 (d). Although it is not very clear in the picture, there exists considerable amount of N_2 in-between the fuel and the air streams, which prevents early combustion in this region. The combustion occurs as the O_2 , together with N_2 , diffuses and mixes with the fuel. The green region close to the inlet shown in the figure can be considered as the region where most of the combustion occurs. The air stream is blocked by the spreading flame and is trapped by the recirculation zones caused by the dump plane. Thus, a majority of the N_2 together with O_2 concentrated in this region.

Figure 5.35 Streamlines originating from air, outer diluent, fuel and inner diluent streams. (a) Side, (b) Perspective view.

Typical streamlines are shown in Figure 5.35 (a) and (b). The streamlines are initialized in air, outer diluent, fuel and inner diluent streams, and are represented by black, blue, red and green colors, respectively. The outer diluent stream, is injected towards the walls of the combustor but is deflected to the center region when it collides with the air stream. The air stream, which is axially aligned in the beginning is deflected initially in the radial direction as a result of this interaction but is later turned towards the center region. The fuel stream appears to be confined to a narrower region and does not penetrate through the diluent stream. The swirling nature of the whole flow field can be seen in Figure 5.35 (b). Except for the air stream both diluent and fuel streams are swirling. The inner diluent, although not initially swirling, is affected by the swirling flow field caused by the fuel and outer diluent streams and follows more or less the same pattern with the fuel stream. The air stream is trapped by the recirculation zone formed by the dump plane and follows a path that is very close to the walls of the combustor.

5.5.3.2 Flame Dynamics Based on Swirl Angle Modification

The time trace data and its frequency spectrum shown in Figure 5.31 and Figure 5.32 correspond to an oscillating flow field with a frequency of approximately 3.0 kHz. Assuming that the whole combustor is a cylinder full of combustion products, acoustic theory predicts first tangential resonant mode as 2.9 kHz, which matches with the dominant frequency detected by our LES computation. The simulations were repeated by changing the swirl angle. The

configuration provided by GE corresponds to a swirl angle between off plane (u) and on plane (v and w) velocity components of the fuel stream as 36° , which corresponds to an axial velocity of 136 m/s. By changing this angle into 22° we have altered the velocity field at the fuel inlet and the axial velocity increased up to approximately 156 m/s. The angle change has been performed linearly as a function of time over a period of 0.6 ms. Figure 5.36 shows the temperature flow field just before and 4.5 ms after the swirl angle change was initiated. As a result of the increment in the axial velocity the flame seems to liftoff. Also, since the flame still does not ignite any closer to the injector plane, the air stream can now penetrate further into the combustor. The maximum temperature values are still occurring on the shear layer between the fuel and air stream, however they do not correspond to a well defined pattern but are affected a lot by the local flow structures.

Figure 5.36 Instantaneous temperature surface plot (a) before and (b) 4.1 ms after swirl modification.

Temperature trace data shown in Figure 5.37 (a) correspond to a highly intermittent evolution for the case without any swirl modification and the majority of the data lies at around 600 K and exhibits spikes as much as 2500 K as a result of ignition at those instances. As the angle is changed, the signal is free from any spikes and lies close to 600 K. The u velocity component shown in Figure 5.37 (b) suggests that due to the increased axial velocity at the fuel stream the velocity field at this location now can attain values as high as 150 m/s.

Figure 5.37 Time trace of temperature and U velocity for variable and constant swirl cases.

5.6 Task 8 (Combustor Design and Validation)

5.6.1 Prototype-1N Experimental Results: Full Combustor

Testing of the full head end was conducted with high-reactivity syngas, consisting of H₂ and CO, with no operability difficulties such as combustion dynamics or flashback (at normal conditions). A fraction of the syngas fuel was sent to the new premixer, while the rest was sent to the existing premix system of the DLN combustor.

A single stable emissions point, plotted in Figure 5.38, was acquired at the design point with the reaction zone temperature just below F-class levels. Emissions were only slightly above the entitlement data (perfectly premixed) for a high-hydrogen syngas fuel obtained in a previous experiment. This is notable, since the head end was run with a non-uniform fuel split, and locally elevated temperatures would be expected to lead to higher NO_x than a uniform head end temperature. For reference, the NO_x data for methane from Leonard and Stegmaier is included on the plot.

This combustion system with new premixer was designed for fuel-flexibility, meaning it should be able to operate with natural gas, syngas, and blends of these fuels. The experimental program included testing the new hardware with natural gas fuel. Combustion dynamic pressures were the same, or even slightly lower in amplitude, than the baseline hardware and were not a difficulty in normal operation. NO_x emissions were only marginally higher than the baseline.

Figure 5.38 Single NOx data point from the present syngas test, with entitlement data included

6 Conclusions

6.1 Task 2 (Design Approaches)

The composition of syngas fuels feeding gas turbines was categorized using five independent parameters: the fraction of combustibles in the fuel, fraction of hydrogen in the combustibles, the fraction of hydrocarbons in the combustibles, the fraction of nitrogen in the inert and fraction of steam in the inert. CO and CO₂ constitute the remainder of the combustibles and inert respectively. Fuels from oxygen blown, air blown, steel mills and co-production plants were considered in this classification. Representative fuels were selected from this categorization and possible ranges of variation of the fuel composition parameters were identified. The NOx and CO emissions from the combustion of the representative fuels were evaluated for seven combustion technologies: diffusion flame with nitrogen diluents, diffusion flame with steam diluents, lean premixed dry-low NOx (DLN), DLN with O₂ enrichment, Rich-burn Quick-quench Lean-burn (RQL), rich catalytic lean burn (RCLTM) and trapped vortex (TVC) combustors. The evaluation was performed using chemical reactor network models that were developed according to the flow physics in these combustor technologies.

A technology scorecard was developed to compare and select technologies for fuel-flexible combustor prototype development. The scorecard included the results of the emissions

prediction using the chemical reactor models as well as qualitative scores on cost of electricity (COE) and reliability-availability-maintainability (RAM) of the different combustor technologies. Based on the technology scorecard, a hybrid matrix was created scoring each combination of technologies on natural gas and syngas performance. Three combinations of technologies were identified for prototype development: Diffusion with steam and DLN, Diffusion with steam and TVC and TVC for both natural gas and syngas. Two prototype concepts were chosen to incorporate the three combination of technologies: A hybrid DLN/diffusion burner and a trapped vortex combustor with passages for diffusion fuel and steam injection

6.2 Task 3 (Syngas fuel flame characterization)

The effect of preheating, CO₂ dilution and syngas fuel content (H₂/CO ratio) have been studied using a laminar jet and burner stabilized, stagnation flame configurations. For room temperature reactants, most of the model predictions are generally in good agreement with the experimental results. For both low and medium H₂ content fuels, the more comprehensive Davis *et al.* H₂/CO and GRI mechanisms provide similar predictions of laminar flame speeds, though the H₂/CO mechanism predictions are slightly higher at lean conditions for the medium H₂ composition fuels. The larger Chen mechanism also is reasonably accurate in its flame speed predictions. The models also predict the measured strained flame speed and strain sensitivity well for low H₂ content compositions. For medium H₂ levels (e.g., 20-50%), however, both the atmospheric and higher pressure data reveal a significant discrepancy between the measured and predicted strain sensitivities at very lean conditions (e.g., $\Phi \leq 0.6$). For high H₂ fuels, the experimental flame speeds are generally higher than the predictions, though the Davis *et al.* H₂/CO mechanism is quite accurate (within a few percent) for equivalence ratios below ~ 0.8 .

With preheated reactants, however, there are noticeable differences between the experimental data and the predictions. For example, the medium H₂ content fuel mixture data are in good agreement with the most of the predictions up to 500 K. As the preheat temperature increases to 700 K, larger discrepancies are observed, especially at lean equivalence ratios. The discrepancies increase to as much as 20% for the predictions with the detailed Davis and reduced Chen 9 species mechanisms. Dilution of the fuel with even 40% CO₂ does not change the degree of agreement between the models and experiments. This indicates that the spectral radiation reabsorption of CO₂ dilution is not a major issue for these mixtures. For the high H₂ content fuels, the predicted flame speeds again increase with temperature faster than the measured values. For low H₂ content fuels, the models also produce similar results, but now they tend to under predict the highly preheated flame speeds. The under prediction is not severe, as the model results are in reasonable agreement with the measurements over most of the lean conditions, though the differences are as much as 10-15% at near stoichiometric conditions. For all the cases studied, the 14 species Chen mechanism predictions at high temperature have reasonably good agreement with the measurements, within the accuracy of the more detailed models. Similarly, the discrepancy between the measurements and the Chen 9 species mechanism predictions are always the greatest. Therefore, the experiments suggest that the reduced 14 species mechanism by Chen is the superior choice for implementing into the LES code for the high temperature reactant gas conditions expected in the gas turbine environment. In

addition with 10% or better agreement with the experiments, the mechanism should not require changes to make reasonably accurate predictions in the LES modeling.

6.3 Task 4 (Systems Modeling)

The Co-generation plant system combined with the combustor level requirements have been defined and ranked. The most important requirements are improved system level efficiency, dual fuel flexibility (co-firing capability), allowance for enhanced fuel variability (Wobbie index), and low emissions (<9 ppm NO_x and CO). The system level evaluation has shown that the Co-generation efficiency is higher for the diffusion combustor concept than the TVC concept. According to the systems evaluation, the hybrid diffusion concept is not able to meet the 9 ppm NO_x requirement with syngas fuels and N₂ diluent addition. In this cycle format, there is not enough available N₂ from the air separation unit to provide the required dilution of the flame temperature. Steam augmentation is included to meet the emissions requirements.

The additional steam augmentation also increases the overall plant efficiency. Another problem with steam diluent addition is the concern for the gas turbine hot gas path (HGP) life, which is expected to be shorter when steam injection is used at lower temperature conditions in order to maintain the same expected HGP life. However, the H₂ content in the EECF syngas are lower than typical syngas due to part of the syngas is converted to hydrocarbon liquid products in the upstream Fisher Tropsch process. As a consequence, the H₂ content in EECF syngas is lower than normal and therefore the H₂O content in the exhaust is lower than normal operation, even with supplemental steam injection. Hence, the diffusion combustor cases do not require operating at lower temperature within these EECF syngas cases and the system evaluation shows a better co-generation efficiency than TVC cases. However, the TVC system shows ~10% increase in plant efficiency when the combustion system is in operation with natural gas.

6.4 Task 5 (Prototype Design)

The purpose of this task is to design two prototypes of a fuel flexible combustor selected from the technologies listed in Task-2. The combustors are to operate them at heavy-duty industrial gas turbine operating conditions.

First, the design and calculations for Prototype-1 are discussed. It is a hybrid of a lean premixed DLN burner for natural gas and a diffusion burner for syngas with diluents injection for NO_x abatement. Important geometric parameters of the diffusion burner were identified through a design of experiments study in conjunction with CFD calculations of the diffusion burner geometry and flowfield. Results show the different possible flame structures from the range of possible tip geometries and their corresponding effect on NO_x emissions, mixing, and the exit temperature profiles. Critical parameters by which to guide the combustor design were identified: NO_x, flame length, exit temperature pattern factor, mixing rates, and temperature of gases impinging on diffusion tip. Cases with shorter flame lengths predicted lower NO_x values in general thereby underlining the importance of high temperature residence times on thermal NO_x formation. Thus, the emissions performance of the nozzle concept is a strong function of the maximum temperatures in the combustor and mixing of the fuel, air, and diluents. The optimized design is a compromise between fuel-air and fuel-diluents mixing to achieve the optimal flame structure for low NO_x performance. The optimal combination of the diffusion

combustor design variables was selected to obtain low NO_x while satisfying the requirements of a short flame length, low diffusion tip temperatures and a flat exit temperature profile. CFD analysis of the design was performed to verify that the combustor requirements are satisfied.

Design of the swizzle for natural gas operation was performed through a parametric study using CFD calculations to determine the air flow-field and mixing at the burner tube exit plane. The shape and dimensions of the vane surface contour was decided based on GE methodology for DLN style premixers. Air-side CFD for the flow around the vane was performed to evaluate the swirling flow characteristics. The velocity profiles coming out of the vanes were found to be consistent with expectations for a lean premixed burner. An optimal strategy for premixed fuel injection was developed and validated with excellent fuel air mixing capability.

Prototype-2, a TVC combustor, was operated with syngas with moderate levels of H₂ at advanced gas turbine operating conditions. The combustor successfully demonstrated ultra-low NO_x emissions (3 ppm) at these conditions in the absence of any significant combustion dynamics. The combustor also demonstrated very high turn-down capability while maintaining very low NO_x, CO, and combustion dynamics levels.

The Prototype-2 TVC syngas combustor has met another significant milestone by demonstrating NO_x emissions of 3 ppm at advanced GAS TURBINE cycle conditions. The hardware also continued to demonstrate robust flashback resistance. Follow-on studies of the TVC must now focus on practical premixer designs. The unique characteristics of the TVC make its premixer requirements different from other GE designs; however, the design can leverage the insights gained from fundamental premixer design studies.

Prototype-1N incorporated full-premixing capabilities for syngas. Single-nozzle rig testing of full-scale syngas premixers indicated operability at engine-realistic conditions for natural gas and syngas fuel. Flashback was observed as the target flame temperature was approached with carbon-free syngas (high-hydrogen) fuel for the baseline nozzle and the nozzle with modified fuel injection. When burner tube and centerbody modifications were made, operability at elevated flame temperatures without flashback was achieved with single digit NO_x emissions.

6.5 Task 6 (Syngas Methodology for Advanced CFD Tools)

The physics of the combustion of synthetic gaseous flames is investigated for laminar and turbulent flow configurations by using DNS and LES. Computations are performed for premixed and non premixed combustion regimes. Flame-vortex and flame-vortex-turbulence interactions were studied using a reduced but multi-step kinetics for CO-H₂ flames. Laminar flame-vortex studies shows that the flame dynamics is highly sensitive to the fuel mixture. H₂ being a highly diffusive and reactive species can follow the flow field better than CO. As a result, the flame front of a H₂ rich syngas mixture is more susceptible to wrinkling and yields an increased degree of misalignment between pressure and density gradients causing generation of local vorticity due to the baroclinic mechanism. This study shows that it is possible that local extinction can be either enhanced or suppressed based on the fuel mixture and the local strain rate (as caused by the vortex).

For a turbulent flow field the interaction between coherent structures and the flame front is not as strong as seen in the laminar study. The vortex sheet is shown to be stretched and loses its strength before being able to induce high level of flame wrinkling. As the background turbulence level decreases, the dependence of the flame dynamics on coherent structures increases and evolves more like a laminar problem.

The LES of the GE syngas combustor shows that the outer diluent stream prevents early combustion and acts as a combustion retarding stream between fuel and air streams. Combustion occurs in the shear layer within pockets of fuel-air mixed regions, and in the global sense, the high temperature region widens up on either side of the centerline. The inner diluent (H_2O) hardly influences the overall combustion dynamics and is trapped within the recirculation zone. The cooling air streams are not very effective for the current inflow conditions as they can not penetrate into the recirculation zones and therefore, provide limited cooling to the walls.

The fuel jet flaps with a frequency of approximately 3 kHz, and this allows the fuel stream to be broken into smaller pockets and enhance mixing so that combustion seems to occur over a wide region. Actually, the flapping frequency is approximately equal to the first resonant tangential mode. Another study by changing the swirl angle is conducted to understand coupling between the flow field and the combustion process. It is shown that as the swirl angle changes the flame lifts off and the frequency of the oscillations also deviates from the resonant tangential mode.

It is clear from this study that most of the flame-vortex-turbulence dynamics seen in this combustor is highly unsteady and therefore, necessitates the use of a LES approach. The current simulations, although limited (due to time and resource constraints) have demonstrated that many subtle unsteady physics for a complex design can be investigated if the full 3D unsteady data is available. However, the accuracy of these calculations cannot be ascertained since there are no data for comparison. Nevertheless, based on our past LES studies we believe most of the physics observed in these simulations are realistic. It is worth noting that the 14-species kinetics model used in these LES also provides some insight into the flame structure caused by both CO and H_2 reaction kinetics. As determined in this study, it is essential to include some detailed kinetics in order to properly capture the physics of syngas combustion in a turbulent environment. The current simulations and results have established a new simulation capability that could be used in the future to further study syngas combustion in complex combustor designs.

6.6 Task 8 (Combustor Design and Validation)

Prototype-1N was further developed for full can combustion testing. A newly-designed head end was successfully operated with syngas fuel in a dry low NO_x (fully premixed) mode. NO_x emissions were only slightly above entitlement levels. The head end (reaction zone) temperature was just below F-class levels. The new premixer exhibited excellent flashback margin at the design condition and also at flame temperatures exceeding the design point for F-class systems. To demonstrate the fuel-flexibility of the new premixer/combustor, operation on natural gas was obtained with a very small NO_x penalty over the baseline (fielded) design, and no significant combustion dynamics were observed.

7 References

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