Fuel Flexible Turbine System (FFTS) Program

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Program Partners:

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Argonne National Laboratory (ANL)

Packer Engineering (Packer)

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Executive Summary

In this fuel flexible turbine system (FFTS) program, the Parker gasification system was further optimized, fuel composition of biomass gasification process was characterized and the feasibility of running Capstone MicroTurbine™ systems with gasification syngas fuels was evaluated. With high hydrogen content, the gaseous fuel from a gasification process of various feed stocks such as switchgrass and corn stover has high reactivity and high flashback propensity when running in the current lean premixed injectors. The research concluded that the existing C65 microturbine combustion system, which is designed for natural gas, is not able to burn the high hydrogen content syngas due to insufficient resistance to flashback (undesired flame propagation to upstream within the fuel injector).

A comprehensive literature review was conducted on high-hydrogen fuel combustion and its main issues. For Capstone's lean premixed injector, the main mechanisms of flashback were identified to be boundary layer flashback and bulk flow flashback. Since the existing microturbine combustion system is not able to operate on high-hydrogen syngas fuels, new hardware needed to be developed. The new hardware developed and tested included (1) a series of injectors with a reduced propensity for boundary layer flashback and (2) two new combustion liner designs (Combustion Liner Design A and B) that lead to desired primary zone air flow split to meet the overall bulk velocity requirement to mitigate the risk of core flashback inside the injectors. The new injector designs were evaluated in both test apparatus and C65/C200 engines.

While some of the new injector designs did not provide satisfactory performance in burning target syngas fuels, particularly in improving resistance to flashback. The combustion system configuration of FFTS-4 injector and Combustion Liner Design A was found promising to enable the C65 microturbine system to run on high hydrogen biomass syngas. The FFTS-4 injector was tested in a C65 engine operating on 100% hydrogen and with the redesigned combustion liner — Combustion Liner Design A — installed. The results were promising for the FFTS program as the system was able to burn 100% hydrogen fuel without flashback while maintaining good combustion performance. While initial results have been demonstrated the feasibility of this program, further research is needed to determine whether these results will be repeated with FFTS-4 injectors installed in all injector ports and over a wide range of operating conditions and fuel variations.

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1. Introduction

1.1 Contract Goals

Capstone Turbine Corporation (CPST) was awarded a research and development contract (DE-EE0001732) by the US Department of Energy to develop and demonstrate a fuel flexible turbine system (FFTS) to be integrated with a small scale biomass gasification system. The FFTS will be a Microturbine-driven, high-speed generator coupled with digital power electronics to produce high quality electrical power. The system will provide electrical power in parallel with the utility grid or provide prime power if no utility grid is available or where service is unreliable. The turbine engine includes an integral heat exchanger that almost doubles electrical efficiency by preheating the compressed air with the exhaust gas to reduce fuel consumption.

1.2 Project Partners: Roles and Responsibilities

Capstone's partners for this project included the University of California at Irvine (UCI), Argonne National Laboratory (ANL), and Packer Engineering (Packer). The roles of each party are:

- (1) CPST: Principal investigator. Responsible for overall development and demonstration with focus on system integration, control, and advanced combustion system development. Combustion development includes: (1) development of advanced injectors for use with typical gasification syngas fuels from different feed stocks — this fuel typically has high hydrogen content and high flame speed — and (2) combustor liner development or modification.
- (2) UCI: Conduct literature survey and preliminary analysis. Provide test support for system and combustion components and conduct fundamental combustion analysis of the combustion performance, including flashback and emissions measurement.
- (3) ANL: Analyze composition of syngas fuel generated by the gasification system to characterize combustion properties, to define fuel specifications, and to provide the demonstration site/laboratory for the project, including site preparation and obtaining test permit from local authorities.
- (4) Packer: Develop gasification system able to gasify different types of renewable agricultural feed stocks and provide fuel for the Microturbine system operation. Gasification fuel must be compliant with the fuel specifications for the turbo-generator.

The development process and division of responsibilities between these parties are shown in Figure 1.

Figure 1: Partner Responsibilities

1.3 Project Scope

After a comprehensive literature review, performance of computational fluid dynamics (CFD) simulations and intensive chemical kinetic simulations to better understand flashback mechanism, turbulent flame speed, and fuel/air mixture reactivity, among other combustion analytical work, a series of experimental studies were performed, using three different experimental platforms: a single axisymmetric injector, a full annular atmospheric combustor (C65), and C65/C200 engines. Several injector design-test-optimization iterations were performed. The experimental studies for injector evaluation and design included: (1) C65 baseline injector tests with natural gas/hydrogen, natural gas/ethane, and natural gas/propane; (2) “cut-back” injector testing with natural gas and hydrogen doping; (3) various diffusion-type injector configuration tests; (4) development of boundary layer flashback resistant injector (high flame speed injector or “FFTS-4” injector); (5) testing of “FFTS-4”; and (6) preliminary CFD analysis of the “FFTS-4” injector. A large amount of valuable data — designed to study the impacts of fuel composition, temperature, pressure, equivalence ratio, and some geometry differences — were collected while further connections between the various test apparatus need to be made. In addition, two new liner designs were completed, one of which was tested in a C65 engine with one FFTS-4 injector burning 100% hydrogen fuel.

The key findings include: (1) the baseline C65 injector was not capable of burning the target fuel without flashback risk; (2) “cut-back” or “diffusion” injectors showed some improvement in flashback resistance over the baseline injectors, but were not capable of burning target fuel with acceptable combustion performance or operability margins; (3) testing of the high-flame speed injector (FFTS-4) performed in a C65 engine — one injector fueled with 100% hydrogen while the other five were fueled with natural gas — showed that the FFTS-4 injector is capable of burning 100% hydrogen without flashback when tested with one of the newly designed combustion liner. Although the current FFTS-4 injector data is limited, it is the likely configuration for high flame speed fuels, like the target fuels of this FFTS project.

This report summarizes the combustion system design work for this FFTS program with a focus on the development of the combustion system, including injector and combustion liner, for high flame speed fuels (typically high hydrogen content), including the details of the analysis, test setups, test data and analysis as well as provide suggestions for next phase of work for the fuel flexible turbine system (FFTS) program.

2. Objectives and Approaches

2.1 Objectives

The primary objective of the program is to develop a Microturbine system to use gaseous fuel resulting from the gasification process of agricultural biomass. These process gases have high hydrogen content — vastly different than natural gas which consists of a majority of methane (CH_4) — and low heating values, but are well known to have high chemical reactivity and high flame speed. In addition, the composition of the fuel may change with the gasification temperature or feedstock types. In general, the fuel composition, reactivity, heating value, and contaminant levels of fuels lead to the selection or optimization of injector or combustor design features that meet or maintain operability over a wide range of operational conditions. Regardless of fuel or operating conditions, for a lean premixed combustion system like that employed in Capstone Microturbine systems, the fundamental combustor operability criteria that must be satisfied include:

- resistance to auto-ignition
- resistance to flashback
- emissions compliance (NO_x , CO, UHC, Smoke)
- acceptable combustion dynamic pressures
- resistance to lean blowout

As a result, the overall combustion system and injector development for FFTS program was focused on operability issues associated with high hydrogen content (high flame speed) fuels. Operability issues include flashback, auto-ignition, lean blow out and combustion dynamics, of which the most problematic issue is flashback. There are four different types of flashback mechanism: (1) boundary layer flashback, (2) core flow flashback, (3) combustion-induced vortex breakdown flashback, and (4) combustion instabilities caused flashback. Core flow flashback and boundary layer flashback are the primary concerns for this project. Thus, the development of the FFTS injectors and combustor has been focused on the understanding and mitigation of these two flashback mechanisms.

General project objectives are:

- (1) Develop a Microturbine system capable of operating on alternative fuels including synthesis gas (syngas) of various compositions (high H_2 and CO)
- (2) Build and demonstrate a prototype turbine-generator system and integrate it with a gasification system for renewable biomass feedstock
- (3) Evaluate and demonstrate the Microturbine system to verify performance and emissions

For combustion development the key direct objectives are:

- Characterization of the fuel generated from the Packer gasification unit ("FFTS" fuel or biomass gasification fuel) — including the fuel composition, heating value, fuel reactivity, particulate matter, and other contaminant levels, among other fuel properties;
- Understanding Microturbine operability issues — such as flashback, lean blowout (LBO), auto-ignition, and combustion dynamics — when using high-hydrogen fuels;

- Develop C65 Microturbine injector to maintain operability and performance for the FFTS fuels.
- Test and validate the injector design in various conditions, ultimately in relevant engine operating conditions;
- Develop an FFTS combustor using the existing C65/C200 combustion architecture — with limited modifications — to support the injector design and operation;
- Test and validate the combustion system design (injector and combustor) in various conditions, ultimately in relevant engine operating conditions.

2.2 Approaches

From a practical point of view, the Capstone C65 Microturbine system was selected from among the Capstone C30/C65/C200 Microturbine product families to be the target development platform and potential commercialization candidate. However, because of similarities between the systems, operating conditions, or combustion architecture, development tests and analysis have been performed for either C65 or C200 engines.

The approaches applied to the development include:

- Comprehensive literature review of flashback, hydrogen fuel combustion, and turbulent flame speed prediction under different operation conditions such as pressure, temperature, and equivalence ratio. A detailed report from UCI is attached in Appendix A: Fuel Flexibility Report.
- Chemical kinetic simulation and combustion analysis to understand turbulent flame speed, auto-ignition time, and reactivity.
- Computational fluid dynamics simulations to simulate flow field and fuel mixing process; used as a design tool and as a tool to reveal injector performance mechanisms.
- Experimental testing which included injector apparatus tests and engine tests as detailed in following sections.
- Model and understand air flow and its distribution within the combustion liner.
- Combustion chamber aerodynamics and chemical kinetics.
- Combustion liner thermal profiling and cooling strategies.
- Combustion performance tuning with air flow distribution.

2.3 Combustion System Design Scope

For the FFTS program, it was determined that the C65 combustion system would be adopted without changes to the igniter, combustion liner envelope, injector envelope, and injector arrangement. Interfaces with other modules, except the interface between nozzle and seal, shall also not be changed. Features that may not be changed include:

- General combustion liner geometry
- Combustion liner shall be mounting method
- Interface of injector with other components
- Number, arrangement, and orientation of injectors

In order to deliver more air to injectors, however, the following features of the liner and the injectors can be changed if needed:

- Dilution and cooling hole sizes
- Location of dilution and cooling holes
- Splitting ratio of air between injector, dilution and cooling holes
- Injector mixing hole dimensions
- Injector mixing hole locations
- Injector fuel distribution holes
- Other dimensional changes that will not change the basic arrangement

2.4 Additional Combustion System Design Considerations

The combustion and fuel injection module performs the following functions:

- Meeting performance requirements to burn a required amount of fuel at required combustion efficiency
- Injector design to meet design requirements such as fuel air mixing profile, velocity profile, and residence time
- Liner design to meet design requirements such as air split ratio and liner life
- Flow splits (internal) design to meet design requirements

3. Experimental Apparatus

The goal of the experimental studies was to evaluate the combustion performance of the designed injectors and to define the conditions at which flashback or lean blow out would occur for target fuel composition and test conditions. The experimental apparatus was directly relevant to Capstone-specific engine and to conditions. For example, C65/C200 engines were used to test fuel variations and injector designs for combustion stability, flashback, or lean blow out. Also, for better visualization and optical access, the annular C65/C200 combustion test apparatus was used to test combustion stability and flame structure at atmospheric conditions. At UCI, the more generic single injector apparatus was used to study flashback mechanisms.

3.1 Test Diagnosis and Data Acquisition

In developing a combustion system for high flame speed fuels, the capability to detect flashback or combustion instability is critical, in addition to other general combustion diagnosis. As a result, the development of a flashback detection tool is essential to this program. The flashback detection tool to be developed will be used in most of the combustion development tests. However, due to cost and reliability considerations, the flashback detection tool will not be required in the final, optimized production system which will be flashback-proof. Other than sensing components, the capability to acquire experimental data at high speed was developed both at Capstone and UCI for injector development testing. For example, the setup of the axisymmetric single injector apparatus and its associated supporting hardware — shown in Figure 2 — is a good example of typical test diagnosis and data acquisition. The test and data system consisted of a National Instruments cRIO-9074 with analog input/output, thermocouples, and high speed analog input modules. The operator interfaced with the cRIO-9074 using a computer and the supporting National Instruments software and drivers. The experiments were controlled by a program written in Labview. For more open single injector or atmospheric annular injector apparatus test, advanced diagnostics such as photodiodes and high-speed camera with UV amplifier and Schlieren imaging were used due to better visual accessibility. However, for engine tests, more traditional detection sensors — thermocouples, for example — were used due to optical access issues. An example of an injector instrumented with multiple thermocouples for flashback detection testing is shown — before being installed for an engine test — in Figure 3. These thermocouples were typically 0.50 mm (0.020") in outer diameter, with fast response.

Figure 2: Axisymmetrical Injector Test Apparatus

Figure 3: Injector Instrumented with Intensive Thermocouples

3.2 Fuel Composition Simulation

3.2.1. Capstone and UCI

To test different fuel compositions, fuel mixing capabilities were available at both Capstone and UCI which delivered the desired surrogate fuel compositions to support the C65/C200 engine and injector apparatus testing. The baseline fuel — natural gas — came from a commercial pipeline while other fuel constituents were supplied from single- or multi-packed cylinders depending on the flow rate required. The pipeline natural gas was periodically analyzed with gas chromatography equipment while the flow rate was measured at 1 Hz frequency during tests. Each fuel stream was accurately metered or controlled with mass flow rate controllers then the gases were fully mixed in a common manifold before delivery to the engine or injector apparatus. The test setup for flashback/combustion stability with a C200 engine for hydrogen/natural gas blended fuels is shown in Figure 4.

Figure 4: CPST Test Setup for Hydrogen Doping Test

3.2.2. Argonne National Laboratory

For the final demonstration of the FFTS program at Argonne National Laboratory (ANL), an integrated microturbine-gasifier system was setup. The setup is shown in Figure 5. A high pressure natural gas (HPNG) C65 unit was used for baseline tests with natural gas. Also, 15 bales of feedstock, four (4) bales of corn stover, and two (2) bags of woodchips were processed, bagged, and stored at ANL for demonstration purposes. After phase 1 safety approvals for operation of the microturbine with natural gas and initial operational tests with natural gas were completed, ANL estimated that the stored feedstocks would be enough to last more than 50 hours for the FFTS demonstration tests using fuel gas generated by the Packer gasification system.

Figure 5: Demonstration Site Setup at ANL

3.3 Generic Single Injector Test Apparatus

The generic axisymmetric injector (shown on the preceding page) simplifies the flow field. The full annular combustor maintains the complexity of the flow field while ignoring pressure effects. The test apparatus was used to examine the effects of various parameters on flashback, including fuel composition, operating conditions, injector materials, and tip temperature, with a focus on fuel composition because of the importance to the design of the FFTS. These results can be used to understand the flashback mechanisms and to develop predictive correlations for the engine environment. The findings are:

- (1) Burner materials, tip temperature, and flame confinement play significant roles in flashback propensity;
- (2) Material with lower thermal conductivity has a greater flashback propensity but slower flame regression inside the tube;
- (3) The difference between flashback propensities was due to different tip temperatures. Critical velocity gradient (g_c) can be predicted fairly well using laminar flame speed calculated using tip temperature.

These observations can potentially be exploited to minimize the negative impacts of flashback in practical applications or improve flashback resistance by changing to materials with higher thermal conductivity.

3.4 Full Annular Combustor Test Apparatus

A combustor from a Capstone C65 Microturbine (natural gas, recuperated Brayton cycle engine) was used for this study. As shown in Figure 6 and Figure 7, the full annular combustor apparatus at UCI includes the primary and dilution zone sections of a Capstone C65 combustor by removing power generator, turbine rotor and recuperator. A C65 engine is typically operated at about four atmospheres at full power, while the full annular apparatus can be only operated at atmospheric condition. However, of primary importance is that the apparatus has the same combustion chamber geometry. As a result, the flow field inside the injector and actual primary zone flow structure can be simulated in the test apparatus, because it is the actual C65 combustion liner, assuming a flow field similarity between C65 engine condition (4 atmospheres) and atmospheric condition. The air was preheated up to 800 °F using an in-line electrical resistance heater. The air ducting delivers combustion air to the primary zone of the C65 system via four supply ports. Efforts were made to control the combustion air distribution to injectors to be uniform within 10%. The fuel supply to each injector was individually controlled in terms of flow and the fuel composition to injector 1 which directly faces the igniter could be controlled.

Figure 6: UCI Annular Combustion Test Apparatus

Figure 7: C6X Annular Combustor Cutaway Drawings

The selected injector configuration of interest — for example, the Capstone current “baseline” injector or the “cut-back” injector — was characterized in the annular test apparatus with three fuel blends. High speed video was used to record the flame activities and structures. Injectors were instrumented with fast-responding thermocouples to detect flashback. In the annular test apparatus, these tests were performed with the aft plane of two injectors where both were lit — one with natural gas and the other with the various fuel mixtures. The rest of the injectors remained unlit. The air flow was set to simulate the lowest combustor liner pressure drop in an effort to create the most favorable conditions for flashback. The air was preheated to 800 °F — or as high as can be reliably reached. Flashback and lean blow out detection was accomplished using visual imaging and the thermocouple instrumented injector provided by Capstone.

3.5 Test Engine

3.5.1. Development Test Engine at CPST and UCI

While the other test tools (e.g., single injector rig, sectional injector rig or full annular combustor rig) and analysis (e.g., chemical kinetic simulation of auto-ignition time, flame speed or CFD flow field simulation) can provide great insights and guidance in designing new injectors and screening new designs, the ultimate verification and qualification of an injector design would be testing the injector sets in a real engine, which is irreplaceable and indispensable. For the FFTS injector design evaluation, the engine would be a C65 or a C200 Microturbine system.

The UCI C65 engine (shown in Figure 8) used in the FFTS program was tested in the Distributed Technology Test Facility at the UCI Combustion Laboratory. The main hardware and software configuration of this C65 engine is shown in the CRMS configuration page screenshot (shown in Figure 9). Relative to the Area B location, the mixing station that allows for changes in fuel composition is located approximately 100 feet away. The distance between the mixing station and the test engine creates some difficulty in performance of inherently dynamic tests such as the current flashback studies because of residence time in the fuel supply line and system delay to fuel composition change requests. However, the experiments could be designed so the fuel composition does not need to be the dynamically-altered variable. The mixing station can combine up to five different gases at a time and was designed to allow for supply to 250 kW power generation devices under nominally steady state operation. Natural gas (NG), hydrogen (H_2), propane (C_3H_8), carbon monoxide (CO), ethane (C_2H_6), carbon dioxide (CO_2) and nitrogen (N_2) are the feed gases.

Figure 8: C65 System at UCI

Figure 9: CRMS Screenshot of UCI C65 FFTS Test Engine Configuration

The capability of the selected injector — for example, a new injector design or the Capstone “baseline” injector — to burn high flame speed fuels — for example methane fuels with increased hydrogen or ethane content — is unclear before engine test. The tests were to operate the C65 engine with instrumented injectors with these high flame speed fuels and use flashback detection tool(s) to find out the “flashback” fuel blends at a set of designed test conditions, such as ambient conditions and power levels. For these characterization tests, power levels to be tested were typically 5, 30 and 65 kW. Three fuel blends of particular interest for the tests were:

- Fuel blend #1: CH₄ + H₂
- Fuel blend #2: CH₄ + C₂H₆
- Fuel Blend #3: CO + H₂

At Capstone’s test facility, C65 and C200 engines were used in a similar manner to test different FFTS injector designs.

- The data collected in the engine test includes but not limited to:

- Test cell /test environment condition
- Fuel composition
- Engine condition (all combustion CRMS parameters shall be recorded)
- Emissions (O_2 , NO_x and CO at minimum)
- Flashback/Stability information (based on selected detection tool/method)

For liner development and verification tests, a C65 natural gas engine was used. The fuel used for testing operability (flashback and LBO) was natural gas and natural gas doped with hydrogen, up to 100% H_2 . Due to availability of hydrogen and injector hardware, screening tests were performed by hydrogen doping on the “injector of interest” while the other five injectors were fueled with natural gas despite the high desirability of running all injectors at 100% hydrogen. Also, only one of the FFTS candidate combustion liners was tested at Capstone with the FFTS-4 injector. Given the favorable results that have been achieved with this FFTS combustion system configuration, it is recommended that more test data is acquired to further optimize the injector and combustion liner design. ANL created the test cell design for the demonstration test.

3.5.2. Demonstration Test Cell at ANL

The final demonstration test of the integrated gasification station and C65 microturbine system were originally planned to be conducted at ANL. The overall system concept is shown in Figure 5 while the actual test cell is shown in Figure 10, the major equipment planned to be used in the demonstration test included:

- Capstone C65 microturbine (C65 MT)
- Gas chromatography (GC) for fuel composition characterization
- Fourier Transfer Infra-Red (FTIR) for emission measurement
- Data acquisition (DAQ) system and related instrumentation box; and
- Horiba MEXA 7100 emission measurement console.

Figure 10: Demonstration Test Cell at ANL

4. Gasification Fuel Characterization

One of the main objectives for this program was to characterize the fuel properties of the gasification fuel. For low emission Microturbine systems, Capstone Microturbine engines use lean premixed combustion technologies to achieve ultra-low emissions for a wide range of fuels, both liquid and gaseous. In lean premixed systems, combustion with a range of fuel blends is affected by fuel reactivity, fuel/air premixer (or injector) configuration, and combustor architecture. Fuel reactivity is determined by the combination of many factors, including auto ignition delay time, laminar/turbulent flame speed, chemical kinetics or reaction rates, and flammability limits as well as its operating conditions. No single parameter is sufficient to fully characterize a given fuel in a given context. All fuel property factors together with the combustion system design — combustion system architecture and injector geometry, for example — determine combustor operability, durability, and the exhaust emission levels. The common fuel constituents and properties for typical gas turbine fuels are shown in Table 1.

Table 1: Common Fuel Constituents and Properties (GT2010-22267)

	Formula	LHV, BTU/ft ³	LHV, BTU/lb.	U/L flammability ratio (60F, 1 atm)
Hydrogen	H ₂	275	51,599	18.41
Carbon Monoxide	CO	321	4,346	5.79
Methane	CH ₄	912	21,524	2.61
Ethane	C ₂ H ₆	1,623	20,437	4.11
Propane	C ₃ H ₈	2,323	19,949	4.26
Butane	C ₄ H ₁₀	3,019	19,674	4.41
Pentane	C ₅ H ₁₂	3,718	19,517	5.13
Hexane	C ₆ H ₁₄	4,415	19,415	
Ethene	C ₂ H ₄	1,502	20,281	10.18
Propene	C ₃ H ₆	2,188	19,696

Among these fuel constituents, the highest fuel reactivity — for example, flame speed or reaction rate — is associated with H_2 , while the lowest is associated with blends of NG with inert gases like nitrogen (N_2) and CO_2 . Combustion system operability can be defined as reliable and stable combustion or stabilized flame contained within the gas turbine combustion chamber in a controlled manner over a wide range of loads and ambient conditions. A Microturbine system is generally required to maintain combustion operability when the load changes dramatically and quickly with an acceptable level of dynamic pressure amplitudes for good system durability. Thus, combustion operability also requires adequate margin to lean blowout to avoid unexpected loss-of-flame events (flameouts) and adequate resistance to flashback to avoid catastrophic hardware damages. However, it is worth noting that combustion stability or operability is also highly associated with the health and smooth control of fuel and air supplies in the event of fuel variation, operating condition changes, or quick load switching.

In order to design a combustion system for the FFTS program, one of the key efforts was to understand the gasification process and the composition of fuel gas generated from the gasification system.

Per Packer's ASPEN modeling, the gas composition of biomass gasification highly depends on the operating temperature of the gasification system. As shown in Table 2, the primary gas constituents of the fuel produced by the gasification system are CO, CO_2 , H_2 , and CH_4 at around 500 °C operating conditions, with 34% CO_2 , 40% CH_4 , 11% H_2 , and 15% CO. Between 500-800 °C operating temperature, the gas composition varies greatly with both CO and H_2 content increasing while CO_2 and CH_4 concentrations decreasing as temperature increases. At 800 °C operating temperature, it was predicted that the primary gas composition would become 1% CO_2 , 3% CH_4 , 47% CO, and 49% H_2 . At the same time, the LHV drops from around 450 BTU/ft³ at 500 °C to about 310 BTU/ft³ with more oxidation and energy conversion at 800 °C. When the gasification system is operated at 800 °C or higher, the gas composition becomes more stable and eventually plateaus. The heating values of the syngas from the process also stabilize.

Figure 11: Packer Engineering ASPEN Model

Table 2: Packer Gasification Fuel Composition Analysis Results

	Feedstock				
Date Performed	12/17/09	01/14/10	11/01/10	11/17/10	11/17/10
Major Component	Corn Stover	Woodchips	Corn Stover	Corn Stover	Woodchips
H ₂	28.60	19.40	42.9	24.3	19.8
CO	25.70	15.00	36.1	25.9	23.3
CO ₂	11.10	7.60	8.49	12.4	15.2
N ₂	22.30	41.80	6.01	18.3	21.7
Methane	7.79	4.96	5.67	11.1	11.5
Oxygen	3.95	11.10	0.2	4.54	3.7
Calculated Gas Properties per ASTM D3588-98(3)					
Relative Density (Dry)	0.7507	0.8345	0.6106	0.7923	0.8474
Gross HV (Dry) (Btu/ft ³)	269.4	169.3	329.6	351.2	356.9
Wobbe Index	310.9	185.3	301.1	394.6	387.7
Net HV (Dry) (Btu/ft ³)	246.1	154	295.9	317.1	323

Table 3: Biomass Syngas Fuel Composition
(Major Components with > 1% mol, Gas Analyzed with Gas Chromatography)

Component	Switchgrass	Corn Stover	Wood Chips
Hydrogen	44.50%	42.90%	41.80%
Carbon Monoxide	31.50%	36.10%	34.80%
Carbon Dioxide	12.40%	8.49%	9.88%
Nitrogen	2.70%	6.01%	4.32%
Methane	7.38%	5.67%	8.21%
Total	98.48%	99.17%	99.01
Relative Density (dry)	0.6148	0.6106	0.6193
Gross HV dry (btu/ft ³)	351.7	329.6	354.2
Net HV dry (btu/ft ³)	319.6	295.9	323.3
Wobbe Index (btu/ft ³)	448.6	421.8	450.1

To further characterize the fuel composition, gas samples were collected at Packer and analyzed at ANL during the gasification development and optimization process. Table 2 shows the fuel compositions for the syngas generated from different biomass feedstocks, namely switchgrass, corn stover, and wood chips during the period of December 2009 to November 2010. As seen from the data, even at the same operating temperature, gasification syngas fuel composition differs for different types of feedstock. However, after the gasification process was further optimized and operating temperature selected, the syngas composition variations became much smaller with H₂ at 41.8–44.5%, CO at 31.50–34.8%, CO₂ at 8.49–12.40%, N₂ at 2.70–6.01%, and CH₄ 5.67–8.21% for different feedstocks as shown in Table 3. The heating values were also analyzed and found to be between 295.9 and 323.3 BTU/ft³, which falls into the low BTU (LBTU) fuel category per Capstone fuel specifications. In order to prepare the syngas for gas turbine use, it was also noted that particulate matter (PM) such as ash and tar in biomass gasification are of great concern to gas turbine application. The Packer gasification system was designed to remove these contaminants to comply with Capstone's fuel cleanliness requirements.

5. Operability Analysis

5.1 Auto-Ignition

Auto-ignition is a spontaneous chemical reaction between fuel and air that occurs without an external ignition source. Higher temperature, higher pressure, and longer residence time make it easier for a fuel-air mixture within the flammability range to auto-ignite. At a fixed temperature, pressure, and fuel-air mixture there is a minimum amount of residence time that is needed for the mixture to auto-ignite, which is called auto-ignition delay time.

Very little information is available for syngas fuels in terms of usage, chemical mechanisms, and combustion behavior. In order to evaluate and understand the auto-ignition properties of the FFTS syngas fuels, UCI conducted a comprehensive literature review and some chemical analysis. Additionally, ANL performed modeling and experimental studies to determine combustion/ignition characteristics of gaseous fuel-air mixture. The ANL effort was to determine the ignition and combustion characteristics of syngas generated in the gasification process with an emphasis on those characteristics relevant to the syngas utilization in a microturbine.

Figure 12: ANL RCM Setup Schematic

Figure 13: RCM at ANL (a) Setup (b) Sample Testing Image ER=0.80, time interval 263

□s; 29.7 Bar, 699K

The ignition boundaries for methane-air mixtures were determined using ANL's rapid compression machine (RCM). The measured values were further compared through CHEMKIN chemical kinetic simulation software using the San Diego chemical reaction mechanism. The ANL RCM setup is shown in Figure 13 in addition to an example of high speed imaging results for measuring flame kernel growth to determine ignition properties. In this program, the ignition and combustion characteristics of the representative biomass syngas were also determined using RCM imaging. The RCM ignition delay time characterization results for methane-air and 50% CO/50% H₂-air mixtures are presented in Figure 14, which indicates that the syngas-air mixture has much shorter ignition delay time after a forced spark ignition. These data are also tabulated in Table 4.

Long-ignition delays: Slow combustion

Short-ignition delays, Fast combustion

Figure 14: RCM Test Results

Table 4: RCM Results for Methane vs. Syngas (Ignition Delay after Forced Ignition)

T2		P2	Equivalence Ratio	Fuel Constituent - Vol%				Ign. Dela	dP/dt
Case #	F	Bar-abs.	-	CH ₄	H ₂	CO	Total	ms	bar/ms
2	1100	4.5	0.5	100	0	0	100	21.68	0.191
4	1100	4.5	0.5	0	50	50	100	4.76	0.779
13	1100	10	0.5	100	0	0	100	77.48	0.091
14	1100	10	0.5	0	50	50	100	7.4	1.0

* ignition delay after sparking, no auto-ignition

For Capstone Microturbine engines, auto-ignition within the injector must be prevented because it will lead to injector hardware damage and combustion system failure. From chemical kinetics simulations, it was found that the air-fuel mixture has a predicted auto-ignition delay time of more than 80 ms, while the residence time of the fuel/air mixture in the injector is much less (2-3 ms). Secondly, literature indicates that experiments demonstrate that the replacement of even small amounts of H₂ with CO in CO/H₂-air mixture leads to inhibition of auto-ignition despite hydrogen's higher reactivity. Thirdly, the auto-ignition temperatures of hydrogen (1085 °F) and CO (1128 °F) are higher than the typical fuels — natural gas and diesel #2 — that Capstone Microturbine engines have been burning successfully for many years without auto-ignition. For example, methane has an auto-ignition temperature of 1076 °F and Diesel #2 has an auto-ignition temperature of 410 °F. As a result, there is high confidence that even at engine conditions (higher temperature/higher pressure), the risk of auto-ignition within the injector is very low.

5.2 Operability Range

5.2.1. Lean Blowout (LBO)

The guiding principle in flame stabilization in both laminar and turbulent flows is that flame speed (turbulent or laminar) matches the local mean flow velocity. LBO occurs when the local mean flow velocity is greater than the flame speed at each point in the flame causing it to physically blow out of the burner. LBO is a major concern in stationary gas turbines where the preferred method of reducing criteria pollutants is lean premixed combustion. Operating a gas turbine near its LBO limit is the current low emission strategy to lower peak flame temperatures and reduce thermal nitrogen oxides (NO_x) emissions. This is also the principal strategy for Capstone's lean premixed combustion technologies to maintain ultra-low emissions. If LBO occurs, the engine requires a restart, incurring costs associated with maintenance, engine life, and availability. Stationary gas turbines operating on NG have been successful at maintaining high reliability, but new fuel concentrations require a re-characterization of LBO behavior. Extensive studies have been performed to examine fuel composition effects of syngas mixtures in this program. From this work there are two main conclusions: (1) H_2 addition extends the LBO limit of CH_4 or other hydrocarbons and (2) correlations depend upon Damköhler number to describe LBO phenomena. Many studies have been performed to improve understanding of LBO with fuels that contain H_2 . Two observations are common in these studies: (1) the addition of H_2 extends the lean operating limit and (2) characterization of LBO has traditionally been characterized by Damköhler number. The majority of the studies do not offer predictive methodologies to establish LBO limits. Those that do offer correlations do so only for swirl stabilized flames, leaving a gap in the characterization of LBO for turbulent jet flames with fuels that contain H_2 . Under the current FFTS program, both LBO and flashback were experimentally tested with UCI's C65 full annular combustion apparatus and in C65/C200 engines both at UCI and Capstone facilities.

5.2.2. Flashback

With fuel variation — particularly the hydrogen content in biomass gasification syngas — and some other operational variations, flashback (FB) has been a significant concern for lean premixed combustion systems like the Capstone C65 engine. Flashback occurs when local flame speed is greater than air/fuel flow speed. The flame stabilization balance is broken and flame propagates upstream toward the fuel injection source. For low NO_x lean premixed combustion in gas turbine conditions, at least four mechanisms of FB have been introduced: (1) core flow FB, (2) boundary layer FB (BLF), (3) combustion induced vortex breakdown (CIVB), and (4) combustion instability induced FB. A C65 injector damaged by a flashback during development tests is shown in Figure 15. Among the four major identified flashback mechanisms, the core flow flashback and boundary layer flashback are believed to be the mechanisms to which Capstone injectors are most susceptible.

Figure 15: C65 Injector Flashback Example

Core flow flashback occurs when the flame speed of the mixture is greater than the core flow velocity, which allows the flame to flashback to an undesired position that may be either too close to the injector or inside the injector, both of which can cause damage to hardware and, eventually, engine failure. In addition, as illustrated below, the boundary layer mechanism causes flashback when the quenching distance of the fuel/air mixture is smaller than the boundary layer thickness, allowing ignition to occur within the low velocity boundary layer. Due to the low velocities in the boundary layer, if ignition can occur the flame will regress provided that the flame speed is greater than the lowest boundary layer velocity outside of the quenching distance. The critical velocity gradient approach (as seen in Figure 17) has been adopted to evaluate the flashback propensity in this study. Higher critical flow velocity means higher propensity of flashback. For turbulent flow, the critical flow velocity gradient was given by (GT2013-94823):

$$g_c = \frac{\partial V}{\partial y} = \frac{\tau_w}{\mu} = 0.03955 u^{-\frac{7}{4}} v^{\frac{3}{4}} d^{\frac{1}{4}}$$

Figure 16: Core Flow Flashback Schematic

Figure 17: Boundary Layer Flashback

Figure 18: Schematic of Critical Velocity Gradient Definition (Lewis & Von Elbe, 1943)

5.2.3. Operability Range for C65 FFTS Fuels

The operability range for a combustion system can be defined as the conditions under which stable combustion can be maintained over a wide range of operating ambient conditions and load ranges. The guiding principle in flame stabilization in both laminar and turbulent flows is that flame speed (turbulent or laminar) matches the local mean flow velocity such that flame structure can be maintained without being blown away, or flashback upstream to fuel supply point. As a result, the operating conditions between LBO and flashback are the operability range for a combustion system. The operability range of a combustion system is determined by fuel properties and combustion system design. When fuel properties and operating conditions are predefined, combustion system design is the key factor to determine operating range.

For this project, the full annular apparatus at UCI was used to test both LBO and flashback with different fuel blends and preheating temperature for combustion air. Thermocouples were the primary measurement tool and were properly instrumented by Capstone to the test injectors, which were installed at the aft plane of the C65 annular test apparatus. The temperature for preheating the combustion air was 550 °F, 650 °F, 750 °F or 850 °F with an in-line electrical heater. The fuels tested were H₂/NG mixtures and H₂/CO mixtures.

Figure 19: C65 Full Annular Apparatus Data for Syngas Fuels

Plotted in Figure 19 are the operability data — equivalence ratio at which LBO or flashback occurs — for H₂-CO fuel. The chart shows LBO and flashback equivalence ratios (ERs or ϕ s) as a function of H₂ content and preheated air temperature. The lower group of lines shows the LBO ERs at different air preheating temperatures while the upper group of lines shows the flashback ERs at different air preheating temperatures. There are four different air preheating temperatures: 550 °F, 650 °F, 750 °F or 850 °F. At each temperature, its corresponding operating range for the injector is the space between the LBO and FB lines. From this set of test data from the C65 full annular apparatus for the C65 baseline natural gas injector running H₂-CO fuel blend, the following observations can be made:

- The hydrogen content in the H₂-CO fuel blend is important for both LBO and flashback ER. At the same air temperature, both LBO and flashback occur at lower equivalence ratio with increased hydrogen contents; that is, combustion reaction can stabilize at leaner condition (LBO at lower ER), while flashback takes place at lower ER as well.
- Hydrogen content change has a greater impact on flashback than LBO, particularly when H₂ < 60% (**Note:** Flashback ER lines have greater slope at low hydrogen content range than LBO lines).
- The air preheating temperatures have great impact on LBO and flashback ER. In general, the higher the temperature, the lower the LBO or flashback ER. This indicates the higher air temperature helps stabilize flame at near LBO conditions such that LBO ER becomes lower. Higher air temperature also increases the propensity of flashback such that injector/combustion system flashback occurs at a lower ER.
- With increased hydrogen content, the combustion system has a smaller operating window — a decreased difference between LBO and flashback ERs, for example — at the same air preheating temperature.
- With increased air preheating temperature, the combustion system has a smaller operating window — a decreased difference between LBO and flashback ERs, for example — at the same hydrogen content.

Given the C65 combustion air is recuperated, the temperature is approximately 1100 °F, much higher than the highest temperature tested (850 °F). The operability of the baseline C65 injector is much smaller when operating on H₂/CO fuel blends. It is projected that the operability range is too small for a practical application. As a result, the existing C65 NG injector and combustion system would not work for FFTS program.

5.3 Emissions

Although there are no emission requirements for the FFTS program, it is highly desired to characterize emissions performance to provide some guidance for the next phase design. As a result, the combustion design still aims to achieve low levels of pollutant emissions, including NO_x and CO among others. For a lean premixed combustion system, emissions strongly depend on the temperature and residence time in the primary zone (PZ). This is particularly true for NO_x , because thermal NO_x mechanism counts for the majority of NO_x production. As a result, in order to maintain a low NO_x level, it is typical to keep a low PZ temperature. However, lower PZ temperature reduces stability and causes high CO emissions. So, the temperature or ER “sweet zone” range is relatively narrow for lean premixed combustion systems. Figure 20 is a chart showing the relationship between NO_x and CO to PZ temperature.

Figure 20: Influence of Primary Zone Temperature on CO and NO_x Emissions
(Ref. Gas Turbine Combustion: Alternative Fuels and Emissions, 3rd Edition)

It is widely believed that both spatial and temporal variation in the fuel/air mixing impact the emissions of NO_x . As a result, efforts should be made to develop an FFTS injector capable of rapid and complete mixing of fuel and air in lean premixed systems — similar to those used in burning natural gas — while incorporating features for increased resistance to flashback. Although different systems have different achievable emission levels due to the design differences, there is a highly cited NO_x “entitlement” emissions chart assuming “perfect” mixing for a premixed natural gas combustion system. This chart is shown in Figure 21. In the design of combustion liner and injector for the FFTS engine, these have been taken into account.

Figure 21: Minimum NO_x Achievable for Lean Premixed Combustion (per Leonard and Stegmaier, 1994)

6. Injector Evaluation and Development

The injector is the key component for the combustion system for the FFTS engine development. In the annular apparatus test — introduced in Section 3.4 — it was found that the existing C65 natural gas baseline injector has poor operability for the target FFTS fuel with 50%CO/50%H₂. Thermocouples were used to detect flashback events during testing. The strategies for developing FFTS injector were:

- Further evaluate the baseline injector in engine tests
- Use CFD (computational fluid dynamics) to understand injector and combustor flow field
- Use CFD to evaluate design strategies for varying flow profiles at the exit of injector
- Develop “cut-back” injector and test under engine condition to evaluate its flashback propensity
- Develop a series of diffusion/premixed hybrid injectors and evaluate the injectors in engine tests
- Develop a new multi-fuel capable, high flame speed fuel injector, which was successfully engine tested with 100% hydrogen, without flashback

6.1 Baseline Injector Engine Test

In addition to the annular apparatus tests discussed in preceding sections, the baseline injector’s ability to burn high flame speed fuels was further evaluated in engine condition. The fuels tested were: (1) NG/C₂H₆ blend and (2) NG/H₂; (3) CO/H₂ fuel blends. A section view of the C65 natural gas baseline injector is shown in Figure 22. Test results are listed in Table 5, Table 6, and Table 7 respectively. Adiabatic flame temperature (AFT) data have been normalized.

Figure 22: C65 NG Baseline Injector

Table 5: Engine Test Results (Baseline Injector, NG/C₂H₆ Blend)

	FUEL TYPE:	C ₂ H ₆ /NG			PLATFORM:	Engine/Baseline Inj.	
Parameters	X_C2	P[atm]	T [K]	φ_inj	S_L* [cm/s]	Normalized AFT [-]	V_inj/S_L
62 kW No Flashback	0.68	4.13	835.7	0.53	87.1	0.995	49.47

Table 6: Engine Test Results (Baseline Injector, NG/H₂ Blend)

	FUEL TYPE:	H ₂ /NG			PLATFORM:	Engine/Baseline	
Parameters	X_H2	P [atm]	T [K]	φ_inj	S_L* [cm/s]	Normalized AFT [-]	V_inj/S_L
65 kW	0.63	4.28	837.0	0.54	171.6	1.020	24.54
60 kW	0.60	4.03	835.0	0.49	138.6	0.973	31.46
59 kW	0.61	3.99	834.7	0.48	138.1	0.967	31.72
30 kW	0.64	2.86	831.7	0.58	238.0	1.057	18.19
20 kW	0.30	2.46	831.2	0.75	208.9	1.161	20.44

Table 7: Engine Test Results (Baseline Injector, CO/H₂ Blend)

	FUEL TYPE:	H ₂ /CO			PLATFORM:	Engine/Baseline	
Parameters	X_H2	P [atm]	T [K]	φ_inj	S_L* [cm/s]	Normalized AFT [-]	V_inj/S_L
62 kW	0.20	4.13	835.7	0.365	80.66	0.943	53.4
39 kW	0.20	3.19	831.9	0.357	85.44	0.932	51.5
30 kW	0.15	2.86	831.7	0.419	107.46	1.004	40.3
20 kW	0.10, 0.17, 0.31	2.46	831.2	0.511	131.59	1.098	32.4

As seen in Table 5, the full power engine test (actual power output was 62 kW) did not detect flashback at test conditions with up to 68% of ethane (C₂H₆). Due to ethane fuel supply issues, testing with NG/C₂H₆ was terminated. For NG/H₂ engine testing, the engine was found to flashback, indicated by temperature rises detected by thermocouples instrumented to various locations of the injectors, at 30%, 64%, 61%, 60%, and 65% for operating at 20, 30, 59, 60, and 65 kW power levels. The NG/H₂ test results demonstrated great margins for the baseline injector for running natural gas fuel at different power levels. CO/H₂ testing revealed that the system was only able to run up to 20%, 20%, and 10-31% H₂ in the CO/H₂ fuel mixtures for 62, 39, 30, and 20 kW respectively. From engine test data, it is apparent that the C65 baseline injector cannot be used for burning FFTS fuel without flashback risk, assuming 50%-CO/50%-H₂ being the design target fuel.

6.2 Injector Design Tools – CFD Simulation

CFD simulation is a useful tool for injector design because of its ability to simulate flow field and the fuel/air mixing process. CFD simulation was used to predict injector exit velocity profile, wake zone inside injector, and fuel distribution at injector exit. The following tasks were performed in FFTS injector development:

- Model four different C65 injector design tools to explore how geometry changes affect flow profile and fuel concentration distribution at injector exit. The goal for the injector configurations was to significantly alter the velocity and fuel distribution exiting the injector so that different profiles could be tested. Test hardware that would have a greater chance of flashback and stability margin differences — which is needed for diagnostic tool development — could then be procured. The goal of the CFD was not to design injectors for production or for the FFTS demonstration. Once diagnostic tools have been developed and determinations of which velocity or fuel distribution features are desirable have been made, then the injectors which contain those features would be designed in a production form. Example results from the CFD simulation are presented in Figure 23 and Figure 24.
- CFD was also used to evaluate four new C200 injector designs, in order to develop flashback resistant injectors for high flame speed fuel like FFTS fuels. Example results from the CFD simulation are presented in Figure 25 and Figure 26.

Figure 23: CFD Fuel Distribution Profile Simulation for Flashback-Resistant C200 Injector Development

Figure 24: CFD Velocity Profile Simulation for Flashback-Resistant C200 Injector Development

Figure 25: CFD Velocity Profile for C65 FFTS Injector Design Tools

Figure 26: CFD Fuel Mass Fraction Profile for C65 FFTS Injector Design Tools

6.3 New Injector “Cut-Back” Baseline Injector Engine Test

After testing the baseline injector in the microturbine engine in the annular test apparatus, as described in Section 6.1, a hypothesis was formed that to reduce flashback risk the elimination of the “intrusion” of the six injectors to the primary zone of the combustion chamber would be helpful to (1) reduce flame anchoring; (2) reduce flow disturbance in PZ and smooth out the flow field; and (3) reduce direct exposure to flame which would result in a cooler injector tip temperature and reduce flashback risk. Shown in Figure 27(a) is the general arrangement of the six injectors in C65/C200 engine while Figure 27(b) shows a visualization of the flame structure of a “cut-back” injector versus a regular C200 natural gas injector when burning natural gas in a C200 full annular test apparatus at Capstone’s test facility.

(a) C65/C200 Injector Arrangement

(b) Cut-back vs. Regular Injector Flame Structure

Figure 27: C65/C200 Injector Arrangement Schematics and “Cut-Back” Injector Flame Visualization

After annular apparatus testing, a set of instrumented “cut-back” injectors were tested in UCI’s C65 engine. A picture was taken to visually compare the baseline C65 injector to the “cut-back” injector. Both injectors are shown in Figure 28. Engine test data are listed in Table 8 and Table 9. The test data provided mixed information: (1) the “cut-back” injector seemed to reduce flashback risk at 20 kW because engine was able to burn 30% NG/70% H₂ fuel mixtures compared to the baseline injector which could only burn 70% NG/30% H₂ and (2) performance of the “cut-back” injector at 30 kW and 60 kW for flashback resistance was worse than the baseline injector.

In addition to NG/H₂ fuel, CO/H₂ fuel was also tested. Comparing data in Table 9 and Table 7, one can draw the conclusion that the “cut-back” injectors did not reduce flashback propensity for running the C65 engine on CO/H₂ fuel.

Figure 28: C65 Baseline (NG) Injector Comparison to “Cut-Back” Injector

Table 8: Engine Test Results (“Cut-Back” Injector, NG/H₂ Blend)

	FUEL	H ₂ /NG			PLATFORM:	Engine/Cutback	
Parameters	X_H2	P [atm]	T [K]	φ_inj	S_L* [cm/s]	Normalized AFT [-]	V_inj/S_L
60 kW	0.50	4.03	835	0.475	179.59	0.973	24.3
30 kW	0.45-0.49	2.86	831.7	0.573	276.9	1.057	15.6
20 kW	0.68, 0.70	2.46	831.2	0.709	373.03	1.159	11.4

Table 9: Engine Test Results ("Cut-Back" Injector, CO/H₂ Blend)

	FUEL TYPE:	H ₂ /CO			PLATFORM:	Engine/Cutback	
Parameters	X_H2	P [atm]	T [K]	ϕ_{inj}	S_L* [cm/s]	Normalized AFT [-]	V_inj/S_L
58 kW	0.23	N/A	N/A	N/A	N/A	N/A	N/A
30 kW	0.14	N/A	N/A	N/A	N/A	N/A	N/A
20 kW	≤ 0.05	N/A	N/A	N/A	N/A	N/A	N/A

6.4 FFTS Injectors #1, #2, #3: Diffusion and Partial Premixed Injectors

6.4.1. Design Considerations

In order to make the C65 system capable of burning high hydrogen content syngas, a re-design of the combustion system (liner and injector) was necessary to make sure that (1) a good air flow split would be achieved to increase the air flow to injectors such that the bulk velocity within the injectors is increased enough to give a higher flashback resistance margin for core flashback — from past C30/C60/C65/C200 experience, it has been established that when the average velocity of fuel/air mixture in the injector is multiple times that of the laminar flame speed of the fuel/air mixture the injector will have good flashback-resistance margin — and (2) a well-designed injector — with proper aerodynamics for a good balance between operability and performance — was developed. In order to combat flashback, the general approaches included:

- (1) Modify combustion liner design to optimize air flow split ratio between combustion air, dilution air, and cooling air such that injectors receive more air to increase bulk velocity within the injector and give higher flashback resistance margin for an increased core flashback resistance.
- (2) Develop new injector concepts and designs such that the internal flow and mixing is optimized to avoid or minimize the formation of a recirculation zone, where flame can stabilize once flashback occurs.
- (3) Reduce fuel concentration in low the velocity zone — particularly in the boundary layer — to make fuel/air mixture less likely or impossible to ignite in these regions.
- (4) Increase flow speed along the adjunction area to manipulate the velocity profile at the injector exit and/or along the inner wall of the injector for increased flashback resistance.

6.4.2. Injector Details

Based on the injector design considerations — listed in Section 6.4.1 — three different designs — denoted as FFTS-1, FFTS-2, and FFTS-3 — were developed and are shown in Figure 29, Figure 30, and Figure 31 respectively. These injectors have the same overall “envelop” as the baseline injector. However, the fuel distribution module in the baseline injector is replaced with a pencil-shaped fuel tube. Details of the central fuel tube are shown in Figure 32. For development injectors, the fuel tube can be moved along the axial direction to change fuel introduction location such that the fuel/air mixture at the injector exit can be varied to test its sensitivity in flashback resistance. For each design, the key features are identified. Changes are incremental.

FFTS-1 (compared to baseline injector):

- Fuel tube has adjustable fuel exit location.
- All eight (8) mixing holes are enlarged from 7.54 mm to 8.56 mm to allow more air flow to injector.

FFTS-2 (compared to baseline injector):

- Fuel tube has adjustable fuel exit location.
- All eight (8) mixing holes are enlarged from 7.54 mm to 8.56 mm to allow more air flow to injector.
- “Fuel distributor” and mixing holes are both moved downstream by 25.4 mm.

FFTS-3 Details (compared to baseline injector):

- Pilot fuel tube can be adjust its fuel exit location
- Mixing holes are changed from eight (8) big holes to 24 holes with 4.94 mm diameter.
- “Fuel distributor” and mixing holes are both moved downstream by 25.4 mm, at same location as FFTS-2.

Fuel Tube Details:

- Total of 20 small fuel injector holes with a diameter of 1.75 mm
- 30 degree tip

Figure 29: FFTS-1 Injector Section View (PN 530007-100)

Figure 30: FFTS-2 Injector Section View (PN 530008-100)

Figure 31: FFTS-3 Injector Section View (PN 530009-100)

Figure 32: Fuel Tube Design #1

The injector features designed to this injector were projected to have following combustion and aerodynamic effects:

- Compared to the full premixed flame in C65 NG system, diffusion flame or partially-premixed flame are expected, with adjustable fuel tube, impact of fuel/air mixing would be revealed.
- More combustion air would be drawn to the injector because of (a) bigger air mixing holes and (b) moving mixing hole downstream.
- Injector can be tested with intrusion to primary zone of the combustor or without by using the "Cutback" version.
- Move the current fuel distributor downstream accordingly to change the level of fuel mixing.

6.4.3.Engine Tests

The engine tests for FFTS-1, -2, and -3 were performed at Capstone's test facility per test plan TP-3001173-000-00. The key testing set up was:

- Modified engine liner designed for FFTS fuels, with about 60% primary zone air split.
- Pilot tube without tip cutoff (Figure 32) or with tip cutoff (Figure 33).
- Each of the injectors was instrumented with at least two thermocouples for flashback detection.
- Portal emissions measurement console TESTO 350 XL was used for CO, CO₂, O₂, and NO_x measurements.
- Liner Configurations: Two different liner configurations were planned to be tested with different air splits to primary zone. The part numbers for the two liner configurations were 529934-100 and 529935-100, and with 158% and 200% air to primary zone respectively (compared to C65 NG system).
- Only one "injector of interest" (installed at loc. #6) was fueled with "test fuel" while the other baseline injectors were fueled with pipeline natural gas.
- Fuels tested were natural gas and NG/H₂ blend.
- Both flashback of the "injector of interest" and the LBO of the system were tested.
- Injector fuel tube was tested at different axial locations (A, B, C, or D) as illustrated in Figure 34.

Figure 33: Fuel Tube (with or without Tip Removed)

Figure 34: Fuel Tube Location Illustration (FFTS-1)

6.4.4. Test Results

For various reasons, only FFTS-1 injector was tested. The main findings from the tests were:

- (1) Fuel Tube Tip Oxidation was observed for the injector configuration with tip on (Figure 35a). However, after the fuel tube tip was removed, no more tip oxidation was observed from FFTS-1 injector, with fuel tube tip at locations # A and #D (Figure 35b)
- (2) FFTS-1 injector was tested to 100% H₂ without flashback for different fuel tube locations.
- (3) LBO was also tested for FFTS-1 injector with all injector fueled with natural gas.
- (4) Further tests were needed to fully understand the performance of FFTS-1 injector.

Figure 35: Configuration: FFTS-1, Fuel Tube Loc. #D, (b) Tip-Cut-off

6.5 FFTS-4 Injector – High Flame Speed Injector

Based on the same considerations specified in Section 6.4.1, another injector was designed for high flame speed fuels — like those syngas fuels specified for the FFTS program — with high hydrogen content. Figure 36 is the cross section view — in its generic form — of a C65 high-H₂ injector (“FFTS-4”). The injector has been further tested in a C65 engine with natural gas blended with hydrogen. The FFTS-4 injector was tested together with the Combustion Liner Design A. These test results are in Section 7.6.

Figure 36: General Multi-Fuel, High Flame Speed Fuel Injector

7. Combustion Liner Design

7.1 Combustion Specification Analysis

Table 10 shows the baseline natural gas C65 system's key ISO condition parameters on which the FFTS system design was based.

Table 10: C65 Natural Gas System Key Combustion Specifications

Parameters	Unit	C65
Combustion Energy	kW	250
Mass Flow - Air	lb/s	1.07
Mass Flow - Fuel	lb/hr	41.97
AFR		91.8
FAR		0.0109
Phi Overall		0.188
Combustor Inlet Temperature	°F	1029
Combustor Outlet Temperature	°F	1750
Max Combustion Exit Temp. (PF=0.2)	°F	1894
Combustor Pressure	psia	69.1
Combustor Pressure Drop	%	2.0

7.2 Flow Area and Geometry Analysis

The combustion liner forms an enclosed chamber wherein extremely high temperature, exothermic chemical reactions take place. The liner not only contains the high temperature gas in the desired space, but a properly designed liner also distributes or directs air to the correct locations, at the correct flow rates, and within the correct velocity range — working with the optimized injectors — so that the combustion design performance targets can be met. The important combustion performance criteria include operability, pollutant emissions, pressure drop, and combustion liner life. Capstone Microturbine systems are Brayton-cycle-based systems with a recuperator to recover heat from turbine exhaust gas to the incoming compressed air for higher efficiency. The pre-heated, compressed recuperator air is used as (1) combustion air as oxidizer, (2) cooling air to achieve the desired component — liner and injector, for example — temperature, and (3) dilution air to mix with high temperature combustion exhaust to generate desired pattern factor (PF), velocity profile, and momentum distribution for the turbine stage.

Flow analysis was performed to understand the current C65 and give direction regarding how to modify the injector and combustion liner for C65 the FFTS demonstration engine. Flow analysis — coupled with other analyses such as combustion chemical kinetics and flow field analysis — was used to design a combustion system geometry that would:

- Achieve desired airflow split to PZ for achieving optimal emissions
- Achieve desired cooling air flow to maintain component temperature at levels that will achieve designed operating life
- Limit pressure drop to the design target — for example, the design target for a natural gas C65 combustion system was 2.0% — to achieve designed performance. As a result, the FFTS engine was designed to maintain same level of pressure drop.
- Have correct jet penetration so dilution air achieves desired pattern factor for optimal turbine stage performance
- Effectively control flow via orifices to give system variability
- Generate preliminary key geometries and dimensions of combustor, injectors, and casing which will be adjusted based on test results

7.2.1. Flow Analysis with One-Dimensional Flow Model

The air flow distribution in the engine is predetermined by the fixed geometry of its components and interfaces. These components include the liner, injectors, injector bellows, and recuperator casing. Figure 37 is the 1-D flow model for C65 combustion system with the design parameters identified in Table 11.

As shown – C65/200 1-D Flow Model

Figure 37: One-Dimensional Flow Model for C65 Combustion Liner

Table 11: One-Dimensional Liner Flow Model Notes and Criteria

Node No.	Node Description	Key Parameter	Design Criteria
1	Recuperator Exit	P, T, flow rate, enthalpy	$\min < T_g < \max$, $m > \min$, $\min < m < \max$
2	Outer Dil. Holes	P, T, flow rate, enthalpy	$\min < m < \max$, $dP < \max$, Jet penetration
3	Combustion & Inner Dil. Air	P, T, flow rate, enthalpy	$dP < \max$, $\min < m < \max$
4	Front Plane Injector Air	P, T, flow rate, enthalpy	$\min < m < \max$, $dP < \max$
5	AFT Plane Inj. & Inner Dil. Air	P, T, flow rate, enthalpy	$\min < m < \max$, $dP < \max$
6	Aft Plane Inj. Air	P, T, flow rate, enthalpy	$\min < m < \max$, $dP < \max$
7	Inner Dil. Air	P, T, flow rate, enthalpy	$\min < m < \max$, $dP < \max$, Jet Penetration
8	Inner Casing Leak	P, T, flow rate, enthalpy	$m < \max$
9	PZ Aft Inj. Section	P, T, flow rate, enthalpy	$\min < T_g < \max$, $\min < t < \max$, $\min < T_w < \max$, $dP < \max$
9.1	Leak -Inj./Liner Interface	P, T, flow rate, enthalpy	$m < \max$
10	PZ Front Inj. Section	P, T, flow rate, enthalpy	$\min < T_g < \max$, $\min < t < \max$, $T_w < \max$, $dP < \max$
10.1	Leak -Inj./Liner Interface	P, T, flow rate, enthalpy	$m < \max$
11	PZ Exit	P, T, flow rate, enthalpy	$\min < T_g < \max$, $\min < t < \max$, $\min < T_w < \max$, $dP < \max$
12	Combustor Exit	P, T, flow rate, enthalpy	$PF < 0.20?$, Mass Momentum Distr.
13	Nozzle Inter-stage Leak	P, T, flow rate, enthalpy	$m < \max$
14	Cooling Slot flow	P, T, flow rate, enthalpy	$\min < m < \max$
15	Leak -Inj./Flange Interface	P, T, flow rate, enthalpy	$m < \max$

7.2.2. Flow Analysis with “Electrical Circuit” Flow Model

It is not practical to measure the flow to each of the flow streams inside the system. A comprehensive study would typically use 3-D CFD simulation to characterize and verify the designed components would meet the designed flow splits. It is also desirable to have a flow model using the “electrical circuit” analogue approach to simulate the flow split as shown in Figure 38. An accurate model would require flow or pressure drop measurements to calculate the “resistor” values component by component, or section by section. The model calculates flow “resistances” (pressure drops) for a number of discrete flow elements, such as wall friction, flow around a bend, and flow through an orifice. For the current FFTS program phase, flow analysis using an “electrical circuit” approach has not been done due to priority and resource limit.

Figure 38: Schematic of 1-D Flow Network for C65

7.3 Combustion System Pressure Drops

One of the high level requirements for the FFTS engine is to maintain higher system efficiency, which passes down to the MEM level with a requirement of not significantly increasing pressure drop. In general, Microturbine efficiency is impacted by the effectiveness or efficiency of all the sub-modules or components, which include the compressor, recuperator group, combustion system, turbine rotor group, and exhaust duct design. However, the impact of combustion system pressure drop on the overall system efficiency is relatively small, per test data and cycle deck analysis. For example, it was predicted that a 1% change in pressure drop — e.g., combustion system pressure increase from 2% to 3% — for a C200 Microturbine system would result in approximately 3 kW change in power and 0.2% change in efficiency. The C65 system architecture is similar to the C200, so the proposed changes of liner and injector design for C65 FFTS would lead to the expectation of some efficiency degradation, but not a significant amount.

7.4 Liner Design

For the FFTS program, flow network analysis and liner design was based on an “effective flow area” approach, which assumed an isothermal condition and 1-D incompressible/ideal gas fluid networks. Flow rate splits are determined by effective passage area which is the smallest geometric area along a passage. Based on combustion analysis, it is required to drive more combustion air to the injector which increases the bulk velocity to mitigate core flow flashback. While overall air flow to injectors is limited by the total area of the six injector exits, the maximum air flow to PZ is 92% by area approximation. At the same time, the liner life requirement and flow pattern control require air flow for liner cooling and flow field optimization. Specific designs were proposed and two liner designs were proposed for the FFTS engine with the following assumptions:

- (1) Flow splits can be approximated with “restricted area” comparison.
- (2) Liner life and flow pattern optimization/maintenance requires approximately 25% of total air flow.
- (3) Liner dilution hole locations will be the same while the size can be changed.

Table 12 lists the result of flow area analysis for the C65 natural gas baseline system. Excluding the floating seals at the interface of injectors and liner, the total effective opening area/flow passage is only 8.57 inch². If the floating seals are included, the effective area would be smaller. By area approximation, the air split of outer dilution holes, the injectors, inner dilution holes, inner dilution slots for a baseline C65 system are 15.54%, 38.76%, 42.12%, and 3.58% respectively, which reasonably agrees with the CFD results.

The two FFTS combustion liner designs are shown in Table 12. Design option A is expected to deliver 60% of total air to injectors while Design B is expected to deliver 76%. In order to drive more air to the injectors for FFTS engine, some of the dilution holes were reduced in size while maintaining the same number of holes. As a result, the total effective area for both designs was significantly reduced from baseline combustion (8.57 inch²) to 5.947 and 4.707 inch² for Design A and Design B respectively.

Table 12: Geometry/Flow Analysis Result for C65 with Proposed FFTS Liner Designs

	C65 NG Baseline	C65 FFTS Design A	C65 FFTS Design B
Inner Dilution Holes			
Number of Holes	40	40	40
Hole Diameter (mm)	8.61	4.859	1.433
Hole Diameter (inch)	0.34	0.191	0.056
Total Hole Area (inch ²)	3.61	1.150	0.100
Inner Dilution Slots			
Number of Slots	24	24	24
Area of Each Slot (mm ²)	8.247	8.247	8.247
Total Slot Area (mm ²)	197.928	197.928	197.928
Total Slot Area (inch ²)	0.307	0.307	0.307
Outer Dilution Holes			
Number of Holes	30	30	30
Hole Diameter (mm)	6.04	5.019	4.471
Hole Diameter (inch)	0.24	0.198	0.176
Total Hole Area (inch ²)	1.33	0.920	0.730

7.5 Engine Test Setup

FFTS-4 injectors designed for C65 FFTS engine were in their general form. The fuel distribution module location can be changed axially as shown in Figure 39. Locations A, B, and C were the three positions tested. The fuel distribution module has 25 fuel injection holes with a diameter of 0.80 or 1.00 mm.

Figure 39: FFTS-4 Injector for C65 Engine Test

Tests were performed to evaluate the flashback and stability capability of the FFTS-4 injector.

The combustion liner is a key combustion system component in the FFTS engine development. In a series of evaluation tests, the baseline C65 natural gas injector and liner were found to have marginal operability in both apparatus and engine tests when using the target FFTS fuel with 50%CO/50%H₂. After the development of the FFTS-4 injector, engine tests were performed in which the baseline natural gas liner was replaced with one of the FFTS liners (as introduced in Table 12). For the engine tests, thermocouples were used to detect flashback events. To summarize, the tested engine configuration had the following key features:

- FFTS Liner Design A: 60% combustion air — based on geometry analysis — delivered via the six injectors
- FFTS-4 injector: dedicated boundary layer air and central multi-fuel distribution module. Refer to Figure 39 for a section view of the injector configuration.
- FFTS-4, the injector of interest, was installed at location #6 only. All other injectors were the baseline C65 NG production injector.
- In flashback testing, only the FFTS-4 injector installed at location #6 received hydrogen doping. The other injectors (if fueled) were running on pipeline natural gas, which was approximately 95% methane.
- In engine flameout/LBO testing, all injectors — including FFTS-4 at location #6 — were supplied with pipeline natural gas if fueled.
- Thermocouples were installed to each of the six injectors for flashback detection.

7.6 Combustion Liner Design A and FFTS-4 Injector Test Results

A series of tests were conducted to evaluate the FFTS-4 injector's operability performance. The two types of FFTS-4 injectors tested were: (1) FFTS-4 injector with 0.80 mm fuel distribution module at location A, closer to the injector exit and (2) FFTS-4 injector with 0.80 mm fuel distribution module at location C, a location more upstream of the injector.

Flashback testing revealed that both FFTS-4 injector configurations tested were capable of burning 100% hydrogen stably without flashback for 6-, 5-, and 4-injector operations at the default TET setting, as shown in Table 13. However, because only one FFTS-4 injector was tested while the other five injectors were the baseline injectors, further testing is required to verify the FFTS-4 injector's flashback resistance, considering the interaction between injectors.

Table 13: FFTS-4 Injector Flashback Test Results

Injector at Loc. #6	Other Injectors	Fuel %H ₂ to Injector At Loc. #6	6 Injectors Flashback Power, kW	5 Injectors Flashback Power, kW	4 Injectors Flashback Power, kW	Oxidation (Visual Inspection)
FFTS-4, Type A, 0.80mm	Baseline	No Flashback at 100%	none	none	none	none
FFTS-4, Type C, 0.80 mm	Baseline	No Flashback at 100%	none	none	none	none

For stability testing, it was found that both FFTS-4 injector configurations — together with 5 C65 baseline production NG injectors — were able to extend flameout power levels to be lower than 20 kW with the exception of FFTS-4, Type C, 0.80 mm injector for 6-, 5- and 4- injector operations at the default TET setting, as shown in Table 14. The results were good, because 20 kW is typically run with 2 or 3 injectors. 4, 5, and 6 injectors being able to run below 20 kW means that the system has good stability margin. However, because only one FFTS-4 injector was tested while the other five injectors were the baseline injectors, further testing is required to verify the FFTS-4 injector stability capability.

In both flashback and stability testing, the before- and after-test visual inspection results — shown in Figure 40 and **Figure 41** — show normal discoloration due to high temperature exposure with no sign of flashback.

Table 14: FFTS-4 Injector Flame-Out Test Results

Candidate Injector at Loc. #6	All other Injectors	Fuel to all Injector % NG	Combustor	6 Injector Flameout kW	5 Injector Flameout kW	4 Injector Flameout kW
FFTS-4, Type A 0.80 mm	Baseline C65 NG Injector	100	1	<20	<20	<20
FFTS-4, Type C 0.80 mm	Baseline C65 NG Injector	100	1	25-20	<20	<20

Figure 40: C65 High-Flame-Speed Injector after 100% H₂ Tests

Figure 41: FFTS-4 Injector Inspection Picture (before and after 100% H₂ Tests)

8. Conclusions and Recommendations

Experimentally, the current C65 natural gas production injector was evaluated for FFTS program application. New injector concepts were developed and tested in a variety of test apparatus with various fuel types — such as natural gas, NG/C₂H₆, NG/H₂, and CO/H₂ fuels — with a focus on injector operability, flashback, and lean blow out. The following results and conclusions can be drawn from the injector development efforts:

- (1) Injector designs for the FFTS system for high hydrogen content biomass syngas should focus on injector operability, particularly on flashback issues.
- (2) Although fuel gas generated from the gasification process varies in fuel composition and other properties, the main constituents are CO and H₂. The design target for the FFTS injector was to be capable of burning 50% CO/50% H₂ fuel blend.
- (3) Among the four identified flashback mechanisms, core flow flashback and boundary layer flashback are of the greatest concern with regard to Capstone's lean premixed injector.
- (4) From experimental testing, it was concluded that the baseline C65 natural gas injector does not have enough flashback margin for burning high hydrogen content fuels.
- (5) Among the newly-developed injector configurations, several injector configurations demonstrated improvement in flashback resistance over the baseline injector. The FFTS-4 injector demonstrated superior operability to burn 100% hydrogen without flashback while maintaining good stability margin in C65 engine testing with a modified liner.
- (6) Injector-only modification may not satisfy the overall design objective to maintain the combustion system robustness while burning high flame speed fuels. Modification or redesign of the combustion liner is required to achieve the overall combustion operability and performance goals — for example, modifications to liner geometry such that more air is introduced via injectors to the primary combustion zone.

A combustion liner — in conjunction with other components — forms the passages for combustion air prior to being introduced to combustion chamber. The air flow split ratio is also determined by the locations and sizing of the dilution holes of the combustion liner. In this report, the background and design approaches for the FFTS combustion liner were introduced. Two different FFTS liner configurations were proposed with 60% and 76% air split to PZ. The preliminary engine test results with FFTS liner A (60% air split to PZ) and FFTS-4 injector were introduced. The following conclusions can be drawn from the combustion liner development efforts:

- (1) An injector-modification-only approach was found to be not satisfactory to meet overall design objectives for FFTS program. Modification or redesign of the baseline C65 combustion liner was required to achieve the overall combustion operability and performance goals for FFTS fuels.
- (2) Design and analysis methodologies were introduced for combustion liner design.
- (3) To support the anti-flashback injector designs for FFTS system, two combustion liner designs with higher PZ air split ratios were proposed.

Preliminary engine test data indicated that the tested FFTS liner A was able to support the FFTS-4 injector in burning high hydrogen fuel (up to 100% H₂). Also, the engine had good stability margin at test conditions.

Given the efforts applied to this FFTS program, significant progress has been made developing the FFTS combustion system (injector and liner). Nonetheless, additional development efforts would further validate the technology for pre-commercial qualification. Recommendations are:

- (1) More comprehensive testing with the FFTS-4 injector to further characterize and optimize product capabilities. This testing would include testing six FFTS-4 type injectors in a C65 or C200 engine burning hydrogen fuels to demonstrate stable operation with high hydrogen content fuel.
- (2) Current liner operability data is limited. More comprehensive testing with the injector designs — the FFTS-4 injector, in particular — would further characterize and optimize the liner's capability. Engine testing should include six FFTS-4 injectors in a C65 or C200 engine, burning hydrogen fuels in all six injectors.
- (3) Draw connections between the data sets from the flashback data collected in experimental testing and chemical kinetics analysis. These connection tasks include: (1) expanding the data base over wide conditions; (2) verifying test data; (3) finding the flashback and LBO correlations of operating conditions and fuel composition; and (4) developing design tools for combustion system under engine conditions.
- (4) Engine testing should simulate a wider range of ambient conditions and a wider range of fuel variations. The current engine tests were performed in typical laboratory conditions available at both UCI and Capstone. Tests were not performed to evaluate different ambient conditions in which the engine would be operated — for example, variations in temperature, elevation, and fuel composition.
- (5) Current tests used the default C65 natural gas control software. Due to the sensitivities of the combustion system — particularly for low emission systems — the combustion control constraints and strategies — TET set-points or injector staging scheme, for example — should be validated or optimized for FFTS fuels.
- (6) Currently, all tests have focused on steady state performance and operability. Transient state tests and optimizations are equally — sometimes more — important. Future development work should include transient tests.
- (7) Because of system similarity, flashback-resistant injectors developed for the FFTS program on the C65 platform may also be considered for applications with other Capstone microturbine systems when burning similar high flame speed fuels. However, additional tests are required to verify performance.
- (8) Emissions sensitivity and other system performance criteria should be further studied with regard to changes in fuel composition.
- (9) FFTS liner B (76% combustion air to PZ) should be characterized for its operability with FFTS-4 injector.
- (10) Liner life evaluation should be conducted by measuring liner temperature distribution.

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9. Appendix A: Fuel Flexibility Report (UCI)

DRAFT
FINAL REPORT

Fuel Flexibility Report

Submitted to Capstone Turbine Corporation

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Executive Summary

This report summarizes the experimental and analysis work completed at UCI in support of Capstone Turbine Corporation's effort under support from the U.S. Department of Energy. The goal of the program is to develop a Fuel Flexible Turbine System (FFTS) that can operate on high levels of hydrogen. UC Irvine's role in the project was to provide test support and also fundamental analysis of the combustion performance including flashback and emissions performance. Supporting the project was cost share from the California Energy Commission which allowed the efforts on more fundamental test rigs to be carried out to compliment and help explain the results observed in test beds specific to Capstone's configurations. The report is organized into a literature review section, a section discussing the experimental facilities at the UCI Combustion Lab, the test results themselves, and the analyses wherein correlations between the different experimental rigs are explored.

Both operability and emissions performance are considered. In terms of operability, autoignition, lean blowoff, and flashback are of primary interest. The reactive nature of hydrogen has been long known to benefit blowoff characteristics, and has been used to extend blowoff limits in many demonstrations. In the present work, blowoff was studied extensively in the full annular rig and a physics based expression was developed that can be used to predict blowoff as a function of fuel composition. Blowoff tests were not conducted in the engine, however, so the generality of these findings must be further evaluated.

However, at the same time, the reactive nature of hydrogen poses significant questions regarding the possibility of autoignition and flashback. Autoignition could present a unique challenge for high inlet temperatures found in recuperated gas turbines, so this operability aspect is examined in this context. Expressions for autoignition were evaluated and a strategy for evaluating autoignition propensity for the conditions of interest is recommended. Application of the methodology indicates that, despite the reactive nature of hydrogen, autoignition should not be an issue for the conditions within the engine. This presumes the premixer flowfield is well developed and largely free from separation or other flowfield features which might lead to locally high residence times.

Flashback propensity is the major challenge with regard to fuel flexibility in low emission systems that rely on lean premixed operation. This is the situation expected with high hydrogen content fuels as is the case for the off gas from a gasifier or other hydrogen containing fuels. It is expected that flashback for the Capstone combustor can occur through turbulent propagation of the reaction into the core of the mixture exiting the injectors and/or through boundary layer propagation. In both cases, understanding the turbulent flame speed is the intuitive key to understanding the phenomena. However, calculation of the turbulent flame speed proves to be difficult due to (1) discrepancies between the experimental data and correlations available and (2) the variation in the correlations themselves. Conservative correlations can be utilized in these calculations, but this may result in some loss in operating range if the correlations are too conservative. In addition to the flame speed, heat transfer, local velocities, reaction rates, and turbulence levels can also contribute to flashback. Hence, correct incorporation of the turbulent flame speed into the overall analysis may also require other considerations.

As a result, flashback analyses incorporating appropriate dimensionless groups, such as Damköhler number, have been carried out in an effort to develop generalized expressions that can correlate engine behavior. Ideally, these expressions can also correlate observations within other experimental platforms which are more cost effective to run and which can provide visual information regarding the reaction. With this motivation, the axisymmetric and full annular combustor rigs played this role to compliment data being obtained on the full FFTS engine. This

has resulted in significant amounts of experimental data generated for the various experimental platforms: axisymmetric single injector, full annular combustor rig, and engine. In spite of this valuable data set that spans fuel composition, temperature, pressure, equivalence ratio, and some geometry differences, only limited connections have been made between the various rigs. Significant effort has been dedicated to assessing connections through many experiments especially with regard to the full annular combustor, which proved difficult to use in flashback testing. However, these data sets have provided a number of statistical correlations that can be used at a minimum to evaluate relative changes in flashback propensity but can also be used for geometries that are very similar to attain higher accuracy estimation of flashback propensity.

The flashback data generated have also exposed a number of interesting physical interactions and trends. In particular, a major observation was the injector tip temperature was typically a function of fuel composition and could be used in laminar flame speed calculations in lieu of gaseous inlet temperature to attain better correlation of data. Extensive evaluations of flashback behavior in the axisymmetric rig were carried out and design guides have been developed. The application of these tools to the full annular rig and engine was attempted with some success.

As part of the overall diagnostic strategy, methods for determining flashback were evaluated. The flashback sensors investigated included a photomultiplier tube, thermocouple, and dynamic pressure transducer. The photomultiplier tube and dynamic pressure transducer showed initial promise but require additional experimentation such that the flashback signal is more robust. The thermocouple is robust in its detection of flashback, however it has a slow response time, which could lead to hardware damage, and also breaks easily and often. Sometimes all the injectors on an injector in the engine would break during a test leaving no flashback detection on that injector. It is very important to use emissions measurements as a secondary detection method to avoid costly damage and loss of data.

In terms of emissions performance, several tests were carried out as a function of fuel composition. These data were used to anchor a reactor network methodology derived from CFD simulations of the engine combustor. The results are used to estimate how hydrogen content impacts NO_x and CO emissions. In general it is observed that the more reactive fuels lead to elevated emission for the baseline injector configuration. The reactor network/CFD approach was successful in predicting the measured trends relative to fuel composition effects on emissions.

1 Introduction

The U.S. Department of Energy has awarded a contract to Capstone Turbine Corporation (CTC) with partners, University of California Irvine (UCI), Argonne National Laboratory, and Packer Engineering, to develop a Fuel Flexible Turbine System (FFTS) that will be integrated with a small scale biomass gasification system. This system will be capable of producing combined heat and power from a variety of potential renewable feedstocks. These processes generally produce fuels that are high in hydrogen content and thus one of the key challenges is to establish a system that can achieve good operability and low emissions while operating on high hydrogen content fuels. In addition, the composition of the fuel may change with feedstock type as well as depend upon the typical needs at the site where such a system may be operated. For example, it may be of interest to operate the system on natural gas to meet energy requirements in times where feedstock is not immediately available. Hence, the development of a fuel flexible system is required to allow the operational profiles that may be encountered. The key technical issues to be addressed to achieve low emissions and high operability include flashback, autoignition, stability, and chemistry of the combustion processes. This project will provide necessary information to address these issues from a theoretical perspective and help bolster the conclusions drawn from the development work being supported by the U.S. DOE.

The focus of this report is on *operability issues* associated with the use of high hydrogen content fuels. This includes autoignition, blowoff, and flashback. Of the various operability issues encountered with high hydrogen content fuels, the most problematic is flashback. This comes as a result of the small quench distances and high flame speeds characteristic of hydrogen. Of the four mechanisms of flashback, the two of greatest concern here are core flow and boundary layer mechanisms. Core flow flashback occurs when the flame speed of the mixture is greater than the core flow velocity, which allows the flame to flashback to an undesired position that may be either too close to the injector or inside the injector both of which can cause damage to hardware and eventually engine failure.

Figure 1: Core flow flashback schematic.

The boundary layer mechanism causes flashback when the quenching distance of the fuel/air mixture is smaller than the boundary layer thickness allowing ignition to occur within the low velocity boundary layer. Due to the low velocities in the boundary layer, if ignition can occur the flame will regress provided that the flame speed is greater than the lowest boundary layer velocity outside of the quenching distance.

Figure 2: Boundary layer flashback schematic

Three experimental platforms were utilized: single axisymmetric injector, full annular atmospheric combustor, and C65 engine. The platforms exhibited diverse complexity ranging from simplistic (axisymmetric injector) to highly complex (engine). The axisymmetric injector was used to fundamentally study the mechanisms of flashback for insight into the results coming from the full annular combustor and engine.

In addition to operability, consideration is also given to understanding how fuel composition impacts pollutant emissions.

2 Literature Review

2.1 Autoignition

The mechanism behind autoignition is a complex overlapping series of chemical reactions and physical processes. Initially the fuel and oxidizer mixture must mix to form a homogenous mixture. If the fuel is initially in a liquid form, atomization and vaporization of the fuel must occur prior to mixing. Contact of the fuel and oxidizer initiates chemical reactions leading to formation of radical species, which consume the fuel and produce even more radicals. This self-accelerating process eventually reaches a critical point where fuel is rapidly consumed, producing a great deal of heat leading to a rapid rise in temperature. This is the moment of autoignition.

The chemistry involved in autoignition can be quite complex and includes tens to hundreds of reactions, depending upon the fuel complexity. Comprehensive chemical kinetic mechanisms can describe the reaction process in detail. However, from an engineering point of view, the details of the individual reactions are less important than knowing the overall rate of the process. Therefore it has been common practice in the past to use a simple global reaction rate of the form: Fuel + Air $\rightarrow$ Products, to describe rates of autoignition. Reaction rates (RR) typically obey the Arrhenius rate form shown in Equation 59:

$$RR = k[\text{fuel}]^m[\text{oxidizer}]^n \quad \text{Equation 59}$$

Where

k is the rate constant which is function of an activation energy and temperature:

$$k = B \exp\left(-\frac{E}{RT}\right)$$

where

B is the pre-exponential factor or coefficient

R is the universal gas constant

E is the activation energy of the overall process

The exponential dependence of the temperature indicates that temperature is by far the most dominant parameter on the rate of reaction. The importance of the fuel and oxidizer quantity is manifested in the reaction orders m and n .

The ignition delay time of a mixture is inversely proportional to the reaction rate. In other words, a fast reaction leads to a short ignition delay, while a slow reaction leads to a long ignition delay. As a result, ignition delay is commonly correlated in the form in Equation 60:

$$\tau \propto \frac{1}{RR} = B^{-1} \exp\left(\frac{E}{RT}\right) [fuel]^{-m} [oxidizer]^{-n} \quad \text{Equation 60}$$

Dividing Equation by the fuel and oxidizer concentration, followed by taking the logarithm of both sides, gives Equation 61:

$$\log(\tau [fuel]^m [oxidizer]^n) = -\log(A) + \frac{E}{R} \cdot \frac{1}{T} \quad \text{Equation 61}$$

This equation is useful when plotting ignition delay data, as will be seen later on. Plots of ignition delay data of the form $(\log \tau)$ vs. $(1/T)$ will yield a straight line whose slope is proportional to the activation energy, E . Also, the intercept of the line with the ordinate axis can be used to determine the pre-exponential factor A , as seen in Figure 3.

Figure 3: Illustration of Ignition Delay Plotted in an Arrhenius Plot. The ignition delay data (dots) form a straight line whose slope is proportional to the activation energy (E) and intercept is proportional to the constant (A). Note that higher temperatures are to the left.

The volumetric molar concentration fuel and oxidizer (typically with units [mol/cc]) can be determined using the ideal gas law shown in Equation 62:

$$[]_i = \frac{X_i P}{RT} \quad \text{Equation 62}$$

In many engineering applications, flow rates, pressures and equivalence ratios are more commonly reported than mixture fractions or molar concentrations. Also the oxidizer is typically air. Therefore, the Arrhenius ignition delay equation can be modified into a more manageable form for industrial use as shown in Equation 63:

$$\tau = \mathcal{A} \exp\left(\frac{E}{RT}\right) P^b \phi^e \quad \text{Equation 63}$$

Here $\mathcal{A}$, b , and e are the pre-exponential factor, pressure exponent, and equivalence ratio exponent respectively. These are not necessarily the same values as B^{-1} , m , and n . Expressions in this form should be most useful to a burner engineer who would like to know the ignition delay time for a given equivalence ratio, burner inlet pressure, and temperature. In this report, expressions for ignition delay time for fuel air will often be given in the form of Equation 63. When these equations are used, the ordinate of the Arrhenius plot is typically the product of the delay times and the pressure, $\tau \cdot P^{-b}$, instead of the fuel and air molar concentrations as seen Figure 3. This approach allows for comparison between results obtained at different pressures. In most studies the pressure dependency, b , is usually found to be near unity.

2.2 Flashback Mechanisms

At least four different flashback mechanisms have been identified (Lieuwen, McDonell et al. 2008). With the general injector design under consideration in the present effort (i.e., “jet flame”), two appear to be of greatest interest/relevance.

2.2.1 Core Flashback

Regarding flashback, the simplest design rule requires that the flow field must not have strong local velocity deficits and that the volumetric flow velocity must be substantially above the turbulent flame speed. Following the reasoning outlined in Lieuwen et al. (2008), given the typical combustor pressure drop of 2-3%, absolute velocities of ≈ 90 -120 m/s are achieved in the burner mixing zone assuming almost isentropic acceleration of the combustion air in the burner. In the case of strong swirl, the axial velocity component, which is relevant for flashback in the core flow of the mixing zone, drops to approx. $u_{ax} \approx 65$ -85 m/s for the same burner pressure drop. The average turbulence level depends mainly on the swirl number in the mixing zone although specific burner design influences this. In the high swirl number designs, usually used for the premixed combustion of natural gas, substantial turbulence is generated in the swirler and the mixing section with mixing zone turbulence levels up to $u'/u_{abs} \approx 10$ -15%. Hence, typical velocity fluctuations in premix burners are not higher than $u'/u_{ax} \approx 14$ -22% or $u' \approx 9$ -18 m/s. Assuming that the flow field is well designed and does not suffer from local wakes with low axial velocity and with excessive turbulence, this leads to the important conclusion that flame propagation in the turbulent burner core flow can only occur if the turbulent burning velocity is substantially higher than the characteristic turbulent velocity fluctuation. For the worst case of maximum swirl, the criteria for flame propagation is then $S_T/u' \approx 4.5$ -7, with the reduction of the swirl number leading to even higher values.

From an engineering perspective, however, one approach to consider is to take that worst case estimates can be provided without considering preferential diffusion, as highly turbulent flow fields provide the worst-case scenarios for flashback due to turbulent flame propagation in the core flow some estimates of the implications of these scenarios can be ascertained. If (1) the turbulent flame speed is approximated by the sum of the laminar flame speed and the local turbulent fluctuations which is reasonable from turbulent burning laws for fast chemistry ($Da \rightarrow 0$) and (2) does not take preferential diffusion into account estimates for the turbulent flame speed can be derived, the value of S_T/u' becomes less than 1.3 to 1.5. Since these values are substantially lower than $S_T/u' \approx 4.5-7$ arrived at above, it seems that the drop of the flow speed below the turbulent burning velocity is not the most critical cause of flashback. However, it is also seen that high turbulence deteriorates the safety margin against flashback. For fuels with low laminar flame speeds (e.g., natural gas) the margin is sufficiently large, whereas fuel with higher laminar flame speeds will have smaller margin. This core flashback may become critical if the velocity field has strong wake regions with excess turbulence stemming from swirler vanes, upstream separation zones and/or the fuel jets. Consequently, a reduction of the swirl below the level usually employed in natural gas burners appears beneficial for the combustion of fuels with high hydrogen content, because this measure reduces turbulence and the turbulent flame speed. In the present injector designs, swirl is minimized, further aiding the reduction of core flow flashback propensity.

2.2.2 Boundary Layer Flashback

Flashback in laminar boundary layers is a classical topic that has been extensively investigated (Lewis and Von Elbe 1943; Putnam and Jensen 1949; Wohl, Kapp et al. 1949; Wohl 1953). An investigation of boundary layer flashback in laminar, syngas fueled Bunsen flames has been detailed by Davu et al. (2005). In turbulent combustion, flame propagation along the burner walls is another key flashback mechanism. Near the wall, the low velocities as well as the turbulence in the boundary layer promote flame propagation upstream. These effects compete with flame quenching due to the heat loss of the burner wall. As flashback limits in laminar flows clearly correlate with the velocity gradient at the wall, the concept of the critical velocity gradient has been developed in the past (Lieuwen, McDonnell et al. 2008) which is a function of the laminar flame speed and the thermal diffusivity, α :

$$g_f \propto \frac{S_L^2}{\alpha}$$

This equation can assess influence of the fuel on flashback in the boundary layer and shows that the laminar flame speed has a substantial influence on the critical velocity gradient required for flashback prevention. The equation implies that the velocity gradient for hydrogen is approximately a factor 10 times that of natural gas.

Whether the critical wall gradient for the corresponding turbulent boundary layer is higher than that for the laminar case depends on the thickness of the quenching distance with respect to the laminar sub-layer (Wohl 1953; Schafer, Koch et al. 2003). Although no generalizations regarding flame propagation in turbulent boundary layers are really available, indications are that proper aerodynamic burner designs produce substantially larger velocity gradients than required to avoid flashback for natural gas. Unfortunately, the same conclusion cannot be made for fuels with high hydrogen content. Based on arguments for the laminar situation, gradients that are 10x greater may be required. As a result, boundary layer flashback is a major area of concern. In present systems, air can be judiciously utilized in the boundary layer to help mitigate conditions that can give rise to flashback. However, a difficulty remains that the

addition of small amounts of air along the wall does not lead to the desired diluted mixtures beyond the lean flammability limit in the critical near wall zones for hydrogen containing syngas. Even with dilution, the laminar flame speed near the wall may be substantially higher than for natural gas without dilution. As a result, keeping the boundary layers as thin as possible is an essential design criterion for syngas burners and, even more important, local separation zones in the mixing zone must be avoided. Particularly critical are diffuser sections near the burner exit, which lead to a rapid increase of the wall boundary layers.

In summary, a major design criterion for the nozzle aerodynamics is that the axial velocity in the nozzle must be as high and as uniform as possible and free of strong wakes. Designs with constant or with slightly conical and accelerating air flow paths downstream of the swirler are the preferred solution. Strong acceleration of the flow bears the danger of flame stabilization upstream near the fuel injector in stoichiometric zones near the fuel jets, once the flame has been able to pass the high velocity area downstream during unexpected events in gas turbine operation like compressor surge and sudden breakdown of the burner mass flow. Thin boundary layers and careful use of air in the boundary layer will be needed to avoid flashback along the boundary layer.

2.3 Flame Speed

For lean premixed combustion strategies, the high flame speed of hydrogen poses perhaps the greatest challenge. This is an issue due to the consideration relative to propagation of the flame upstream into a premixing zone which will result in high emissions and potentially destruction of the hardware. From a fundamental view point, flame speeds can be rigorously analyzed in the laminar regime. The laminar flame speed, S_L , is a constant quantity that can be determined for a specific gas mixture that is unchanging at the same conditions. The turbulent flame speed, S_T , however, is a rate of consumption of mass per unit area divided by the unburned gas mixture density. This quantity is dependent upon the turbulence properties of the field, along with the flame-stabilizing method. As with characteristics of any turbulent flow, the turbulent flame speed is highly dependent on the specific conditions including geometry, resulting in difficulty of measurement or repeatability (Glassman 1996). A typical expression for S_T based on turbulent fluctuations and laminar flame speed is given by:

$$\frac{S_T}{S_L} = 1 + \left(\frac{2u'}{S_L} \right)^2$$

where u' is the average fluctuating velocity (Lewis and von Elbe 1987).

Because of the many issues involving direct determination of the S_T , many studies focus on the determination of S_L because of its evident importance in the turbulent quantity. This will be discussed in more detail in Section 2.3.2.1.

Two major factors influence the assessment of the flame speed relative to phenomena like flashback. First, flame speeds of mixtures (as opposed to pure components) and/or at conditions of interest are not widely available. Second the inability to accurately predict turbulent flame speeds for arbitrary mixtures and conditions poses an especially challenging problem. Nonetheless, the grounding of all turbulent flame speed expressions is in the laminar flame speed. As a result, it is useful and necessary to consider the laminar flame speed as a starting point.

2.3.1 Laminar Flame Speed

Unlike diffusion flames, flame flashback can occur for premixed laminar flames. Flashback involves the physical propagation of the flame upstream of the designated anchor point and into the premixing region that is not designed to endure high temperature reactions. For a Bunsen flame, flashback occurs when the flame velocity is greater than the unburned gas velocity. Flame speeds vary largely with fuel composition, from 40 cm/s for CH_4 to 240 cm/s for H_2 . Because the fuels of interest are mixtures of widely varying compositions, the resulting flame speeds also occur on a large range, giving rise to the issue of flame flashback.

The laminar flame speed (S_L) of a mixture is defined as the propagation rate of the flame relative to the unburned gas mixture in the normal direction. Figure 4 shows a tube open on both ends with unburned gases moving through the combustion wave. Also termed “burning velocity”, the laminar flame speed is defined for a one-dimensional, planar, adiabatic, steady, unstrained laminar flame.

Figure 4: Definition of laminar flame speed (S_L)

The laminar flame speed can be viewed in two ways dependent upon the coordinate system: 1) a freely propagating flame in a tube with the coordinate system fixed to the combustion wave, or 2) a flat flame stabilized on a burner. In terms of the continuity equation, laminar flame speed is defined as:

$$\rho_u S_L A = \rho_v S_L A = \rho_b v_b A$$

where the subscripts u and b describe the characteristics of the unburned and unburned gases.

For the inner premixed cone of a Bunsen flame, the laminar flame speed is defined as:

$$S_L = v_u \sin \alpha$$

where α is the cone angle, as shown in Figure 5.

For an actual flame cone, S_L only occurs at one distance (y_A) from the wall of the burner, which is called the anchoring point of the flame (Lee and Chung 1997). At the anchoring point, $v_u(y_A) = S_L$, but $v_u < S_L$ at all other radial distances.

Figure 5: The laminar flame speed of a stationary premixed flame cone is equal to the velocity normal to the velocity of the unburned gas ($v_{u,n}$)

Although numerous studies have been performed determining the laminar flame speeds of pure gases such as H_2 , CO , and CH_4 , much less data can be found for mixtures simulating syngas for use in gas turbine applications. An experimental investigation has been performed to determine the burning velocities of various mixtures of H_2 , CO , and CH_4 with air (Scholte and Vaags 1959). In the study, the burner method was used, where the laminar flame speed is defined as $S_L = v_u \sin \alpha$ and Schlieren or shadowgraph imaging is used to determine the cone angle (Glassman 1996). The maximum values for laminar flame speed (S_{max}) are given for the specific H_2/CO mixtures at g_{max} , which describes the percentage of fuel gas in the fuel/air mixture, as shown in Table 1. The described study provides a baseline for flame speed measurements of syngas composed of only H_2 and CO , but lacks data for fuels containing inert gases such as CO_2 or H_2O , which are often found in mixtures used for gas turbine applications.

Table 1: Maximum burning velocities for H_2/CO flames (Scholte and Vaags 1959)

Fuel Composition		S_{max} cm/s	g_{max} % by volume
H_2	CO		
0	100	13.6	-
0.55	99.45	23.5	52
3.0	97	52	51
10.5	89.9	82.5	51
24.1	75.9	115.5	50
43.3	56.7	157	48
69.7	30.3	224.5	44
100	0	281	42.2

A later study further investigated the laminar flame speeds of H_2/CO systems for the purpose of examining the $CO + OH$ reaction for flame modeling codes (McLean, Smith et al. 1994). The experimental method used in the study involved measuring the flame speeds of expanding spherical flames with high speed Schlieren cine-photography (Dowdy, Smith et al. 1991). In the

study, a relationship between flame speed and flame radius was determined, and the flame radius is extrapolated to infinity to determine the laminar flame speed at the condition of zero stretch. Six different stoichiometric $\text{H}_2/\text{CO}/\text{air}$ flames were examined with fuel compositions ranging from 0-100% H_2 . Data obtained was compared with previous studies by Scholte and Vaags (1959), and showed closed agreement for 95% CO + 5% H_2 lean mixtures, with increasing disagreement for richer mixtures. Conversely, the correlation for 50% CO + 50% H_2 declines at leaner mixtures. The major reasoning for these observations is attributed to the spherical bomb versus burner experimental techniques, as well as the accuracy of the original measurements by Scholte and Vaags (1959).

Another study was performed to determine the effect of hydrogen and methane addition to the flame speed and extinction rates of CO/air flames at atmospheric pressure (Vagelopoulos and Egolfopoulos 1994). The counterflow twin-flame technique develops a relationship between strain rate and velocity, and the strain rate is extrapolated to zero to determine the laminar flame speed. The mole fraction of hydrogen in the fuel/air mixture for the study was ranged from 0 to 0.07, where the mole fractions of the fuel (H_2 + CO) studied were 0.14, 0.17, and 0.20 of the total fuel/air mixture. Results showed that the laminar flame speed increased with the addition of small amounts of hydrogen due to the added H radicals accelerating the CO oxidation reaction. But with the addition of larger amounts of hydrogen, the shift was away from the CO oxidation reaction and toward the kinetics of hydrogen, decreasing the significance of the CO oxidation reaction in the overall reaction rate.

A more recent study investigating the laminar flame speeds of H_2/CO mixtures included the effect of CO_2 dilution and increased preheat temperatures at lean conditions (Natarajan, Lieuwen et al. 2007; Natarajan 2008; Natarajan, Kochar et al. 2009). The laminar flame speeds of $\text{H}_2/\text{CO}/\text{CO}_2/\text{air}$ flames were determined by the cylindrical tube method, in which the propagation rate of the flame through a cylindrical tube full of combustible as open on one end is measured. The study analyzed premixed laminar flames at equivalence ratios ranging from 0.6 to 1.0 at preheat temperatures up to 700 K. Validation experiments were first performed in which data was compared with previous measurements taken by McLean et al. for 95% CO + 5% H_2 and 50% CO + 50% H_2 fuel compositions. Good correlation with previous studies was found, implying accuracy of the chosen technique. The 95:5 and 50:50 CO/H_2 mixtures were then analyzed with dilution up to 20%. This resulted in the decrease of laminar flame speed with increased CO_2 dilution, as predicted by numerical methods, with deviations of up to 30-40% from predicted values at lean conditions.

An experimental and numerical analysis was recently performed to determine the relationship of laminar flame speed with several parameters such as equivalence ratio, pressure, and preheat temperature (Braun-Unkhoff, Kick et al. 2007). The investigation was performed for an H_2/CH_4 mixture as well as with two specific biogenic syngas mixtures produced from: 1) the gasification of corn silage, and 2) the gasification of ethanol. The experiment used the burner method, and flame images were obtained with a CCD camera and the laminar flame speed was calculated from the unburned gas velocity and cone angle. The results showed good trend agreement with detailed, reduced, and modified in-house numerical predictions, with under predictions of up to 10%.

In summary, many studies have been performed analyzing the laminar flame speeds of various fuels including syngas mixtures of H_2 , CO , CO_2 , and CH_4 as well as pure hydrogen. Although variation between these studies may come from the various experimental methods used, the trends are consistent and within reasonable error, and generally follow numerical predictions. As a result, it is reasonable to utilize chemical reactor principles to reasonably estimate laminar

flame speed. Again, particular mechanisms that are best suited for the conditions of interest must be used to get reasonable results.

2.3.2 Turbulent Flame Speed

As mentioned above, the common practice approach relative to turbulent flame speeds is to combine laminar flame speed information with some estimate of the turbulent velocity fluctuations. Flame speeds depend on fuel composition for both laminar and turbulent flame speeds (Lipatnikov and Chomiak 2005). For this reason, calculations of S_T by extrapolating data from other fuels, which have similar laminar flame speeds and from experiments with similar turbulence intensities u'/S_L , may not be applicable. An excellent example is the work by Kido, et al. (2002) where measured turbulent flame speeds for a variety of H_2 , CH_4 , and C_3H_8 mixtures combined specifically to generate the same laminar flame speed varied by nearly a factor of ten.

The reason for these fuel effects is uncertain. Some have suggested that correlations can be made with thermo-diffusive effects. For example, differences in the relative rates of mass diffusion (of the deficient species) and/or thermal diffusion affect the local laminar flame speed and the tendency of the flame to become spontaneously wrinkled (even in the absence of turbulent fluctuations). If differential diffusion processes are significant, then this could be expected to be very significant in syngas fuels, because of the large differences in diffusivity of the various fuel components. In lean flames, the effect leads to a positive correlation between the diffusivity of the fuel and the turbulent burning velocity. If the turbulence level is very low this effect may become significant in syngas flames as the hydrogen concentration increases, but it is probably much less important in highly turbulent flames.

Figure 6: Measured Turbulent Burning Velocities for Fuels with Similar Laminar Flame Speeds (Kido, Nakahara et al. 2002).

2.3.2.1 Turbulent Flame Speed Estimation

As mentioned above, it is really the turbulent flame speed that is relevant to determination of flashback in the present system. In this section, additional details are given regarding the approach for determining the turbulent flame speed.

At this point in the literature it is evident that at least four definitions of turbulent flame speed (S_T) exist:

1. $S_{T,LD} = \text{Local Displacement Speed} = \vec{U}_f - \vec{U}_r$
2. $S_{T,GD} = \text{Global Displacement Speed} = \frac{\partial r_f}{\partial t} - \vec{U}_r$
3. $S_{T,LC} = \text{Local Consumption Speed} = S_{L0} I_0 \int_{-\infty}^{+\infty} \Sigma \partial \eta$
4. $S_{T,GC} = \text{Global Displacement Speed} = \frac{\dot{m}_r}{\rho_r A_T}$

where,

$\vec{U}_f = \text{flame velocity}$ $\vec{U}_r = \text{reactant velocity}$

$r_f = \text{average expanding rate of flame kernel}$

$S_{L0} = \text{unstretched laminar flame speed}$

$I_0 = \text{stretch factor}$

$\Sigma = \text{flame surface density}$

$\eta = \text{direction locally normal to flame brush}$

$\rho_r = \text{density of reactants}$

$A_T = \text{mean flame area corresponding to a prescribed } < c > \text{ contour}$

$< c > = \text{reaction progress variable}$

$\dot{m}_r = \text{mass flow rate of reactants}$

These speeds are measured utilizing various experimental methods. For example, the measurement of $S_{T,GD}$ requires a flame kernel with no edges typical of that seen in a spark-ignited flame within a combustion vessel. In the literature, there are discrepancies between the data obtained for the various definitions. Distinguishing between these various definitions and to what flame geometry they are applicable assists in explaining some of these discrepancies (Cheng 2009). However, there are even discrepancies in the data gathered for the same S_T definition using the same experimental approach. This has been shown to be due to differences in how certain variables were varied during the experiment (Filatyev, Driscoll et al. 2005). Work done by Cheng (2009) offers in depth analysis of why the various data is different and recommends using measurements obtained with a flame geometry similar to that in the particular application when estimating flashback behavior (2009). Therefore, those well known correlations within the literature will be discussed along with experimental data gathered for flame geometries similar to that under consideration here (axi-symmetric envelope (Bunsen) flame).

Among the first equations developed for the calculation of turbulent flame speed were developed theoretically by Damköhler (1947):

$$S_T = S_L + u'$$

And Schelkin (1943):

$$\frac{S_T}{S_L} = \left[1 + \left(2 \frac{u'}{S_L} \right)^2 \right]^{0.5}$$

where,

$$u' = \text{fluctuating velocity component.}$$

Lefebvre (1998) uses these equations for the section on turbulent flame speeds in Gas Turbine Combustion. These expressions were developed without the four different definitions outlined above in mind, but they most closely correspond to a $S_{T,LD}$ or $S_{T,LC}$ definition.

Other theoretical expression were developed by Yakhot (1988) and Bradley (1992) and also correspond to a $S_{T,LD}$ or $S_{T,LC}$. Yakhot's correlation is shown below.

$$\frac{S_T}{S_L} = \exp \left[\left(\frac{S_T}{S_L} \right)^2 / \left(\frac{u'}{S_L} \right)^2 \right]$$

Bradley's expression is shown below.

$$\frac{S_T}{S_L} = 1.52 \frac{u'}{S_L}$$

These expressions represent attempts to establish an equation that could be used for various mixtures and flame geometries, however, as stated before discrepancies exist between these equations and experimental data. Figure 7 summarizes the sensitivity of the estimated turbulent flame speed using these different expressions.

Figure 7: Summary of correlations from the literature for a constant $S_L=0.34$ m/s.

Much work has been done on the measurement of turbulent flame speeds for various fuels, however, the data available concerning hydrogen and syngas fuels is limited. The data are limited even further by the fact that most of the measurements have been done using spark-ignited flame kernels in constant volumes ($S_{T,GD}$). These data are not applicable to the C65 due to the differing flame geometries. Figure 8 illustrates how the data measured in this way varies significantly from the other methods that more closely resemble what is occurring within the C65 combustor.

Kido, et al. (2002) (Figure 6) is shown as representative of $S_{T,GD}$ measurements since it has been referenced often in turbulent flame speed discussions. Both experiments shown above were performed at atmospheric conditions ($T=298$ K, $P=1$ atm). The data taken by Littlejohn, et al. (2010) was measured using a low-swirl burner for which $S_{T,LD}$ measurements were made. This definition of turbulent flame speed more closely resembles that of a C65 flame compared to that of a $S_{T,GD}$ measurement, however, it does not best approximate it. Therefore, they will not be focused on, and the correlation in the figure above will be taken as representative of these $S_{T,LD}$ measurements.

The $S_{T,GC}$ is most applicable to the C65 engine and will be the focus of the following paragraphs. $S_{T,GC}$ is usually associated with Bunsen flames because this particular definition can only be measured using a Bunsen flame where the reactants must pass through the flame brush and cannot escape around the edges (Cheng 2009).

Figure 8: Kido, et al. (2002) data collected using spark-ignited flame kernel shown here with symbols ($S_{T,GD}$). Correlations obtained using low swirl burner ($S_{T,LD}$) (Littlejohn, Cheng et al. 2010). From (Cheng 2009).

From the definition of $S_{T,GC}$, the mass flowrate and density of the reactants must be known in addition to the mean flame area corresponding to a specified contour which is associated with the reaction progress variable. The area is usually determined by assuming certain points within the flame are associated with a particular reaction progress variable, which then allows determination of the flame front surface area. The error associated with this assumption as determined by Venaketswaran, et al. (2009) is 3%.

Halter, et al. (2007) measured $S_{T,GC}$ for various H_2/CH_4 compositions and pressures (1, 3, and 5 atm). All of the measurements were performed at 298 K with an inlet bulk flow velocity of 2.1 m/s. The equivalence ratio was also kept constant at 0.6. There was no measurement of the turbulence intensity with these experiments. The turbulent global consumption speed was determined using the cone method in the same manner as Kobayashi et al. (1996). The results are shown in Figure 9.

In order to know what the $S_{T,GC}$ is doing with respect to pressure and hydrogen content, S_L must be known. Since it is well known that the S_L will increase with increasing hydrogen content, the $S_{T,GC}$ must be increasing with increased hydrogen content as well because the $S_{T,GC}/S_L$ ratio increased. However, it is more difficult to determine whether $S_{T,GC}$ has increased or decreased with pressure because the laminar flame speed for these same mixtures decreases with increasing pressure. After calculating the laminar flame speed for each respective mixture and

pressure using the chemical kinetics software DARSv2.0 or ChemkinPRO with various detailed chemistry mechanisms GRI Mech 3.0, it becomes clear that the pressure dependence of $S_{T,GC}$ is not straightforward. It increases with pressure from 1 to 3 atm but decreases from 3 to 5 atm. Further, the behavior of $S_{T,GC}$ depends upon the mixture, i.e. the pure methane mixture increases while the mixtures containing hydrogen do not. Figure 10 illustrates this below.

Figure 9: Dependence of $S_{T,GC}/S_L$ ratio on hydrogen content and pressure for H₂/CH₄ mixtures (Halter, Chauveau et al. 2007).

Figure 10: $S_{T,GC}$ dependence on pressure and hydrogen content for H₂/CH₄ mixtures. Adapted from Halter, et al. (2007).

The results shown in Figure 10 for pure methane differ from Kobayashi et al. (1996) where it was shown that the dependence of turbulent flame speeds on pressure for methane-air mixtures is weak as seen in Figure 11. The direct comparison of the data from the two publications is not possible due to the lack of turbulence intensity measurements by Halter (2007), but these conflicting results clearly indicate the need for more experimental data concerning the effect of pressure on turbulent flame speed. However, it is apparent that the ratio $S_{T,GC}/S_L$ does indeed increase with increasing pressure.

Figure 11: Experimental $S_{T,GC}$ data for various pressures for methane from Kobayashi et al. (1996).

Venaketswaran, et al. (2009) determined $S_{T,GC}$ using Bunsen flames at atmospheric conditions for several H_2/CO mixtures and then compared them to some correlations present in the literature. The turbulence intensity was varied for several different mixtures, equivalence ratios, inlet bulk flow velocities, and laminar flame speeds. The results show that the $S_{T,GC}$ increases with an increase in hydrogen content as well as with an increase in turbulence intensity. The mean flow velocity also leads to an increase in the $S_{T,GC}$ by increasing the turbulence intensity. The equivalence ratio sweeps revealed that leaner mixtures lead to lower $S_{T,GC}$. For all the variations, the data fell mostly within the boundaries of the two correlations: Schelkin (1943) and Yakhot (1988). Some of the data are shown in Figure 12 below for conditions summarized in Table 2.

Table 2: Investigated parameter space for Venaketswaran, et al. (2009).

	Constant S_L				ϕ Sweep					CH_4
U (m/s)	4, 10, 30, 50				4, 10, 30, 50					4, 10, 30
H_2 (%)	30	50	70	90	30	60				0
ϕ	0.59	0.53	0.50	0.46	0.7	0.8	0.4	0.6	0.8	0.9
S_L (m/s)	0.34				0.48	0.59	0.15	0.51	0.90	0.34

Figure 12: $S_{T,GC}$ data compared with several correlations in the literature for varying turbulence intensity for various H_2/CO mixtures and inlet bulk velocities at constant laminar flame speed (0.34 m/s). Adapted from Venaketswaran, et al. (2009).

Daniele, et al. (2009) also determined $S_{T,GC}$ for various H_2/CO mixtures but using a combustor with an expansion geometry for pre-heated and pressurized conditions ($T=673$ K, $P=5$ bar). The inlet bulk velocity, mixture composition, and equivalence ratio were varied. These variations were also accomplished in Venaketswaran, et al. (2009) and the trends in $S_{T,GC}$ agree. Direct comparison of the data is difficult due to the different representations, pressures, mixtures, etc. used in the two publications. However, the trends in the two publications were similar: higher equivalence ratio leads to higher $S_{T,GC}$, higher inlet bulk velocity leads to higher $S_{T,GC}$, and higher hydrogen content leads to higher $S_{T,GC}$. When looking at similar mixtures at similar equivalence ratios, it is apparent that the $S_{T,GC}$ results from Daniele, et al. (2009) may be higher than those from Venaketswaran, et al. (2009) which may indicate an increase with increasing pressure due to the different pressures each experiment was performed, but each experiment was also performed at different temperatures making it difficult to be sure what effect pressure has. This

needs to be verified further. The addition of N₂ to the H₂/CO mixture was also implemented in Venaketswaran, et al. (2009) but had little effect on the $S_{T,GC}$ as seen in Figure 13 where the measurements of mixtures 2 and 4 almost sit on top of each other.

To conclude, the literature provides a general idea of the qualitative trends with respect to the variation of various parameters such as equivalence ratio, temperature, inlet bulk velocity, turbulence intensity, hydrogen content, and diluent content with the exception of pressure for which there is not yet definitive data as to the response of S_T to variation in pressure. The various trends are as follows: leaner conditions results in a slower S_T , higher hydrogen content causes an increase in S_T , increases in inlet bulk velocity lead to increased S_T , and the addition of diluents does not have a marked effect on S_T . The correlations present within the literature can be used to develop an envelope of possible S_T for a given set of conditions as was evidenced by the Venaketswaran, et al. (2009) data where there were correlations marking the lower and upper bounds of the experimental data (See Figure 14). Despite this possible use of the present correlations in the literature, the lack of experimental data for which direct comparison is possible for the flame geometry of interest (Bunsen) motivates experiments where the conditions and measurements can be compared directly among many different operating conditions.

Figure 13: $S_{T,GC}$ data for various mixtures and equivalence ratios with inlet bulk velocity of 40m/s, $T=673K$, and $P=5$ bar. Adapted from Daniele et al. (2009).

Figure 14: Comparison of several different correlations from literature to gathered data for a constant $S_L = 0.34$ m/s (Venaketswaran, Marshall et al. 2009).

To illustrate one possible approach to using the turbulent flame speed is illustrated in Figure 15. This represents a “hybrid” methodology as used by Wang et al., to estimate boundary flashback for hydrogen flames produced by macrolaminar injectors. In this case the pressure dependency of methane flames was applied to hydrogen flames along with laminar flame speed dependency for hydrogen. This “mis-matched” correlation, while admittedly requiring assumptions, was applied in conjunction with CFD analysis of the injector boundary layer flow. Of 45 conditions studied, 9 exhibited flashback and the analysis using the correlation along with the CFD was predicted in each case.

Figure 15: Hybrid Approach for Estimating Boundary Layer Flashback (Wang, McDonnell et al. 2009).

2.4 Fundamental Axisymmetric Bunsen/Jet Flame Flashback Studies

In 1943, Lewis and von Elbe published a journal article entitled “The Structure and Stability of Burner Flames”, which was the first major publication to look at flashback (and blow off) and attempt to explain and predict this phenomenon (1943). Lewis and von Elbe suggested using the critical boundary layer velocity gradient as the parameter that dictates whether flashback (and blow off) will occur or not. Since flashback occurs when the burning velocity exceeds the gas velocity somewhere in the flow, for steady fully developed laminar flows in tubes, the region most susceptible to flashback would be near the wall where there is a low velocity region in the boundary layer due to the no-slip condition at the wall. In fact, the no-slip condition causes a zero velocity region at the wall surface where flashback would occur for fuels with even the lowest burning velocities if it were not for the additional flame quenching effects caused by the wall (radical destruction and cooling). These flame quenching effects of the wall cause the burning velocity to decrease near the wall and at some point nearer the wall a flame cannot exist at all due to the wall quenching effects (i.e., burning velocity = 0). This description of flashback allows one to define the critical velocity gradient (curve 2 of Figure 16 as the velocity gradient at which flashback occurs. For laminar flows, this critical velocity gradient is defined in terms of the volumetric gas flow rate (Q) as $g_f = \frac{4Q}{\pi R^3}$. Given this definition, experimentally determining the critical boundary layer velocity gradient for laminar flames was as simple as measuring the volumetric gas flow rate at flashback.

Figure 16: Simplified description of flashback for laminar flames in a fully developed pipe flow. Curve 1: Flashback. Curve 2: Flashback limit. Curve 3: Flame will move downstream where it will either restabilize or blowoff (Lewis and Von Elbe 1943)

Lewis and von Elbe's experimental set up consisted of various one meter long pyrex tubes with different diameters but all had the same wall thickness of 1 mm. For each diameter, the critical velocity gradients were measured for various premixed natural gas-air compositions by decreasing the flow rate until flashback occurred (see Figure 17). The critical velocity gradient showed some promise in that for some tube sizes the critical velocity gradients were nearly the same throughout the equivalence ratio sweep, however, the range of tube sizes for which this occurred was quite small (0.577 – 1.417 cm). The diameters that did not show any collapsing to a single curve were those that approached the quenching diameter of 0.315 cm (0.333 and 0.389 cm) and those that began to show effects of turbulence near stoichiometric conditions (1.55 cm). The burner tube wall temperature was not controlled during these experiments but was monitored and also cooled between experiments. It was found that for wall temperature increases of 100 C, there was little to no effect on the results. Measurements of the critical

velocity gradient at blow off were also measured for various natural gas-air compositions. The surrounding atmosphere was also varied for these experiments and included CO₂, O₂, Air, N₂, and He. The surrounding atmosphere was found to have a profound effect on the blow off limits with differences between each gas. The velocity of the surrounding gas (co-flowing) was also varied and was found to not have an appreciable effect on the blow off limit. Some additional interesting observations involved the curious instability of flames on the smaller diameter tubes where the flame would tend unpredictably toward extinction or flashback. Additionally for larger tubes, the blow off critical velocity gradient curve would asymptotically approach the flashback critical velocity gradient curve.

Figure 17: Critical velocity gradients of flashback for various concentrations of natural gas in air (Lewis and Von Elbe 1943)

In 1945, von Elbe and Mentser furthered the initial studies in Lewis and von Elbe (1943) by studying tilted flames for hydrogen-air, hydrogen-oxygen, and acetylene-oxygen mixtures. Tilted flames are those flames that have partly regressed into the burner tube and restabilized in that partly regressed state as is shown in Figure 18. These researchers gathered critical boundary layer velocity gradient data for the aforementioned mixtures at points when tilted flames occur and points when full flashback occurred. It was found that the boundary layer velocity gradients for tilted flames were not independent of diameter for the range of tube diameters considered here (0.108-0.33 cm) unlike the critical velocity gradients for full flashback (although it was found that in Lewis and Von Elbe (1943) the critical velocity gradient at flashback was only independent of tube diameter over a small range of diameters). The occurrence of these tilted flames extend the range of unstable flames, since once these flames occur full flashback will undoubtedly occur shortly thereafter due to wall heating unless the wall is cooled which is not typical in practical applications. Von Elbe and Mentser also presented an equation based on the velocity gradient at which the tilted flame occurs, the burning velocity of the mixture, and the burner tube diameter that equals a constant. This constant is not supposed to vary as burner

tube diameter is changed and for the burner tube diameters investigated experimentally here, this constant was found to be nearly constant showing that this equation may hold some promise. Blow off velocity gradients were also measured for the various mixtures, and flame back pressures and burning velocities were measured for the acetylene-oxygen mixtures. It was found that the flame back pressure for acetylene-oxygen mixtures (5.5 cm of water) can be much larger than the flame back pressures for natural gas-air flames (0.01 cm of water, calculated).

Figure 18: Tilted flame flow lines as recreated from particle tracks (von Elbe and Mentser 1945)

Wohl, et. al., also investigated the stability limits of open flames on tubes (1949). These researchers focused on butane-air mixtures. The flashback velocity gradient was measured for a 0.4 inch tube in different surrounding atmospheres (air and CO₂). The surrounding atmosphere was found to not have an effect on the flashback velocity gradient. Interesting observations and discussions with regard to the shape of flames at flashback for very lean flames in tubes were made. Flat and meniscus shaped flames could be observed before flashback for some of the very lean butane-air mixtures. Additionally, flashback velocity gradient measurements were made for a nozzle configuration with an exit diameter of 0.37 inches (contraction ratio 1:29), and more interesting observations were made with regard to the flame shape at different conditions. When these researchers compared the flashback velocity gradient results from a 0.37 inch nozzle to a 0.37 inch tube, the flashback velocity gradients were nearly the same for the different configurations despite the much different flame shape for each configuration at rich equivalence ratios. The majority of this publication focuses on blow off of butane-air flames (also some blow off results for city gas (Newark, DE)-air flames). Experiments to determine the stability limits of Newark, DE city gas-air and butane-air mixtures were also performed where the flame was in an enclosure.

Reiter and Wright performed experiments to obtain the stability limits of propane-hydrogen-air mixtures (1950). The experimental setup consisted of a several burner tube materials (pyrex, stainless steel 304, and silica) where the burner tube was cooled by air. The tube diameters varied from 0.573 to 1.34 cm. The stability limits are reported in boundary layer velocity gradient form. The tube material was found to have some slight effect on the flashback and blowoff critical velocity gradients.

Grumer, Harris et al., prepared a report for the Bureau of Mines entitled "Fundamental flashback, blow off, and yellow tip limits of fuel gas-air mixtures" which investigated the stability limits of various hydrogen, carbon monoxide, methane, and other hydrocarbon mixtures (1956). These data were reported in critical velocity gradient form and were all done with no preheating

of the mixture. Tube materials were pyrex glass and metal. Tube diameters typically varied from 0.2 – 1.2 cm with the largest diameter being 1.4 cm. The burner tip was not cooled directly but after each test the tip was allowed to cool back to room temperature before the next test. An important observation from these data was that critical velocity gradients for flashback and blow off of various hydrocarbon mixtures could be predicted based on the weighted average of all the critical velocity gradients of each component in the mixtures just as is done when determining other properties such as the heating value. However, this was only possible with hydrocarbons. Carbon monoxide and hydrogen mixtures did not display this behavior. Noncircular and sharp edged, short port burner geometries were also examined with the determination of critical velocity gradients as well as the appropriate friction factors for the given geometry (rectangular, square, triangular, sharp edged/short port). It was also found that there was some dependence of the friction factor on the fuel composition (i.e., different for CH_4 and H_2 -CO mixtures). Finally, the effect of preheat of the fuel-air mixture on the flashback and blow off velocity gradients was also investigated. Although these measurements and analyses were only done for methane-air mixtures, the correlation devised showed some promise in prediction of the temperature effect on the flashback and blow off velocity gradients. Joseph Grumer authored several publications reporting flashback and blow off velocity gradient data as well as reporting on the various prediction methodologies discovered during the experiments for the completion of the Bureau of Mines Report. In 1952, Grumer had two publications in the Journal, Industrial and Engineering Chemistry, wherein he described in one publication a simple critical velocity gradient prediction methodology for tube burners with no preheat (Grumer, Harris et al. 1952) and in the other he simply reported stability limit data from the experiments for various methane, hydrogen, and carbon monoxide mixtures (Grumer and Harris 1952). In 1954, Grumer published information from the Bureau of Mines report work wherein he described the methodology of predicting the temperature effect on the flashback and blow off gradients albeit only for methane-air and propane-air mixtures (Grumer and Harris 1954).

Dugger gathered flashback and blow off velocity gradient data for propane-air mixtures in a brass tube 1.56 cm in diameter with a water cooling jacket (1955). Dugger also preheated the propane-air mixtures to various levels (306, 422, 506, and 617 K) and also maintained the wall temperature such that it was within 10 K of the preheat temperature. As one would expect the preheating decreased the flashback resistance (i.e., increased the flashback velocity gradient). Dugger also discusses the penetration distance of quenching effects as calculated from the division of the flame speed by the flashback velocity gradient and how these penetration distances differ from measurements of quenching distances between parallel plates and cylindrical tubes (in fact the quenching distance measurements made in cylindrical tubes and parallel plates also differ from one another as well). This topic was also previously discussed in von Elbe and Mentser (1945). Attempts to predict the flashback velocity gradient were also made in this publication and followed the methods of Grumer and Harris (1954).

Figure 19: Effect of initial mixture temperature on flashback and blow off velocity gradients for propane-air flames in tubes (Dugger 1955)

Bollinger and Edse performed experiments to determine the flashback velocity gradients of hydrogen-oxygen mixtures (1956). These experiments were performed on burner tubes of various materials (copper, inconel, monel, nickel, and stainless steel) with and without wall cooling for diameters ranging from 0.31 – 1.417 cm. The effect of whether the burner was indoors or outdoors was also examined. When the burner was inside, the flashback velocity gradient was 25% higher at the peak than when the burner was outdoors. However, the burner tip temperature for the indoors condition was lower than when the burner was outdoors for all the equivalence ratios tested suggesting that this ambient effect does not have to do with the burner tip temperature. Further experiments and analyses were needed here before a conclusion could be made. The flashback velocity gradients were found to be dependent upon tube diameter which is different from previous work where the flashback and blow off velocity gradients were found to be independent of tube diameter (Lewis and Von Elbe 1943). This work, however, involved mostly turbulent flows since hydrogen-oxygen mixtures were being investigated, and in previous works laminar flows were involved. The burner tip temperature was measured for the uncooled tubes at flashback for some of the tests, and it was found that the burner tip temperature at flashback would increase with hydrogen concentration (equivalence ratio) and varied with the tube material as well (i.e., stainless steel with the highest tip temperatures and copper with the lowest tip temperatures). The effect of wall cooling on flashback was also investigated, and as expected, the tubes with cooling had lower flashback velocity gradients. A nozzle configuration was also tested, and the use of the nozzle provided much lower flashback velocity gradients when compared to that of the straight tube configuration. In fact, shadowgraph photos (not shown in publication rather only mentioned) were taken of the nozzle flames, and from these photos it was observed that the flames appeared laminar in nature despite Reynolds numbers suggesting turbulent flow.

Miller and Setzer performed experiments investigating the stability of n-butane/nitrogen dioxide flames (1957). Tube diameters of 0.396 – 1.026 cm were used and the tubes were water cooled. The wall temperature was also varied from 20-280 C. Polyhedral flames were observed

under some conditions, and laminar flame speed measurements were made with direct photographs and shadowgraphs with the results compared to each other.

Kurz produced two publications in 1957 that dealt with stability limits of Bunsen type flames. The first publication reported stability limits of mixtures of ethylene, propane, and iso-butane (Kurz 1957). A co-flowing inert shielding gas was utilized to exclude the entrainment of ambient air. The tube diameter used for this first publication was 1.75 cm and included a water cooled burner tip. Only laminar flames were observed. It was found that for these hydrocarbons the flashback volumetric flow rate could be predicted based on adding the ratios of the particular gas flow rates and some standard gas flow rate. Kurz's second publication extended these investigations by examining the effects of different factors on flashback (1957). The effect of the tube diameter (1.75, 3.05, 11.1, 17.5 cm) was investigated, and it was found that the tube diameter does not have an effect as long as the velocity gradient is used as has already been shown previously by Lewis and von Elbe in 1943. The effect of the shielding gas composition was also investigated. The shielding gas composition will only affect the blow off limits where the effects on flashback limits are negligible.

Fine prepared reports to the National Advisory Committee on Aeronautics in 1956 and 1957. The report in 1956 presented stability limits of hydrogen-air flames at reduced pressures for several equivalence ratios and also measured laminar flame speeds for these mixtures (Fine 1956). Fine's experimental set up consisted of a tube (0.546 – 1.459 cm) that was enjoined to a combustion chamber which is different from many of the previous work where the tube was open to the surrounding atmosphere. The burner tip was cooled with a water jacket. Fine also approached the flashback limit much differently than any of the previous publications in which either or both the fuel and air flow rates were increased or decreased respectively until flashback occurred. Fine actually began the experiments at some sub atmospheric pressure and increased the pressure (at constant mass flow) of the combustion chamber until flashback occurred. The equivalence ratio was varied from 0.8-2.25 during these experiments. The laminar burning velocity of these hydrogen-air flames was found to vary proportionally with pressure to a power of 0.23. The laminar flashback velocity gradient of these hydrogen-air flames was also found to vary proportionally with pressure to a power of 1.35. Fine's second report to the National Advisory Committee on Aeronautics extended the stability limits to include both laminar and turbulent hydrogen-air flames at reduced pressures (Fine 1957). The tube diameters considered in this report are slightly larger than in the previous report (1.016 – 1.89 cm). The burner tip was again cooled, and the approach to flashback was the same as in the previous report. The equivalence ratios investigated were 0.5 – 3. The pressure exponent for the flashback velocity gradient was the same for both the laminar and turbulent flows. The turbulent flashback velocity gradients were about 2.8 times that of the laminar flashback velocity gradients. This difference was presumed by Fine to occur mostly due to a decrease in the penetration distance rather than an increase in burning velocity (burning velocities were measured). Fine also produced a journal publication in 1958 summarizing some of the results from these two reports in addition to presenting additional data acquired with same experimental set up and procedure with several different mixtures (Fine 1958). These mixtures included two fuels (hydrogen and propane) with several different oxidants (50/50 O₂/N₂, 20.6/79.4 O₂/He, 20.6/79.4 O₂/Ar). The data here were only presented for equivalence ratios of 1 and 1.5 for the hydrogen mixtures and 0.85 and 1 for the propane mixtures. Fine did observe tilted flames at certain conditions although tried to avoid them. Fine then also performed some experiments investigating the effect of initial temperature on the flashback of laminar and turbulent flames (Fine 1959). In this publication, a similar experimental set up was used with a 1.016 cm tube although the tube was now also heated such that the gas temperature could be adjusted while the burner tip temperature was also monitored. Hydrogen, propane, and ethylene fuels were

used with oxidant mixtures of air and 50/50 O_2/N_2 . The same approach to flashback was used as in Fine's previous works. Fine determined that there was an exponential dependence of the flashback velocity gradient on temperature. Fine also produced some correlations relating the critical flashback velocity gradient to the stream velocity, pressure, and temperature.

Grumer published another paper in the journal Jet Propulsion that reported some turbulent flashback velocity gradient data for natural gas-air flames (Grumer 1958). The tube sizes Grumer was using here were 0.944 – 7.62 cm. He also examines his new data alongside data already gathered by Bollinger and Edse (1956) and von Elbe and Mentser (1945). Grumer looks into whether using tilted flame events to predict turbulent flashback events is possible, however, in the end, he dismisses this because he concludes that in turbulent flashback core flow fluctuation may actually be precipitating flashback rather than the laminar sublayer of the boundary layer although he doesn't present evidence to support this conclusion.

Yamazaki and Tsuji also presented data on turbulent flames for a city gas with the composition CO, 13.9; H₂, 26.9; CH₄, 15.3; Cn Hm, 5.1; O₂, 1.9; CO₂, 3.3; and N₂, 33.6 % (1961). The experimental set up consisted of a nozzle configuration as opposed to a straight tube with a contraction ratio of 2.5:1. The exit diameter was 75 mm. Mean velocities at flashback and blow off were measured for these city gas-air flames for various levels of turbulence as produced by several different perforated plates. The turbulence levels and velocity distributions were also measured. Yamazaki and Tsuji conclude from these experiments that the stability limits especially at flashback cannot be explained only by the conventional boundary velocity gradient concept when the boundary layer at the burner port is thin. Additionally, it was found that concave flames can exist over a wide range of equivalence ratios and these concave flames flashback from the center instead of the burner rim as the flow rate is reduced. This was deduced with the use of schlieren photography at 64 frames/sec.

Khitrin, Moin et al., also examined turbulent flashback for hydrogen-air, methane-oxygen, and methane air flames (1965). In addition to these turbulent experiments, Khitrin, Moin et al., also gathered flashback velocity gradient and laminar burning velocity data for several different preheat temperatures for methane-oxygen flames (burner tube diameters 18-25 mm). Preheating was accomplished through heating the burner tube. Preheat temperatures varied from 20-400 C. The temperature of the burner tip was maintained at a temperature near the preheat gas temperature. Flashback experiments were also conducted on a nozzle configuration, and these yielded some interesting results. The button/meniscus shaped flames observed in (Wohl, Kapp et al. 1949) were also observed here. The contraction ratio was varied and as the ratio of inlet to outlet diameter was increased the flashback velocity also increased considerably. It was also observed that if the nozzle was extended with washers to decelerate the velocities near the wall then the shape of the flame could be changed from flat to more conical, and in fact, they observed a step change in flashback velocities at a particular nozzle extension height. For the turbulent flame experiments for hydrogen-air mixtures, the tube diameter was varied from 18-38 mm. From these data, it becomes clear that the diameter does not affect the flashback velocity for turbulent flashback as it does in laminar cases (used laminar data from Von Elbe and Mentser for diameters of 5.06mm and 2.941mm). This was also observed for methane-air and methane-oxygen mixtures although not shown explicitly in the paper. Another observation from the data is that for the hydrogen-air mixtures the peak of turbulent flashbacks is shifted toward leaner conditions than the peak of laminar flashbacks and the burning velocity (this "anomaly" did not occur for the methane mixtures). Khitrin attributes this shifting due to the lower Lewis number of hydrogen since this shifting does not occur for the methane-air and methane oxygen turbulent flames. For the methane-air and methane-oxygen turbulent flashback events, Khitrin presents a correlation based on the Reynolds and Peclet

(flame speed based) numbers, however, no correlation is presented for the hydrogen-air flames (and these hydrogen-air data are also presented in separate plots with different axes definitions).

Ball, Putnam et al., (1978) provided the U.S. Department of Energy with a report containing flashback velocity gradient, burning velocity, and quenching distance measurements for several different syngas fuels. The tube diameters were varied from 6.25 mm to 22.2 mm, however, most of the measurements were made for tube diameters of 6.25 mm. The burner tube walls were cooled with a water jacket. These data for flashback velocity gradient, burning velocity, and quenching distance were then entered into the dimensionless group $\frac{G\delta}{S}$, where G is the velocity gradient, δ is the quenching distance, and S is the burning velocity. This dimensionless group had a constant value of 2.5 for all fuel compositions except those where either CO or H₂ was absent and the methane content was high. For these compositions, the value was around 2. This dimensionless group was also discussed in a brief communication by Putnam in the journal *Combustion and Flame* (Putnam, Ball et al. 1980). Some other interesting observations included the need for a chimney (diameter=54mm and 180mm tall) due to the air currents generated from the exhaust hood affecting the results. Sharp flashback was also not observed for slow burning velocity fuels rather a slow regression down the tube would be observed. Other researchers had previously observed this as well.

Wierzba, Oladipo et al., performed experiments with a tube confined by a rectangular 132x132mm combustion chamber (Wierzba, Oladipo et al. 1993). These experiments differed from previous work in that a pilot flame was used, which was located 70 mm from the combustor inlet (pilot flame fuel did not affect results so methane or ethylene were used). The fuel concentration was increased while maintaining a constant velocity until flashback was observed either by eye (combustor had windows) or thermocouple. Fuel mixtures included H₂/CH₄, H₂/C₂H₄, and H₂/C₃H₈ mixtures.

Dam, Love et al., and Davu, Franco et al., also produced laminar flashback data for various syngases, however, their experimental setup was under laminar conditions and very similar to previous works with the exception of the acoustic excitation (Davu, Franco et al. 2005; Dam, Love et al. 2011).

Eichler, Baumgartner et al., presented experimental data for a 40 mm diameter tube in which the tube exit was confined and unconfined (2011). The tube diameter of 40 mm was chosen to minimize the interaction between the two boundary layers and also because the results could be compared to the 38 mm data produced by Khitrin, Moin et al. (1965). The only fuel considered here was hydrogen, and a pilot flame was used to stabilize the flame although the pilot flame was turned off as the point of flashback was approached such that the pilot would not influence the results. The pilot temperature and glass tube temperature were monitored, and it was found that the pilot temperature would vary significantly when the pilot flame was used therefore cooling of the pilot burner (essentially the tube exit tip) such that it was within 40-60 C. The tube exit was confined by a 30mm long, 44 mm diameter ceramic tube. Flashback was induced by increasing the fuel flow while holding air flow constant. The process was monitored with an ICCD (OH*) camera, which was used to detect when flashback occurred. The data showed that confined tube burner flames showed a higher propensity for flashback than unconfined tube burner flames. The data for the unconfined tube burner flames also compared well with those results from Khitrin, Moin et al., (1965). Additional experiments were performed in confined rectangular ducts with a similar piloting and flashback approach strategies. The flashback velocity gradient data from these confined rectangular ducts showed similar values compared to those from the confined tube burner geometry.

This literature review has shown that a large amount of laminar flashback for Bunsen-type flames data with various fuel compositions and at various wall temperatures has already been gathered. Some turbulent data has also been cataloged, but to a much lesser extent. Additionally, much of the previous work focused on smaller diameter tubes (< 1 inch) where turbulent effects were less prevalent.

2.5 Additional Studies Using More Complex Experimental Setups

Developing a system that can properly combust syngas and other high H_2 content fuels in a manner that is clean, efficient, and reliable requires additional technology. State-of-the-art stationary gas turbines operate in an LPM fashion, which introduces a number of operability issues. The combustor must reliably hold a flame through various conditions so it does not experience FB or LBO. These issues are exacerbated when operating on syngas fuels due to variations in fuel properties and lack of understanding of their interactions with flow field dynamics. This section identifies previous work done to address operability issues pertaining to FB and LBO with a focus on not only classical work, but also current work in alternative fuels.

Lean Blowout

The guiding principle in flame stabilization in both laminar and turbulent flows is that flame speed (turbulent or laminar) matches the local mean flow velocity (Turns 2000). LBO occurs when the local mean flow velocity is greater than the flame speed at each point in the flame causing it to physically blow out of the burner (Lieuwen and Yang 2009). A laminar flame anchored at a position will lift off if the exit velocity is sufficiently high (Turns 2000). As the flame propagates away from the burner rim it is no longer controlled by heat loss and sink of radicals to the wall. As a result, the laminar flame speed increases creating a new stabilization point until the flame reaches a distance where outside air is entrained diluting the mixture and reducing the flame speed to its LBO limit (Glassman 1996). In turbulent flames, characterization of LBO behavior is closely associated with the Damköhler number or ratio of residence and chemical time scales. It is debated as to which controlling process most accurately describes the LBO phenomena. Although in general it is viewed as the inability to balance the rate of entrainment of reactants into the recirculation zone.

LBO is a major concern in stationary gas turbines where the preferred method of reducing criteria pollutants is LPM combustion. Operating a gas turbine near its LBO limit is the current low emission strategy to lower peak flame temperatures and reduce thermal nitrogen oxides (NO_x) emissions (Lieuwen, McDonell et al. 2008). If LBO occurs the engine requires a restart incurring costs associated with maintenance, engine life, and availability (Schefer 2003). Stationary gas turbines operating on NG have been successful at maintaining high reliability, but new fuel concentrations require a re-characterization of LBO behavior.

Extensive studies have been performed to examine fuel composition effects of syngas mixtures. From this work there are two main conclusions: (1) H_2 addition extends the LBO limit of CH_4 or other hydrocarbons, (2) correlations depend upon Damköhler number to describe LBO phenomena.

Griebel et al. (2006) studied LBO limits in a premixed combustor stabilized by recirculation from a sudden expansion geometry consisting of coaxial quartz tubes ($D_{inlet}=25$ mm, $D_{expansion}=75$ mm) for preheat temperatures of 673 to 773 K. Inlet bulk velocities are varied from 32 to 80 m/s at pressures between 5 and 14 bars. Fuel mixtures consisted of 0-20% H_2 by volume in methane. Results indicate that addition of H_2 lowered the LBO fuel/air ratio by 10% for 20% H_2 addition. The reason for the extension in flammability limit is attributed to the increase in

OH^* radical concentration that leads to higher global reaction rates along with higher flame speed.

Daniele et al. (2009) reports on LBO and NO_x emissions for four syngas mixtures designed to represent coal, refinery residues, biomass, and co-firing of syngas with NG. Experimental results are carried out in the same high pressure vessel as Griebel et al. (2006) with preheats of 673 K, bulk velocities of 40-80 m/s and pressures between 5-15 bars. Detection of LBO is accomplished with chemiluminescence at a sampling rate of 1200 Hz and analysis done in both time and frequency domains. Results show that higher percentages of H_2 in the mixture allow for leaner EQs. Also, there is a significant difference in behavior between fuels with/without methane which the author attributes to higher laminar flame speeds of H_2 containing syngas mixtures over methane. Another observation is the mixture with methane was more sensitive to inlet velocity and pressure than the pure syngas mixtures.

Schefer, Wicksall, and Agrawal studied LBO limits of H_2/CH_4 flames in a lean premixed swirl stabilized combustor at standard conditions (Schefer, Wicksall et al. 2002; Schefer 2003). Their papers investigate the effect of H_2 addition to methane in regards to the stability, emissions, and flame structure. Their experimental setup is a swirl stabilized flame within a quartz housing operating at atmospheric conditions. From a stability standpoint, results showed that flames at higher air flow rates stabilized at higher adiabatic flame temperatures due to the higher strain rate in the flame at larger fuel-air flow rates. Flame shape photographs showed that the swirler created two flow separation zones located downstream of the centerbody and another at the combustor wall. Addition of H_2 created a stable flame in the corner of the second separation zone that was significantly shorter indicating more rapid combustion. Once again, LBO is decreased by adding H_2 into methane for mixtures with up to 40% H_2 by volume. An emphasis is placed on the chain branching reaction $H + O_2 \leftrightarrow OH + O$ in regards to extinction. Schefer et al. (2002) argues that H_2 enrichment increases OH^* radical concentration leading to increases in specific reaction rates.

Yoshimura et al. (2005) explored how emissions and stability are affected through the addition of H_2 under lean premixed conditions. In the study, the relative amounts of H_2 , up to 50% by volume, are compared to both the stability limits and the ability to achieve both low CO and NO_x . It is stated that the addition of H_2 to NG will result in an increase in the burning velocity and lower LBO limits, which will in turn decrease thermal NO_x emissions. This research is motivated by the broadening of the flammability limits through the addition of H_2 that from an emissions standpoint is beneficial since NO_x is reduced from the increase in burning velocity and lower flame temperatures. The experimental setup consisted of a model combustor made from a simple tube, quarl, and pilot tube that swirl stabilized blends of NG and H_2 .

Compositions of the main fuel and pilot fuel varied to investigate stability and emissions. For the main fuel, compositions varied from 0-50% H_2 and an upper limit of pilot flow of NG was set as roughly 10% of the total fuel flow. Results indicated that with the piloted flame NO_x emissions were around 8.6ppm (corrected to 15% O_2), but without the pilot emissions remained around 1.6ppm (corrected). This demonstrates that the pilot was a significant source of NO_x and eliminating or adjusting its composition might be useful in reducing NO_x emissions. CO emissions followed a typical "bucket" behavior where the lower temperatures quenched the reaction causing higher emissions and higher temperatures caused disassociation of CO_2 generating elevated CO. Results show that NO_x emissions are not strongly affected by the main fuel composition and mainly generated by the pilot.

Stability effects showed that the addition of H_2 extended the temperatures at which LBO occurs, thus increasing the range that low emissions can be obtained. H_2 mixed into NG

improved CO emissions and flame stability, specifically the combustor operated at 200K cooler versus pure NG, while also doubling the operational range over which both low NO_x and CO emissions are achieved. Results also demonstrated that greater H₂ ratios are better for performance of the combustor and reduction of its emissions. The results also emphasized that the pilot has more influence on performance than the composition of H₂ in the mixture.

The research also studied how OH^* intensity changes with composition and flowrate for the pilot flame. Results indicated that half the pilot flow stability increases initially until the H₂ percentage increases. In the case of 50% H₂ by volume the pilot reaction became shorter and the volume of unburned fuel decreased.

Zhang et al. [63] and Noble et al. (2006) both investigated LBO limits in H₂/CO/CH₄ mixtures in a swirl stabilized combustor for varying pressures from 1.7 to 4.4 atm, temperatures from 300 to 470 K, and fuel compositions covering the entire space. Results are consistent with previous studies that the dominating factor in LBO is the H₂% in the fuel. This work evaluates various methods of correlation including Lewis number, AFT, flame speed, and chemical residence time. Two models of flame stabilization are investigated: one utilizing a well-stirred reactor (WSR) approach, and the other investigating a propagation based mechanism. Conclusions from the study indicate success with the WSR correlating H₂/CH₄ data, but not H₂CO. On the other hand, the propagation based approach achieved success with pure CO, H₂CO, H₂NG, CH₄/CO and deviates at pure mixtures of H₂ or CH₄. Both approaches clearly depend on laminar flame speed so concluding which model describes the data best is not possible. Noble et al. extends the analysis and correlates data with Damköhler number to predict LBO ratios to within 10%. Note that this approach is still based on a WSR to calculate the residence time at LBO.

Strakey et al. (2007) also reports on the extension of LBO limits in a swirl stabilized combustor while using Damköhler number based approaches where the chemical residence time is based off the extinction limit of a WSR. Results are consistent with those in the literature demonstrating an extension of the LBO limits. This paper illustrates a method of predicting LBO utilizing a WSR by first establishing an effective residence time with pure NG based upon an experimental result. The effective residence time is then anchored for the WSR while the composition of H₂ is increased. Finally, the EQ at LBO is found and it coincides with the experimental result validating the methodology.

Development of physics based correlations has been difficult because of a lack of understanding of LBO, especially the dynamics and flame characteristics at the stabilization point. Many physical considerations have been used in correlating LBO, but they all lead to the same form of correlation in terms of a Damköhler number, $Da = \tau_{chem}/\tau_{res}$ (Shanbhogue, Husain et al. 2009). The generally accepted idea is that LBO occurs when the characteristic chemical time becomes longer than the characteristic residence time (Noble, Zhang et al. 2006). Due to the wide band of turbulent time scales that exists within combustors it is possible for oxidation of different fuel elements to occur in different combustion regimes. Whether premixed flames in highly turbulent environments exhibit flamelet or WSR properties is debatable (Shanbhogue, Husain et al. 2009). However, using WSR approaches have shown success in correlating LBO behavior for both regimes. Establishing the chemical kinetic time scale is key for evaluating LBO limits (Ni, Zhang et al. ; Schefer, Wicksall et al. 2002; Noble, Zhang et al. 2006; Strakey, Sidwell et al. 2007; Shanbhogue, Husain et al. 2009). The methodology for calculation of the chemical kinetic time scale may vary. Comparison of the chemical kinetic time scale determined from the laminar flame speed (S_L) and thermal diffusivity of the mixture ($\tau_{chem} = \alpha/S_L^2$) with the chemical kinetic time scale at LBO calculated using a WSR

demonstrates that the two are interrelated for mixtures of H_2/NG and H_2/CO , with the exception of high CO mixtures (Ni, Zhang et al.). The relationship between the two chemical time scales is the foundation upon which LBO is correlated using a WSR.

Many studies have been performed to improve understanding of LBO with H_2 containing fuels. From these studies two observations are common: (1) addition of H_2 extends the lean operating limit, (2) characterization of LBO has traditionally been characterized by Damköhler number. The majority of the work does not offer predictive methodologies to establish LBO limits. Those that do offer correlations only do so for swirl stabilized flames leaving a gap in the characterization of LBO for turbulent jet flames with H_2 containing fuels.

Table 3: Summary of LBO literature related to syngas mixtures

Author	Year	Group	Stabilization	Temperature (K)	Pressure (atm)	Inlet Velocities (m/s)	Composition by Volume	Correlation
Daniele	2008	PSI	Sudden Expansion Recirculation	673	5-15	40-80	H ₂ /CO/CH ₄ : 20,20,60 H ₂ /CO: 50,50 H ₂ /CO: 33,67 H ₂ /CO/N ₂ : 40,40,20	none
Schefer	2002	Sandia	Swirl	300	1	8-22	H ₂ /CH ₄ : 0-40	none
Wicksall	2005	OK	Swirl	300	1	10	H ₂ /CH ₄ : 0-40	none
Schefer	2003	OK	Swirl	300	1	12-80	H ₂ /CH ₄ : 0-40	none
Strakey	2007	NETL	Swirl	580	1-8	40-80	H ₂ /NG: 0-80	WSR
Yoshimura	2005	UCICL	Swirl	672	1	1.55 (w/o preheat, reaction)	H ₂ /NG: 0-100	none
Zhang	2005	GT	Swirl	300,470	1.7-4.4	93-186	H ₂ /CH ₄ /CO: 0-100, 0-100, 0-100	WSR/Flame Speed
Noble	2006	GT	Swirl	300,470	1.7-4.4	36-72	H ₂ /CH ₄ /CO: 0-100, 0-100, 0-100	WSR/Flame Speed
Griebel	2006	PSI	Sudden Expansion Recirculation	673-773	5-14	32-80	H ₂ /CH ₄ : 0-20	none

Flashback

Schäfer et al. (2003) studied both turbulent and wall FB of kerosene-air flames at atmospheric conditions in a test rig outfitted with optical access. Kerosene was injected and atomized before entering a premixing duct with a diameter of 4.1 cm and a length of 55 cm. Laser Doppler Anemometry (LDA) collected velocity data at the inlet to the combustor at conditions close to FB. Results indicated a strong dependence on EQ, with maximum values for the critical velocities occurring close to stoichiometric conditions. Furthermore, the model for FB through the boundary layer in laminar flames was suitable for predicting FB for Re numbers between 3000 and 6500. In several cases, velocity gradients at the wall were sufficiently large so that FB through the boundary layer could not occur, but instead occurred through the main flow. The author purports the previously presented idea of a competition between turbulent flame speed and velocity in the main flow using a turbulent flame speed correlation based on experimental results.

The recent interest in utilizing H_2 rich fuel streams in gas turbines has generated a number of papers investigating FB with syngas compositions. Daniele et al. (2009) investigated FB for a 50/50 H_2/CO mixture with pressure varying from 2-15 atm. Bulk velocities varied from 40 m/s to 152 m/s while preheat ranged from 577K to 674K. Flame stabilization was accomplished by flue gas recirculation from sudden expansion geometry. Conclusions from this work indicate that FB through the boundary layer was present and showed a strong dependence with pressure. FB propensity was independent of the bulk velocity and mitigated most by the reduction of inlet temperature. Based upon an analysis of laminar flame speed S_L and preheat temperature the author concludes that S_L is the main parameter influencing FB propensity when varying preheat temperature. Furthermore, based on a phenomenological analysis pressure dependence was attributed to the decrease of the quenching distance.

While Daniele et al. (2009) focused on one particular synthesis gas mixture, Noble et al. (2006) tested FB with varying syngas composition. Testing was performed in a pressure vessel with upstream mixed fuel and air going through a changeable centerbody and swirler. Conditions covered the entire spectrum of compositions for $H_2/CO/CH_4$ mixtures at two different pressures, 1.7 and 4.4 atm. Preheat temperatures ranged from 300K to 470K and velocity ranged from 36-72 m/s. FB detection was accomplished using thermocouples mounted at different locations along the vessel. Two distinct FB events occurred, rapid flame propagation into the premixer and anchoring temperature rise. Interestingly, results showed H_2 percentage independence for FB at fuel compositions less than 60%, but LBO EQ was a strong function of H_2 composition. FB results indicated that leaner EQs at lower flow velocities increased the propensity for FB. In several cases FB occurred even when the flame speed was never high enough to propagate upstream leading to the postulation that vortex breakdown is one of the FB mechanisms present. Diagrams with hypothesized flow streamlines in the vicinity of the flame and circulation bubble are shown to illustrate vortex breakdown at higher pressures. Moreover, using the flame temperature correlation versus H_2 percent removed the variability seen in plotting FB EQ versus H_2 percentage.

2.6 Engine Studies

Other researchers have operated gas turbines on high hydrogen content fuels. Most of these previous works have focused on non-premixed combustion systems (Conrad and Corrington 1957; Nomura, Tamaki et al. 1981; Sampath and Shum 1985; Tomczak, Benelli et al. 2002; Juste 2006; Cocchi, Provenzale et al. 2008; Cocchi and Sigali 2010). Some work with regard to

the operation of premixed systems on high hydrogen content fuels has also been carried out (Minakawa, Miyajima et al. 1997; Farina, Perry et al. 2009; Perry, Farina et al. 2009; Therkelsen, Werts et al. 2009). General Electric and Siemens researchers have also investigated premixed combustion systems for operation of gas turbines on high hydrogen content fuels (Lacy, Ziminsky et al. 2008; Bradley and Fadok 2009).

The combustion system of concern in the present application is a premixed system with direct jet injection to the combustor. This configuration differs from most of the previous cases investigated previously in the literature with the exception of (Therkelsen, Werts et al. 2009). These researchers investigated hydrogen fueling of the same engine to be investigated in this work, a Capstone C65 engine. The previous work of (Minakawa, Miyajima et al. 1997) investigated a premixed combustion system for use in microturbine application as well, however, the flames were bluff body stabilized and the premixer velocities were much higher than under consideration in this work. Farina et. al. (Farina, Perry et al. 2009) and Perry et. al. (Perry, Farina et al. 2009) investigated premixed, high swirl combustion systems whereas the system under investigation here has low swirl.

2.7 Summary

Fuel flexibility research has been performed at various levels of complexity (i.e., atmospheric rigs to full scale engine tests). These works have led to important insights related to flashback but clear connections and correlations that effectively relate flashback on simplified atmospheric rigs to engines do not yet exist for those engines with jet flame configuration.

3 Experiments and Results

3.1 Overview & Methodology

The goal of these experiments was to produce a design tool that allowed engineers to estimate the conditions at which flashback and lean blow out would occur for various fuel compositions. Ideally the design tool would also allow for various pressures, temperatures, materials, etc., however, the phenomena of flashback is very complex and involves an extremely diverse set of parameters. Therefore, the purpose of this design tool was relegated to Capstone specific equipment. The axisymmetric injector simplifies the flow field while the full annular combustor maintains the complexity of the flow field while eliminating pressure effects. The connection of these two experimental platforms to each other and ultimately to the engine will provide necessary insights as well as provide Capstone engineers with a methodology to predict flashback phenomena using simplified (i.e., much less expensive) experiments.

3.2 Axisymmetric Single Injector

The goal of these experiments is the examination of the effect of various parameters on flashback while emphasizing the effect of fuel composition because of its importance to the design of the Fuel Flexible Turbine System. These results can then be used to more fully develop predictive correlations for the engine.

3.2.1 Data Acquisition and Control System

The flashback studies have been performed using a data acquisition and control set up as shown in Figure 20. The setup consisted of a National Instruments cRIO-9074 with analog

input/output, thermocouples, and high speed analog input modules. The operator interfaced with the cRIO-9074 using a computer and the supporting National Instruments software and drivers. The experiments were controlled by a program written in Labview. This program allowed for special capabilities such as holding the adiabatic flame temperature constant while varying air flow rate. Several mass flow controllers (Alicat Scientific) allowed for independent control of the fuel constituents and air flow rates. Thermocouples were also used to monitor and control various temperatures. The heating of the injector wall (quartz tube) in Phase I required use of heat tape wrapped around the tube, which resulted in loss of some visual access for some of the experiments. A photodiode and/or microphone were also used to detect the moment at which flashback occurred. A high speed camera was also utilized for visualization of the highly dynamic process of flashback.

Figure 20: Schematic of the axisymmetric single injector rig and associated supporting hardware

The experiments investigated the effect of preheat, injector material, injector tip distance (See Figure 24), and enclosure diameter on flashback. Investigation of the differences between the flashback of attached and lifted flames was also completed. The axisymmetric single injector rig needed modifications to allow for preheat, various enclosure diameters, and additional injector tip temperature measurements. A new enclosure holder plate was designed and manufactured for these purposes (Figure 21). The new plate was made of stainless steel to allow for high preheat temperatures similar to those experienced in recuperated Brayton cycles where inlet air temperatures of 1000-1300 F are possible (the FFTS system, i.e., Capstone C65, is a recuperated Brayton cycle).

Figure 21: Modified enclosure holder plate

Four small holes near the injector exit were included for use as pilot fuel injection (Figure 21). Several different sets of grooves were introduced on the face of the enclosure holder plate. One set of grooves allows for the placement of thermocouples on the outer wall of the injector tip. The thermocouples placed in these grooves will be set in place using epoxy, which will also help with thermal contact to the outer wall of the injector tip. The other set of grooves allow for three different sizes of enclosure diameter to be evaluated. This is important because significant differences between unconfined and confined flames were observed in Phase I as well as in the literature (Eichler, Baumgartner et al. 2012).

The addition of an air heater was required to provide the capability of preheating the inlet air temperature to the injector. A 4 kW Sylvania heater (PN 038823) was used for this purpose. Insulation was also added to the long stainless steel tube that allows for premixing and flow conditioning below the injector. The control of the heater outlet temperature is accomplished by PID control of the power supplied to the heater via an SCR power controller. The installation of this heater is capable of supplying air at temperatures of 1000 F at a flow rate of 470 SLPM.

More thermocouples were also added to advance the temperature monitoring near the injector tip and the enclosure holder. The figure below shows the alignment of thermocouples. The tip temperature was calculated by average the values measured by TC1 and TC3. The TC2 was used to detect the flashback event and it was robust and reliable to tell the flame regression. TC4-TC7 were used to measure the temperature distribution on the plate. All of the TCs employs TJ36-CAXL-020U-12 provided by Omega Engineering, Inc. The diameter of the sheath is 0.50 mm (0.020").

Figure 22 Alignment of the thermocouples

3.2.2 Fuel Selection

The fuel selection is driven by the practical perspective that only those fuels with high hydrogen content, i.e. high flame speeds, pose a high risk for flashback in practical systems which is the target application for the design guides developed in this project. As a result, the variation for the hydrogen composition is 25-100%. No mixtures with lower than 25% hydrogen content will be studied because of their much lower flame speeds. The variation in methane and carbon monoxide content to be studied is 0-75%. Table 4 shows the seven fuel mixtures that will be studied in each set of tests.

Table 4 Fuel compositions

H ₂	25	50	75	25	50	75	100
CO	75	50	25	0	0	0	0
CH ₄	0	0	0	75	50	25	0

3.2.3 Flashback Studies

The flashback studies focused on determining the specific effects of preheat temperature, injector tube material, enclosure diameter, higher adiabatic flame temperatures (i.e. higher equivalence ratio), and lifted versus attached flames. The procedure at which flashback is approached in each set of tests is such that the adiabatic flame temperature will be held constant as the air flow rate is decreased until flashback occurs with the exception of the investigation of lifted versus attached flames where flashback will be induced by increasing equivalence ratio rather than decreasing air flow rate while holding the equivalence ratio constant. It must also be stated here that quasi-steady state conditions will be established while moving toward the flashback condition.

3.2.3.1 Study of Effect of Inlet Temperature, Adiabatic Flame Temperature, and Injector Material

The preheat temperature of interest is 867 K similar to what is seen in the Capstone C65 engine. The air heater installed for this study is capable of 1000 K but only for small flow rates, and with the flow rates needed in this study, the preheater was only able to achieve 810 K. In addition to studying the effect of preheat temperature on flashback, the effect of the injector material was investigated since previous publications have observed that a change in the tube material can drastically affect the critical flashback velocity gradient (Bollinger and Edse 1956), and given that the injector material in a practical application will be a metal alloy and the injector material used for visualization purposes is quartz, the effect of the tube material should be studied. The effect of the adiabatic flame temperature was also studied. The following describes the conditions for these experiments:

- Preheat temperatures of 300, 450, 588, and 810 K for each fuel composition in Table 4 at adiabatic flame temperatures of 1700 and 1900 K with both injector materials (quartz and Stainless steel 316)

These experiments will provide valuable information relating to the effect of preheat temperature on flashback in addition to the tube material effect on flashback. The tube material effect will provide insight into the heat transfer processes from the flame to the injector tip that may be affecting flashback.

3.2.3.2 Study of Effect of Enclosure Diameter

The effect of enclosure diameter was investigated for pure hydrogen and 50% H₂- 50%CH₄. No preheat was included in these experiments. One large and one small enclosure were tested to determine the effect on flashback for AFTs of 1700 and 1900 K.

3.2.3.3 Specific Study of Effect of Tube Diameter

The injector tube diameter was varied between a 1 inch OD and 0.5 inch OD tube for several fuel compositions. Flashback was approached by holding the AFT constant at 1700 K and decreasing the air flow rate.

3.2.3.4 Specific Study of Effect of Fuel Concentration Profile

The fuel compositions considered here were 100% H_2 , 50% $H_2/50\%CO$, 50% $H_2/50\%CH_4$, and CH_4 . The effect of the fuel concentration profile was accomplished through variation in the axial position of the fuel injector module as shown in Figure 23. The position directly affected the mixedness of the injector, i.e. when the fuel injector module was close to the exit plane there was the least mixing. For each fuel composition the fuel concentration profile (axial position of fuel injector module) was varied between four levels, varying from poorly mixed to well mixed. The same strategy as in the previous section was implemented here. The adiabatic flame temperature was held constant (1700 K) throughout thereby determining the appropriate equivalence ratio. The air flow rate was decreased until flashback was encountered.

Figure 23: Schematic showing how fuel concentration profile will be varied

3.2.3.5 Specific Study of Diluent Effect

The effect of diluents was also investigated. Many fuels, especially those from landfill or anaerobic digestion processes have significant quantities of either CO_2 or N_2 . However, because diluents will generally result in greater flashback resistance, only limited testing was needed to establish the general trend with diluent addition. As a result, CO_2 was added in three amounts (0%, 7.5%, 15%) to four fuel compositions: 100% H_2 , 50% $H_2/50\%CO$, 50% $H_2/50\%CH_4$, and CH_4 . The fuel concentration profile was flat (premixed) for each case. For each fuel composition, CO_2 was added, and as in the previous sections, the air flow rate was decreased until flashback occurred with the adiabatic flame temperature being held constant (1700 K).

Nitrogen was also added in three amounts (0%, 25%, 50%) to four fuel compositions: 100% H_2 , 50% $H_2/50\%CO$, 50% $H_2/50\%CH_4$, and CH_4 . These tests also required the fuel concentration profile to be flat (premixed) for each case. For each fuel composition, N_2 was added, and as in the previous sections, the air flow rate was decreased until flashback occurred with the adiabatic flame temperature being held constant (1700 K).

3.2.3.6 Specific Study of Higher Hydrocarbon Effects

The effect of higher hydrocarbons was also investigated. This was accomplished in the same manner the effect of diluents was determined. Some syngas fuels have significant quantities of higher hydrocarbons. As a result, for this test, ethane was added in three amounts (0%, 12.5%, and 25%) to four fuel compositions: 100% H_2 , 50% $H_2/50\%CO$, 50% $H_2/50\%CH_4$, and CH_4 . The fuel concentration profile was flat (premixed) for each case. For each fuel composition, the

air flow rate was decreased until flashback occurred with the adiabatic flame temperature being held constant (1700 K).

3.2.3.7 Study of Lifted versus Attached Flames

The investigation of lifted and attached flames consisted of selecting two fuel compositions that could yield both attached and lifted flames. The fuel compositions chosen for this study were 50% H₂- 50%CO and 50% H₂- 50%CH₄. High speed OH* images will be taken while each flame mode flashes back allowing observations to be made of the mechanism of flashback for lifted and attached flames. Flashback will be approached by adjusting equivalence ratio rather than air flow rate.

3.2.3.8 Study of Effect of Injector Standoff Distance

The effect of the distance between the injector tip and the enclosure holder plate (see Figure 24) on flashback was investigated for imaging purposes at the injector tip. Since the enclosure holder plate is opaque, imaging of the flame propagation into the injector near its tip is not possible if the enclosure holder plate is flush with the injector tip, i.e., the distance between the injector tip and enclosure holder plate is zero. However, if the enclosure holder plate could be moved downward several centimeters, high speed OH* imaging of the flame as it begins to regress into the injector would still be possible. Therefore, it is proposed that this distance be varied for a fuel composition of pure hydrogen with an AFT=1700 K for an injector tip distance of 2 cm.

Figure 24 Schematic describing distance between the injector tip and enclosure holder plate

3.2.4 Inlet Temperature, Adiabatic Flame Temperature, and Injector Material Effects for various H₂/CO and H₂/NG Mixtures

Figure 25 and Figure 26 show the results from the investigation of the effect of inlet temperature, adiabatic flame temperature, and injector material. Figure 25 shows the flashback (critical) air flow rate versus the inlet air temperature for the various fuel compositions, AFTs, and injector materials under consideration. Figure 26 shows the injector tip temperature at flashback versus the inlet air temperature for the various fuel compositions, AFTs, and injector materials under consideration. These two figures can be complicated to look at as a result of the

amount of information they contain. However, this does not preclude the observation of the general trends. Each data point corresponds to the average of several tests in which air flow rate was decreased until flashback was observed. Error bars were not large enough to be seen due to the symbol size and were therefore omitted. The legend specifies (in this order) the injector material (stainless or quartz); the nominal fuel composition (%H₂-%CO-%CH₄); and the adiabatic flame temperature. Some of the tests could not be completed as a result of the preheater minimum air flow rate requirement to prevent damage to its heating coils. This minimum air flow rate is shown in Figure 25 as a red dashed line. In fact those data near the minimum air flow rate required testing with a different test procedure where flashback was induced by increasing equivalence ratio while holding air flow rate fixed. This was required because for AFTs of 1700 and 1900 K the flashback air flow rate was below the minimum air flow rate of the preheater. Therefore, the equivalence ratio (EQ) needed to be increased above 1900 K as can be seen in the legend for those data that required this EQ increase flashback approach procedure. The same data shown in Figure 25 are plotted in Figure 26 but instead of showing the flashback air flow rate as the response the flashback tip temperature is shown as the response.

Several general observations can be made from Figure 25 and Figure 26. The most obvious and most interesting observation is that as inlet temperature increases the critical air flow rate decreases. This result at first seems contrary to what would be expected, however, it is important to realize that since AFT is being held constant the EQ of the mixture is being adjusted as inlet temperature increases such that constant AFT is attained. A second noteworthy observation is that the injector tip temperature at flashback does not necessarily increase as inlet temperature increases although it does so in most cases. This is also somewhat unexpected. Hydrogen content also strongly affects the injector tip temperature with higher hydrogen content leading to higher tip temperatures. It is interesting to note that the injector tip temperatures are lower than the inlet temperature once the inlet temperature is increased above 600 K. Other observations, seen in Phase I, are also present here such as when hydrogen content increases the flashback propensity increases.

The effect of injector material and AFT can also be seen in Figure 25 and Figure 26. The quartz injector led to higher flashback propensity (i.e., higher critical air flow rate) than the stainless steel injector for the same fuel composition, AFT, and inlet temperature. This may be a result of the higher thermal conductivity of the stainless steel injector which thereby allows increased heat transfer to cool the injector tip. This hypothesis is somewhat supported by the typical observation of cooler injector tip temperatures of the stainless steel injector versus the quartz injector for the same fuel composition, AFT, and inlet temperature. However, there are some instances where the tip temperatures were not affected by the injector material (e.g. 100% H₂, 1900K AFT, and 810 K preheat). The effect of AFT on the flashback propensity was that any increase in AFT would increase the flashback propensity and injector tip temperatures. This effect was expected and can be observed in Figure 25 and Figure 26. It should also be noted that the difference between the flashback propensity (and tip temperatures) of two AFT levels for the same fuel composition is greater at higher inlet temperatures.

Attached and lifted flames are also present throughout these experiments. Attached flames are defined as those flames that are anchored very near the injector exit plane whereas lifted flames are defined as flames anchored some distance from the injector exit plane. Figure 25 and Figure 26 shows what combinations of fuel composition, AFT, and inlet temperature result in lifted flames. The lifted flames have lower flashback propensity than attached flames. The tip temperature of lifted flames is also typically lower than the tip temperature of the attached flames as one would expect. These flames are studied further in the section 3.2.10.

Figure 25: Critical air flow rates vs. inlet temperatures with different fuels, AFTs and injector materials

Table 5: Conditions in Figure 25 that FB happened at the minimum flow rate and approached by increasing AFT

Material	H2%	CO%	CH4%	Inlet temp [K]	Initial AFT [K]	FB AFT [K]	Flame mode
stainless	25	0	75	294	1700	1850	lifted
stainless	25	75	0	294	1700	1778.8	lifted
stainless	50	0	50	294	1700	1710	lifted
stainless	25	0	75	449	1900	2188.5	lifted
stainless	50	50	0	449	1700	1907.5	lifted
stainless	50	0	50	449	1900	2012.3	lifted
stainless	25	75	0	588	1900	2070	lifted
quartz	25	75	0	294	1700	1722.3	attached
quartz	25	0	75	294	1700	1792.2	lifted
quartz	50	0	50	294	1700	1710.2	lifted

Figure 26: Tip temperatures at FB vs. inlet temperatures with different fuels, AFTs and injector materials

3.2.5 Enclosure/Confinement Diameter

The study of the effect of enclosure diameter on flashback propensity was done systematically by varying the diameter of the enclosure. The results are shown in Figure 44 for lifted flames and in Figure 27 for attached flames (100% H₂) at various preheats and AFTs. It is clear from these results that the enclosure size has an effect on lifted flames but little effect on attached flames.

Figure 27: Systematic investigation of effects of enclosure sizes

3.2.6 Tube Diameter

Figure 28 shows the experimental results from the study of the effect of the tube diameter on flashback air flow rate. As one would expect, the flashback air flow rate for the smaller tube is lower than the air flow rate for the larger tube because a lower air flow rate will be needed with a smaller tube to achieve a similar velocity as in a larger tube, and since velocity is the important parameter with regard to flashback, Figure 29 shows the injector exit velocity versus percent hydrogen in the fuel for the two tube diameters. The velocity for the two tube diameters differ slightly in that the smaller tube has a somewhat lower velocity.

Figure 28: Experimental results from investigation of tube diameter effect on flashback air flow rate

Figure 29: Injector exit velocity vs. percent hydrogen in fuel for a larger and smaller tube diameter

3.2.7 Injector Exit Fuel Concentration Profile

For the specific study of the effect of fuel concentration profile, the various fuel supply tube settings needed to be selected such that three additional levels of mixing were achieved in addition to the perfectly premixed results from the previous sections. This was accomplished via trial and error using measured injector exit fuel concentration profiles for several different fuel injector tube lengths such that the various levels of mixing desired were achieved.

A flame ionization detector (FID) fed by an iso-kinetic probe was used to measure the fuel concentration profile at the exit of the injector for the various fuel tube lengths. This was performed for a fuel of 100% natural gas (Irvine natural gas has 96% CH₄ content). The different fuel supply tube configurations were identified by the mixing length, which has been defined as the distance from the exit of the fuel supply tube to the exit of the injector (See

Figure 23 and Table 6). Measurements were taken at two different air flow rates (10 and 100 SLPM) in order to see the effect of the air flow rate on the fuel concentration profile, and as one can see from Figure 30 through Figure 32, the air flow rate has a small effect on the fuel concentration profile. These measurements were repeated twice for each air flow rate.

Table 6: Different mixing lengths to achieve different levels of mixing.

M1 – mixing length 1
M2 – mixing length 2
M3 – mixing length 3

Figure 30: Injector exit fuel concentration profile (measured) for a mixing length of 5.5 inches and for air flow rates of 10 and 100 SLPM

Figure 31: Injector exit fuel concentration profile (measured) for a mixing length of 4 inches and for air flow rates of 10 and 100 SLPM

Figure 32: Injector exit fuel concentration profile (measured) for a mixing length of 2.5 inches and for air flow rates of 10 and 100 SLPM

Figure 33: Experimental results from investigation of the effect of fuel concentration profile on flashback

Figure 33 displays the experimental results from the investigation of the effect of fuel concentration profile on flashback air flow rate. The plot is labeled in a similar fashion as previous plots in that the nominal compositions are defined in the legend as H2-CO-CH4. The

M1, M2, or M3 designation following the composition refers to the 2.5, 4, 5.5 inch mixing length, respectively. Pure natural gas cases are shown for M1 and M2 because flame stabilization could be achieved for pure natural gas with mixing lengths of M1 and M2 due to the presence of rich regions near the center of the injector exit plane.

Figure 34 shows the effect of wall temperature on these experimental results since it is not held constant for all tests. Variation of the fuel concentration profile appears to have the most pronounced effect on the 100% hydrogen cases. As the boundary layer fuel concentration is reduced the propensity for flashback is also reduced, which is what one would expect. However, this effect does not seem to hold for 50/50 H₂/CH₄ mixtures as is shown in Figure 33 and Figure 34. Upon looking only at Figure 33, the fuel concentration profile does seem to have an effect for the 50/50 H₂/CO cases, but taking into account the wall temperature, as is done in Figure 34, this is shown to not be the case.

Figure 34: Experimental results from the investigation of the effect of fuel concentration profile with the wall temperature effect on flashback air flow rate explicitly shown

3.2.8 Diluent Addition

Figure 35 and Figure 37 show the experimental results from the study of the effect of CO₂ and N₂ dilution of the fuel for these fuel compositions: 50/50 H₂/CH₄, 50/50 H₂/CO, and 100% H₂. The legend notation is again similar to those of previous sections where the nominal composition is specified with the first three elements as H₂-CO-CH₄ and the last element is the percent diluent added to fuel composition giving H₂-CO-CH₄-CO₂ for Figure 35 and H₂-CO-CH₄-N₂ for Figure 37. In both Figure 35 and Figure 37, the equivalence ratio is shown on the x-axis rather than the percent hydrogen in the fuel because this shows how the equivalence ratio (EQ) is changing as diluent is added to the fuel. As diluent is added the EQ must increase such that an adiabatic flame temperature of 1700 K is maintained, however, due to imperfect fuel control the EQ in Figure 35 and Figure 37 are not always increasing compared to the no diluent cases. Again the wall temperature effect must be taken into account as has been done in

previous sections and is accomplished by Figure 36 and Figure 38. In looking at Figure 35, Figure 36, Figure 37, and Figure 38, one can conclude that the effect of diluent addition has little effect on the air flow rate at which flashback occurs. A possible explanation for this is that the small increase in EQ such that the adiabatic flame temperature is maintained at 1700 K offsets the decrease in flame speed that comes from the diluents addition. This explanation does require further analysis that involves calculation of flame speeds.

Figure 35: Experimental results from the investigation of the effect of CO₂ addition to the fuel on flashback air flow rate

Figure 36: Experimental results from the investigation of the effect of CO₂ addition to the fuel with the wall temperature effect on flashback air flow rate explicitly shown

Figure 37: Experimental results from the investigation of the effect of N₂ addition to the fuel on flashback air flow rate

Figure 38: Experimental results from the investigation of the effect of N2 addition to the fuel with the wall temperature effect on flashback air flow rate explicitly shown

3.2.9 Higher Hydrocarbon Addition

Figure 39 shows the experimental results from the study of the effect of hydrocarbon (ethane) addition to these fuel compositions: 50/50 H₂/CH₄, 50/50 H₂/CO, and 100% H₂. The legend notation is again similar to those of previous sections where the nominal composition is specified with the first three elements as H₂-CO-CH₄ and the last element is the percent ethane added to the fuel composition giving H₂-CO-CH₄-C₂H₆. In Figure 39, the equivalence ratio is shown on the x-axis rather than the percent hydrogen in the fuel because this shows how the equivalence ratio (EQ) is changing as ethane is added to the fuel. As ethane is added the EQ must change such that an adiabatic flame temperature of 1700 K is maintained, however, due to imperfect fuel control the EQ in Figure 39 and Figure 40 has some variation for equivalent fuel/ethane mixtures. Again the wall temperature effect must be taken into account as has been done in previous sections and is accomplished by Figure 40. Unlike the addition of diluents, the addition of ethane results in a major reduction of flashback air flow rate for the 100% H₂ case and less so for the other fuel compositions, 50/50 H₂/CO and 50/50 H₂/CH₄.

3.2.10 Lifted Flame

The specific study of the effect of lifted flames versus attached flames on flashback propensity was performed for three fuel compositions: H_2 , 50/50 H_2/CO , and 50/50 H_2/CH_4 . Figure 41 shows images of the different flame modes. For this study, flashback was approached differently than in the previous study. Instead of holding the AFT constant as in the previous section, the AFT was increased as air flow rate was held constant until flashback occurred. After each increase in AFT, thermal equilibrium was achieved before increasing AFT again.

Figure 41: Comparison between lifted and attached flame 50% H_2 -50% CH_4

High speed intensified OH^* video of the flashback process was captured for the different fuel compositions in the different flame modes (i.e., attached v. lifted). Figure 42 and Figure 43 show several still images that have been extracted from the high speed videos for a fuel composition of 50% H_2 – 50% CH_4 for the lifted and attached flame modes. Figure 42 shows flashback for an attached flame mode. The first image shows the flame in the attached mode prior to flashback, The second image shows the onset of flashback as manifested by the regression in the boundary layer of the left side of the tube. The third image shows a tilted flame as has been described by other researchers (von Elbe and Mentser 1945). The last image shows the flame has nearly regressed fully into the injector.

Figure 42: Intensified OH* images of FB for fuel composition of 50% H₂- 50%CH₄ (attached flame)

Figure 43 shows flashback of a flame in the lifted mode prior to flashback. The first image shows the lifted flame before flashback occurs. The position of the lifted flame in the enclosure fluctuates up and down. As flashback is approached this fluctuation intensifies until finally one side of the lifted flame attaches to the burner rim. Then the flame transitions to an attached mode for only a moment before fully regressing into the injector. It seems as though flashback is still occurring primarily through the boundary layer mode of flashback.

Figure 43: Intensified OH* images of FB for fuel composition of 50% H₂, 50%CH₄ (lifted flame)

Figure 44 presents the tests that investigate the effects of enclosure size and flame type on flashback AFT and flow rate. Two protocols are applied to approach the critical FB point: increasing AFT (test protocol #1) or decreasing flow rate (test protocol #2). The motivation of this figure is to compare lifted and attached flame modes and their effect on flashback. However, there are also some data included here that show how the enclosure size affects lifted flames and their flashback events significantly. These data are the H₂/NG mixtures (diamonds)

in Figure 44. One can see that the larger enclosure size with a lifted H₂/NG flame will result in lower flashback propensity. This is an important observation regarding lifted flames.

Then in order to compare lifted and attached flames H₂/CO mixtures were investigated. From these H₂/CO data it cannot be fully concluded that lifted flames reduce flashback propensity. As the flow rate is increased the required AFT for flashback also increases, and this trend is shown with each set of data in Figure 44. The dark green diamonds, which represent the lifted H₂/CO flames, have a flatter slope than the attached H₂/CO flames (red crosses) and as a result the dark green diamonds (lifted) intersect the red crosses (attached) at a point which suggests that there is a point where lifted flames may not decrease flashback propensity. It is clear however, that before this intersection lifted flames do decrease flashback propensity for a given flow rate. The light green diamonds are also data from H₂/CO experiments, but in these experiments the lifted flame actually stabilized as an attached flame while approaching flashback. The new point of stabilization as an attached flame is what is shown a light green diamond in Figure 44.

Figure 44: Investigation of effects of enclosure size and flame type on FB AFT and FB air flow rate (Test protocol #1: FB onsets with increasing AFT and fixed flow rate; #2: FB onsets with decreasing flow rate and fixed AFT)

3.2.11 Standoff Distance

The effect of the distance from the injector tip to the enclosure holder plate (See Figure 24) on flashback was also investigated. These tests were performed only with the quartz tube, 100% H₂, and AFT=1700 K. The distance was varied to 2 cm in order to identify an effect. This study was motivated by the desire to visualize the propagation of the reaction into the injector tube with the high speed OH* intensifier which is not possible in the normal setup due to the enclosure holder plate. Figure 45 shows several still images taken from the high speed intensified OH* video of the flashback process. The red arrow indicates the location of the

enclosure holder plate. These images nicely show the propagation of the flame into the injector through the boundary layer mechanism. The air flow rate at which flashback occurred in these tests was higher than those tests where the enclosure holder plate was at the injector exit. Therefore, this test setup leads to higher flashback propensity.

Figure 45: Intensified OH* images of FB for fuel composition of 100% H₂ (attached flame with an ordinary enclosure and lower enclosure plate level)

3.3 Full Annular

A combustor from a Capstone C60 Microturbine (NG recuperated Brayton cycle engine) was used for this study. The engine normally operates at a pressure of approximately four atmospheres, but the combustor has been modified to run at one atmosphere by the removal of the turbo machinery to allow optical access. Moreover, the air inlet ports are strategically located in the modified combustor to better simulate actual engine flow conditions. The combustor primary zone air enters through six injectors tangentially opposed on two different planes (Figure 47). Of primary importance is the ability of this test rig to simulate flow fields and primary zone structures as would be found in the microturbine generator (MTG). For example, due to the large scale recirculation zone formed by tangential injection of the primary air, entrainment of dilution zone air into the primary zone reduces the calculated fuel/air ratio. To the extent possible gas turbine conditions are recreated in the combustor to investigate combustion instability phenomena.

Figure 46: Annular combustor test rig

Figure 47: C60 annular combustor cutaway drawings: (a) 3D view of combustor showing two planes of injectors, (b) bottom plane, (c) overhead view of both planes

To detect FB and LBO limits an instrumented C60 NG injector outfitted with three different types of sensors was used. The first principle is detection of temperature changes at different points of the injector during a FB/LBO event. Figure 49 shows the locations of the thermocouples placed along the injector. The second principle of detection is the use of a pressure to detect a change during FB and LBO. Figure 49 indicates the position of the pressure port routed with an 1/8" in. tube through the fuel inlet section of the injector of the injector and exposed to the premixing zone. During FB the pressure within the premixer rises due to hot gases at higher density produced within a smaller area. Alternatively, during LBO the absence of a flame means no convective or radiative heat transfer back into the premixer so the gas density is lower and subsequently pressure decreases. However, the change in pressure is not as evident for LBO as it is for FB. The last detection approach is flame chemiluminescence which is the electromagnetic radiation emitted from the de-excitation of electronically excited species that are formed via chemical reactions during combustion. Thus, chemiluminescence provides information about the conditions in the reaction zone including whether the flame is flashbacked or blown out. This instrumented injector features a Fiberguide Industries Superguide G, High OH for UV visualization (Part# CB14370) fiber optic probe inserted through the fuel inlet section of the injector. By design, the probe captures chemiluminescence at a conical angle within the

injector when the flame propagates into the premixer. Conversely, during LBO the flame extinguishes and chemiluminescence signal ceases.

Figure 48: Instrumented flashback/lean blowout C60 Capstone OEM injector

Figure 49: OEM natural gas injector instrumented with thermocouples, pressure probe, and fiber optic

Given the stochastic nature of the combustion phenomena in question it was necessary to discern between the variation expected from the results to the influence of experimental factors. After initial tests produced unrepeatable results an evaluation of different testing protocols was performed. The objective of these protocol tests was to identify factors that lead to inconsistent results. From this investigation several underlying factors were found to be influencing results including, injector tip temperatures, thermal equilibrium, step change of EQ, and re-ignition. Studies on injector tip temperature have shown that for lean fuel mixtures FB occurs at a constant burner-tip temperature for any given H_2 concentration, if the thermal conductivity and wall thickness are held constant regardless of the burner diameter (Bollinger and Edse 1956). Results coincided with this observation, thus care is taken during tests to allow injector tip temperatures to reinitialize to equilibrium after a FB event. Furthermore, the entire combustor must be given sufficient time after ignition to reach a condition of thermal equilibrium otherwise varying levels of heat can be transferred to the incoming air (which first flows around the combustor before entering the combustor itself) and hence causes unwanted variation in temperatures. Overcoming this challenge involved preheating the combustor until the surface temperature reaches a nominal value. The rate at which the EQ is changed also affects FB and LBO limits so sensitivity tests were conducted to determine suitable values. A rate of 0.01/60sec change in EQ achieved a balance between causing too large of a temperature fluctuation when the EQ changes and sufficient time for temperatures to re-equilibrate. Figure 50 plots H_2/CO FB and LBO data with standard deviations to show how consistent results are with the established protocol. At several H_2 concentrations data repeated at exactly the same EQ indicated by the lack of standard deviation bars. Issues with ignition only had to be taken into account for compositions in which the margin between LBO and FB was small. Finding a region of stability proved difficult as small fluctuations in air or fuel control could cause either FB or LBO. Tests conducted at these mixtures had to be reignited quickly if such an event occurred to try and maintain thermal equilibrium. Once a flame stabilized for some time then the test was carried out as described:

1. Allow preheat temperature to plateau with no more than a 1 degree rise every minute
2. Set second injector to EQ of 0.73 and light off then set both injectors to 0.73 and allow combustor to warm up for a period of 15 minutes
3. Monitor combustor surface temperature and injector temperatures ensuring that they are close to equilibrium
4. Set composition of H_2 let injector temperatures plateau and incrementally change EQ by 0.01 every 60 seconds
5. After the flame extinguishes, allow the preheated air to flow through the combustor for 2 minutes until all the injector temperatures reach identical values
6. Relight and repeat steps 4-6

Figure 50: Plot of H₂/CO FB and LBO with standard deviation

With the protocol established a comparison of the operating limits for different fuels is accomplished by operating the combustor until it reaches the FB and LBO limits. Tests to determine the stability maps are conducted by setting a preheat temperature, combustor pressure drop, and fuel composition. Complications arose from the need to keep the flow rate, combustor pressure drop, and temperature constant while changing EQ. MFCs are programmed to adjust to variability in air flow rate to maintain a constant EQ. Inlet air temperatures remained relatively constant, but small adjustments were made to account for variability caused by higher reaction temperatures. For the data shown in the results, flow rate, pressure drop, and temperature remain constant to 2.5%, 10%, and 1%, respectively. Note that the pressure drop fluctuation is inherently higher due to the temperature variations while increasing or decreasing EQ.

Identifying the LBO limit is done audibly and visually then confirmed by a sudden reduction in injector temperatures. Higher compositions of H₂ produced LBO that was triggered immediately as the EQ changed. In other cases, LBO occurred at a constant EQ with a gradual reduction in tip temperatures until the flame could no longer be sustained. Attachment of the flame at the rim of the injector for H₂/NG occurred approximately at 15% H₂ with no transition to a lifted flame before LBO. Compositions below 15% ignite in a lifted mode and LBO occurs over a longer period of gradually decreasing temperature. No ambiguity exists in identifying the LBO limit, however, in certain mixtures between 50 to 80% H₂/NG FB occurs while performing LBO. The cause of these events is suspected to result from various instabilities, such as fluctuations in the fuel flow rate as it responds to slight variations in the inlet air flow rate. In addition, inherent disturbances in pressure create instantaneous changes in the flow field altering the reaction stoichiometry leading to variations in the heat release. Study of these “dynamic” stability events is beyond the scope of this paper and subsequently results are not presented for FB during LBO.

Detection of FB is done by utilizing an instrumented injector consisting of three thermocouples (type K) with two located at opposite ends of the tip and the other in the injector air holes (Figure 49). The tangential placement of the injector in the primary zone causes one side to protrude farther into the primary zone causing higher temperatures at this tip location. The associated thermocouple on the side that extends farther into the combustor is designated as the “hot” thermocouple and the one on the opposite side is referred to as the “cold” thermocouple. A thermocouple placed at the inlet of the preheated air is simply referred to as the “air” thermocouple. The injector also features a pressure probe in the premixing zone to measure the change in pressure during FB. Furthermore, FB, which involves rapid flame propagation upstream into the premixer, produces an audible change in pitch indicating to the operator that FB has occurred, which is then verified by a corresponding temperature rise.

Defining a consistent definition of FB is difficult because different compositions generated FB in different ways. FB behavior for H_2/NG mixtures always consisted of rapid propagation of the flame upstream. As shown in Figure 51a, this is reflected by a dramatic change in the slope for the “hot” thermocouple temperature profile. Visual observations confirm a rapid displacement of the flame front from the anchored position. For H_2/CO mixtures with more than 50% H_2 FB occurred similarly to H_2/NG . However, as demonstrated in Figure 51b at 50% H_2 , FB resulted in a gradual rise in the “hot” thermocouple. FB is reported for the exponential rise in tip temperature when temperatures on the “hot” thermocouple surpass 1144 K.

Figure 51: (a) “Hot” thermocouple temperature response for rapid propagation into premixer for H_2/NG at 80, (b) “Hot” thermocouple temperature response for gradual propagation into the premixing zone for H_2/CO 50/50 mix

Testing was conducted with two injectors on plane A, where one injector had a varying composition and varying local EQ while the other injector was fueled with NG at a constant EQ of $\Phi=0.7$. Plane B injectors were not fired for any of the results reported. Preheated air is constantly being fed through both planes of injectors and inner and outer dilution holes. In summary of the testing protocol the combustor air flow splits between the various dilution and primary zone holes were found to be close to those splits at engine operating conditions. Preheat temperatures can reach a maximum of 811 K, but for a majority of tests 672 K was chosen in order to compare to previous results. Total air flow rates ranged from 0.115-0.127 kg/s, corresponding to a nominal combustor pressure drop of 1%. Fuel consisted of mixtures of NG/H_2 and H_2/CO with fuel blending accomplished using two MFCs (Alicat MC Series) to mix fuel to a desired composition far upstream then inject it into the fuel-air premixing zone. Mixing

the fuel far upstream is done to allow sufficient mixing time to create a homogenous fuel mixture before it is introduced to the injector in Figure 49. While creating the stability maps shown in later sections, several observations regarding how FB occurred are reported. These observations will be discussed in later sections with experimental data to support conclusions. FB behavior witnessed in these experiments can be categorized into three different types: rapid upstream propagation, slow movement of the flame position into the injector tip, and rapid propagation upstream while decreasing EQ.

3.3.1 Equivalence Ratio Sweeps

Figure 52 shows operating limits for H_2/NG mixtures for a 672 K preheat temperature. An apparent drop in the operability margin is observed past 40% H_2 content where FB begins to occur readily. Tests performed at 40% H_2 yielded one FB result at 0.59 while the other test increased the EQ up to 0.8 without FB. Below H_2 concentrations of 40% FB tests are limited by hardware temperatures so EQs are run to a maximum of 0.8 without FB. It is unknown whether higher EQ would eventually induce FB, but the shift in the trend is evident. Each point was repeated twice during testing to ensure it was repeatable and random points were retested on different dates to ensure repeatability. For compositions between 50-80% H_2 in NG, the margin between FB and LBO is almost non-existent. In fact, a 0.01 change in the EQ resulted in either FB or LBO depending upon the direction of the change. In many instances the injector would FB during LBO tests and vice versa. On the upper end of H_2 concentration (90-100%) the stability margin starts to reappear slightly.

Figure 53 illustrates the operating limits for H_2/CO between FB and LBO for 672 K. LBO follows a roughly linear downward trend as the concentration of H_2 is increased. This observation is consistent with previous work of Schefer (2003), Strakey (2007), and Noble (2010) in that increasing the concentration of H_2 extends the lean limit to lower EQ. FB exhibits the same behavior except that instead of being linear, an increasingly steep dependence upon EQ is observed at higher concentrations of H_2 . This is most evident for H_2/CO . Drop off in the FB EQ at higher H_2 concentration is more apparent for H_2/CO than for H_2/NG . The range of operability for H_2/CO is greater than that for H_2/NG for H_2 concentrations of 40-90%. In addition, for lower concentrations of H_2 the operability is improved. For H_2 concentrations below 40% FB did not occur since the maximum allowable hardware temperatures were approached as a result of increasing EQ.

Figure 52: Operability map for single injector preheat 672 K varied H_2/NG composition and EQ (ϕ)

Figure 53: Operability map for single injector preheat 672 K varied H_2/CO composition and EQ (ϕ)

3.3.1.1 Injector Interaction

Results in this section pertain to the scenario where both injectors on the bottom plane (Figure 47) change composition and EQ simultaneously. Operating limits for H_2/CO mixtures shown in Figure 54 indicate an extension of the LBO limit in the two injector scenario. In terms of FB limits, varying both injectors has no effect. Again as expected, EQs descend downward as the concentration of H_2 in the fuel increases. For LBO, the drop in EQ is shifted downward by approximately the same value for each composition. It is suspected that the extended LBO limit is due to the increase of H_2 in the primary zone of the combustor generating radicals that support the stability of the local reaction zones. FB limits exhibit no shift and the decrease in the operating EQ limit has an identical slope in both scenarios.

Tests conducted with two injectors simultaneously varying on the bottom plane with H_2/NG , shown in Figure 55, indicate a shift to lower EQ at which both the LBO and FB occur as H_2 concentration is increased. LBO in H_2/NG has identical behavior to H_2/CO in the simultaneously varying injectors case where EQ for LBO is decreased. FB behavior does not correspond with H_2/CO two injectors varying simultaneously, instead EQs at FB decrease similar to LBO. Again, a narrow range of operability for H_2/NG is observed as indicated by the small gap between FB and LBO. An interesting observation is that the flame is more easily stabilized than the single injector case and is not subject to a lack of operability at all H_2 concentrations. Figure 55 shows a comparison of the two injector varying versus the single injector varying cases, demonstrating a slightly wider operating EQ range for simultaneous variation of two injectors. However, for two injectors with mixtures greater than 60% H_2 , a seemingly stable flame would occasionally FB raising uncertainty as to whether a true operability region exists, or if FB is simply delayed.

Figure 54: Operability map comparison of two simultaneously varied injectors to single injector for H_2/CO with 672 K preheat

Figure 55: Operability map comparison of two simultaneously varied injectors to single injector for H_2/NG with 672 K preheat

3.3.1.2 Preheat Effects

The effects of preheat are investigated in Figure 56 and Figure 57 with an expectation that preheat will produce FB at lower EQs and the LBO margin will be extended with greater preheat. LBO margins for H_2/NG suggest that at lower preheat temperatures the addition of H_2 has a greater effect on LBO. This dependency is most apparent at H_2 concentrations below 50%. In addition to greater sensitivity to H_2 , there is a lack of operating margin for H_2/NG in the non-preheated (300K) case that is not seen with H_2/CO . Figure 57 demonstrates that a stable region between FB and LBO limits exists with H_2/CO , whereas Figure 56 clearly shows no operating margin for either preheat case with H_2/NG indicating a dependency on fuel type. Note the variability of the data in Figure 56 for the 300K case which has inconsistent FB behavior, especially at 73% H_2 , where the EQ at FB deviates from the trend by increasing with additional H_2 . This discrepancy in the trend is attributed to difficulty in stabilizing the flame within a small margin of operability and also to the increased sensitivity to the EQ set point. Furthermore, there is a question as to whether this is indeed a “real” FB limit or induced by instabilities caused by operating near the LBO limit. These same inconsistencies are not present for H_2/CO because the wider operating region facilitated flame stabilization and made it less sensitive to dynamic changes.

Figure 56: Flashback and lean blowout limits for H_2/NG at 672K and 300K

Figure 57: Flashback and lean blowout limits for H_2/CO at 672K and 300K

Figure 58 and Figure 59 show the calculated AFTs for the experimental FB and LBO data in Figure 56 and Figure 57. Recall that Figure 56 and Figure 57 showed the effect of preheat on FB and LBO EQs for various H_2 concentrations. The calculation of AFT for H_2/CO mixtures revealed that AFT at FB and LBO does not vary as inlet air preheat is changed from 300 K to 672 K (see Figure 57 and Figure 58). However, for H_2/NG mixtures, the AFT at FB and LBO did

still depend on the preheat temperatures although to a lesser extent (see Figure 56 and Figure 59). This further illustrates the differences between the two sets of mixtures. Other researchers have found that the AFT can be used to correlate FB data while these same researchers showed difficulty using the calculated laminar flame speed to meaningfully correlate the same data that correlated well when using AFT as a correlating parameter (Littlejohn, Cheng et al. 2010). Comparison of Figure 53 and Figure 54 shows a perplexing observation that the margin of stability of H_2/NG is almost non-existent whereas H_2/CO has a clear gap between FB and LBO. The expectation here is that higher flame speeds along with higher AFTs of H_2/CO will promote a decrease in the stability margin compared to NG. In contrast to the present work, results from Noble et al. (2010) show a clear gap between H_2/CO and H_2/NG . Their experimental setup featured a swirl stabilized flame unlike the jet flame studied in the current work. It is not entirely clear whether the lack of operability margin for the H_2/NG case in the current work is a result of the lack of swirl or a function of the geometry of the combustor.

Figure 58: H_2/CO AFT at flashback and lean blowout for preheat temperatures of 672K and 300K

Figure 59: H_2/NG AFT (T_{ad}) at flashback and lean blowout for preheat temperatures of 672K and 300K

Effects of preheat are shown in Figure 56 and Figure 57, which as stated previously higher preheats correspond to FB and LBO occurring at lower EQ compared to the non-preheated case. The tendency is that the preheat increases the reaction zone temperature and diffusivity, while decreasing the unburned density causing an increase in the laminar flame speed (Turns 2000). However, Noble et al. demonstrated that the laminar flame speed is not an

important parameter in characterization of FB. Instead, Figure 58 and Figure 59 shows that AFT associated with FB and LBO conditions collapses onto a single value mainly at H_2 concentrations $>60\%$. Figure 58 indicates that the FB and LBO limits occur at a fixed AFT for a given percentage of H_2 in the fuel. Comparing Figure 56 and Figure 59 for H_2/NG , again the gap in EQ between preheats is diminished when plotted by AFT. LBO data show that air preheat does not affect FB and LBO EQ values at higher H_2 concentrations, but does affect FB and LBO values at lower H_2 concentrations. The implication of this observation is that the AFT is an important parameter in developing predictive methodologies for FB and LBO limits at varying preheats, especially at high H_2 concentrations.

3.4 C-65 Engine Experiments

The engine was tested in “Area B” of the Distributed Technology Test Facility at the UCI Combustion Laboratory (see Figure 60). Relative to the Area B location, the mixing station that allows for changes in fuel composition is located approximately 100 feet away. The distance between the mixing station and the Area B location creates some difficulty in performing inherently dynamic tests such as the current flashback studies. However, the experiments could be designed in a way that the fuel composition does not need to be the dynamically altered variable. This section goes over these facilities that are associated with the engine tests.

Figure 60: Plot Layout for Distributed Technologies Testing Facility (DTTF) at UC Irvine.

A data acquisition system is available for the “test pad” where the engine is installed with the capability for 32 temperature measurements, 4 high speed voltage measurements (100 kHz), emissions measurements, and fuel flow rate measurements. Two sets of instrumented injectors

have been used on the engine. The only difference between the second set and the first set is that there are only three thermocouples on the second set (hot, cold, air) where on the first set there were more. Each set can be used interchangeably since the hot and cold temperatures are used here for flashback detection. Thermocouples are also used to measure the stack exhaust temperature, and their numbering scheme is shown in Figure 61.

Figure 61: Thermocouple placement for exhaust stack measurements.

A schematic of the mixing station is shown in Figure 62. It is important to understand some of the key features and constraints of the mixing station relative to subsequent discussions. The mixing station can mix together up to 5 different gases at a time and was designed to allow for supply to 250 kW power generation devices under nominally steady state operation. Natural gas (NG), hydrogen (H₂), propane (C₃H₈), carbon monoxide (CO), ethane (C₂H₆), carbon dioxide (CO₂) and nitrogen (N₂) are the feed gases. Due to review of typical fuels available for DG systems, utilization of H₂ and C₃H₈ is mutually exclusive, and utilization of CO and C₂H₆ is mutually exclusive, thus up to only 5 gases at a time may be mixed.

The mixing station works by passively measuring the flow rate of the main energy-containing constituent in the fuel mixture, known as the “anchor fuel”, and then controlling the flow rates of the remaining constituents based on gas concentration set points inputted by the user. For example, if the user wants to flow a 50% NG, 25% CO₂ and 25% N₂ mixture, and the generator requires 10 SCFM (standard cubic feet per minute) of NG to meet its power output set point, the fuel mixing system will measure the 10 SCFM natural gas flow rate and control the CO₂ and N₂ flow rates to 5 SCFM each. The anchor fuel bypasses the control valve so its flow rate can be passively measured.

All other flows beside the “anchor fuel” flow are each independently controlled, where flow rate is measured by a mass flow meter and controlled with a pneumatically actuated control valve. There are two options for controlling flow. First, a proportional-integral-derivative (PID) feedback loop may be engaged and “tuned” to the requirements of a specific test. Second, the control valve positions may be set directly via the user interface. The user specifies the following before operating the system:

7. Two lines can flow two different gases one of which must be selected depending upon the desired output mixture. The user must select H₂ or C₃H₈, and CO or C₂H₆. Valves 136 and 137 will be appropriately actuated. The PID set points for the 122-142 and 123-

143 feedback loops will be automatically adjusted according to the gas selected by the user.

8. The user must choose the “anchor fuel”. This is the main energy-containing fuel mixture constituent. The choices are NG, H₂ or C₃H₈. If it's NG, valve 131 will divert NG flow around valve 141 and valve 132 will divert H₂ or C₃H₈ through valve 142. If the anchor fuel is H₂ or C₃H₈, valve 131 will divert NG flow through valve 141 and valve 132 will divert H₂ or C₃H₈ around valve 142.
9. The user must then set the concentration set points for all gases other than the “anchor fuel” if PID control is to be used, or the user must manually control each control valve by entering control valve settings.

Figure 62: UCI Mixing Station.

The procedure for testing is determined by limitations on the mixing station in addition to Capstone's direction in performing tests. Previously, the engine was shutoff when a sharp temperature rise occurred on the injector tip temperature. This temperature rise would eventually plateau and whether or not this is truly flashback was questionable, so to overcome this uncertainty the direction was to wait until the air temperature thermocouple would achieve a rapid rise in temperature similar to those seen by the tip temperature. In the case of testing with H₂/CO, the engine needed to be started on a mixture of NG with CO₂ to achieve a low BTU gas compatible with the “fuelty=1” setting. After allowing the engine to warm up the switch is made to make CO the baseline fuel in preparation for blending hydrogen. Procedure is as follows:

1. Start engine on NG or NG/CO₂ if testing H₂/CO
2. Blend in hydrogen
3. Incrementally increase hydrogen percentage every ~2.5 minutes
4. Observe rapid temperature increase in air thermocouple
5. Shutdown engine

3.4.1 Flashback Results

Date	Power [kW]	Injector Design	% H2 at Flashback [based on <u>air</u> temp; +/- 3%]	% H2 at Flashback [based on <u>tip</u> temp; +/- 3%]
01/27/11	20	Baseline,NG	30	
01/28/11	20	Baseline,NG	28	
02/23/11	20	Baseline, CO	10	
09/20/12	20	Baseline, CO	17*	
09/27/12	20	Baseline, CO	31.6**	
04/21/11	20	Cutback,NG	70	70
10/21/11	20	Cutback,NG	68	68
05/09/11	20	Cutback,CO	5	11
05/26/11	20	Cutback,CO	<5	8
12/20/10	30	Baseline,NG	61	
02/22/11	30	Baseline, CO	15	
02/23/11	30	Baseline, CO	15	
04/29/11	30	Cutback,NG	49	70
10/26/11	30	Cutback,NG	47	
10/27/11	30	Cutback,NG	45-48	
05/13/11	30	Cutback,CO	14	19
03/04/11	39	Baseline, CO	20	
12/10/10	65	Baseline,NG	59	
03/30/11	59	Baseline,NG	61	
03/30/11	60	Baseline,NG	60	
03/23/11	62	Baseline, CO	20	
04/29/11	60	Cutback,NG	50	73
10/27/11	59	Cutback,NG	52	
05/20/11	58	Cutback,CO	23	23

Note: Data in Red are those data for which the cutback injectors were damaged

*TET=1100 & FUELTY=1 so 4 injectors on. **TET=1000 & FUELTY=1 so 4 injectors on.

4 Operability Analysis

Where possible, the goal of these experiments was to produce a design tool that allowed engineers to estimate the conditions at which autoignition, flashback and lean blow out would occur for various fuel compositions. Ideally the design tool would also allow for various pressures, temperatures, materials, etc., however, the phenomena of flashback is very complex and involves an extremely diverse set of parameters. Therefore, the purpose of this design tool was relegated to Capstone specific equipment. The axisymmetric injector simplifies the flow field while the full annular combustor maintains the complexity of the flow field while eliminating pressure effects. The connection of these two experimental platforms to each other and

ultimately to the engine will provide necessary insights as well as provide Capstone engineers with a methodology to investigate flashback phenomena.

4.1 Autoignition

Autoignition can be predicted using both correlations and comprehensive modeling.

The ignition delay times from various researchers using flow reactors and shock tubes are shown in Figure 63 (Snyder, Robertson et al. 1965; Peschke and Spadaccini 1985; Blumenthal, Fieweger et al. 1996; Wang, Olivier et al. 2003; Beerer and McDonell 2008; Santoro 2009). Peschke and Spadaccini, as well as Santoro, used flow reactors, while the other investigations used shock tubes. The temperature dependency of hydrogen is quite unique. At the highest temperatures (above 1,200 K), the activation energy is very low (16 kcal/mol) but gradually rises as the temperature drops below 1,000 K. In the lower-temperature region below 900 K, the activation once again reduces. This would suggest a complex interaction between many factors (chemical or physical) unlike the alkane work, which generally exhibited constant activation energy throughout the entire temperature range studied. The current study was conducted at lower pressures than the work of Peschke and Spadaccini (1985), which may explain the relatively longer ignition delay times observed. The flow reactor work of Santoro (2009) was performed at pressures only slightly higher than the current study, and the agreement between the two studies is very good. Interestingly, all three flow reactor studies show activation energies as little as 3 to 8 kcal/mol, indicating a very small temperature dependency. Noteworthy is that Peschke and Spadaccini observed autoignition as low as 660 K, while the current study and Santoro et al. only observed autoignition at temperatures above, roughly, 750 K. Unfortunately no explanation for these differences could be determined.

Figure 63: Comparison of Flow Reactor Results from Beerer and McDonell (2008; “current study”) to the Flow Reactor Results of Peschke and Spadaccini (1985) and Santoro et al. (2009), and the Shock Tube Results of Snyder et al. (1965), Blumenthal et al. (1996), Slack (1977), and Wang (2003).

For the low-temperature, high-pressure conditions typical of premixed conditions for reciprocating engines or gas turbines, the behavior of the ignition delay time appears to be

relatively insensitive to temperature. Data obtained recently agrees well with the flow reactor work from Peschke and Spadaccini (1985), thus it appears the correlation presented in Equation 72 is appropriate in these regimes (i.e., 600 to 800 K up to 23 atm). For convenience, this is provided in Equation 72:

$$\tau(s) \cdot [O_2]^{0.50} [F]^{0.25} = 1.29 \times 10^{-7} \exp\left(\frac{3985}{T}\right) \quad \text{Equation 72}$$

Hydrogen autoignition was modeled using the Galway mechanism (Petersen, Kalitan et al. 2007). The simulated ignition delay curves for pressures between 1 and 10 atm are shown in Figure 64. Hydrogen's ignition delay times are seen to be highly dependent upon both the pressure and temperature. At higher temperatures (above 1,100 K), the overall activation energy for all pressures is roughly 17 kcal/mol. When the temperature is lowered to around 1,000 K, the activation energy increases to roughly 100 kcal/mol, while below approximately 900 K the activation energy reduces to 45 kcal/mol. The activation energy for each region is labeled in Figure 64. The transition from one region to another is pressure dependent. The simulation predicts that the transition from one activation energy region to another will shift to high temperatures with increasing pressure. At higher temperatures, the delay times decrease monotonically with increasing pressure. But in the 100 kcal/mol region the reverse is true. In the 45 kcal/mol region, the ignition delay times are seen to once again monotonically decrease with increasing pressure.

The shock tube data obtained by (Snyder, Robertson et al. 1965; Bhaskaran, Gupta et al. 1973; Slack 1977; Blumenthal, Fieweger et al. 1996; Wang, Olivier et al. 2003), also exhibit an activation energy transition as a function of pressure and temperature. Quantitatively, the shock tube data and simulation are in agreement in the high-temperature (17 kcal/mol activation energy) region. However, the shock tube ignition delay times at lower temperatures, after the transition from the 100 kcal/mol activation energy region, are several times shorter than the simulation. Also perplexing is that all of the flow reactor work (the current work; Santoro et al. 2009; Peschke and Spadaccini 1985) report ignition delay times orders of magnitudes shorter than the simulation's. The activation energy of the flow reactor data is roughly 3 to 8 kcal/mol—much less than the simulation's 45 kcal/mol.

Figure 64: Comparison of Experimental Work to Homogenous Simulations Using the Kinetic Mechanism from the Galway Group

The reason for these discrepancies is not known with any confidence and is still an open question. The short ignition delay times for the shock tube at intermediate temperatures are reminiscent of the methane results from (Huang, Hill et al. 2004; de Vries and Petersen 2007). One could possibly argue that the non-idealities present in low-temperature shock tube data from hydrocarbons fuel experiments also effect hydrogen (Dryer and Chaos 2008). However this does not explain why the flow reactor results disagree with the simulation. In spite of this, the dominant chemistry involved in hydrogen autoignition is believed to be well understood and can explain some of the trends observed in the simulation and experimental data (Yetter, Dryer et al. 1992).

At high temperatures, the chain branching of the system is dominated by the elementary reaction: $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$. This reaction has an estimated activation energy of 16.4 kcal/mol (Mueller 2000), which is similar to the overall activation energy of the hydrogen simulation at high temperatures (17 kcal/mol). The O and OH radicals formed from this step react with the following branching reactions (Equation 94 and Equation 96) to further increase the radical pool:

The fast radical formation from these reactions results in very short ignition delay times for mixtures in the branched chain explosive region. Upon crossing into the thermal/chain explosive region, the recombination reaction $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$ competes for H radicals and produces the HO_2 . The HO_2 radicals formed react with themselves or with molecular hydrogen to form H_2O_2 , which decomposes into two reactive OH radicals (Equation 97 through Equation 99):

The radicals formed from this sequence can combine with the previous reaction steps to increase the radical pool. However the addition of this latter reaction sequence reduces the overall rate of reaction. These reactions are, however, highly exothermic, which can increase the system's temperature to the point that the system passes back into the branched chain explosive region (Yetter, Dryer et al. 1992). This exothermic process provides the name for this region's name; that is "thermal/chain" explosive region.

The activation energy of the hydrogen peroxide decomposition reaction is 45.5 kcal/mol, which is quite close to the overall ignition delay activation energy in the lower temperature range (45 kcal/mol). The similarity of the dominant elementary reactions in the branched chain explosive region and thermal explosive region to the overall activation energy of the hydrogen ignition delay at high and low temperature, respectively, suggest a relationship between them. To demonstrate this relationship, the pressures and temperatures where the transition from the 17 to 100 kcal/mol occurs in Figure 64 (marked as white circles) are also plotted on the hydrogen/oxygen explosive limits chart in Figure 65 (again marked as white circles). The pressure and temperature of this transition region fall on the extended second-limit boundary, as seen in Figure 65. Hence the transition from the 17 to 100 kcal/mol region is a result of crossing the extended second limit. It is curious that the overall activation energy does not transition directly from 17 to 45 kcal/mol. No definitive reasons as to why the system temporally exhibits a region of 100 kcal/mol could be found.

Figure 65: Hydrogen-Oxygen Explosion Limit Chart with Experimental Test Conditions Identified. The shaded region represents typical gas turbine combustor inlet temperature and pressures.

Identifying the dominant reaction steps helps explain some of the trends seen in Figure 64. At high temperatures, where ignition delay times are inversely proportional to pressure, all the simulated initial conditions of the fuel/air mixture are within the branched chain region. On the other hand, around 1,000 K the ignition delay time is seen to be shorter at 1 atm than at higher pressures (2, 4, 10 atm, etc..) which is a result of the 1 atm event starting in the relatively fast branched chain region, while the other events start in the slower thermal/chain explosive route. Once all the simulations are all within the thermal/chain explosive region (about 800 K), the ignition delay is once again seen to be inversely proportional to pressure. The pressure relation is a result of the hydrogen-peroxide decomposition step itself being directly proportional to pressure. This complex behavior should make one wary of extrapolating hydrogen correlations to pressures and temperatures well outside the region in which they were derived, as the dependency can change rather dramatically.

All flow reactor testing was performed in the region close to the third limit, which divides the thermal/chain explosive region from the non-explosive region in Figure 65. The shock tube data span both the thermal/chain explosive region and the branched chain region. Like the simulation, the experimental data points also show a large increase in the activation energy upon crossing the extended second limit. The high temperature shock tube data (in the branched chain explosive region) both qualitatively and quantitatively agree with the simulation. However, the shock tube and flow reactor ignition data (for mixtures of fuel and air with initial conditions within the thermal/chain explosive region) are overpredicted by simulation.

The model's ability to reproduce the alkane ignition points at intermediate temperatures would hint that similar agreement could be obtained with hydrogen (Beerer, McDonell et al. 2010). However, this clearly is not true. Because the disagreement only occurs in the thermal/chain region where HO_2 and H_2O_2 is dominant, one may draw the conclusion that the discrepancy could be due to uncertainties in these specific elementary reaction rates. However, Sabia et al. (2006) analyzed these reactions using sensitivity analysis and concluded that unrealistic modifications to the rate constants would be required in order to better match the experimental work of Snyder et al. (1965). Also any large modification to the reaction rates would almost certainly affect the simulation's ability to predict alkane ignition delay as well. Dryer and Chaos (2008) agree with this conclusion and argue that the short measurement ignition delay times are an experimental artifacts. For the case of low-temperature shock tube experiments, they cite Voevodski and Soloukhin (1965) along with Meyer and Oppenheim (1971). Both studies observed, through high-speed photography, that hydrogen ignition features randomly spaced ignition kernels in the end gas at these intermediate temperature regions, rather than a clean spatially uniform homogenous event behind the shock. They believed that the inhomogeneous ignition at intermediate temperatures (in the thermal explosive region) were due not purely to chemical kinetics but also to small mixture inhomogeneity in species concentration or temperature. Pang et al. (2009) have also suggested that boundary layer build up or bifurcation of the shock could also create these inhomogeneous regions in shock tube that could lead to early ignition events.

The low activation energy of the flow reactor data from the three flow reactor studies (Beerer and McDonell, 2008; Santoro 2009; and Peschke and Spadaccini 1985) is low and is rather suspicious. The repeatability of hydrogen ignition delay times has been reported to be poor in comparison to alkane fuels. It is possible that some unknown mechanism could be initiating the autoignition event in hydrogen; say perhaps static electricity build up or possible catalytic effect with the wall. Dryer and Chaos (2008) also suggest that the finite time for mixing in the venturi could alter the rate the radical pool grows during the induction period. Hydrogen is perhaps much more sensitive to any small perturbations in the plug flow. Further work is still definitely warranted in this region, as many questions still remain unanswered.

From a high level perspective, while the discrepancies noted above are intriguing, it is of primary interest to understand if ignition delay poses a concern in the actual engine. In terms of commercial application, the hatched region in Figure 65 represents the inlet temperature and pressure conditions where most gas turbine premixer currently operate. Unfortunately this hatched region falls in the area where all these hydrogen autoignition discrepancies occur. The ramifications of these results for hydrogen and, for reference, alkanes, on commercial application are discussed in the next section.

In order to demonstrate their applicability, the correlations for pure methane, ethane, propane (Beerer, et al., 2010), and hydrogen (Peschke and Spadacinni, 1985) were used to evaluate the ignition delay time at premixer inlet conditions for a number of gas turbines in commercial use today including the Capstone C-60. These delay times indicate how long of a mixing time can be tolerated before autoignition occurs if one of these engines were to hypothetically use one of these fuels in operation.

As an example, the Solar Mercury 50 has a premixer inlet temperature and pressure of 880 K and 9.9 atm. The correlations estimate the ignition delay of methane, ethane, and propane at these conditions to be 266 ms, 123 ms, and 82 ms, respectively. Therefore the premixing time for the Mercury 50 should not exceed the delay time calculated here for each fuel. In most engines the mixing time is typically 1–5 ms (Lieuwen, McDonell et al. 2008), so the delay times

calculated here suggest that autoignition does not pose a significant problem in most cases. However, this simple analysis involves numerous assumptions. As stated by Lieuwen et al. (2008):

“The time scales associated with physical mixing in the current low emissions is on the order of 1 to 5 milliseconds, based on the bulk velocities and premixer volumes. However, it should be recognized that the complex aerodynamics associated with swirl, separation, and strong gradients can make it difficult to assign a single time scale to represent the physical premixing time in a given system. Even if a very small fraction of the mixture has a longer residence time, spontaneous ignition of that mixture can lead to ignition of the entire mixture within the premixer.”

The engine application analysis illustrated in Table 7 implies that the premixer design has aerodynamically “smooth” passages without any large recirculation zones or wake regions. Given these assumptions, this study finds that such fuels (assuming they are clean, dry, in the gaseous phase, and contaminant free) should not pose a significant hazard in terms of premixer autoignition for future gas turbines.

Table 7: List of Current Commercial Engines with their Approximate Combustor Inlet Pressure and Temperature, along with Estimations of Ignition Delay Times for Pure Methane, Ethane, and Propane at Specific Inlet Conditions

Engine	Pressure	Inlet Temp	τ (msec) CH ₄	τ (msec) C ₂ H ₆	T (msec) C ₃ H ₈	τ (msec) H ₂
	atm	K	CH ₄	C ₂ H ₆	C ₃ H ₈	H ₂
GE 9H *	23	705	2,036	6,213	2,421	85
Solar Taurus 65	15	670	6,205	33,277	11,264	153
Solar Taurus 60	12.3	644	13,232	112,220	33,876	221
Solar Mercury 50 **	9.9	880	346	123	82	59
GE LM 6000	35	798	289	251	134	35
Siemens V-94.3A*	17.7	665	5,835	34,082	11,293	141
Siemens V-94.2*	12	600	38,988	786,278	191,174	336
Capstone C60 **	4.2	833	1,477	859	506	140
Alstom G24/26 EV Burner *	30	815	264	188	105	35
Alstom G24/26 SEV Burner ***	15	1,300	1.65	0.07	0.104	0.003

* Inlet estimated from ideal gas isentropic compression

** Recuperated Engine Cycle

*** Re-heat burner, used CHEMKIN and Galway Mechanism to calculate τ with $\phi = 0.6$

τ for alkanes calculated from correlations in Beerer et al. (2011)

τ for hydrogen calculated from correlations in Pescke & Spadaccini (1985)

4.2 Lean Blow Off

4.2.1 Full Annular

4.2.1.1 Lean Blowout Prediction via Perfectly Stirred Reactor (PSR)

Chemical reactor networks (CRNs) have been applied to a variety of combustion topics, such as determining overall reaction kinetic rates, NO_x formation, and turbulent flame phenomena (Turns 2000). PSRs idealize mixing behavior such that they simulate a situation where combustion products are back-mixed with reactants so quickly that the reaction zone is distributed uniformly in the control volume. For the combustor in this experiment the exhaust gas recirculation promotes turbulent mixing of reaction zones that produce back-mixing conditions that approach the stirred reactor idealization. Success in correlating behavior for lean blow out with a PSR has been shown by several authors (Ni, Zhang et al. ; Noble, Zhang et al. 2006; Strakey, Sidwell et al. 2007).

Evaluation of LBO using a CRN is carried out following the approach of Strakey et al. (2007). This method involves performing PSR simulations for the experimental conditions (i.e., inlet temperature, EQ, etc.) at which LBO occurred for a composition of pure NG where the residence time is varied until extinction. An experiment is performed in order to calibrate an “effective” residence time of a PSR. This “effective” residence time is then used to predict LBO as the concentration of H_2 in the fuel is increased. In the experiment two injectors on the first plane are fired in the combustor, but for the purposes of the PSR analysis only the local EQ of the injector flowing H_2/NG and H_2/CO are considered for these simulations. In other words, the EQ of the primary zone is not being used. Hence, it is being assumed that the injectors are independent from one another. Also, no heat losses or diffusion effects are considered in the PSR model so the residence time that is calculated relies on the empirical data of the pure NG extinction limit. Figure 67 shows the residence time at extinction to be 0.053, 0.064, and 0.063 for Galway C5 (Bourque, Healy et al. 2008), Galway nC5 (Healy, Kopp et al. 2010), and GRI Mech 3.0 chemical kinetic mechanisms, respectively. This effective residence time at the extinction limit is then fixed in the PSR and EQ is varied until a reaction can no longer be sustained. LBO in the PSR is defined as the EQ at the point of lean extinction.

Figure 66: PSR lean blowout approach schematic

The approach to determining LBO limits is as follows:

- 1) Perform computational experiment on “standard” fuel (100% NG) to determine LBO EQ
- 2) Vary the residence time of a PSR with the “standard” fuel until extinction occurs
- 3) Set the effective residence time at LBO for the standard fuel and vary composition of fuel into the PSR
- 4) Vary EQ until lean extinction limit of the PSR is reached

Figure 67: Residence times for lean blowout limits for different mechanisms

Figure 68 plots the actual and predicted LBO limits of the PSR analysis for H_2/NG fuel mixtures. Results agree relatively well for all mechanisms, especially at the lower and upper limits. Between 30-70% H_2 there are some issues with under predicting the result slightly. This occurs because the experimental data at these points are unstable so finding a stable flame to run for an extended period of time to achieve LBO without FB is difficult. At the start of the tests the EQ is set very close to the LBO limit because this is the only point where a semi-stable flame is possible for an extended period of time. These compositions blow out right as the EQ decreases. In the latter points that agree the EQ are set farther above the LBO limit and allowed to gradually approach the limit which might account for the better agreement in the model. Also important to note is that inlet temperatures to the PSR are taken from the injector inlet “air” thermocouple temperatures along with flow rates right before LBO. Despite slightly under predicted values for several compositions, this approach well predicts LBO for H_2/NG mixtures at 1 atm, consistent with results from Strakey et al. (2007).

An attempt was made to apply this same procedure to correlate H_2/CO mixtures with limited success. Figure 69 illustrates the shortcomings of using a PSR to predict LBO limits with H_2/CO . For high concentrations of CO the calculated values diverge from the experimental value and only attain reasonable agreement at concentrations of H_2 above 70%. The reason why a PSR cannot predict LBO behavior in H_2/CO mixtures is because the two timescales (τ_{res}, τ_{chem}) do not correspond to each other at high concentrations of CO. In other words, the “effective” residence time (τ_{res}) calculated from the experimental LBO limit in the PSR is not related to the chemical residence time (τ_{chem}). Therefore, the residence time at lean extinction will not be consistent with the one observed with added H_2 . This conclusion follows that of Zhang et al. [63] where the time scales of $H_2/CH_4/CO$ mixtures are all closely interrelated, except at high concentrations of CO.

Figure 68: Comparison of mechanisms for H2/NG for predicting lean blowout limits at 672K

Figure 69: H2/CO attempt at predicting lean blowout limits using a PSR at 672 K

4.2.1.2 Lean Blow Out Correlation via Damköhler Number

Many correlations found throughout the literature reduce to a Damköhler number where $\tau_{chem} = \alpha/S_L^2$. The example presented here uses the same data as the previous PSR example

except that the calculation for τ_{chem} is approached in a different manner. Establishing an interchange criterion to accommodate different fuel mixtures is inherent in the calculation for τ_{chem} , since it relies on thermal diffusivity and laminar flame speed. Damköhler number also requires a calculation of a flow timescale, τ_{flow} , which is taken here as the diameter of the injector (pre-sudden expansion recirculation length) divided by a corrected burned gas temperature ($U_b = U_o(T_{ad}/T_{unburned})$). This correction term accounts for the change in temperature due to combustion of fuels with varying concentrations of H_2 and change in unburned gas temperature from recuperated preheating. One drawback of this approach is that the laminar flame speed must be calculated for the mixture and there are often difficulties in obtaining convergence with lean H_2 mixture concentrations. Noble et al. (2006) observed similar difficulties and instead used a chemical residence time based upon a PSR extinction limit. Despite the practical limitations of the approach the methodology is still valid and warrants discussion.

The following steps are taken to correlate data from the experiment using a Damköhler number approach:

- 1) Obtain thermal diffusivity, α , of the fuel-air mixture using a transport properties calculator at LBO conditions
- 2) Calculate laminar flame speed, S_L , either via kinetics software such as CHEMKIN or obtain values from literature
- 3) Correct for burned gas velocity such that the properties of the combustible mixture are taken into account ($U_b = U_o(T_{ad}/T_{unburned})$)
- 4) Decide on a characteristic length scale applicable to the combustor in question. For the example demonstrated here the length scale is taken to be the diameter of the premixer.
- 5) Calculate the Damköhler number according to Equation 1 :

$$Da = \frac{\tau_{res}}{\tau_{chem}} = \frac{DS_L^2}{U_b \alpha} \quad (1)$$

Figure 70: Damköhler number calculation at LBO for H₂/CO

Figure 70 demonstrates the calculation of the Damköhler number for H₂/CO based upon LBO limits. The trend indicates that LBO occurs when the Damköhler number approaches unity which happens to be theoretical limit where LBO occurs in bluff body flames (Glassman 1996). Alternatively, this number can be presented as the limit where it is no longer possible to balance the rate of entrainment of reactants into the recirculation zone when viewed as a PSR. In addition to Damköhler number, both τ_{chem} and τ_{res} are shown to characterize the effects of the flow properties and laminar flame speed. τ_{res} remains relatively constant and is only influenced by the unburned gas temperature U_b due to the change in AFT. However, increases in U_b due to AFT increases are counteracted by the fact that LBO occurs at leaner conditions so the points change only marginally as the concentration of H₂ in the fuel mixture increases. Damköhler number at both 0% and 90% H₂ deviate the most due to the calculation of S_L at these points. Pure CO did not converge because GRI MECH was designed for hydrocarbon fuels meaning that an absence of H₂ in the mixture would not allow the kinetic mechanisms to simulate properly therefore a 99:1 ratio of CO to H₂ was used to circumvent the problem. Between 0% and 10% H₂ there is a considerable jump in S_L reflected by the decrease in τ_{chem} . This effect occurs as a result of additional H₂ creating a pool of OH^* radicals that accelerate the reaction $CO + OH^* \rightarrow CO_2 + H$. Again there is a counteracting effect from the extension of the lean extinction limit so that flame speeds remain relatively constant through the entire range of H₂ composition.

Correlation of the LBO limits for H₂/CO mixtures with Damköhler number is more effective than using a PSR reactor because of the practical limitations in establishing a reliable “effective” residence time in the PSR to calibrate the mixture at high CO concentrations. Evaluating the flame speed at high concentrations of CO also presents challenges as seen from the stark deviation between 0-10% H₂ in Figure 70. Despite some limitations at the lower end

this approach still remains the most consistent approach for evaluation of LBO of H_2/CO mixtures. The competing methodology of using a WSR for H_2/CO mixtures is only comparable at high concentrations of H_2 (Figure 69).

Figure 71: Damköhler number calculation at LBO for H_2/NG

Figure 71 presents the calculation of the Damköhler number for H_2/NG mixtures at the LBO limit. There is a reasonable correlation of LBO with Damköhler number shown by LBO occurring at a constant value of ~ 2 . τ_{chem} steadily increases over the range of 0-60% H_2 then begins to increase more dramatically from 60-100%. Flame speeds at LBO decrease with additional H_2 due to the extension of the LBO limit allowing for lower EQs. τ_{res} stays relatively constant only increasing slightly from a decrease in AFT. From a theoretical point of view, a decrease in flame speed is slowing the chemical reaction processes and the decreasing AFT is altering the burned gas temperature increasing mixing time, therefore LBO occurs when these residence times approach one another. However, since AFT and S_L are tied to the concentration of H_2 in the fuel they adjust τ_{chem} and τ_{res} accordingly so that LBO occurs at a constant Damköhler number.

Given the large order of magnitudes seen in Figure 70 and Figure 71 the precision of using Damköhler number in a practical sense comes into question. Stable operating conditions could coincide with the Damköhler number at LBO meaning that is not sensitive enough as a prediction tool. Results presented in Figure 68 show close agreement with EQ which is a more practical term in describing the operation of a gas turbine within its fuel space. To establish Damköhler number as a suitable LBO prediction tool a study of its sensitivity is performed below.

This analysis of the sensitivity to Damköhler number is taken from the point of view of a design engineer using the Damköhler number gain insight into the expected LBO behavior with addition of H_2 . First of all, the calculation to correlate with Damköhler number required knowing

different parameters such as, thermal diffusivity, preheat temperature, laminar flame speed, and mixing residence time all at the point of LBO. To reduce the number of variables needed in this prediction tool several assumptions are made under the premise that the combustor is in normal operation with a hydrocarbon fuel where conditions are likely to be known.

Assumptions

- 1) Damköhler number remains constant and is equal to the number predicted for the pure hydrocarbon fuel
- 2) Mixing residence time remains constant
- 3) Preheat temperature does not vary
- 4) Thermal diffusivity is that of the pure hydrocarbon fuel

With these assumptions in place the next step is to determine where each composition crosses the predicted Damköhler number at LBO. A simulation with CHEMKIN is run to identify which EQ yields the expected Damköhler number at LBO for each composition. Figure 72 shows relatively good agreement between actual and predicted values using this approach. Furthermore, the questionable sensitivity of the Damköhler number is addressed as values which deviate far from the expected value do not translate into a significant deviation in EQ. The reason for this behavior can be described by Figure 73 that plots how Damköhler number changes with varying EQ and composition. The horizontal line in Figure 73 is the expected Damköhler number at LBO for pure CO. Increasing $H_2\%$ means that the Damköhler number is more sensitive to changes in EQ due to the strong dependence on laminar flame speed. Consequently, at higher $H_2\%$ the curves lie closer to one another with a steeper slope making LBO more forgiving in its prediction values. With an increase in CO the flame speed is not affected as strongly by EQ and predicting the LBO limit becomes more difficult because EQ ratio spans a much wider range so the constant Damköhler number assumption does not hold as strongly. For mixtures with small amounts of H_2 (<5%) this methodology cannot calculate the expected LBO limit, but is still more effective than using a WSR. This limitation can be explained by the 5/95 and 1/99 H_2/CO ratios in Figure 73 where Damköhler number is hardly affected by increases in EQ. It appears that this is a result of the kinetic mechanism not capturing the effect of a small addition of H_2 into the CO mixture since the experimental LBO EQ for pure CO is not substantially far from that of the 10/90 H_2/CO (0.42 compared to 0.4, respectively). In summary, the stated assumptions produce a fit of the data that meets the goal of predicting LBO with a reasonable degree of accuracy over the range of 10-100% H_2 .

Figure 72: Actual versus expected LBO EQ for H_2/CO assuming Damköhler number=1.09

Figure 73: Damköhler number EQ LBO simulations H_2/CO

Having considered H_2/CO mixtures the next step is to consider if this method can accurately evaluate LBO limits for H_2/NG . Actual versus predicted results in Figure 74 indicate better agreement than data shown for H_2/CO in Figure 72. These results are comparable to the type of agreement seen in Figure 68 when using a WSR to predict LBO limits. Figure 75 illustrates that the reaction kinetics lend themselves to better agreement between experimental and predicted results for H_2/NG over H_2/CO because Damköhler number is more sensitive to changes in EQ for H_2/NG than H_2/CO at all H_2 concentrations between 0-100%. Therefore, obtaining an accurate prediction for H_2/NG is centered on calculating the correct Damköhler number. With H_2/CO the constant Damköhler number assumption makes it less forgiving to varying $H_2\%$ since small changes in Damköhler number translates to large changes in EQ. H_2/NG LBO is better predicted than H_2/CO using Damköhler number since it is strongly dependent on changes in EQ meaning that the constant Damköhler number assumption is more suitable for H_2/NG than H_2/CO .

Figure 74: Actual versus expected LBO EQ for H_2/NG assuming constant Damköhler number=2.91

Figure 75: Damköhler number EQ LBO simulations H₂/NG

Up to this point all the Damköhler number results have only been for the testing protocol of firing one injector at an EQ of 0.7 with NG and the other varying EQ and composition. The underlying assumption is that there is no interaction between the injectors because the barrier of additional dilution air from the unfired injectors. While this assumption may hold for FB, the comparison of LBO limits shows a small decrease (Figure 54, Figure 55). Also, there is an undeniable change in the preheating temperature and burnt gas stoichiometry from switching to two injectors fired with constant EQ and H₂ concentration. To further evaluate the robustness of the Damköhler number as a prediction tool, data taken for H₂/CO with a modified testing protocol are considered.

Results in Figure 76 for both injectors simultaneously varying H₂% and EQ indicates that Damköhler number changes by approximately one order of magnitude. This decrease in Damköhler number with increasing H₂ has also been shown by Noble et al. (2006) where values dropped by a factor of 100. One fundamental difference is that Noble et al. (2006) used τ_{chem} of a WSR and here it is calculated based on flame speed. The non-linear drop off in Damköhler at high concentrations of H₂ is not as pronounced as Noble's experiment, but still large enough to cause a clear deviation in the trend as shown by Figure 77. Considering that this data set does not include a LBO value for pure CO the Damköhler number of the 30% H₂ result is set constant for the prediction. Previous results with only one injector varied also illustrate a slight drop in Damköhler number with increasing H₂ although less pronounced than the case considered here. In contrast to the single injector varying case the result deviates at higher concentrations of H₂ instead of achieving a better fit. The lack of fit is due to the change in the operating range that affects the exponential dependencies of flame speed, Damköhler number, and EQ. With the two injectors simultaneously varied LBO occurs at lower EQs where flame speed is not as strongly dependent on EQ, therefore the range of EQ is wider and the constant Damköhler number assumption lends itself to larger deviations.

The change in Damköhler number with increasing H_2 may be due to preferential diffusion effects that lead to appreciable changes in the turbulent flame speed of mixtures. Lewis number describes the ratio of thermal to species diffusivity which has been identified as an important parameter influencing flame structure and stability. Addition of H_2 significantly decreases the flame Lewis number meaning that reactants diffuse more rapidly toward the reaction zone in comparison to the amount of thermal energy loss through conduction back to the fresh reactants leading to an increase in reaction zone temperature (Lieuwen and Yang 2009). Results depicted in Figure 77 suggest the deviation at higher H_2 concentrations is tied to preferential diffusion effects increasing reaction rates generating larger chemical residence time and lowering the Damköhler number at LBO. To correct for this deviation of EQ a similar approach to Noble (2006) is taken where EQ ratio is adjusted by a ratio of diffusivities. For this work the following Lewis number for a mixture is defined as:

$$Le_{mix} = \frac{\alpha}{\sum_{k=fuel} A_k D_{km}} \quad (2)$$

Where A_k is the percentage of heat release due to the fuel k relative to that of the entire mixture. Adjustment to the EQ ratio is suggested to be in the form of:

$$\Delta\phi = C * \ln(Le) \quad (3)$$

$C = 0.02$ yielded the corrected Lewis number fit shown in Figure 77 that corrects for the deviation in the predicted trend with increasing H_2 concentration. Although this correction produced a better fit of the data (root mean squared error of 0.007 compared to 0.019), it adds complexity to the prediction methodology. The use of the correction factor is justified past H_2 concentrations of 50% where the residuals begin to significantly increase. Another point to consider in using the correction factor is the accuracy needed in the EQ for stable combustion. Maximum deviation is at 90% H_2 where the residual is 0.03, but this value may be large relative to the EQ operating range.

In summary, the use of the Damköhler number as a predictive methodology is viable if the previously stated assumptions are made. These assumptions circumvent the need for LBO conditions and require only the conditions of the combustor operating on a hydrocarbon fuel. One limitation was identified with H_2/CO at very lean conditions with high H_2 concentration where the constant Damköhler assumption led to a deviation in actual versus predicted values. A correction factor involving the Lewis number was applied and predicted values show a reasonable fit to experimental data. In addition to the identification of limitations, studies of the sensitivity of the Damköhler number to the EQs in question show that it is capable of capturing LBO behavior with varying fuel compositions. Although the Damköhler number at LBO varied based upon the protocol of the experiment and fuel types, the methodology used in the different scenarios was able to produce a predictive fit to the experimental data, thus making the Damköhler number a suitable candidate as a fuel interchange parameter for transitioning gas turbines to operate with high H_2 content fuels.

Figure 76: Damköhler number calculation at LBO for H_2/CO mixtures with two injectors simultaneously varied

Figure 77: Actual versus expected LBO EQ for H_2/CO mixtures with two injectors simultaneously varied assuming constant Damköhler number=0.60

4.3 Flashback

4.3.1 Axisymmetric

4.3.1.1 Critical Gradient Framework

The theory of laminar boundary layer FB (BLF) as proposed by Lewis and von Elbe defines a “critical” velocity gradient as the velocity gradient at the wall when BLF occurs (Lewis and Von Elbe 1943). This critical gradient is defined from the flame’s ability to propagate upstream through the boundary layer only if the burning velocity (S_L) exceeds the local flow velocity (V). However, the wall provides quenching effects that resists flame propagation near the wall. The quenching distance is defined as that distance from the wall where a reaction can no longer exist. Shown in Figure 78, the penetration distance, d_p is defined as the distance from the wall to the point where the flow velocity profile tangents with the burning velocity profile. It also approximates the position where the burning velocity starts to decrease due to the quenching effect of the wall (von Elbe and Mentser 1945). Therefore when the quenching distance (d_q) exceeds the penetration distance (d_p), FB cannot occur. These relationships are summarized in E- 1 and E- 2. Given that the velocity profile can be assumed to be linear near the wall, E- 3 results from the combination of E- 1 and E- 2. E- 3 provides a theoretical prediction for the critical velocity gradient that can be determined based on inlet conditions. E- 4 to E- 8 show the derivation of turbulent boundary layer velocity gradient (g). g is defined in E-4. According to the definition of shear stress, g is also the ratio of shear stress τ to dynamic viscosity μ . For a flow $Q = \pi R^2 \bar{u}$ through a tube with a length of L and a diameter of R , the shear stress at the wall (τ_o) can be obtained by measuring the pressure gradient along the tube (E- 5). In a turbulent flow, the relationship between the pressure gradient and the flow rate is usually determined empirically. The laws of flow resistance address this connection, and the dimensionless coefficient of resistance, λ^* , is defined in E- 6. In 1911, H. Blasius developed an empirical equation for λ^* (E- 7) after analyzing various experimental results using Reynolds’ law of similarity (Schlichting and Gersten 2004). Combining these equations leads to an expression for the velocity gradient in the boundary layer of a turbulent flow through a tube in terms of bulk flow parameters as shown in E- 8. The derivation provides insights not evident from the equation itself. For example, the bulk velocity in E- 8 is derived from the pressure gradient (E- 6) and the coefficient of resistance (E- 7). But the equations for these two parameters do not directly account for temperature changes, which is a key focus of the current research. Additionally, the temperature varies across the diameter of the tube as a result of preheating and heat transfer through the injector wall. Accordingly, the velocity gradient can be modified to account for the temperature effects as, the elements in E- 8 are based on a specified temperature. For example, as a result of preheat, E- 9 shows a straightforward revision to the flow bulk velocity. The kinetic viscosities and densities are also updated accordingly. It is noted that these treatments assume heat loss is negligible and the temperature is uniform across the tube exit.

Figure 78 Schematic of the definition of the critical velocity gradient (Lewis and Von Elbe 1943)

$$V \sim S_L \quad \text{E- 1}$$

$$d_p \sim d_q \quad \text{E- 2}$$

$$g_c \equiv \frac{V - 0}{d_p} \sim \frac{S_L}{d_q} \quad \text{E- 3}$$

$$g \equiv \frac{\partial V}{\partial y} = \frac{\tau_0}{\mu} \quad \text{E- 4}$$

$$\tau_o = \frac{p_1 - p_2}{L} \frac{R}{2} \quad \text{E- 5}$$

$$\frac{p_1 - p_2}{L} \equiv \frac{\lambda^*}{d} \frac{1}{2} \rho \bar{u}^2 \quad \text{E- 6}$$

$$\lambda^* \equiv 0.3164 \left(\frac{\bar{u} d}{\nu} \right)^{-1/4} \quad \text{E- 7}$$

$$g = \frac{0.03955 Re^{0.75} \bar{u}}{D} = \frac{0.03955 \bar{u}^{1.75} \rho^{0.75}}{\mu^{0.75} D^{0.25}} \quad \text{E- 8}$$

$$V = V_{standard} \frac{T_{inlet}}{T_{standard}} \quad \text{E- 9}$$

4.3.1.1.1 Quenching distance (d_q)

The quenching distance and whether it is greater than the boundary layer thickness and/or penetration distance is significant in the determination of whether FB will occur as discussed above. According to Turns et al. (Turns 1996), quenching distance can be defined as that diameter of a circular tube where a flame can no longer propagate and extinguish. The criterion for the situation in which a flame is quenched by a cold wall is further defined as when the rate of heat release by chemical reactions inside the slab is less than the rate of heat loss through the slab by conduction. As a result, the expression of quenching distance is developed as shown by E- 10, where T_u and T_w denote the inlet and wall temperature, respectively. The term “b” is an arbitrary constant introduced by Turns et al. (Turns 1996) that is defined as the ratio of the local temperature gradient near the wall to that averaged through thermal boundary layer. In the current research, the constant $2\sqrt{b}$ is assumed to be 1. The tip temperature, T_{tip} , is also taken as the wall temperature when calculating the quenching distance.

$$d_q = \frac{2\alpha\sqrt{b}}{S_L} \sqrt{\frac{AFT - T_w}{AFT - T_u}} \quad \text{E- 10}$$

4.3.1.2 Statistical Model

To add further insight into the parameters that impact FB, analysis of variance (ANOVA) was carried out. Only statistically significant terms are retained in the correlation based on those with p-value less than 0.0001. As the critical velocity gradient, g_c , is a traditional way to correlate boundary layer FB (Bollinger and Edse 1956; Caffo and Padovani 1963; Khitrin, Moin et al. 1965; Eichler, Baumgartner et al. 2011; Eichler, Baumgartner et al. 2012), it was selected as the response for flashback tendency for the statistical model.

The first statistical model (E- 11) expresses g_c in terms of fuel composition, inlet temperature, and AFT. The model does not account for material effects and yields an R^2 value of 0.7901. Figure 79 compares the predicted values (E- 11) with the measured values. It is noted that the data from the stainless steel and quartz tube experiments diverge, indicating that material effects are significant. With this model, the quartz data are underestimated while the stainless steel tube data are overestimated. This reveals that quartz injectors result in higher FB propensity than in stainless steel injectors.

To further quantify material effects, analysis of variance was performed separately for quartz (E- 12) and stainless steel tubes (E- 13). The correlations are significant with an R^2 of 0.9702 and 0.9485 for quartz and stainless steel, respectively. As seen in Figure 80, the prediction of the statistical model is much better than without accounting for the injector material.

Table 8 Units for parameters correlated

	Unit		Unit
Fuel Composition	[-]	EQ	[-]
Temperature	[K]	S _L	[cm/s]
Thermal Diffusivity	[cm ² /s]	d _q	cm

$$g_c = (283.12H_2 + 23.07CO - 51.50CH_4 + 314.13H_2 \cdot CH_4 + 0.076H_2 \cdot T_{inlet} - 0.277H_2 \cdot AFT)^2 \quad \text{E- 11}$$

$$g_{c_quartz} = (324.45H_2 + 31.91CO - 75.43CH_4 + 416.75H_2 \cdot CH_4 + 0.07H_2 \cdot T_{inlet} - 0.32H_2 \cdot AFT)^2 \quad \text{E- 12}$$

$$g_{c_stainless} = (224.18H_2 + 9.36CO - 45CH_4 + 232.63H_2 \cdot CH_4 + 0.0331H_2 \cdot T_{inlet} - 0.213H_2 \cdot AFT)^2 \quad \text{E- 13}$$

 Figure 79 Model predicting g_c without consideration of material effects

It was noted that the tip temperature for the quartz injector was higher than that for the stainless steel injector, all other parameters being equal. This difference between the two injector materials is hypothesized to be a result of the different thermal properties of the two materials. Therefore, as a strategy to incorporate the effects of materials, the tip temperature is selected as a parameter for inclusion in the ANOVA. E- 14 is the resulting model when incorporating the factor of tip temperature for various inlet temperatures. E- 15 represents a simplification for only non-preheated cases.

Figure 80 Models predicting g_c : quartz tube (blue diamonds) and stainless tube (red triangles)

Figure 81 and Figure 82 show that the correlations of E- 14 and E- 15 better predict the critical velocity gradient compared to E-11 as shown in Figure 79. The R^2 values are 0.9108 and 0.9717 for E- 14 and E- 15, respectively. It is also noted that AFT was *not found* to be significant and is thus not included in the correlations. Thus introducing the tip temperature as a factor reasonably captures the material effect. However, that the correlation predictive power is improved when only non-preheated cases are analyzed suggests some phenomena are still missed in this model.

$$\begin{aligned}
 g_c = & (210.25H_2 - 35.23CO - 149.97CH_4 \\
 & + 0.135H_2 \cdot T_{inlet} \\
 & - 0.783H_2 \cdot T_{tip} \\
 & + 0.315CH_4 \cdot T_{tip})^2
 \end{aligned}
 \quad \text{E- 14}$$

$$\begin{aligned}
 g_c = & (261.74H_2 - 30.69CO - 188.38CH_4 \\
 & - 0.8H_2 \cdot T_{tip} + 0.424CH_4 \\
 & \cdot T_{tip})^2
 \end{aligned}
 \quad \text{E- 15}$$

Figure 81 Models predicting g_c with tip temperature instead of inlet temperature

Figure 82 Models predicting g_c with tip temperature for non-preheated cases

The statistical models developed correlate the FB propensity, g_c , with operational inputs (i.e., fuel compositions, inlet temperature, tip temperature, and AFT) well. The tip temperature is found to effectively capture the injector material effect, which verifies the connection between thermophysical properties and FB propensity. However, the statistical model is limited with respect to providing insight into the physical nature of FB. Therefore, a deeper physical analysis is necessary and is addressed in the following section.

4.3.1.3 Physical model

While the previous correlations are useful as an indicator of how the factors studied impact FB, they do not yield a physical interpretation. As a result, it is desired to develop a model based more on the physical phenomena that are known to influence FB. The purpose of a physics based model is to establish the relationship between the FB propensity and various physical, thermal, geometric, and chemical properties of the system such that the effect of changing fuel composition on FB propensity can be better understood. To maintain consistency with previous work, g_c is again selected as the model response and the inputs to the model are various physical-chemical parameters, such as laminar flame speed (S_L), quenching distance (d_q), thermal diffusivity (α), etc. The following sections will discuss in detail the various model inputs considered as well as the developed correlation.

4.3.1.3.1 Single parameter model (laminar flame speed)

The laminar flame speed is an intrinsic parameter of a fuel/mixture and is intuitively connected to flashback propensity as it can be, in principle, used to estimate flame propagation rates. It is a function of fuel composition, AFT, and unburned temperature. In this analysis, the laminar flame speed is calculated using the PREMIX code package (Kee RJ 1985) within Chemkin Pro release 15082. The kinetic mechanism used is GRI 3.0 (Gregory P. Smith).

Laminar flame speeds were calculated using the tip temperature and the preheat temperature as the inlet temperature input to PREMIX. This was done in an effort to identify the significance this would have on correlating the critical velocity gradient with the laminar flame speed. Table 9 summarizes the R^2 values for linear correlations between laminar flame speed and critical velocity gradient. The critical velocity gradient was also calculated using both the tip temperature and preheat temperature (i.e., to calculate parameters such as viscosity and density that are used to determine the critical velocity gradient). As seen in Table 9, the inlet temperature based laminar flame speed ($S_{L_{inlet}}$) cannot correlate the g_c results. However, the

tip temperature based flame speed (S_{L_tip}) does a reasonable job. Furthermore, the g_c based on tip temperature (g_{c_tip}) shows a slightly better correlation than the inlet temperature based g_c (g_{c_inlet}).

Table 9 Comparison of temperature selection for S_L and g_c calculations

R^2	S_{L_inlet}	S_{L_tip}
g_{c_inlet}	0.0895	0.8105
g_{c_tip}	0.0188	0.8432

E- 16 is the linear correlation between g_{c_tip} and S_{L_tip} corresponding to the R^2 value of 0.8432 shown in Table 9. Figure 83 shows the predicted values from E- 16 versus the actual values. Although some scatter is evident, this correlation predicts the critical gradient fairly well. This result supports the observation and intuition that FB propensity is strongly dependent on the flame speed, but it also illustrates that the flame speed used must be calculated using the appropriate temperature.

$$g_{c_tip} = -6055.28 + 174.73S_{L_tip}$$

E- 16

Figure 83 Model of single parameter correlation (laminar flame speed based on tip temperature)

To further assess systematic contributions to the scatter shown in Figure 83, Figure 84 shows the g_{c_tip} versus S_{L_tip} , for the various cases tested. As shown, significant variation results from differences in fuel composition and injector material. As found from the analysis of variance, the effect of AFT is not significant upon inspection of Figure 84. This indicates that the laminar flame speed calculation is taking the AFT variation into account sufficiently.

As the laminar flame speed reasonably correlates g_c for a given material, separate correlations were developed for each injector material as shown in E- 17 and E- 18. These correlations yield much better R^2 values, 0.9597 and 0.9248 for E- 17 and E- 18, respectively

than that for the material independent correlation shown in E- 16. These correlations show that the laminar flame speed based on tip temperature can predict the FB propensity fairly well for a given injector material. This is somewhat unexpected since the behavior of turbulent FB is predicted using a laminar flame property. One potential explanation is that the use of tip temperature as an input to the laminar flame speed calculation includes information that results from the turbulent heat transfer and combustion.

Figure 84 g_c versus the laminar flame speed calculated with tip temperature

$$g_{c_quartz_tip} = -3998.8 + 197.97S_{L-tip} \quad \text{E- 17}$$

$$g_{c_stainless_tip} = -957.35 + 98.76S_{L-tip} \quad \text{E- 18}$$

4.3.1.3.2 Multiple Parameter Correlations

The correlation of g_c and laminar flame speed appears promising, however, the effects of quenching (which also includes injector material properties) are not accounted for. In order to capture these effects other factors were introduced as inputs (i.e., thermal diffusivity and quenching distance), and an ANOVA was again performed. Additionally, all parameters included in the analysis were both based on tip temperature and inlet temperature. All terms that yielded p-values greater than 0.0001 were eliminated. The parameter elimination process revealed that only terms that were calculated using tip temperature were statistically significant. This reaffirms the significance of the tip temperature.

E- 19 presents the resulting correlation which has an R2 value of 0.9367. All parameters are normalized by reference values shown in Table 10. Figure 85 illustrates the superior performance of the new model compared to those presented above.

$$\begin{aligned}
 g_{c_tip} = & (155 + 122.9 \frac{\alpha_{tip}}{\alpha_0} + 1340.8 \frac{d_{q_tip}}{d_{q0}} - 212 \frac{T_{tip}}{T_0} - 49 \frac{S_{L_tip}}{S_{L0}} \\
 & + 74 \frac{\alpha_{tip} T_{tip}}{\alpha_0 T_0} - 8549 \frac{d_{q_tip} S_{L_tip}}{d_{q0} S_{L0}} \\
 & - 31.1 \frac{T_{tip} S_{L_tip}}{T_0 S_{L0}})^2
 \end{aligned}
 \quad \text{E- 19}$$

$$g_{c_tip} = 92.28 \left(\frac{\alpha_{tip}}{\alpha_0} \right)^{2.04} \left(\frac{S_{L_tip} d_{q0}}{S_{L0} d_{q_tip}} \right)^{0.328}
 \quad \text{E- 20}$$

Table 10 Definition of reference values

	Definition	Value
S_{L0}	Maximum laminar flame speed of Methane	44.8cm/s(Glassman 1996)
d_{q0}	Quenching distance of CH ₄ /Air at EQ=1	0.25cm(Barnett and Hibbard 1957)
α_0	Thermal diffusivity of air at 1 atm and 300K	22.5E-6 m ² /s (Incropera 2002)
T_0	Ambient temperature	300K

Figure 85 Comparison of actual values v.s. predicted values by multi parameter model (E- 19)

The model in E- 19 correlates the data well using physics based parameters. However, the physical meaning of the correlation itself is not obvious. As a result, additional parameter

analysis was carried out to refine the model in a manner that allows more straightforward interpretation.

Given the relationship (see E- 3) between the critical velocity gradient, the laminar flame speed, and the quenching distance as proposed by Lewis and von Elbe (Lewis and Von Elbe 1943), another form of a physics based model was developed. The laminar flame speed and quenching distance are combined, generating the model with an R^2 value of 0.895, shown by E- 20. The predicted and actual g_c values are shown in Figure 86

Figure 86 Comparison of actual values v.s. predicted values by multi parameter model (E- 20)

E- 20 indicates a better correlation than E- 16. However, evidence of material effects can still be seen from the scatter in the results. Recalling the models developed previously (shown in Figure 81 and Figure 83), the material influence was captured but not fully. This leads to the conclusion that the large difference in flashback propensity between steel and quartz may not be explained by the tip temperature alone. Another effect originating from the material itself may be present, e.g. a third-body or catalytic effect.

The expression in E- 20 allows interpretation that is consistent with intuition and previous understanding of FB. For example, smaller quench distances indicate higher FB propensity. Mixtures with higher diffusivity will be more prone to FB. And mixtures with higher flame speeds will be more prone to FB. Again, it is emphasized that use of the correct mixture temperatures for assessing these properties is very important. For practical systems, ascertaining the burner tip temperature may be difficult. However it could be estimated from CFD, inlet temperatures, or other means. It also provides an insight that FB prevention may be achieved by cooling the burner rim. To help explore this, the next section presents a heat transfer model that may allow a mechanism for ascertaining the tip temperature based on other known boundary conditions.

Finally, it should be pointed out that the above correlations were developed based on the data collected from the specific burner setup, thus they may not be universally applicable. To investigate such limitations, parallel research has been carried out (Duan, Shaffer et al. 2013).

4.3.1.3.3 Heat Transfer Analysis of Material Effects

The previous statistical and physical analyses affirm that the injector tip temperature and injector material affect FB propensity significantly. It was observed that FB occurred more readily with a quartz injector and that the tip temperature of the quartz injector at FB was higher

than the stainless steel injector (Figure 87). As a result of the observed effect of injector material on FB, a conceptual heat transfer model is developed to more thoroughly investigate the material effect on FB and injector tip temperature. For this initial investigation, pure hydrogen cases without preheat are considered.

Figure 87 Tip temperature of pure hydrogen flame without preheating

Figure 88 characterizes the heat transfer within the injector wall. The external heat input, i.e. from the enclosure plate and flame, $\dot{Q}$, is balanced by the forced convection, Q_{conv} , and the conduction downward through the solid wall, Q_{cond} . E- 21 shows the energy balance equation. The natural convection is negligible compared to forced convection. E- 22 defines the time rate of change of the system (control volume) energy. As equilibrium is reached, this term approaches zero. E- 23 and E- 24 present expressions for conduction and convection, respectively, where T_0 denotes the ambient temperature. In the current analysis, the inlet temperature is also assumed to be same as that of ambient. Given the steady state analysis, E- 21 through E- 25 are combined to get the ordinary differential equation, shown by E- 26. Using the boundary condition in Table 11 an analytical solution can be found for this ordinary differential equation as shown in E- 27. For a given fuel composition, flow rate and equivalence ratio, the convective coefficient h and heat input, $\dot{Q}$ are both constant. Therefore, according to E- 28, with the third boundary condition applied, this relationship results: $(T_{tip} - T_0) \propto 1/\sqrt{\delta k}$. This indicates that, with larger thermal conductivity and wall thickness, the tip temperature will be smaller. Additionally, given that the tip temperature is proportional to the square root of the thermal conductivity, the tip temperature is not directly proportional to the thermal conductivity.

Figure 88 schematic of the heat transfer within injector wall

$$\dot{Q} = \dot{Q}_{cond} - \dot{Q}_{conv} \quad \text{E- 21}$$

$$\dot{Q} = CA_{sect}(x_2 - x_1)\rho \frac{\partial T}{\partial t} \quad \text{E- 22}$$

$$\dot{Q}_{cond} = -kA_{sect} \left[\frac{\partial T}{\partial x} \Big|_{0 \rightarrow 1} - \frac{\partial T}{\partial x} \Big|_{1 \rightarrow 2} \right] \quad \text{E- 23}$$

$$\dot{Q}_{conv} = 2\pi R_1 h(x_2 - x_1)(T - T_0) \quad \text{E- 24}$$

$$A_{sect} = \pi R_1^2 - \pi R_2^2 = \pi(R_1 - R_2)(R_1 + R_2) \approx 2\pi R_1 \delta \quad \text{E- 25}$$

$$\frac{\partial^2(T - T_0)}{\partial x^2} - \frac{h}{\delta k}(T - T_0) = 0 \quad \text{E- 26}$$

Table 11 Boundary condition employed for the heat transfer analysis

$x \rightarrow \infty$	$T = T_0$
$x \rightarrow 0$	$T = T_{tip}$

$x \rightarrow 0$	$-kA_{sect} \left. \frac{\partial T}{\partial x} \right _{x=0} = \dot{Q}$
-------------------	---

$$(T - T_0) = (T_{tip} - T_0)e^{-x\sqrt{\frac{h}{\delta k}}} \quad \text{E- 27}$$

$$\dot{Q} = kA_{sect} \left. \frac{\partial T}{\partial x} \right|_{x=0} = 2\pi\sqrt{\delta kh}(T_{tip} - T_0) \quad \text{E- 28}$$

4.3.1.4 Summary and Conclusion

The current study carried out experimental study to survey the various parameter effects on FB propensity, including fuel composition, AFT, inlet temperature and injector material. The results were analyzed using statistics based tools. Further physical analysis was conducted and it is followed by a qualitative heat transfer analysis. Several observations have been made:

1. Better correlations can be obtained if the tip temperature is used as the representative temperature (inlet temperature).
2. The physical correlations suggest that the FB propensity is strongly influenced by the laminar flame speed when calculated based on the injector tip temperature. The correlation was improved by adding additional parameters.
3. Both in the statistical and physical models, the discrepancy caused by injector materials was mitigated substantially by employing tip temperature.

Based on these findings, the following conclusions are drawn:

1. The FB propensity strongly depends on tip temperature, which is determined by thermal physical properties of the burner material.
2. Proper temperatures should be chosen to predict FB propensity. Critical velocity gradient can be predicted fairly well using laminar flame speed calculated using tip temperature.

4.3.2 Full Annular

4.3.2.1 Flashback Correlation via Turbulent Propagation Rate

Predicting FB in laminar flows has been thoroughly researched with an established theory to explain the phenomena. This theory does not translate over to turbulent flows and there is still debate on how FB occurs. Difficulty lies in determining a turbulent flame speed since it is coupled to turbulent flow conditions that vary in space and time. In addition, a consistent definition of turbulent flame speed has yet to be discovered and is usually defined by the flame stabilization mechanism. Often assumptions are made based upon the turbulent combustion regime that the reaction encompasses and correlations of turbulent flame speed pertain only to that region. To satisfy an industry need for valid turbulent flame propagation rates designers are turning to empirical formulations from trends of data in the literature. Often these formulations have significant limitations making them valid in specific combustion regimes on a

single fuel type. Furthermore, there is no specific link of the turbulent flame speed to the various FB mechanisms such as, core or boundary layer.

The methodology explored in this section utilizes turbulent flame speeds in the literature applied to FB conditions within the annular combustor operating on H₂/CO mixtures. H₂/NG mixtures are not explored because of the observation/suspicion that FB occurs as a result of instabilities near the LBO limit. Turbulent flow properties are assumed from typical measured values for similar burners found in the literature. Research emphasis into this methodology is focused on linking turbulent flame speed to FB conditions with varying fuel composition. Again, it is important that the methodologies be developed around information readily available from commercial gas turbines. For example, requiring visualization of the flame is not practical to commercial combustors. Steps to this approach are as follows:

- 1) Establish turbulent flow properties of the reaction zone either through CFD, experiments, or reasonable assumptions
- 2) Obtain a reliable means of correlating turbulent flame speed S_T for different burner geometries
- 3) Determine a link from S_T to FB mechanisms (core, boundary layer, CIVB, instability induced)
- 4) Investigate the effects of fuel composition

Knowledge of turbulent flow properties depends on which correlations are used for S_T . Most correlations in the literature require turbulence intensity u' and some call for turbulent Reynolds number Re_T . S_T correlations in this section focus on experimental data presented by Venkateswaran et al. (2011). This experimental work is investigated because parameters affecting S_T are systematically varied for different H₂/CO ratios with a turbulent Bunsen flame. Although the authors show how results compare to other existing correlations, there is no empirical correlation. To overcome this limitation, response surface methodology is used to generate a statistical model based on experimental data.

Creating a response surface methodology was accomplished using the design of experiments software, Design-Expert® by Stat-Ease, Inc. Results create a statistical correlation between S_T/S_L (response) and various parameters (input): H₂%, bulk velocity U_o , u'/S_L , and tube diameter. Figure 89 demonstrates an example of a typical response surface generated by the software showing the interaction of u'/S_L and H₂% at a particular U_o . Figure 90 highlights that the model is well suited to the experimental data without any values, or group of values, not easily predicted by the model. A statistical expression generated from the data is shown in Figure 91 for the 20 mm diameter which calculates S_T/S_L for FB in the annular combustor. The correlation developed by Daniele et al. (2011) will be used to calculate S_T .

$$\frac{S_T}{S_L} = a \left(\frac{u'}{S_L} \right)^{0.63} \left(\frac{L_T}{\delta_L} \right)^{-0.37} \left(\frac{P}{P_o} \right)^{0.63} \left(\frac{T}{T_o} \right)^{-0.63} ; a = 337.5$$

It must be noted here that this correlation does not depend on laminar flame speed. This conclusion results from the fact that the quenching distance is equal to the thermal diffusivity

divided by laminar flame speed, $\delta_L = \frac{\alpha}{S_L}$. If this is substituted into the above expression, the following results:

$$S_T = a(u')^{0.63} \left(\frac{L_T}{\alpha}\right)^{-0.37} \left(\frac{P}{P_0}\right)^{0.63} \left(\frac{T}{T_0}\right)^{-0.63}$$

This expression is independent of laminar flame speed. In spite of this, the analysis was completed because this expression still has some variation with fuel composition through the thermal diffusivity and it was developed using several different fuel compositions.

Several assumptions are listed below which are necessary to apply the correlation and the response surface to FB data.

Assumptions

- 1) u' is considered to be 10% of U_o
- 2) Integral length scale l_o is equal to the one determined by Daniele et al. (2011)
- 3) Burner diameter effect between 20 mm for Venkateswaran et al. (2011) and 25 mm for Capstone OEM injector is negligible

Figure 89: Response surface created from experimental data of Venkateswaran et al. (2011)

With these assumptions, the turbulent premixed combustion regime the flame resides in can be determined to evaluate whether the correlations coincide with the regime in which the FB data exist. FB for H_2/CO two injector varied configuration is characterized by strongly wrinkled

flames in the Borghi diagram depicted in Figure 92. All points appear confined to a small region in the diagram without any large influences. FB results from Daniele et al. (2009) are also included in the diagram illustrating that their results for a premixed jet flame burner spans a range of combustion regimes from strongly wrinkled flames through thin reaction zones ending in flamelets in eddies. The trend is that pressure drives the results upwards along the u'/S_L axis due to the decrease in S_L from pressure (see Figure 103). Decreasing values along the l_o/δ_L axis is again mainly a result of decreasing S_L . Therefore, since flame thickness can be approximated by the thermal diffusivity divided by the laminar flame speed of the mixture, a decrease in S_L means greater flame thicknesses. Venkateswaran (2011) data are also shown in Figure 92 depicting that they span the region between strongly wrinkled flames to thin reaction zones. Note that these data are not FB data and only results of turbulent flame speed measurements. The experiment designed for these measurements revolved around keeping S_L constant, therefore movement along the u'/S_L axis is due to increases in u' from greater bulk velocities.

Figure 90: Graph of predicted response values versus the actual response values

$$\begin{aligned}
& \text{Diameter} \quad 20\text{mm} \\
& S_T/S_L = \\
& +5.27288 \\
& -0.16269 * \%H_2 \\
& -0.028632 * \text{Bulk Velocity (m/s)} \\
& -0.031473 * u'/S_L \\
& +4.22787\text{E-}003 * \%H_2 * \text{Bulk Velocity (m/s)} \\
& +3.87055\text{E-}003 * \%H_2 * u'/S_L \\
& +6.54489\text{E-}004 * \text{Bulk Velocity (m/s)} * u'/S_L \\
& +2.48323\text{E-}003 * \%H_2^2 \\
& +5.66076\text{E-}003 * \text{Bulk Velocity (m/s)}^2 \\
& +0.014902 * u'/S_L^2 \\
& -8.19835\text{E-}005 * \%H_2 * \text{Bulk Velocity (m/s)} * u'/S_L \\
& -6.15043\text{E-}006 * \%H_2^2 * \text{Bulk Velocity (m/s)} \\
& -2.72118\text{E-}006 * \%H_2^2 * u'/S_L \\
& -2.50323\text{E-}005 * \%H_2 * \text{Bulk Velocity (m/s)}^2 \\
& +4.68454\text{E-}005 * \%H_2 * u'/S_L^2 \\
& -8.22047\text{E-}004 * \text{Bulk Velocity (m/s)}^2 * u'/S_L \\
& +8.69231\text{E-}004 * \text{Bulk Velocity (m/s)} * u'/S_L^2 \\
& -1.31982\text{E-}005 * \%H_2^3 \\
& +1.40094\text{E-}004 * \text{Bulk Velocity (m/s)}^3 \\
& -4.78399\text{E-}004 * u'/S_L^3
\end{aligned}$$

Figure 91: Statistical expression for S_T/S_L with 20mm tube based on data from Venkateswaran et al. (2011)

The next step in the approach is to apply the correlations for S_T/S_L on the FB data to establish the link between S_T and FB. High concentrations of H_2 at atmospheric pressure lead to large S_L and consequently a small value for u'/S_L . Figure 93 portrays a response surface for an averaged u'/S_L where the standard deviation is 0.11 for all H_2 concentrations. S_T/S_L at low u'/S_L values is a strong function of bulk velocity meaning that the appreciable increase in the burning rate is due to turbulence and not additional H_2 .

Figure 92: Borghi diagram of FB data for Daniele et al. (2009), H₂/CO two injector varied data, and S_T measurements from Venkateswaran (2011)

A green line across the response surface indicates where H₂/CO mixtures with two injectors varied FB data lies. Corresponding 2-D plots in Figure 93 display FB results with respect to either H₂% or bulk velocity. These plots illustrate that without the 3D response surface the decrease in S_T/S_L may be misinterpreted as dependent on H₂% where in fact bulk velocity is the key factor. What the model fails to capture is that decreases in bulk velocity are an indirect result of increased H₂%. Bulk velocity within the combustor is tied directly to the preheat temperature of the incoming recuperated air, therefore a reaction with lower AFT creates lower bulk velocities. Reactions with high H₂ concentrations have lower AFTs at FB meaning that bulk velocities are lower and more prone to FB. Recall that the test protocol is to ignite at a specific H₂ concentration near the lean operating limit, for that reason the bulk velocity is lower and increases only as a function of AFT. Then it is expected that increased H₂ concentration will cause FB to occur at lower S_T/S_L as shown in Figure 93. Support for FB dependency upon AFT is presented in Figure 94 showing linear dependency of FB upon AFT that diminishes as the H₂ concentration increases. The linearity of the plot promotes the idea that lower AFT decreases preheat temperatures which lowers the bulk velocity of the injector making it more prone to FB because AFT is a direct function of preheat. Main conclusion of this result is that variables which affect bulk velocity will have the greatest impact on the FB propensity for the response surface generated from experimental FB data.

Figure 93: Response surface generated for H₂/CO two injector varied FB with averaged u'/S_L

Figure 94: Turbulent flame speed at FB dependency on AFT

Given the complex interactions between a variety of parameters that affect FB, an index which quantifies FB propensity would be a useful design tool. Conventional wisdom is that higher turbulent propagation rate translates to higher FB propensity. However, S_T/S_L is not an all encompassing factor to measure FB propensity, merely another variable with its own interactions. Until a theory to describe turbulent FB physically is developed, empirical formulations can serve the industry need. A FB propensity index should be developed around variables known to influence FB such as,

$$FB = f\left(\frac{S_T}{S_L}, u', U_o, T_b, P\right) \quad (4)$$

These variables are plotted against $H_2\%$ concentration in Figure 95 all demonstrating a slight decrease at approximately identical slope, with the exception of u'/S_L . Each of these variables interact with one another, but the goal is determine how each of them are affected by the addition of H_2 and how such changes affect FB. Creating a robust index of these variables relies on accurate determination of interactions between these factors so that a robust FB index can be developed. An example of a simple FB propensity index is given as,

$$FB_{index} = \frac{S_T}{u'} * \frac{T_{ad}}{T_{unburned}} * \frac{U_o}{U_{max}} \quad (5)$$

This index uses the interaction of S_T/S_L and u'/S_L to obtain the first term of Equation 5 obtained from the response surface. The second term of Equation 5 is derived from the observation of the dependency of FB on AFT, especially for varying preheats. The last term in Equation 5 is

included based on experimental results and large dependency seen in the response surface shown in Figure 93. Results for FB using this index are plotted in Figure 96 demonstrating a linear fit with a $R^2 = 0.95$. While this index has severe limitations such as, no effect of pressure, developed around one data set, applicable to one combustion regime, it still remains promising as a methodology to quantify FB.

Figure 95: Parameters influencing FB as a function of H_2 concentration

Figure 96: Flashback propensity index

The FB propensity index presented in Figure 96 quantifies the likelihood of FB within each data set. However, a correlation that collapses the data in Figure 96 would provide a more comprehensive index of FB propensity amongst the test protocols and preheat levels. To achieve a collapsed form, the first step is to realize that the weighting of terms in Equation 5 are arbitrarily predetermined when normalizing. An adjustment is made to each term in the index to obtain Equation 6, which collapses the data as depicted in Figure 97. Exponents in Equation 6 have no physical basis and are selected only to provide the best fit of the data. To illustrate the applicability of this index to other data sets, FB data from Daniele et al. (2009) are plotted using the weighted index showing a reasonable fit considering the lack of a pressure effect term.

Given the complexities in predicting FB in turbulent combustion regimes, the index quantifies FB propensity for engine design. The index illustrates how different conditions affect FB in comparison to the other data sets. For example, the 300K data in Figure 96 has a lower FB propensity when compared to other data, but when weighted the propensity increases reflecting the effect of reduced velocity from lower preheat. A correlation of the data for different sets indicates that future points taken between the range of conditions tested should evaluate their propensity with reference to the experimental conditions. Results are plotted as a function of $H_2\%$ to maintain consistency with other methodologies while recognizing that it is a dominant factor. This correlation is currently only suited to H_2/CO mixtures and future work is to expand its utility to operate with dimensionless interchange parameters to account for other fuel types.

$$FB_{index} = \left(\frac{S_T}{u'}\right)^{2.82} * \left(\frac{T_{ad}}{T_{unburned}}\right)^{5.45} * \left(\frac{U_o}{U_{max}}\right)^{-1.28} \quad (6)$$

Figure 97: Weighted flashback propensity index

4.3.2.2 Flashback Correlation via Damköhler Number

Applying a Damköhler number to FB prediction as a function of fuel composition has been investigated previously in laminar premixed flames by Kurdyumov et al. (2007). Their experiments focused on propane and methane in an uncooled tube burner. The work focused on identifying the dominant parameters that control the critical conditions for FB and developing a simplified theoretical model. The main non-dimensional parameter describing wall FB was given by the authors in the form of a critical Damköhler number,

$$Da_c = \frac{S_L^2}{Dg_c} \quad (7)$$

where D is the fuel diffusivity at reference temperature. Simulation work revealed that the Lewis number and heat loss to the wall were the most influential factors on Da_c .

Expanding on the work of Kurdyumov et al. (2007), this investigation seeks a Damköhler number correlation for FB relevant to turbulent conditions. The expression in Equation 7 is not applicable in this case because of the laminar regime limitation so Damköhler number is calculated by Equation 1. Identical steps taken in Section 4.2.1.2 to calculate Damköhler number are applied to FB data. Figure 98 presents FB results for H_2/CO demonstrating that FB occurs at an approximately constant $Da = 10.81$ with a standard deviation of 1.28 for concentrations of H_2 between 30-90%. FB at pure H_2 has an order of magnitude drop in Damköhler number seemingly as a result of different kinetics from the lack of CO. 90% H_2 has an average $S_L = 211 \text{ cm/s}$ compared to $S_L = 86 \text{ cm/s}$ for 100% H_2 .

Figure 98: Damköhler number at FB for H₂/CO

Observation of constant Damköhler number at FB is an interesting result that can be used to apply assumptions necessary for a predictive methodology. Similar assumptions to those in Section 4.2.1.2 to predict Damköhler number for LBO are stated below for FB.

Assumptions

- 1) Damköhler number remains constant at FB for all H₂ concentrations
- 2) Change in mixing residence time is insignificant
- 3) Preheat temperature taken at the lowest H₂ concentration for which FB occurs and remains constant
- 4) Thermal diffusivity is equal to the lowest H₂ concentration for which FB occurs and remains constant

With these assumptions, only the lowest H₂ concentration for which FB occurs needs to be known. This is different from the approach with LBO because combustors designed to operate with NG do not readily FB without significant variation to normal conditions, therefore H₂ must be added before FB occurs. For H₂/CO the lowest concentration of H₂ for which FB occurred was 30% increasing by 10% intervals.

Prediction values are determined as a function of preheat, residence time, and thermal diffusivity using the 30% H₂ experimental results. Preheat is taken from a thermocouple at the

inlet air and residence time is calculated as the injector diameter over burned gas velocity ($U_b = U_o(T_{ad}/T_{unburned})$). Thermal diffusivity is evaluated with a transport property calculator. Figure 99 graphs Damköhler number as a function of varying EQ with the assumptions in place showing a squared dependency with S_L . Lower H_2 concentrations have lesser slopes so Damköhler number does not increase as rapidly with EQ. Other terms in the calculation of Damköhler number such as, thermal diffusivity, burned gas temperature, and characteristic diameter are held constant. Predictions are made by determining where composition lines cross $Da = 9.23$ corresponding to the upper limit for FB at 30% H_2 . Comparison between the simulation and the actual values in Figure 100 depicts a relatively good fit of the data, although slightly under predicted. The largest deviation away from $Da = 9.23$ was 11.23 at 60% H_2 translating into a difference of .04 in EQ. Data between 1 and 2 injectors is consistent showing no change in FB behavior between the two burner configurations. At 100% H_2 the calculated Damköhler number in Figure 98 is below the other values indicating that it will not predict accurately, yet the comparison between the actual and predicted value remains close. In the experimental data a disproportionate drop-off in EQ exists from 90% to 100% (see Figure 53) that is captured in the calculation of S_L . A drop in S_L is suspected to be a result of the absence of CO so that the kinetics only take into account mechanisms involving H_2 . Analogous to how small additions of H_2 dramatically increase reaction rates, small amounts of CO may lead to significant decreases in kinetic rates explaining the disproportionate trend in EQ. Nonetheless, the predicted and actual results correspond to one another upholding the constant Damköhler at FB assumption.

Figure 99: Damköhler number EQ FB simulations H_2/CO

Figure 100: Actual versus expected FB EQ for H_2/CO assuming constant Damköhler number=9.23

To garner further understanding of the effect of S_L on the prediction of FB with Damköhler number two different cases are shown in Figure 101 and Figure 102. Variation of Damköhler is a function of S_L that changes with EQ and $\text{H}_2\%$ as indicated in both figures. Figure 101 is anchored to 30/70 H_2/CO with FB occurring at $S_L = 263 \text{ cm/s}$. As the H_2 concentration in the fuel is adjusted, FB still occurs at $S_L = 263 \text{ cm/s}$, but the EQ corresponding to this flame speed changes. Where the EQ that matches $S_L = 263 \text{ cm/s}$ accurately predicts the experimental FB EQ for the concentration of H_2 in the fuel. $S_L = 263 \text{ cm/s}$ can be thought of as an “effective flame speed” anchored to an experimental result at 30/70 H_2 . Figure 101 anchors the result to 80/20 H_2/CO with an “effective” $S_L = 215 \text{ cm/s}$. Again, the adjustments to EQ produce results that well coincide with experimentally determined FB EQ. For instance, a comparison of 50/50 H_2/CO in Figure 101 and Figure 102 demonstrates a different slope with EQ, yet with their respective “effective” flame speeds the predicted EQ at FB are identical.

To summarize how the Damköhler number is used to predict FB, the first step is to calculate Damköhler number at FB and confirm that FB occurs at a constant value across all H_2 concentration levels. Using this observation obtained from experimental data the factors responsible for variation of Damköhler are then investigated illustrating that S_L is most significant. S_L is then varied for different $\text{H}_2\%$ and EQ while other conditions are held constant until the critical Damköhler number at FB is reached. This procedure requires that only one experimental FB condition be known or determined to predict the EQ at which fuels containing other H_2 concentrations will FB.

Figure 101: Laminar flame speed variation with EQ for 30/70 H₂/CO

Figure 102: Laminar flame speed variation with EQ for 80/20 H₂/CO

4.3.3 Connecting Full Annular Data to Engine Data

Work conducted on the annular combustor is done to develop methodologies capable of predicting FB and LBO in numerous combustion systems. However, these methodologies must first be verified on the system for which it was designed. This proof is necessary to ensure that assumptions and experimental methods for the atmospheric combustor corroborate the behavior of combustion phenomena in the engine. A verification of the methodology on a commercial gas turbine will demonstrate its usefulness in predicting catastrophic FB events, thus creating a roadmap for transitioning a gas turbine to operation on high H_2 content fuels.

Figure 103: Laminar flame speed and mass burning rate as a function of pressure for 50/50 H_2/CO fuel mixtures at $\phi=0.6$ and 300 K (Natarajan 2008)

The major issue in adapting results from the atmospheric annular combustor to the engine is the change in pressure. Figure 103 plots the decrease in S_L with pressure for a 50/50 H_2/CO mixture at an $EQ = 0.6$. Decrease in the laminar burning velocity suggests less FB propensity, but as also indicated by Figure 103 increased density corresponds to an increase in the mass burning rate. Increase in mass burning rate is a result of additional turbulence adding to flame wrinkling and generating more reaction area (Natarajan 2008). These effects are coupled with decreases in thermal diffusivity and S_L with pressure. Furthermore, the additional pressure has significant changes on the operability range between FB and LBO. Creating a new map for comparison to annular data to infer the pressure effect is not possible due to a lack of control over conditions, therefore an alternative strategy is necessary.

The proposed strategy is to use characteristic features of FB within the annular rig to deduce how the engine will behave. For example, one significant characteristic is that FB occurred at a single Damköhler number for various conditions. This creates a link between H_2 concentration and FB that accounts for expected differences in EQ. Without this link the analysis would be left comparing FB at 10% H_2 in the engine to the minimum FB concentration of 30% H_2 in the annular combustor. Instead, it can be inferred that if the annular combustor were at pressure, it would FB at the same Damköhler number at 30% and 10% H_2 , thus linking

the engine to the annular combustor. Accomplishing the goal of linking the annular combustor the engine is to best match inlet conditions and then to simulate the effect of pressure.

Conditions that the annular combustor can replicate are inlet velocity, AFT, and burner configuration. It is unable to achieve engine preheat temperatures or operate at pressure. At power levels below 20 kW the engine fires only two injectors at a local EQ near stoichiometric to supply enough fuel to keep the primary zone from lean extinction from the additional air of the other four injectors. High local EQs create an environment susceptible to FB, especially with added effects of preheat and pressure. Engine control logic is centered around maintaining a constant turbine exit temperature by adjusting the amount of fuel inlet to the injector according to its heating value. Engine tests are conducted by starting the engine on NG and transitioning it to CO then adding H₂ until FB. During tests the concentration of H₂ in the fuel is controlled by a mixing station and the engine adjusts to accommodate the change in heating value. Conditions for FB in the engine are compared in Table 12 to conditions within the annular combustor for H₂/CO. Bulk velocity and preheat approximately match engine conditions, while pressure, AFT, and thermal diffusivity vary.

Table 12: Comparison of FB between annular combustor and engine experiments

Platform	% H ₂	% CO	Φ FB	u (m/s)	Tpreheat (K)	AFT (K)	Flame spd. (cm/s)	Mix Therm Diff (cm ² /s)	Pressure (atm)
Annular	30	70	0.64	50	719.6	2272	263	1.18	1
Engine	10	90	0.73	45	812	2468	206	0.53	2.45

As shown by Table 12, FB in the engine occurs at a H₂ concentration of ~10.3% at the same injector velocity, and higher temperatures. However, higher preheat and AFT do not explain the difference between FB at 10.3% and 30% H₂. Pressure is the underlying factor leading to the significant difference in FB in the engine compared to the annular combustor. To account for the pressure effect on FB and still maintain a comparison across fuel compositions Damköhler number is corrected for pressure. The definition of the Damkohler number below shows a correction for pressure to S_L using CHEMKIN and modification to the thermal diffusivity with a transport properties calculator. Diameter is unchanged and the burned gas velocity U_b remains comparable so no correction is applied to these terms. Thermal diffusivity is plotted as a function of pressure in Figure 104 at FB conditions. Thermal diffusivity drops from ~1.3 to ~0.5 over a pressure range of 1-2.45 atm. H₂ compositional effects and variation in preheat temperature have little influence on thermal diffusivity for the conditions considered. S_L is also varied for pressure at FB conditions in demonstrating more dramatic decreases with increasing H₂ concentration. Flame speeds at concentrations between 30-60% group closely with one another then exhibit a significant decrease at 70% that continues through 90%. Combination of thermal diffusivity and flame speed leads to an increase in Damköhler number for concentrations between 30-60% (Figure 106). Past 60% the decrease in thermal diffusivity is comparable to the decrease in flame speed which cancels the effect of each and creates no appreciable change in the Damköhler number. FB in the annular combustor at high H₂% begin to deviate away from engine preheat conditions for preheat and AFT making these conditions unsuitable for an accurate comparison between the two platforms. Nonetheless, there exists a

relatively wide range of $H_2\%$ for which one can adjust Damköhler number for pressure in a manner that well predicts the FB limit in the engine.

$$Da = \frac{\tau_{res}}{\tau_{chem}} = \frac{DS_L^2}{U_b \alpha}$$

Figure 104: Thermal diffusivity as a function of pressure

Figure 105: Laminar flame speed corrected for pressure

Figure 106: Damköhler at FB corrected for pressure

Example of predictive capability

Having established that the FB limit corrected for pressure in the annular combustor approaches the experimental result gathered from engine testing the next step is to investigate its predictive capability. The methodology to account for pressure within the engine is as follows:

- 1) Perform experiment on annular combustor matching preheat, bulk velocity, and AFT to obtain EQ and H₂% at FB
- 2) Determine thermal diffusivity for conditions at FB corrected for pressure
- 3) Correct laminar flame speed for pressure using CHEMKIN
- 4) Calculate expected FB Damköhler number corrected for pressure
- 5) Match Damköhler number of the engine based on operability schedule needed to maintain constant heat input to expected FB Damköhler number from the annular combustor

FB conditions from the annular combustor in Table 12 generate an expected FB Damköhler number of 13.33 in comparison to that of 14.67 determined in the engine, as shown in Figure 106. Damköhler number is a dimensionless parameter and it must be translated to a more useful factor such as, H₂% or EQ at FB. Fortunately, the engine is designed to maintain a constant turbine exit temperature or constant heat input, consequently, determining EQ for changing fuel compositions can be calculated from normal operation on NG. Figure 107 plots the expected Damköhler number using engine preheat of 830 K (NG at 20 kW) with EQ and H₂ constrained by constant heat input. The constant heat input line represents the Damköhler number calculated with 830 K preheat at an EQ and H₂% needed to maintain the same heat input as NG. Engine FB represents where FB occurred in the engine. The expected Damköhler line corresponds to the 13.33 value predicted from annular combustor data corrected for pressure. Annular data adjusted for pressure predicts FB at 9% H₂ and actual FB occurred at 10% indicating that the methodology is capable of capturing the effects of pressure on FB between test platforms. While this is only for one data point tests within the engine have consistently repeated with a small margin of error at different power levels.

When plotted versus laminar flame speed, FB is expected at a flame speed of 202 cm/s in the engine at pressure, which is lower than the flame speed of 263 cm/s observed in the atmospheric combustor. FB in the engine occurs at nearly the same flame speed of 200 cm/s as depicted in Figure 108. FB flame speeds at pressure for 30-60 H₂% all predict FB around 200 cm/s then deviate greatly above >60% H₂ making them unable to forecast engine FB. This means that pressure corrected annular combustor data <60 H₂% can be used to anticipate FB in the engine. There is great agreement between the predicted flame and actual flame speed at FB demonstrating that the calculation is able to capture effects of pressure on FB.

Figure 107: Damköhler number versus H_2 at corrected pressure

Figure 108: Laminar flame speed at FB for annular combustor and engine

As a methodology for determining FB limits in the engine with H₂/CO using a pressure corrected Damköhler number is appropriate. Results show FB occurs at a consistent Damköhler number regardless of H₂ concentration in the fuel for the annular combustor. The implication of the constant Damköhler result is that it provides a method of comparing FB limits between across fuel compositions. Coupling this result with a correction on the laminar flame speed and thermal diffusivity for pressure grants the capability to replicate engine results. Thermal diffusivity had little change among compositions and preheats, but strong effect of pressure. Laminar flame speed had both effect on pressure and H₂%, especially past 60% H₂. These effects combine to generate an increase in the Damköhler number with pressure that serves as the prediction value. To validate the methodology a constant heat input attribute of the engine is used to calculate the EQ for given H₂% in the fuel. Using a nominal engine preheat with the calculated EQ for different H₂% Damköhler number is plotted to determine where it matches the predicted value from the annular combustor. Data shows agreement between annular combustor predicted and actual engine Damköhler numbers. However, this is only one data point from the engine, so additional data were obtained to assess the validity of this methodology. The next section describes these additional data and the comparison to the predictions from the pressure corrected full annular data.

4.3.3.1 Additional Reduced TET Engine Experiments and Issues

These results seem promising, and further experimental tests were performed to evaluate this methodology for connecting the full annular rig to the engine. These additional engine tests would consist of running the engine on H₂/CO mixtures at 20 kW with reduced TET settings (i.e., 2 injector operation in order to match injectors on in the previous test shown in Figure 107 and Figure 108 but while also having variation in the injector EQ). However, conducting these experiments at reduced TET settings proved highly difficult while maintaining 2 injector operation (i.e., maintaining the FUELTY=3 setting for high Btu fuels wherein 2 injectors would be on at 20kW). This resulted from the test procedure. The test procedure for H₂/CO mixtures at 20kW would first begin with starting the engine on natural gas with the FUELTY=3. Then after the engine had warmed up, the fuel would be switched over to CO. Once everything settled after this fuel switch, H₂ could then be blended into the CO until flashback occurred. For these reduced TET tests, an additional step would then occur where the TET was then decreased (to either 1100 or 1000 F). During this step, the air flow would increase and as opposed to the fuel flow decreasing to reduce TET, the fuel flow was increased to compensate for the increasing air flow rate. This resulted in higher pressure drops as had been observed at higher loads when running on pure CO. In fact at higher loads, it was necessary to switch to FUELTY=1 (low Btu setting) in order to achieve the load setting without hitting the Wenergy max in the software and the fuel control valve fully open. In the case at hand, the engine could operate on pure CO at a reduced TET, but the issues arose when beginning to blend H₂. In order to initiate H₂ flow, the CO valve would need to close for pressure to equalize at the downstream mixing plenum before H₂ would flow. As this process occurred, the engine fuel control valve would then need to increase as the supply pressure decreased. Eventually it would reach 100% open without any H₂ being blended. If TET was increased to 1120 F this issue could be averted, but then the mixing station could not successfully blend the H₂ smoothly. Tests could be run with success under 4 injector operation (FUELTY=1 low Btu), and given the apparent independent interaction of the injectors in the full annular test rig seen in the injector interaction experiments (See Section 3.3.1.1), it was hypothesized that the injectors would interact minimally under 4 injector operation and the data from the 4 injector operation could be compared with the 2 injector operation.

Using the methodology described in Figure 107 and Figure 108 and adding the new 4 injector data to Figure 108, Figure 109 can be created to verify the methodology. As can be seen in Figure 109, the methodology does not work for the 4 injector engine data. This may be a result of injector interaction or that the methodology is inadequate. Without more data (i.e., lower TET) at 2 injector operation, it is not certain if the methodology works.

Figure 109 Damköhler number versus H₂ at corrected pressure with new engine data

4.3.4 Engine Data – Statistical Analysis

The original intent was to develop correlations for predicting flashback in the engine as a function of fuel composition that would provide Capstone with an easy to use expression.. This was to be developed for an improved injector design. However, a final configuration was not available for such testing. Despite this, the engine data collected throughout these research efforts on the baseline injector was considered. It is noted that these data were not gathered following a statistically developed matrix, yet the results were evaluated for development of a correlation. However, after a attempting analysis of the data, it was realized that the necessary analysis of variance (ANOVA) would not be meaningful for a couple reasons. The injector staging introduces discontinuities that make using the over different power levels inappropriate. If focus was only given to one power level, then there simply would not be anything varying as an input since the experiments were run by varying the power level and hydrogen content. In spite of these issues, an ANOVA was performed but the resulting equations had deficiencies and therefore are not reliable.

The baseline injector data is shown in Table 13 for reference here.

Table 13 Engine test results for baseline injectors used in ANOVA and CFD analyses

Test ID	%H ₂	%NG	%CO	Inj. #	Power [kW]	Engine Pressure [kPa]	Preheat Temperature [K]	Total air flow rate [kg/s]	EQ	Inj. Velocity (m/s)
1	31.3	68.7	0	2	20	249	816	0.312	0.918	55.7
2	33.2	66.8	0	2	20	248	811	0.310	0.920	55.4
3	10.3	0	89.7	2	20	249	812	0.302	0.729	62.2
4	61.1	38.9	0	4	30	289	947	0.349	0.507	61.0
5	15.8	0	84.2	4	30	289	814	0.346	0.375	54.7
6	15.4	0	84.6	4	30	289	858	0.341	0.375	56.8
7	20.3	0	79.7	4	39	322	864	0.393	0.409	59.9
8	61	39	0	6	59	404	848	0.489	0.424	53.9
9	60.3	39.7	0	6	60	409	847	0.489	0.427	53.3
10	20.3	0	79.7	6	62	420	841	0.479	0.347	53.4
11	59.7	40.3	0	6	65	432	845	0.504	0.439	51.9
12	31.6	0	68.4	4	20	249	795	0.369	0.313	64.9
13	25.6	0	74.4	4	20	249	841	0.327	0.319	60.7
14	15.6	0	84.4	4	20	249	845	0.326	0.312	60.7
15	16.6	0	83.4	4	20	249	848	0.327	0.316	61.2

4.3.5 Coupled CFD/Gradient Theory Analysis

Beyond the development of a simple correlation for predicting flashback, a more sophisticated approach was also explored involving the use of CFD to estimate wall boundary gradients and turbulence levels. These values can, in principle, be coupled to critical gradient concepts associated with quench distance and turbulent flame propagation rates to assess flashback propensity. A key issue here is the need to define an appropriate flame speed as has been discussed above. However, several expressions can be evaluated and compared to assess sensitivity of the results to this parameter and engineering judgment made relative to what to use.

The same baseline injector data presented in Table 13 are used in these analyses. 15 tests have been conducted with various fuel composition and power load. The data shown in this table represents the critical condition when flashback happens. The data are labeled using test ID in the order by which tests were taken. It should be noticed that the measured injector inlet temperature of the 4th test is much higher than the average value. Also the variation in hydrogen content at flashback of the last four tests is due to different protocols to determine flashback events (i.e., using tip temperature or air hole temperature to define flashback).

(a) Inlet temperature

(b) Tip temperature

Figure 110 Engine data bulk velocity v.s. laminar flame speed (point in red circle is an outlier) (a) S_L calculated based on inlet temperature; (b) S_L calculated based on tip temperature

Figure 110 presents the raw data when flashback events happen. The critical bulk velocity is plotted versus calculated laminar flame speed. This plot represents the straightforward attempt to correlate flashback parameters using a fuel property. Different test conditions are labeled in the plot, showing the effects of fuel type in mixture and injector numbers. The laminar flame speed in plot (a) and (b) are based on inlet temperature and measured burner tip temperature, respectively. Comparing these two plots, the temperature selection to determine laminar flame speed does not significantly affect the trend. Higher laminar flame speed tends to increase flashback propensity. However, limited data between the groups with two and four injectors

prevents a solid conclusion. Also, it should be noted that the NG-#4 data shows an abnormal behavior compared with the other points. As mentioned before, the measured inlet temperature of this case is high and thus is considered an outlier.

The correlation shown in Figure 110 is weak, and, therefore, in the following sections, more detailed analysis using CFD is conducted.

4.3.5.1 CFD Modeling

Figure 111 (a) presents the geometry used for the CFD simulation. It is consistent with the one used for the CRN analysis (Section 5.1.1.2). The only difference is that the injectors are extruded outward to simulate the flow in the injector. The first version of meshes is shown by Figure 111 (b). Meshes are generated based on element size of 1 mm, which yields around 1 million elements.

Figure 111 Schematic of the geometry and mesh used for CFD simulation

Figure 112 Mesh sensitivity check

A mesh sensitivity check is also conducted. The results are presented in Figure 112. Flow field in one injector is compared, which is calculated based on standard $k-\epsilon$ model with enhanced wall treatment. Mesh adaption based on velocity gradient was employed to refine meshes. Figure 112 shows two rounds of adaption were carried out, generating a two million and a three million mesh. Comparing the velocity distribution along the radius, the change from two million mesh to three million is not significant. Therefore, it is unnecessary to further refine the mesh, and the final mesh used in the following analyses is three million. Figure 113 shows an example of velocity fluctuation (U') distribution on an injector exit plane. U' is calculated via E- 29 for four different mass flow rates. The distance to center points is normalized using the radius of the outlet.

$$k \approx \frac{3u'}{2} \quad \text{E- 29}$$

To further post-process the simulation results, a local coordinate system is defined on each injector outlet. Shown by Figure 114, the origin point is fixed on the center of the injector outlet. The normal direction, $\vec{n}_i$, of the i th injector outlet and $\vec{X}$ of the global coordinate are used as two axes of the local coordinates. $\vec{Y}_i$ is further defined as the direction perpendicular to $\vec{n}_i$ and $\vec{X}$. Therefore, each point on the outlet plane can be described as (α, r) , where r denotes the magnitude of the vector from the center to this point and α denotes the angle between r and $\vec{X}$. Therefore, $\alpha=90^\circ$ means upwind to the flow recirculation inside of the annular combustor, whereas $\alpha=270^\circ$ means downwind.

Figure 115 and Figure 116 further illustrate the velocity magnitude and fluctuation velocity distribution in terms of (α, r) on an injector. The variation with respect to α suggests that potential interaction between injectors.

Figure 113 Calculated fluctuation velocity distribution on the injector outlet with normalized mass flow rate

Figure 114 Definition of the local coordinator system (n_i - x - y_i) for i th injector inlet

Figure 115 Fluctuation velocity distribution on 1st injector plane in terms of (α , r)

Figure 116 Velocity magnitude distribution on 1st injector plane in terms of (α , r)

4.3.5.2 CFD Assisted Flashback Analysis

The methodology employed in this research was first proposed by Wang et al. (2009). Figure 117 illustrates this approach. The flow velocity curve is calculated using CFD simulation and it intersects with the turbulent flame speed curve. The intersection point is defined as the critical thickness, d_c . It defines the region where the flame is able to propagate upstream. The quenching region is defined by the quenching distance, d_q , and is the region where the flame is quenched. Therefore, boundary layer flashback is the result of competition between the quenching distance and critical distance, i.e. only if quenching distance is smaller than critical distance, flashback will occur.

Figure 117 Schematic of the definition of critical distance d_c

Specifically, here are the steps of this methodology (Wang, McDonell et al. 2009):

1. Collect data from CFD simulation, such as fluctuation velocity and flow velocity;
2. Plug in the turbulent flame speed expressions, calculate the turbulent flame;
3. Find the border where burning velocity starts to be larger than the flow velocity, defined as critical distance (d_c);
4. Calculate the quenching length scale (d_q);
5. Compare the d_q and d_c ;

Therefore, in addition to the CFD simulation it is also necessary to calculate turbulent flame speed and quenching distance in this methodology. Table 14 summarizes the turbulent flame speed formulas used in these analyses.

Table 14 Summary of turbulent flame speed formula

Source	Formula	note
(Daniele, Jansohn et al. 2011)	$S_T = a(u')^{0.63} \left(\frac{L_T}{\alpha}\right)^{-0.37} \left(\frac{P}{P_0}\right)^{0.63} \left(\frac{T}{T_0}\right)^{-0.63}$	Global consumption rate, P ₀ =1 atm, T ₀ =1 K, L _T =0.5R
(Cheng 2009)	$S_T = S_L + a \cdot u'$	Local displacement rate, a=3.15 for hydrogen and a=1.73 for methane
(Kobayashi, Tamura et al. 1996)	$\frac{S_T}{S_L} = 5.04 \left(\frac{P}{P_0}\right)^{0.2} \left(\frac{u'}{S_L}\right)^{0.38}$	Global Consumption Rate
(Zimont 2000)	$S_T = A \cdot u'^{3/4} S_L^{1/2} \alpha^{-1/4} L_T^{1/4}$	Global Consumption Rate

Quenching distance is related to the thermal thickness, d_{q0} , which is defined as shown by E- 30 (Turns 1996). It represents the flame thickness and equals the ratio of thermal diffusivity and laminar flame speed. In order to determine the real quenching distance, Ballal et. al conducted extensive work, and pointed out that the quenching distance is related to the minimum ignition energy (Ballal and Lefebvre 1977). The final expression suggested by this publication for quenching distances of turbulent flames is shown in E- 31. However, the quenching distance in Ballal's work was defined as the minimum distance between two sparks for flame ignition. This could be significantly different than the wall quenching effects in practical jet flames. As a result, another quenching distance expression is proposed (Turns 1996), as shown by E- 32.

$$d_{q0} \equiv \frac{\alpha}{S_L} \quad \text{E- 30}$$

$$d_q = \frac{10 \cdot \alpha}{S_T - 0.63 \cdot u'} \quad \text{E- 31}$$

$$d_q \propto \frac{\alpha}{S_L} \sqrt{\frac{AFT - T_{inlet}}{AFT - T_{tip}}} \quad \text{E- 32}$$

In order to understand the parameters that dominate flashback, a sensitivity analysis was conducted wherein the hydrogen content was increased and decreased from the measured flashback condition at each of the 15 engine conditions. This was done in order to see which

parameters changed most and in what direction. This is helpful here because it is reasonable to assume that increasing hydrogen content increases flashback propensity therefore one can see how each of the parameters changes relative to flashback propensity.

Hydrogen Content Sensitivity Analysis

In this section, hydrogen composition varies to represent flashback and non-flashback scenarios. According to the test protocol, flashback events are approached by increasing hydrogen composition in the fuels with constant heat input and TET. Therefore, the higher flashback propensity condition is defined as the fuel with 30% higher hydrogen composition. In contrast, the cases with 30% less hydrogen composition are considered as the lower flashback propensity condition (or non-flashback scenario). The fuel flow rate is also adjusted to provide constant heat input. On the other hand, air flow rate is relatively unchanged if heat input is the same. Therefore, the equivalence ratio is not kept constant if the fuel composition is changed.

Figure 118 presents the calculated variation of laminar flame speed due to the increase or decrease of hydrogen composition in the fuels. The values are normalized using the baseline cases when flashback events were observed in the engine tests. The baseline conditions are also presented in the Table 13. As shown by Figure 118, increase in hydrogen content increases laminar flame speed as one would expect. The variation range is generally around 20% to 30%. However, the increases are very significant for four cases (test 4, 8, 9 and 11). It should be noticed that the conditions of these cases are quite identical. They are all hydrogen and methane mixtures and the hydrogen composition is higher than 50%.

Figure 118 Variation of S_L due to increase/ decrease of H_2 composition in the fuels

Similarly, Figure 119 presents the variation of thermal diffusivity. As shown by the plot, the variation of thermal diffusivity is not as significant as that of laminar flame speed. For most of the cases, variation is no more than 10%. It is because the mixture properties are more determined by air properties in the lean fuel mixtures than fuel. Significantly higher variations are also observed for the four cases that showed higher S_L variation. Figure 120 presents the

variation of the thermal thickness, which is defined as the ratio of thermal diffusivity over laminar flame speed. This variation is indicative of the variation of the quenching distance.

Figure 119 Variation of thermal diffusivity due to increase/ decrease of H₂ composition in the fuels

Figure 120 Variation of thermal thickness due to increase/ decrease of H₂ composition in the fuels

Thickness of flashback region

E- 34 defines the thickness of flashback region as d_{FB} . It represents the comparison between the relative scale of quenching distance and critical distance. Theoretically, flashback happens if $d_{FB} < 0$. Given the stochastic nature of flashback and turbulent combustion, the critical d_{FB} should fluctuate in a region near zero, and larger d_{FB} suggests higher possibility of flashback. Therefore, d_{FB} could be taken as an indicator of flashback propensity.

$$d_q = A \cdot d_{q0}$$

E- 33

$$d_{FB} = d_q - d_c$$

E- 34

Table 15 presents the calculated d_{FB} of all test cases. The superscript of + and – denote fuels with 30% more or less hydrogen, respectively. All d_{FB} are normalized using radius, R. The quenching distance is estimated according to E- 33. However, the ratio of d_q and d_{q0} is still undetermined. As shown by E- 32, it could be affected by temperature, geometry, etc. In the current research, the A is tuned to yield d_{FB} of 0 for each test, and it is plugged into E- 34 to determine d_{FB}^+ and d_{FB}^- respectively. As shown in Table 15, the methodology can predict flashback well when looking at large swings in hydrogen content.

Table 15 Flashback event prediction using Daniele et al. (2011) turbulent flame speed formula (+/- 30% hydrogen)

Test ID	X_H2	X_NG	X_CO	Inj. #	A ($d_{FB}=0$)	d_{FB}^+/R [%]	d_{FB}^-/R [%]	Prediction
1	0.313	0.687	0	2	7.387	-0.070	0.061	Y
2	0.332	0.668	0	2	7.400	-0.079	0.068	Y
3	0.103	0	0.897	2	7.349	-0.150	0.217	Y
4	0.611	0.389	0	4	5.908	-0.537	0.297	Y
5	0.158	0	0.842	4	3.436	-0.140	0.205	Y
6	0.154	0	0.846	4	3.943	-0.154	0.219	Y
7	0.203	0	0.797	4	5.251	-0.174	0.225	Y
8	0.61	0.39	0	6	3.210	-0.511	0.342	Y
9	0.603	0.397	0	6	3.255	-0.487	0.342	Y
10	0.203	0	0.797	6	3.939	-0.130	0.183	Y
11	0.597	0.403	0	6	3.535	-0.458	0.307	Y
12	0.316	0	0.684	4	2.524	-0.195	0.264	Y
13	0.256	0	0.744	4	3.027	-0.205	0.272	Y
14	0.156	0	0.844	4	2.474	-0.164	0.208	Y
15	0.166	0	0.834	4	2.614	-0.172	0.212	Y

Table 16 shows that for a smaller change in hydrogen content this methodology is not able to predict flashback as well. Table 17 and Table 18 show similar results but using the Zimont (2000) turbulent flame speed formula. Similar observations can be made regarding these Zimont results.

Table 16 Flashback event prediction using Daniele et al. (2011) turbulent flame speed formula (+/- 10% hydrogen)

Test ID	X_H2	X_NG	X_CO	Inj. #	A ($d_{FB}=0$)	d_{FB}^+/R [%]	d_{FB}^-/R [%]	Prediction
1	0.313	0.687	0	2	7.387	0.076	0.126	F
2	0.332	0.668	0	2	7.400	0.127	0.181	F
3	0.103	0	0.897	2	7.349	0.221	0.364	F
4	0.611	0.389	0	4	5.908	-0.241	0.011	Y
5	0.158	0	0.842	4	3.436	0.001	0.121	F
6	0.154	0	0.846	4	3.943	0.206	0.348	F
7	0.203	0	0.797	4	5.251	-0.174	-0.055	F
8	0.61	0.39	0	6	3.210	-0.172	0.097	Y
9	0.603	0.397	0	6	3.255	-0.223	0.022	Y
10	0.203	0	0.797	6	3.939	-0.219	-0.127	F
11	0.597	0.403	0	6	3.535	-0.286	-0.074	F
12	0.316	0	0.684	4	2.524	0.096	0.248	F
13	0.256	0	0.744	4	3.027	-0.215	-0.075	F
14	0.156	0	0.844	4	2.474	-0.064	0.053	Y
15	0.166	0	0.834	4	2.614	-0.129	-0.003	F

Table 17 Flashback event prediction using Zimont (2000) turbulent flame speed formula (+/- 30% hydrogen)

Test ID	X_H2	X_NG	X_CO	Inj. #	A ($d_{FB}=0$)	d_{FB}^+/R [%]	d_{FB}^-/R [%]	Prediction
1	0.313	0.687	0	2	13.507	-0.179	0.143	Y
2	0.332	0.668	0	2	13.575	-0.197	0.167	Y
3	0.103	0	0.897	2	13.474	-0.385	0.528	Y
4	0.611	0.389	0	4	10.252	-1.283	0.671	Y
5	0.158	0	0.842	4	4.885	-0.255	0.367	Y
6	0.154	0	0.846	4	5.915	-0.306	0.428	Y
7	0.203	0	0.797	4	8.452	-0.374	0.466	Y
8	0.61	0.39	0	6	4.216	-0.919	0.582	Y
9	0.603	0.397	0	6	4.248	-0.886	0.568	Y
10	0.203	0	0.797	6	5.437	-0.236	0.329	Y
11	0.597	0.403	0	6	4.678	-0.813	0.516	Y
12	0.316	0	0.684	4	3.475	-0.355	0.469	Y
13	0.256	0	0.744	4	4.385	-0.403	0.499	Y
14	0.156	0	0.844	4	3.364	-0.290	0.373	Y
15	0.166	0	0.834	4	3.618	-0.314	0.383	Y

Table 18 Flashback event prediction using Zimont (2000) turbulent flame speed formula (+/- 10% hydrogen)

Test ID	X_H2	X_NG	X_CO	Inj. #	A ($d_{FB}=0$)	d_{FB}^+/R [%]	d_{FB}^-/R [%]	Prediction
1	0.313	0.687	0	2	13.507	-0.007	0.126	Y
2	0.332	0.668	0	2	13.575	0.145	0.285	F
3	0.103	0	0.897	2	13.474	0.383	0.726	F
4	0.611	0.389	0	4	10.252	-0.865	-0.232	F
5	0.158	0	0.842	4	4.885	-0.150	0.067	Y
6	0.154	0	0.846	4	5.915	0.274	0.557	F
7	0.203	0	0.797	4	8.452	-0.619	-0.352	F
8	0.61	0.39	0	6	4.216	-0.513	-0.016	F
9	0.603	0.397	0	6	4.248	-0.637	-0.174	F
10	0.203	0	0.797	6	5.437	-0.642	-0.448	F
11	0.597	0.403	0	6	4.678	-0.785	-0.361	F
12	0.316	0	0.684	4	3.475	0.008	0.307	F
13	0.256	0	0.744	4	4.385	-0.634	-0.356	F
14	0.156	0	0.844	4	3.364	-0.277	-0.048	F
15	0.166	0	0.834	4	3.618	-0.412	-0.172	F

Quenching and Critical Distance Comparisons

The d_q and d_c is compared in this section, and the sensitivity of these two distances to $\pm 30\%$ hydrogen content changes (i.e., increased/decreased flashback propensity) is discussed in this section.

Figure 121 illustrates the sensitivity of d_c to different turbulent flame speeds. As fuel composition changes so does the turbulent flame speed. Since the flow velocity is more likely determined by the air flow rate, the velocity profile does not change too much if the heat input is constant. If hydrogen composition in the fuel mixture increases, the turbulent flame speed curve moves from S_{T1} to S_{T2} . Accordingly, the intersection point moves inward and upward. Since the flow velocity distributes linearly near the wall, the variation of d_c due to turbulent flame speed change

can be determined by dividing turbulent flame speed change using velocity gradient (g). The calculation is shown by E- 36, E- 37 and E- 38.

Figure 121 Schematic of sensitive analysis on turbulent flame speed effect

$$\Delta d_c \equiv |d_{c2} - d_{c1}| \quad \text{E- 35}$$

$$\Delta S_T = |S_{T2} - S_{T1}| \quad \text{E- 36}$$

$$\Delta d_c = \frac{\Delta S_T}{g} \quad \text{E- 37}$$

$$g = \frac{0.03955 Re^{0.75} \bar{u}}{D} \quad \text{E- 38}$$

$$\Delta d_q = |d_{q2} - d_{q1}| \quad \text{E- 39}$$

On the other hand, the quenching distance variation is calculated via E- 33 and E- 39. The coefficient, A , is defined as ratio between quenching distance and thermal thickness. According to E- 31, the magnitude of A is around 10. To estimate the turbulent flame speed, the ratio of turbulent flame speed and laminar flame speed presented in the previous publications are employed (Daniele, Jansohn et al. 2011; Venkateswaran, Marshall et al. 2011). The magnitude of velocity fluctuation is estimated to be 5 m/s according to CFD simulation (Figure 113). In this case, magnitude of S_T/S_L ratio is estimated to be 10. Table 19 summarizes these estimations.

Table 19 Estimated magnitudes for the quenching and critical distances comparison

	S_T/S_L	U' [m/s]	d_q/d_{q0}	g [1/s]
magnitude	10	5	10	500000

Figure 122 Comparison between the variation of d_q and d_c due to $\pm 30\%$ H_2 change

Figure 122 shows the comparison between the variation of d_q and d_c due to $\pm 30\%$ H_2 difference. It can be seen that the change of quenching distance is more significant than that of critical thickness. This observation suggests that flashback propensity variation due to fuel composition change in a jet flame based engine is more likely determined by the wall quenching effects.

5 Engine Emissions Analysis

This section analyzes the emissions measurements made during the engine tests at UCI. Chemical reactor network analyses were also performed to further this analysis.

5.1 Emissions

Throughout these tests the engine emissions were measured and logged. Given the transient nature of these tests and the lag in the emissions measurements due to the flow delay between the exhaust stack and the PG250 gas analyzer, these measurements are better suited for the analysis of trends due to fuel composition changes and design modifications. The fuel composition effect will be examined first with the design modification effect being analyzed second.

5.1.1 Baseline Injector

5.1.1.1 Measurements and Single Perfectly Stirred Reactor Analysis

Figure 123 and Figure 124 illustrate the effect of the anchor fuel (CO vs. NG) on the pollutant emissions at various engine loads. The NO_x emissions under carbon monoxide fueling of the microturbine are slightly higher than they would be under natural gas operation. A much larger effect on the CO emissions is observed although only at a load level of 30 kW. At 30 kW, the CO emissions are reduced significantly by operating on carbon monoxide. The trend in emissions versus the engine load are similar between the two anchor fuels demonstrating that the injector staging plays a significant role in spite of fuel changes.

Figure 123 NO_x emissions for baseline injectors before blending in hydrogen

Figure 124 CO emissions for baseline injectors before blending in hydrogen

In an effort to apply straightforward simulation tools to this problem, a simple chemical reactor was setup to assess how hydrogen addition impacts emissions. Chemical kinetic simulations were performed using Chemkin to investigate the effect of hydrogen addition to the two anchor fuels (CO and NG) at several different loads (20, 30, 60 kW). A single perfectly stirred reactor (PSR) module was used to simulate the primary zone of the combustor in the microturbine. The kinetic mechanism used was GRI Mech 3.0 since the nitrogen chemistry of this mechanism is more fully developed and verified than some of the other kinetic mechanisms available. Additionally, it has been concluded by previous researchers that this mechanism is sufficient for

syngas analyses at temperatures above 1000K (Chacartegui, Torres et al. 2011). The appropriate flow rates, reactor volume, and equivalence ratios for each fuel mixture were used in these simulations to best approximate the overall primary zone conditions. Comparing the measurements to those results from the simulations reveals that these kinetic PSR simulations do not predict the engine emissions trends. However, this was not the goal of these simulations. Rather the motivation of these simulations is to examine the effect of hydrogen addition and compare these trends from the simulations to the experimental measurements.

The simulated emissions from the kinetic PSR model are shown in Figure 125 and Figure 126. The trend that is likely first observed is that when switching anchor fuels from natural gas to carbon monoxide one should expect an increase in both NO_x and CO emissions although the level of this increase diminishes at higher hydrogen content. Another major observation is that the addition of hydrogen to natural gas results in an increase in NO_x emissions and a decrease in CO emissions whereas when hydrogen is added to carbon monoxide both the NO_x and CO emissions are decreased. The rate of change in emissions for each % addition of hydrogen is different between the two anchor fuels. The rate of change in NO_x and CO emissions for an anchor fuel of carbon monoxide is highest at low levels of hydrogen addition whereas the rate of change in NO_x emissions for an anchor fuel of natural gas is nearly the same at both high and low levels of hydrogen. However, the rate of change in CO emissions for an anchor fuel of natural gas is highest at high hydrogen content which is the opposite of the carbon monoxide anchor fuel case.

The PSR simulation emission trends concerning only the switch of anchor fuels (no hydrogen addition) do not agree with those trends from the engine measurements. For example, the use carbon monoxide as an anchor fuel instead of natural gas results in only small increases in NO_x and CO emissions rather than the large increases suggested by the simulations, and in fact for the 30 kW load level, the CO emissions are decreased significantly rather than increased.

Figure 125 NO_x emissions versus percent hydrogen content in the fuel from PSR simulations engine specific operating conditions

Figure 126 CO emissions versus percent hydrogen content in the fuel from PSR simulations engine specific operating conditions

To further compare the emissions trends from the PSR simulations to the experimental data, Figure 127 and Figure 128 were compiled. Figure 127 and Figure 128 show the percent change in the NO_x and CO emissions as the percent hydrogen in the fuel was increased from 0% to the hydrogen content just before flashback. These figures were compiled in order to compare how the addition of hydrogen altered the NO_x and CO emissions for the two anchor fuels (NG and CO). The first thing to notice from Figure 127 and Figure 128 is that the trends in the experimental data agree somewhat with the trends in the PSR simulations. There are some data points that should show an increase or decrease in emissions according to the PSR simulations but rather show no change, which is better agreement than if there were a decrease instead of a increase or vice versa. The response of the engine emissions to hydrogen addition to natural gas shows an increase in NO_x and a decrease in CO if one were to ignore the responses that show no change. Likewise for the hydrogen addition to carbon monoxide, if one were to ignore the emissions responses with no change then the addition of hydrogen to carbon monoxide would cause a decrease in both NO_x and CO, which agrees with the trends seen from the PSR simulations. However, there is one experimental data point (H₂/CO at 20kW) that shows a directly opposite trend from the PSR simulations, i.e., the CO emissions should decrease as hydrogen is added to the anchor carbon monoxide fuel according to the PSR simulations (Figure 125 and Figure 126) but the experimental data show that in fact the CO emissions increase when hydrogen is blended into carbon monoxide at a 20kW load

To more specifically examine each of the cases and their comparison to the PSR simulation trends, the response of the pollutant emissions to hydrogen addition to natural gas at 20kW is examined first. With regard to the CO emissions for this case, the experimental data show no change in emissions where the PSR simulations suggest a slight decrease. This may not be significant disagreement because the hydrogen content before flashback is below 50% where the PSR simulations showed that hydrogen addition to natural gas only resulted in a small decrease in CO emissions for lower hydrogen contents (<40%). However, the fact that the NO_x emissions do not increase as hydrogen is added does not agree with those trends from the PSR simulations. It should also be noted here that several publications contain experimental data showing an increase in NO_x as hydrogen is added to natural gas (or another baseline fuel) (Tomczak, Benelli et al. 2002; Juste 2006; Cocchi, Provenzale et al. 2008) or substituted for the original fuel (Nomura, Tamaki et al. 1981; Sampath and Shum 1985; Therkelsen, Werts et al. 2009). However, other publications show experimental data with sub 1 ppm NO_x measurements after several design modifications (Minakawa, Miyajima et al. 1997; Farina, Perry et al. 2009). Additionally, it should also be noted that when hydrogen is blended into carbon monoxide at

20kW there is no increase in NO_x engine emissions and an increase in engine CO emissions. These experimental results differ from the PSR simulation trends that suggest a large decrease in both NO_x and CO emissions for similar hydrogen content seen in the experiment.

At 30 kW the decrease in CO emissions from the engine as hydrogen is added to both the carbon monoxide and natural gas anchor fuels agrees with the trend observed from the PSR simulations (Figure 126). The increase in NO_x emissions from the engine as hydrogen was added to natural gas agrees with the trend seen in the PSR simulation results (Figure 125), however, this increase is nonexistent for the carbon monoxide anchor fuel and hence is different from the decrease seen in the PSR simulation results (Figure 125).

There is further disagreement between the engine measurements and the PSR simulations at the full load natural gas cases. For the natural gas as anchor fuel cases, there is an increase in NO_x which agrees with those PSR simulation trends (Figure 125) but the engine CO emissions do not agree with the corresponding PSR simulation trends where increased hydrogen content should lead to decreased CO emissions. Although for the full load case of carbon monoxide as the anchor fuel tests, the engine NO_x and CO emissions trends do agree with the PSR simulation trends since the addition of hydrogen leads to reduced NO_x and CO emissions from the engine. Given that the emissions trends from the PSR simulations do not agree well with the measured engine emissions for several of the cases suggests that a more complex network of reactors that describe the combustor more accurately (e.g., the fuel staging is very important but with only one PSR the staging effects are lost) must be used in order to predict the emissions trends accurately. It must also be noted that even more complexity would need to be added in order to predict the changes in emissions as a result of the design modification discussed in the next paragraph.

Figure 127 Percent change in NO_x emissions as hydrogen is blended from 0% to hydrogen content just before flashback for the baseline injector design

Figure 128 Percent change in CO emissions as hydrogen is blended from 0% to hydrogen content just before flashback for the baseline injector design

5.1.1.2 Reactor Network Analysis

To provide a more detailed examination of the emissions, a more sophisticated reactor network was developed based on CFD analysis of the combustor. The work presented above made assumptions regarding the nature of the combustion zones which were useful to help estimate trends, but the level of agreement with the measured results indicated a need for refinement of the approach.

A more sophisticated approach was taken relying upon CFD simulations of the combustor as a means to divide the combustor into appropriate individual reactors. Both CFD and CRN models take into account the air/fuel splits across the six injectors and the distribution of air jets in the dilution zone. The dilution zone includes two air streams, the inner air jets and the outer air jets, which cool the exhaust gases before they are supplied to the turbine. Information regarding air split is proprietary.

An intelligently designed chemical reactor network must be an accurate representation of the flow patterns and mixing characteristics of the device it represents. In a CRN, the flow and flame patterns in the combustion volume are divided into zones represented by a reactor. Each reactor requires several inputs, such as composition of the reactants, residence time, reactor volume, temperature, pressure, flow rate, and distribution of the recirculation patterns. That information can be obtained from previous experimental results and from CFD simulations. Since the reaction structure inside a turbine's combustion chamber is not visually accessible for the experimenter, the CFD results have shown to be particularly suitable to gain details about those reaction structures. For that reason, the flame profiles, volume of the reactors, residence time, and recirculation patterns were obtained from the CFD results.

At full load (60 kilowatts electrical, kWe) the six nozzles inject a mixture of fuel and air into the combustion chamber. The turbine operating at full load on natural gas (in this case pure CH_4) was the model base to set up the chemical reactor network. Important variable such as the residence time, volume of each reactor, and temperature after the core of the reactions, were extracted from the CFD results of the turbine at full load. Figure 129 shows the temperature contours at the first and second plane. These contours were obtained for the turbine combustor running at full load. It is possible to see in Figure 170 the six injectors and the characteristic

conic section of an attached premixed flame (blue region). Both the CFD and CRN simulations assume a perfect premixing of fuel and oxidant.

Figure 129: Temperature Contours of a Turbine Combustion Chamber. The computational model shows the temperature profiles at full load (60 kWe). Note the two planes of injectors indicated in the figure.

The chemical reactor network presented in Figure 130 depicts the flow distribution extracted from the CFD analysis. The first block (or Block 1) includes the total mass flow inlet of premixed gas that is necessary to achieve an electrical power output equal to 60 kWe. The flow rate of premixed gas was set using the actual thermal efficiency at full power. In the same block, the flow rate is divided into three blocks (blocks 2, 4, and 5). Since the turbine configuration displays flame symmetry, it was possible to set a block of two perfectly stirred reactors (PSR) to represent each pair symmetrical flames. Each pair of flames is grouped into blocks 2, 4, and 5, and is represented by two PSRs in series.

The first reactor of the series represents the primary reaction zone, or the core of the reactions, where the effects of the surroundings are negligible; the second reactor in each block symbolizes a post-flame zone, which is a region at high temperature where the first PSR injects its combustion products; additionally, blocks 4 and 5 account for the effect of the exhaust gases that were produced in Block 2. The splitter in the CRN divides the exhaust products from Block 2 into three flow streams; two of these portions are directed toward the two second PSRs of the fourth and fifth blocks. In that manner, the effect of the exhaust gas that comes from the plane of two injectors is accounted for with this CRN configuration. Conversely, this CRN does not consider an interaction between flames that are located within the same plane. Analysis of the CFD results indicates that, in the plane of two injectors, little interaction between the reaction zones occurs. However, the products from the combustion in the plane of two does interact with the reactions associated with the injectors in the plane of four. The exhaust recirculation effect (both from the preceding flame and from the preceding plane) is accounted for by using a portion of the exhaust gases from Block 2. Block 6 represents a post-flame region where the streams of all the previous reactors are mixed again before they are diluted with air coming from Block 7 (the dilution air inlet). Finally, Block 8 accounts for the mixing process and the reactions after the dilution air is injected. Nitrogen oxide and CO emissions corrected to 15 percent O_2 are analyzed in the exhaust products of Block 8.

Figure 130: Example of a Combustion System Divided into Several Chemical Reactors

To evaluate the performance of the CRN, simulations were compared with measured NO_x results over a range of loads corresponding to the “6-injector” stage range. The CRN developed and shown in Figure 130 was used to predict the NO_x emissions levels from 54 to 60kW load under the situation where all 6 injectors are fired.. A comparison of the results is shown in Figure 131. The results demonstrate very good agreement.

Figure 131: Predicted NO_x Emissions Over Full Load Stage with 6 Injectors Operating.

On the basis of this agreement, the role of added hydrogen and carbon monoxide is explored by varying the composition of the fuel over a range of conditions. In addition, while systematic emissions studies were not carried out with varying fuel composition, some results were obtained for several mixtures which can be used to directly compare the results of the CRN. The CRN can then be used to provide an estimate of how fuel composition impacts emissions.

A numerical experiment to estimate the effect of varying the fuel composition on the NO_x emissions was carried out using the CRN methodology. The NO_x emissions of various mixtures of CH₄, CO and H₂ were tested. Since the reaction mechanism (GRI-Mech 3.0) is designed to model natural gas combustion (including NO formation and reburn chemistry), we restricted the minimum concentration (mole fraction) of CH₄ to be at least 30%. The fuel blends used for the analysis are presented in Table 20. The table also presents the NO_x emissions in parts per million by volume (ppmv) and corrected at 15% O₂. In addition, notice that the equivalence ratio is variable for each mixture and its value is calculated to hold an adiabatic flame temperature equal to 1850K; for the calculation of the adiabatic flame temperature, it is taken into account that the air is preheated with a heat recuperation system up to 830K; those conditions are similar to those found in the combustion chamber of the engine. By holding constant the adiabatic flame temperature and the power input, we guarantee the temperature at the turbine entrance to remain constant, while conserving the original power output. Also, the effect of the fuel composition on the engine efficiency is assumed to be independent of the fuel composition.

It is noteworthy that at constant temperature 1850K, the equivalence ratio lowers with the addition of either CO or H₂ to the baseline fuel (100% CH₄). It means that the mixtures of CH₄ with either gas are leaner when compared to the pure methane. For the same concentration of CO or H₂, the addition of CO to CH₄ presents a more important effect on reducing the equivalence ratio compared to the addition of H₂. However, a leaner mixture does not necessarily entail lower NO_x emissions. In this case, the emissions of NO_x increase when adding either CO or H₂; but the effect of the addition of CO is more efficient at enhancing the

production NO_x compared to the addition of H_2 . This result indicates that the chemistry of the reactions have a substantial effect on the formation of NO_x and the intermediate radicals that are formed when the fuel is mixed with CO have a more active participation on the NO_x pathways. Figure 132 presents the contour plot of the equivalence ratio as a function of the triple mixture of CH_4 -CO and H_2 .

Table 20. Fuel mixtures and prediction of NO_x using the CRN.

CH_4	H_2	CO	Equivalence ratio	NO_x
Mol fraction	Mol fraction	Mol fraction	-----	ppmv @ 15 % O_2
0.767	0.117	0.117	0.4598	9.3
0.65	0	0.35	0.4505	10.4
0.3	0.35	0.35	0.4254	12.9
0.3	0.233	0.467	0.4254	13.8
0.3	0.467	0.233	0.429	12.1
0.65	0.35	0	0.4596	9.25
0.3	0.7	0	0.435	10.9
0.533	0	0.467	0.4415	11.8
0.65	0.35	0	0.4575	9.4
1	0	0	0.468	8.4
0.533	0.233	0.233	0.447	10.5
0.3	0	0.7	0.4158	26.45

Design-Expert® Software
Component Coding: Actual
ER @ 1850AFT
● Design Points
0.468
0.4158

X1 = A: CH_4
X2 = B: H_2
X3 = C: CO

Figure 132. Contour plot of the equivalence ratio as a function of the triple mixture of CH_4 -CO and H_2 . For all the mixtures, the equivalence ratio sets an adiabatic flame temperature (AFT) equal 1850K.

The results of NO_x emissions for the triple mixture are presented in Figure 133. Notice that the emissions of NO_x are the highest when the fuel is mixed with CO and the maximum is found for 70% CO and 30% CH₄ (26.5 ppmv at 15% O₂). The minimum NO_x emissions are predicted for the case of 100% CH₄ (8.4 ppmv at 15% O₂), while the blend 70%H₂ – 30%CH₄ mixture presents an intermediate value (10.9 ppmv at 15% O₂). Table 21 shows measurements of NO_x at full load, and for several blends of natural gas/H₂ and CO/H₂. The column labeled as “NO_x before blending in H₂ [ppmv @15%O₂]” shows the results of NO_x emissions for the engine running at full load on the baseline fuel. In this case, the baseline fuels were either natural gas or CO. For the natural gas baseline case the NO_x emissions measured at the stack were observed to be 4-5 ppmv at 15% O₂. When CO was used as baseline fuel, the NO_x emissions were observed to increase up to 13 ppmv @15%O₂. Furthermore, it was observed that the addition of H₂ to CH₄ increases the production of NO_x, from from 4-5 ppmv @15%O₂ to 7-8 ppmv @15%O₂ while adding H₂ to CO reduced the production of NO_x from 13 to 6 ppmv @15%O₂, (see the last column on the right “NO_x before flashback [ppmv @15%O₂]”. These trends are consistent with those indicated by the CRN analysis. However, while the CRN methodology displays similar trends for NO_x emissions when the fuel composition is varied, the level of accuracy might be improved by building a CRN for each mixture, this is necessary since the characteristic variables (residence time, volume, temperature, composition) of each reactor vary with the fuel composition. This could be accomplished with further work using the measured results.

Figure 133. Contour plot of the NO_x emissions as a function of the triple mixture of CH₄-CO and H₂.

Table 21. Measurements of NO_x at full load for several blends of natural gas/H₂ and CO/H₂

Power [kW]	Baseline fuel	% H ₂ at Flashback +/- 3% (based on tip)	NO _x before blending in H ₂ [ppmv @15%O ₂]	NO _x before flashback [ppmv @15%O ₂]
59	NG	61	4	7
60	NG	60	5	8
62	CO	20	13	6
65	NG	59	5	8

To help understand why hydrogen addition increases NO_x in the case of natural gas, while it decreases NO_x when added to CO, Figure 134 shows the concentration of NO_x formed through different pathways. The production of NO_x through the NNH and prompt mechanisms are almost constant and relatively low for all the blends, and only for the highest concentration of 70% CO the NO_x formed through the NNH route seems to increase from 0.4 to 1.6 ppmv @ 15% O₂. It is observed that the presence of CO can enhance NO_x formation through the N₂O and thermal mechanisms as both mechanisms include the “O” radical as intermediate species to produce NO. As the concentration of CO in the fuel is raised, the CO molecule reacts and is divided into C and O radicals, those radical end up producing NO through the following paths:

- Zeldovich mechanism

- N₂O mechanism

On the other hand, the addition of H₂ to the fuel also increases the production of NO_x, and the N₂O mechanism is more significantly affected. In this case the molecule of H₂ increases the reactivity of the O₂ molecule and enhances the production of more O radicals, when compared to the case of pure CH₄.

Figure 134. NOx formation pathways for mixtures of natural gas with H₂ and CO.

5.1.2 Modified Injector

The effect of the injector design modification is now discussed. Figure 135 and Figure 136 show how the injector design modification affected the change in emissions as hydrogen was added to the anchor fuel. The design modification has the most significant effect on the NOx emissions at 30kW when comparing the emissions response to hydrogen addition to natural gas for the baseline injector and the modified injector. However, at this same load not much difference between the baseline and modified injectors is observed when examining the CO emissions response to hydrogen addition. For the 20 and 60kW loads, the design modification leads to a larger increase in NOx emissions and a larger decrease in CO emissions when compared to the emissions responses of the baseline injector for hydrogen addition to natural gas. It is also interesting to compare the changes caused by switching anchor fuels shown in Figure 127 and Figure 128 to the changes in emissions caused by injector design changes in Figure 135 and Figure 136. By doing this it can be seen that both the modification in design and switch in anchor fuels result in significant emissions changes as hydrogen is blended into the anchor fuel.

Figure 135 Percent change in NOx emissions as hydrogen is blended from 0% to hydrogen content just before flashback for the two injector designs

Figure 136 Percent change in CO emissions as hydrogen is blended from 0% to hydrogen content just before flashback for the two injector designs

6 Summary and Conclusions

Three experimental platforms were utilized in these flashback studies to support the design of the FFTS: axisymmetric single injector, full annular atmospheric combustor, and the C65 engine. The diversity in complexity among these different platforms allowed insights to be made that otherwise wouldn't have been possible using only the engine.

Single axisymmetric injector experiments were carried out to investigate the effects of (1) fuel composition, (2) injector geometry (i.e., injector diameter, enclosure diameter, standoff distance), (3) addition of diluents, (4) addition of higher hydrocarbons, (5) injector wall/tip temperature, (6) injector mixedness, (7) preheat, (8) adiabatic flame temperature, and (9) injector material on flashback in an axi-symmetric injector. The experimental setup consisted of

the injector, which was a clear quartz (that allowed for visualization of the interior of the injector) or stainless steel tube, and a quartz enclosure that was used for flame stabilization since some of the lower flame speed fuel compositions could not be made to stabilize on the injector tip alone (the quartz enclosure was removed when using the schlieren imaging techniques). The enclosure plate holder was designed such that various enclosure diameters could be investigated while also allowing various temperature measurements to be made. Schlieren imaging techniques and OH* intensified imaging were relied upon for visualization of the flame. The test procedure was typically the same throughout all the axisymmetric single injector experiments, i.e., the flame temperature was held constant while the air flow rate was decreased until flashback occurred. Reasonable correlation between the critical flashback gradient and the physical parameters, quenching distance and laminar flame speed, was achieved by using the injector tip temperature for any temperature terms in the determination of these physical parameters. In addition, the heat transfer occurring in this flame/tube/enclosure/plate system was analyzed using a simplified heat transfer model in order to more thoroughly investigate the effects of each mode of heat transfer since the experimental results showed that injector tip temperature played an important role and was dependent on fuel composition.

Full annular combustor experiments were performed with the motivation to connect this rig to the engine since the full annular combustor rig is much less expensive to run especially when considering the cost of carbon monoxide. The experiments consisted of varying equivalence ratio for various mixtures of hydrogen/carbon monoxide and hydrogen/natural gas until flashback or lean blow off was achieved. Significant time and effort were spent on ensuring accurate flow through the rig. These experimental results were then correlated using Damköhler number and turbulent flame speed. The Damköhler number correlated these data well, however, when connecting the engine data to full annular rig data, the Damköhler number proved insufficient.

The engine experiments were time consuming, difficult, and costly when carbon monoxide mixtures were being evaluated due to the high cost of carbon monoxide. These experiments involved the UCI Combustion Laboratory mixing station and the C65 engine. Changes made at the mixing station could significantly affect engine operation in some instances, making some data very difficult to attain. Several engine experiments also resulted in injector damage due to loss of thermocouples for detection of flashback without the emissions analyzer operating as backup flashback detection. In spite of all these challenges, a data set with measurements made at 20kW, 30kW, and 65kW were made for hydrogen/natural gas and hydrogen/carbon monoxide mixtures. These data were used in conjunction with computational fluid dynamic modeling of the C65 combustor to test a flashback prediction methodology (Wang et al. 2009) as well as gain more insight into the physical parameters driving flashback. The test of the flashback methodology could predict whether flashback would occur for large changes in hydrogen content, however, could not make these predictions for smaller variations in hydrogen content. This analysis did yield interesting results that showed quenching distance being the parameter that changes most with fuel composition implying that an accurate quenching distance correlation is very important.

Emissions data were also gathered during some of the engine experiments. These data were sufficient to test the predictive capabilities of chemical reactor networks in chemical kinetic software developed using computational fluid dynamics simulations. The chemical reactor networks were shown to be able to predict the trends in emissions changes as a function of fuel composition change, however, these chemical reactor network simulations could not predict with accuracy the values.

7 References

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8 Appendix

8.1 Challenges

8.1.1 Full Annular Experiments

During shakedown testing it was recognized that air was flowing asymmetrically in the combustor upon visual inspection of the flame. This problem needed to be resolved since distribution of flow within in the combustor is assumed to be asymmetrical and split according to CFD calculations. Figure 137 shows a video screenshot of H_2/CO flowing identical flowrates of 2.35 SCFM, yet the luminous zone of the flame are indicative of different EQs. The reaction on the left side of the combustor in Figure 137 with a bright orange luminous zone indicates a deficit in air flow at that location resulting in a rich flame. On the other hand, the flame on the right side of Figure 137 is less luminous and light blue suggesting a lean flame. Also, the structure of the flames is vastly different since the luminous orange flame is shorter wider at the base of the injector whereas the lean flame is longer and thinner at the base. This test was repeated on a H_2/NG mixture shown in Figure 138 with 0.77 SCFM flow through each injector. Again, there is asymmetrical behavior explained by the luminous flame on the left-hand side of the combustor while the flame on the right is barely visible.

Figure 137: Video screenshot of H_2/CO asymmetrical flow

Figure 138: Video screenshot of H_2/NG showing asymmetrical flow

Asymmetrical flow in the combustor was identified to be occurring from a leak between the combustor casing and recuperator housing generating a flow deficit on one side of the combustor. To remedy the leak a Cotronics seal (Part # 954-OD-1) designed with a thermal expansion rate close to that of stainless steel was applied between the gap. Another Contronics seal (Part# 907GF-6) was also applied just above the inner dilution holes where the turbine nozzle normally press fits into. These seals were chosen for their ability to accommodate for the thermal expansion the combustor cycles through during testing. Flow symmetry across the six injectors was verified post-sealing using a pitot probe and a flame ionization detector (Horiba FIA-236) in order to ensure that results are not skewed by leaks or asymmetric flows. Pitot probe measurements were taken at the center of each injector as an estimate of the average flow velocity and then converted to a flow rate using the exit area of the injector. With the flame ionization detector a metered flow of NG and air is provided to the injector and measurements

for composition are taken at the exit plane of the injector. Based upon the expected composition and the actual composition calculated from the flame ionization detector an asymmetry in the flow of the combustor can be calculated.

Initial FID results confirmed poor symmetry between the two injectors as shown in the “pre-seal” row of Table 22. “Post-seal” results match closely with those calculated from theoretical flow splits and are symmetrical. Table 23 compares the pitot probe and flame ionization detector results demonstrating agreement between the two measurement types along with identical flow rates out of each injector.

In summary, asymmetry and rich reaction zones were discovered in the combustor and attributed to a leak between the combustor casing and recuperator housing. The leak was filled using high temperature ceramic sealant and diagnostic tests confirm that flow in the primary zone was symmetric.

Figure 139: High temperature seals

Table 22: Performance of high temperature seals in rectifying asymmetry

	Injector 1		Injector 2	
	ϕ [Expected]	ϕ [Actual]	ϕ [Expected]	ϕ [Actual]
Pre-seal	0.40	0.56	0.39	0.49
Gap seal	0.38	0.32	0.38	0.31
Inner dilution seal	0.37	0.36	0.37	0.35
Post-testing seal	0.38	0.38	0.38	0.38

Table 23: Symmetry of all injectors post-sealing procedure

Injector	1	2	3	4	5	6
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Pitot Probe %	16.9	16.68	15.97	15.97	16.45	15.48
FID %	17.12	17	16.38	16.66	17.67	16.1

8.1.2 Engine Experiments

When applying the mixing station to the engine tests, a number of challenges arose. The first involved oscillations in the flow rate out of the natural gas compressor. These oscillations hindered the station's ability to mix natural gas with another gas when natural gas was selected as the anchor fuel. The oscillation in the natural gas flow rate would cause the set point for the blend gas to oscillate which resulted in large oscillations in the gas composition. The compressor was tuned several times with no improvement in these oscillations. Finally, the placement of a regulator between the compressor plenum and the mixing station decreased these oscillations in natural gas flow rate to an acceptable level.

The second challenge arose from the poor controllability of the hydrogen flow rate given the default PID parameters and control valve stem configurations (See Figure 140). Fortunately, with appropriate adjustment of the PID parameters and proper control valve stem selection reasonable control of the hydrogen flow rate was attained. However, there remains smaller amplitude oscillations that result only when mixing hydrogen (when mixing other gases such as CO₂ and NG these oscillations do not occur).

Figure 140: Example of poor controllability of the hydrogen flow rate when mixing natural gas and H2

A third challenge was a result of the request for 100% CO testing. With the original design, CO could not be selected as the anchor fuel. Therefore, a hardware or software modification was needed to address this limitation. A software modification was thus made (by the company that originally set up the control software for the mixing station). In the modification the CO line was switched to the natural gas line since the requirement was mixing of hydrogen and CO. However, some challenges still remain with regard to operating the engine on pure CO, which are a result of the original hardware being designed for use of natural gas as an anchor fuel not CO. This is a problem because of the much lower Btu content of CO, which requires much higher volumetric and mass flow rates. In particular, problems with the original pressure regulators have been the most limiting. Future work requires replacement of these regulators, but the short term fix has required increased upstream pressures.