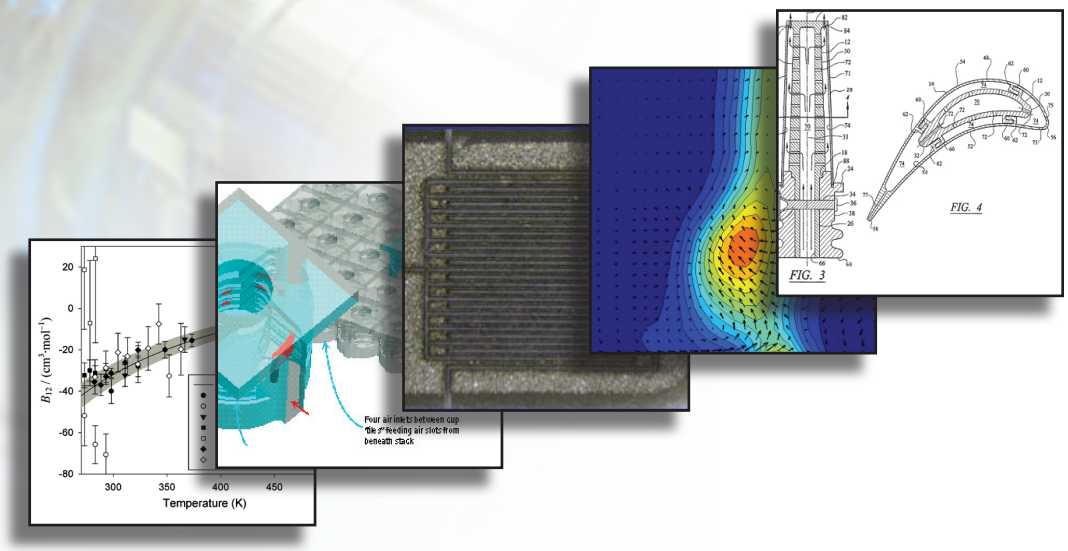
U.S. Department of Energy • Office of Fossil Energy
National Energy Technology Laboratory

Office of Fossil Energy Advanced Turbine Program

FY 2007 Annual Report

Turbines for Coal Based Power Systems that Capture Carbon



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2007
OFFICE OF FOSSIL ENERGY
ADVANCED TURBINE PROGRAM

September 2007

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I. INTRODUCTION

I. Introduction

On behalf of the Office of Fossil Energy, the Advanced Turbine Program is pleased to present the FY 2007 Advanced Turbine Program Annual Report. This report summarizes current progress towards meeting the goals of power production from coal that is clean, efficient, and less costly.

Background and Technology Status

Turbines are a proven technology for power generation. This is typified by the shear number of turbines in use today. Turbines find use in a wide range of applications: turbines for propulsion in the aviation industry, steam turbines in pulverized coal combustion boilers, MW-scale turbines for shaft work and electric power, turbines for use as compressors, microturbines for small-scale power generation, and gas turbines in simple and combined cycle (CC) applications. Turbine technology is responsible for the vast majority of power production in the U.S. and the world. For the past 25 years, increases in power generation, in terms of added capacity, have been dominated by natural gas fueled turbines in the CC configuration (a gas and steam turbine coupled together). This growth in natural gas CC applications is due to unprecedented performance in terms of cost, efficiency, emissions and power density when compared to any other utility-scale power generation system.

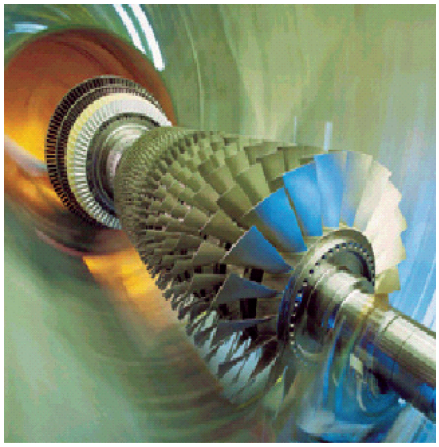


Photo courtesy of Siemens Power Generation, 2007

Gas turbine technology for electric power generation continues to advance in response to ever more demanding performance requirements. This advancement has been achieved in part because of cost-shared research and development (R&D) partnerships between industry and the government. These partnerships strive to advance turbine technology and performance beyond what the industry is expected to achieve on its own in terms of efficiency, emissions and cost. This advanced performance with accelerated availability to the marketplace has direct and tangible benefits to the public in terms of lower cost of electricity and reduced emissions of criteria pollutants.

A successful example of government-private sector partnership was the U.S. DOE Office of Fossil Energy's (FE's) Advanced Turbine System (ATS) Program, the precursor of the Advanced Turbine Program. The ATS Program helped bring to the marketplace the H-class gas turbine combined cycle, a steam-cooled turbine allowing operation at firing temperatures of 2,600°F and capable of achieving a CC efficiency of 60%. At the time of its commercial deployment, the H-class gas turbine was the largest CC system ever commercially deployed, with high efficiency and single-digit NOx emission capability. Turbine systems, components, and know-how demonstrated through the ATS Program have also resulted in an advanced G-class machine achieving similar temperatures with air cooling. Likewise, the performance of existing F-class machines has advanced with firing temperatures in excess of 2,500°F. All of these systems are now commercially deployed with public benefits of reduced emissions (criteria pollutants and carbon dioxide, also denoted as CO_2, which is a greenhouse gas) and lower cost per unit of power produced.

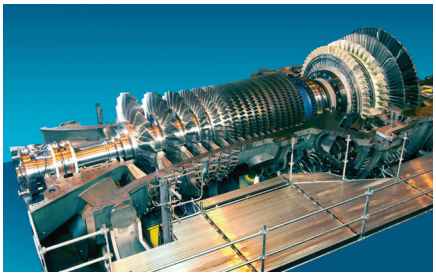
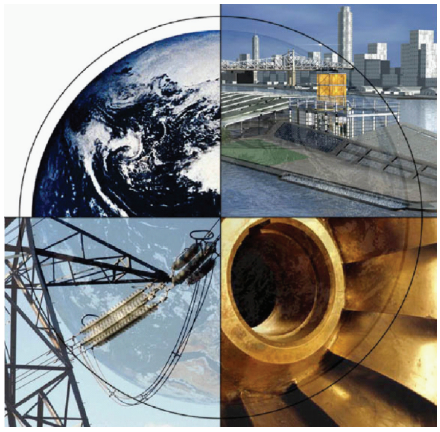


Photo courtesy of GE Energy

The President of the United States and the Department of Energy are committed to using coal in ways that are cleaner and more efficient. The technological progress of recent years has created a new opportunity for coal. Aggressive goals have been developed to lead the industry to a new, affordable breed of coal plant – a near-zero emissions plant that generates power and produces high-value fuels such as hydrogen with minimal impact on the environment.



Advanced turbines are an essential component of this new breed of coal plant. With gas turbines these new power plants will produce electricity and hydrogen from coal while capturing and sequestering the produced carbon dioxide. To realize the full potential of these coal plants in meeting the nation's energy goals, progress must be made on hydrogen fueled turbine performance to reduce emissions, increase efficiency and reduce cost.

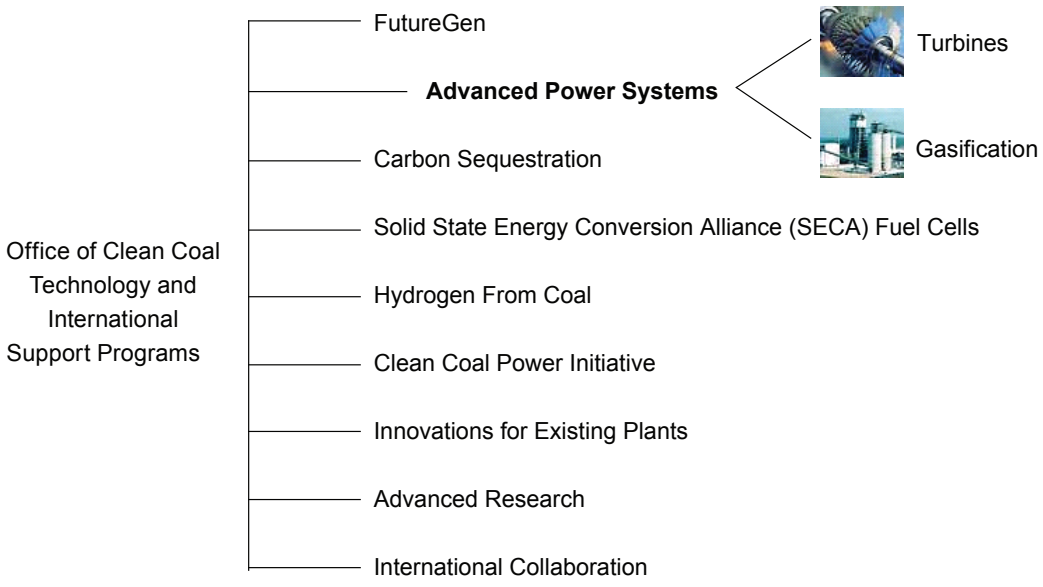
There are significant scientific and engineering challenges associated with meeting increasing demands on turbine technology when using hydrogen fuels derived from coal. For example:

- Hydrogen fueled combustor performance is being optimized for low NOx and high stability operation. Simultaneously, turbine inlet temperatures are being increased to realize higher efficiency, creating the need to protect the turbine's hot gas path components from heat damage.
- Combustion research is exploring the fundamental science of low NOx hydrogen combustion.
- Hydrogen combustor concepts that use physical mixing, catalysts and diluents are being engineered to minimize flash back, flame holding, instability and NOx production.
- Differences in the properties of the working fluids produced by hydrogen-air or syngas-oxygen combustion will also require new technologies related to turbine components, in the areas of materials as well as cooling.

To meet these challenges, the Advanced Turbine Program is implementing a research program to develop turbines for IGCC systems that capture CO_2.

Office of Fossil Energy and Advanced Turbine Program Goals

The U.S. Department of Energy's Office of FE manages a portfolio of research programs directed to demonstrate advanced coal-based electric power generation with near-zero emissions. These programs are designed to provide low-cost technological solutions to high-level Presidential initiatives that include the Climate Change, Clear Skies, FutureGen and Hydrogen Initiatives. Programs managed by the Office of FE's Office of Clean Coal are depicted in the figure below.



In response to these presidential initiatives, the Office of FE Office of Clean Coal has developed a strategic plan that lays out goals for three distinct time horizons. These goals include:

1. By 2010, develop advanced coal-based power systems capable of 45–50 percent efficiency at <$1,000/kW (in 2002 dollars).
2. By 2012, develop technologies for capture and sequestration of carbon dioxide that result in less than 10 percent increase in the cost of electricity in an IGCC-based plant and less than 20 percent increase in the cost of electricity for pulverized coal boilers.
3. By 2015, demonstrate coal-based energy plants that offer near-zero emissions (including CO_2) with multi-product production.

An additional primary objective of the Advanced Turbine Program is to support the FutureGen Initiative. The FutureGen Initiative is a project to validate the technical feasibility and the economic viability of producing electricity and hydrogen from coal, while capturing and sequestering the CO_2 generated in the process. In 2012, the FutureGen project is to begin operation of a nominal 275-megawatt (MW) prototype plant that will produce electricity and hydrogen with near-zero emissions. Advanced turbine technology is critical to the success of FutureGen and the achievement of the FutureGen goals.

The Advanced Turbine Program is organized into four areas: H_2 fueled turbines for IGCC applications, oxy-fuel turbines for IGCC applications, MW-scale H_2 fueled turbines and CO_2 compression technology. This annual report presents the status of projects addressing these topics and progress towards the goals and objective outlined above.

Advanced Turbine Program's Objectives

The Advanced Turbine Program will contribute to the 2010 goal above by meeting the following objectives:

- Efficiency: Demonstrate 2–3 percentage points improvement above the baseline[1] for CC performance for an IGCC syngas-fueled system.
- Cost: Demonstrate a 20–30% reduction (below the baseline) in CC capital cost, plus enhanced value for lower cost of electricity.
- Emissions: Demonstrate combustor emissions with 2 ppm NOx (@15% O_2) in simple cycle exhaust.

It is expected that the contributions to the 2010 goals will carry over and contribute to the 2012 goal for IGCC-based power systems that capture carbon. The main challenge here is that the machine will now be fueled by pure hydrogen (100% of the turbine energy input from hydrogen). Additionally, the Advanced Turbine Program plans to contribute to the 2012 goal by providing advanced and highly integrated CO_2 compression technology to reduce the compression penalty (auxiliary load) by 30-40%.

In supporting the FutureGen Project, the Advanced Turbine Program takes the approach to provide a turbine with the latest advances made through pursuing the 2010, 2012, and 2015 goals. This will allow installation of the most advanced hydrogen-fueled turbine at the FutureGen project. It is envisioned that this turbine could be installed with a pre-planned technology improvement philosophy. This approach would allow the machine to be optimized in the field for combustion, firing temperature and other performance-enhancing components or subsystems, and would allow for a machine fueled with 100 percent hydrogen to operate with the highest efficiency and lowest NOx emissions, validating Advanced Turbine Program contributions to 2010 and 2012 goals.

The Advanced Turbine Program will contribute to the 2015 goal above by meeting the following objectives:

[1] Baseline efficiency is defined in "Development of Baseline Performance Values for Turbines in Existing IGCC Applications," Richard A. Dennis, Walter W. Shelton, and Patrick Le, Proceedings of GT2007, May, 2007.

Efficiency:

- Hydrogen turbine CC with 3-5 percentage points improvement (total above baseline).
- Oxy-fuel turbine-based IGCC system with 40-50% efficiency (higher heating value).

Cost:

- Competitive cost of electricity for near-zero emission systems.

Emissions:

- H_2 turbine-based IGCC demonstrated with 2 ppm NOx (@15% O_2).
- Oxy-fuel turbine-based IGCC with near-zero emissions (>99% turbine exhaust captured and sequestered implying near-zero emissions of CO_2 and criteria pollutants).

Multiple Products:

- H_2 turbine-based IGCC with higher capacity gasification to allow balancing between power and fuels production.
- Oxy-fuel turbine based IGCC operating on hydrogen-depleted syngas producing power with hydrogen as a by-product.

2007 Annual Accomplishments

The Advanced Turbine Program made significant accomplishments in FY 2007 in the areas of NOx emissions, combined cycle efficiency improvement and cost reduction.

NOx Emissions: In separate projects using hydrogen as fuel, both GE and Siemens demonstrated the potential to reach the 2 ppm NOx goal at the lower range of firing temperatures.

Combined Cycle Efficiency Improvement: Improved plant and machine efficiencies were demonstrated in IGCC and turbine system studies using increased turbine firing temperature. Mechanical and aerodynamic turbine airfoil designs have been conceptualized to further improve turbine performance using syngas and hydrogen. Improved flow leakage and part cooling also have potential to increase turbine efficiency.

Cost Reduction: The increases in turbine performance and efficiency described in the preceding will result in combined cycle power islands with significantly higher power output, resulting in lower cost per kilowatt.

The accomplishments discussed in this report provide the initial steps towards producing efficient commercial hydrogen turbines. The improvements identified above are being incorporated into new turbine concept designs. Using these turbine concept designs, IGCC plants have been modeled that reach the 2010 and 2015 Advanced Turbine Program goals using hydrogen as fuel.

Project Highlights

The following projects highlight progress made in the Advanced Turbine Program during FY 2007.

Hydrogen Turbines for FutureGen

- GE Energy conducted the first full-scale, multi-nozzle test on premixed high hydrogen fuel. The test demonstrated strong operability relative to dynamics, flameholding, and flashback and showed that very low NOx levels are achievable.
- Siemens Power Generation demonstrated approximately 40% spallation life improvement over the state-of-the-art thermal barrier coating system with new modified bond coats and substrates.

- GE Global Research demonstrated 3 ppm NOx emissions and low CO at advanced gas turbine conditions using a novel trapped vortex combustor.
- Lawrence Berkeley National Laboratory designed and tested a low-swirl combustor injector capable of firing hydrogen at temperatures of interest with low single-digit NOx.
- Precision Combustion Inc. has selected the Solar Turbines, Inc. Taurus 70 engine as the development platform for assessing their rich catalytic lean-burn (RCL) hydrogen combustion system for low cost and high efficiency.
- Siemens Power Generation has identified catalytic coatings with acceptable light-off and fuel conversion capabilities on natural gas, syngas and high hydrogen fuels.

Advanced Oxy-Fuel Turbines

- Siemens Power Generation has completed conceptual designs of high pressure and intermediate pressure turbines, and identified critical areas to develop ahead of the detailed design. High level risk analysis, economic analysis and market demand simulation of power generation using oxy-fuel turbine technology has been completed.
- Clean Energy Systems, Inc. (CES) determined through systems modeling that the long-term (2015) CES oxy-syngas cycle can attain coal-to-grid higher heating value (HHV) cycle efficiencies of 35% with 99+% CO_2 capture.

Advanced Research

- The National Energy Technology Laboratory demonstrated flashback detection by combustion control and diagnostics sensor (CCADS) with fuel blends from 30–80% hydrogen in an industrial scale lean premixed combustor with optical access. Flashback detection with CCADS was demonstrated to be much faster than conventional thermocouple based systems.
- Ramgen Power Systems, Inc. operated their Rampressor at a pressure ratio of approximately 7.9:1 and a mass flow of approximately 2.43 lbm/s without the optimization of the geometry, boundary layer techniques and tip clearance.
- Southwest Research Institute identified an optimum compression concept that provides a 25% power savings and an alternative pumping arrangement that provides a 30% power savings, which combine for total power savings up to 35%.
- Princeton University showed that syngas ignition properties in the mild ignition regime are controlled by the formation of HO_2 and H_2O_2 and the decomposition of H_2O_2, and are subject to significant perturbations by fluid dynamic, mixing, and catalytic effects.
- Case Western Reserve University investigated the reaction kinetics of $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$ by *ab initio* calculations and master equation modeling, and derived a rate expression for this reaction.
- MesoScribe Technologies, Inc. demonstrated Direct Write thermal spray technology with the capability to fabricate thermocouples, heat flux sensors, thermopiles, and strain gages within thermal barrier coatings for use at high temperature.

NETL's University Turbine Systems Research

- The University of Central Florida has developed a new and improved model to predict ignition delay for hydrogen fuels for potential use in combustor design.
- Tests at Brigham Young University show that a transition temperature of ~975°C exists where an abrupt increase in deposition occurs; above this temperature, the deposition rate increases with temperature.

Following is a summary status for each project managed through the Advanced Turbine Program. The scope, objectives, status and accomplishments are reported for each project. The Advanced Turbine Program is encouraged by the technical progress made this year and the prospects for continued advancements in the coming year are good, paving the way to achievement of the goals and implementation of FutureGen.

II. HYDROGEN TURBINES FOR FUTUREGEN

II.1 Advanced IGCC/H_2 Gas Turbine Program

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Subcontractors:
- GE Global Research Center, Niskayuna, NY
- GE Aviation, Cincinnati, OH

Objectives

The primary objective of this project is to develop the technology for a fuel flexible (coal-derived hydrogen and syngas) gas turbine that achieves key DOE performance goals:

- Efficiency (45-50% combined cycle efficiency)
- Emissions (less than 2 ppm NOx at 15% O_2)
- Capital cost (less than $1,000/kW in 2003 dollars)

Accomplishments

- Conducted the first full-scale, multi-nozzle test on premixed high hydrogen fuel – this test demonstrated strong operability relative to dynamics, flameholding, and flashback and also showed that very low NOx levels were achievable.
- Developed design of experiments evaluation around the key nozzle parameters that have been identified through early modeling and experimentation – this experimental evaluation is making great progress and some very strong results have been achieved such as:
  - Testing of high hydrogen fuels at temperatures higher than previously achievable – GE has been able to test these nozzles at the high flame temperatures required in order to drive towards the efficiency goal of the program by operating at higher firing temperatures.
  - NOx levels near entitlement have been achieved – with these new nozzles, GE has been able to achieve NOx levels very near the entitlement level at the high temperatures required for this project.
- Developed laboratory test conditions that replicate actual operation in an integrated gasification combined cycle (IGCC) environment – this important step provides the foundation for the materials and coating evaluation that will occur as part of this project.
- Downselected to the two most promising Gen II environmental barrier coating (EBC) systems for further evaluation.
- Completed IGCC performance analysis to determine the effect of variable exhaust gas recirculation.
- Evaluated IGCC make-up water requirements for six turbine design cases with and without carbon capture.

Introduction

As demand for electricity continues to grow in the United States, there is a clear interest in reducing our dependency on foreign sources of energy. Coal is our most abundant domestic fossil energy resource. In an IGCC plant, coal can be converted into a gas (synthesis gas or syngas). This process also lends itself well to carbon capture and storage whereby the strong greenhouse gas, carbon dioxide, can be captured and stored rather than released into the environment. The resultant gas (either syngas or "carbon free" syngas – i.e., high hydrogen fuel) can be burned in gas turbines to generate electricity.

In order to more cleanly and more efficiently burn both syngas and high hydrogen fuels, improvements in gas turbine technology are required. GE's advanced turbine program addresses key technology development needs required to achieve specific DOE performance goals relative to emissions, efficiency, and capital cost. The project is comprised of two phases: Phase I, which began in October 2005 and concludes this September, is focused on conceptual design and technology development. The output of Phase I is a downselection of the key technologies that will be further applied and developed at the component level in Phase II. The four-to-five year Phase II effort will be focused on validating the technologies at a component level.

Approach

The project is comprised of three main technical focus areas (combustion, turbine/aero, and materials) plus a systems level activity. The systems level approach translates the integration of technology improvements into plant performance and investigates the various system trade-offs and their impact on overall plant performance. The combustion element of the project is

focused on improving combustion technology to achieve the DOE NOx emissions target of 2 ppm NOx. Work in this area addresses the challenges of developing a combustion system that can burn both syngas and high hydrogen fuels to produce extremely low NOx emissions while avoiding flameholding, flashback, and dynamics issues. The turbine/aero element of the project addresses specific turbine technology improvements to address the efficiency targets that have been identified by the DOE (45-50% combined cycle efficiency). The materials portion of the project is focused on applying materials technology to enable the turbine to operate reliably at higher firing temperatures in the IGCC environment. This includes evaluation of advanced alloys and coatings, including targeted use of ceramic matrix composites (CMCs) with EBCs. In summary, this comprehensive project addresses the technology development needs for advanced gas turbines for IGCC and FutureGen-type applications while targeting the specific goals identified by the DOE relative to emissions, efficiency, and capital cost.

Results

In Phase I of the project, a heavy emphasis has been placed on combustion technology development. In late December 2006, GE conducted the first full-scale, multi-nozzle test on premixed high hydrogen fuel at E class conditions – this test demonstrated strong operability relative to dynamics, flameholding, and flashback and also showed that very low NOx levels were achievable. Images from that test are provided in Figure 1. Future planned full-scale, multi-nozzle tests will drive conditions to F class and beyond.

This year, GE designed the first generation of nozzle prototypes capable of achieving gas turbine conditions on high hydrogen fuels without flashback. These Gen I prototypes are approaching the entitlement for emissions as established through earlier perfectly premixed tests completed on the project (see Figure 2). The project continues to work on achieving parity in terms of reliability between high hydrogen fuels and natural gas; this is the focus of the Gen II designs to be tested later this year.

Beyond the combustion area of the project, some important progress has been made in the materials area. Based on early IGCC field hardware evaluation and IGCC fuel sampling work done as part of this project, GE successfully developed laboratory test conditions that replicate the IGCC environment. This test will serve as the basis for the planned material/coating test project that will enhance materials selection to best achieve DOE goals.

In the systems area of the project, several important studies have been performed this year. For example, this project evaluated the impact of carbon capture on IGCC

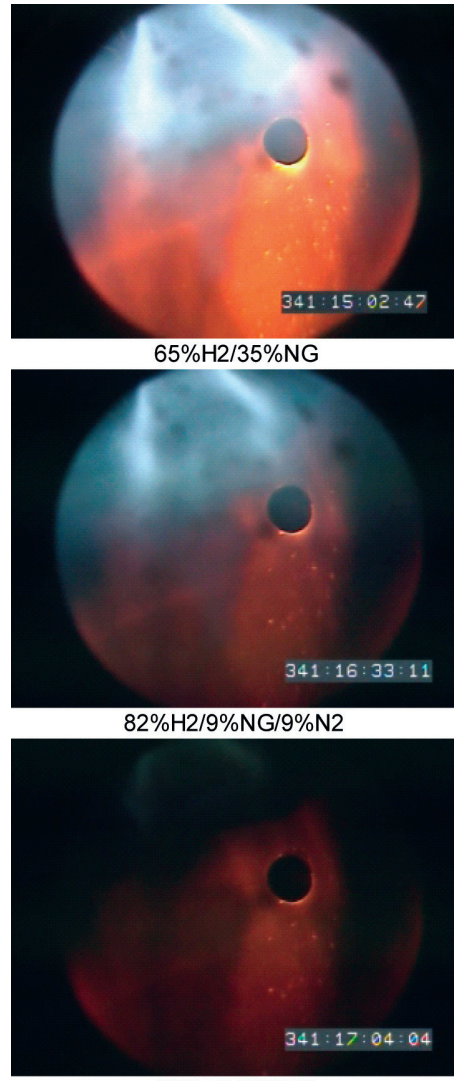

FIGURE 1. Flame Images from the Full-Scale Multi-Nozzle Test

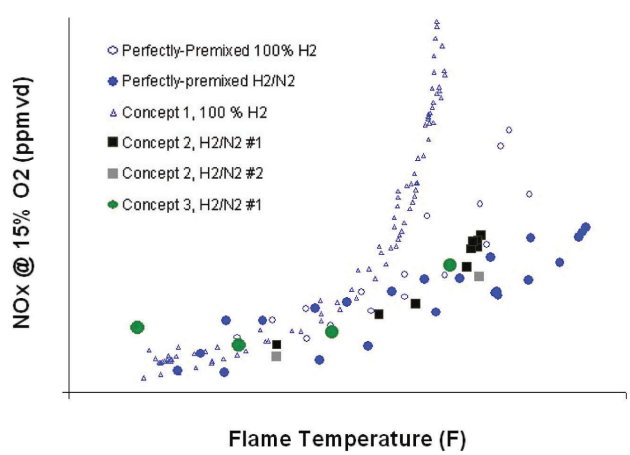

FIGURE 2. Sampling of NOx Data Gathered as Part of the Current DOE Project

plant performance. From this study, it can be seen that there is a significant IGCC performance benefit for reducing carbon capture to 85% versus 90%. A separate systems analysis also identified the performance impact of exhaust gas recirculation. IGCC make-up water requirements were also evaluated for cases with and without carbon capture – studies identified that IGCC make-up water requirements are about three times higher for gas turbine design cases with hydrogen fuel as compared to gas turbine designs with syngas fuel.

Conclusions and Future Directions

At this point of the project, GE is nearing the conclusion of Phase I of the project and three main conclusions can be made:

1. The project is well aligned with the DOE vision relative to emissions, efficiency, and capital cost.
2. The project is broad and is addressing key gas turbine technology development needs for syngas and high hydrogen fuels.
3. The project is making very strong progress in the combustion area towards the aggressive DOE NOx target of 2 ppm.

In Phase II of the project, the focus will be to validate the various technologies being explored at the component level. For example, by the end of Phase II, the goal would be to have an advanced combustion system that achieves 2 ppm NOx for a full-scale, multi-nozzle configuration. This combustion system would:

- Demonstrate syngas operability for DOE's 2010 goal.
- Demonstrate syngas and high H_2 operability for DOE's 2015 goal.

Similarly, in the turbine area, the goal would be to have validated turbine and materials technologies such that:

- GE demonstrates technology for 2-3% pts combined cycle efficiency improvement by 2010.
- GE demonstrates technology for 3-5% pts combined cycle efficiency improvement by end of Phase II for 2015 target.

In a currently un-awarded Phase III portion of the project, the focus would be on field validation of technologies at FutureGen (or another suitable site). Additionally, GE would complete detailed design and build of a prototype turbine that achieves:

- Emissions of 2 ppm NOx
- A 45-50% combined cycle efficiency
- Reduced capital cost

FY 2007 Publications/Presentations

1. Dustin Davis et al, "The Effect of Fuel Density on Mixing Profiles in a DACRS Type Premixer: Experiments and Simulation", ASME Turbo Expo 2007, May 14–17, 2007.

II.2 Advanced Hydrogen Turbine Development

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Subcontractors:
- Florida Turbine Technologies, Jupiter, FL
- Agillis, Jupiter, FL
- Combustion Science & Technologies, Orlando, FL
- University of Central Florida, Orlando, FL
- University of Florida, Gainsville, FL
- Georgia Institute of Technology, Atlanta, GA
- Texas A&M University, College Station, TX

Objectives

- To develop a conceptual design of the Advanced Hydrogen Turbine that meets the Department of Energy (DOE) 2015 program goals to improve combined cycle (CC) plant efficiency by 3-5 percentage points above state-of-the-art systems and reduce NOx emissions to 2 ppm with competitive cost of electricity.
- To ensure DOE intermediate goals of 2-3 percentage points improvement and reduction of CC plant capital cost by 20-30% over state-of-the-art are demonstrated by 2010.
- To conduct necessary materials, combustion, and turbine cooling feature tests to establish feasibility of identified concepts and select the most promising concepts for further development in Phase 2.
- To develop a plant conceptual design basis for use in evaluating the performance improvements of the Advanced Hydrogen Turbine technologies.
- To establish a plan for technology infusion to the FutureGen and 2010 platforms so that they will directly benefit from the advancements made in this project.

Accomplishments

- Approximately 40% spallation life improvement over the state-of-the-art thermal barrier coating system was demonstrated with new modified bond coats and substrates.
- An increased annulus turbine showing significant improvement in turbine efficiency with high mass flow was found to be feasible.
- Proof-of-concept full-scale rig test of an advanced combustion concept demonstrated very promising results in terms of NOx emissions and stability.

Introduction

Siemens Power Generation was awarded a contract by the DOE for Phases 1 and 2 of the Advanced Hydrogen Turbine Development project in October, 2005. The DOE Advanced Power Systems overall goal is to conduct research and development necessary to produce CO_2 sequestration-ready coal-based integrated gasification combined cycle (IGCC) power systems with high efficiency, near-zero emissions and competitive capital cost. The two-phase (with possible extension to three-phase) program will develop a hydrogen turbine based on the successful SGT6-6000G technologies. This advanced technology model was selected as the starting point due to its high firing temperature, output power and efficiency, as well as its novel secondary air and turbine cooling systems.

Fiscal year (FY) 2007 activities focused on identifying the required technologies, preparing technology development plans, carrying out cycle optimization studies, estimating plant cost and developing component conceptual designs.

Approach

Siemens has developed an overall project strategy that supports the DOE program goals and future commercialization. The path forward is a stepped approach which ensures the DOE intermediate (2010) and long-term (2015) goals are addressed. Beginning in FY 2008, Phase 2 will include advanced technologies development, down-selection and validation. In Phase 3, if awarded, the final product manufacturing specifications will be completed and the engine will be manufactured and installed in a FutureGen type IGCC plant for validation testing to demonstrate the project's commercial viability and that the DOE program goals have been achieved.

Results

In FY 2007, thermal barrier coating (TBC) system concepts were identified. A review was carried out on the development of high temperature capable TBCs

(Thermal Barrier Coating Conceptual Design, DOE Milestone No. 5) and was completed in December, 2006. A validation plan has been generated to ensure success in advanced coating systems development.

DOE Milestone No. 6 was accomplished with the completion of Baseline Combustor Testing. Full-scale testing was conducted using the baseline F-class diffusion flame combustor with modification. This enhanced diffusion flame combustor was tested with natural gas, hydrogen and syngas at various conditions. Satisfactory results were obtained and will be utilized as a baseline to which other designs will be compared.

Considerable progress was made on the advanced combustion designs through rig testing. Proof-of-concept full-scale rig test at elevated temperature demonstrated lower NOx emissions and combustion dynamics compared to current premix systems (see Figure 1).

Emissions and capital cost studies have been conducted which conclude CO_2 emissions in lb/MWhr (see Figure 2), NOx emissions in lb/MWhr, and plant capital cost in $/kW are reduced with increased plant efficiency, compared to current state-of-the-art (SOTA).

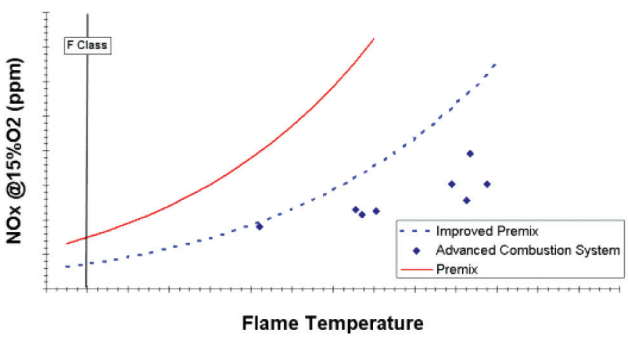

FIGURE 1. NOx Emissions Reduction with Advanced Technology

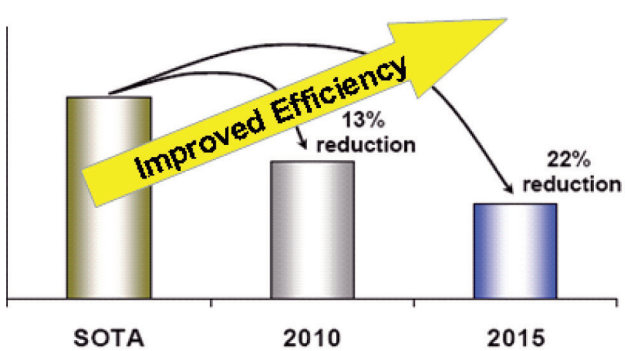

FIGURE 2. CO_2 Emissions Reduction with Advanced GT Technology

DOE Milestone No. 7 was accomplished producing a plant conceptual design. Plant efficiency calculations support a proposed two-step approach to meeting DOE intermediate (2010) and long-term (2015) efficiency goals (see Figure 3).

Results of a customer survey of industry experts, IGCC developers, operators and technology managers were obtained. Plant availability, capital cost and technology demonstration was concluded to be the major concerns for IGCC developers.

Significant progress was made through collaboration with universities in the areas of combustion kinetics modeling and testing (see Figure 4) as well as experimental data to support the advanced turbine cooling concept design.

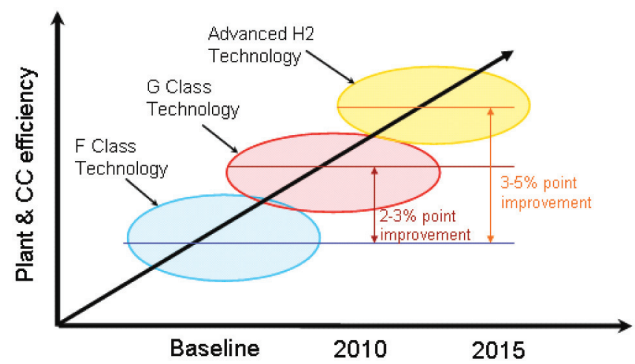

FIGURE 3. Proposed Two-Step Approach to Meet DOE Efficiency Goals

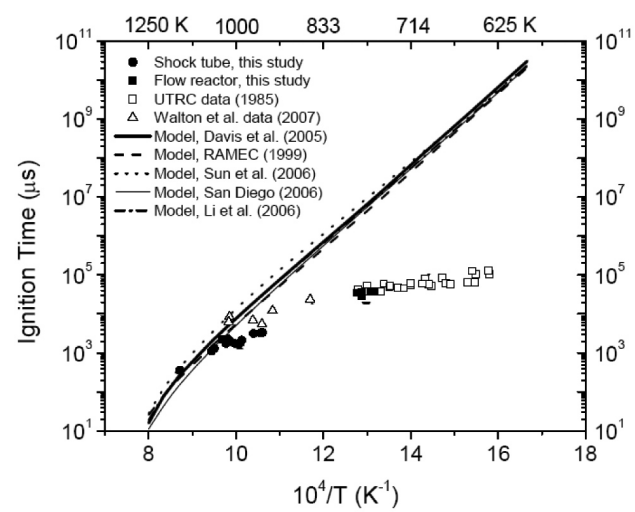

FIGURE 4. Ignition Delay Test Data and Comparison to Current Model

Conclusions and Future Directions

Based on the selected engine design point range, preliminary studies were carried out on an advanced compressor design to provide the required stage number and flow path geometry. The conceptual design utilized the existing advanced compressor design, with additional stages added to the rear to reach the target pressure ratio. A range of pressure ratios was also investigated and the implication on stage count was assessed. The next step will be 2D and 3D analyses and compressor design initiation.

A key component in successfully developing a fuel flexible hydrogen turbine is the combustion system. To achieve the very challenging program emission goal at the elevated firing temperature and pressure ratio, several competing combustion concepts, such as diffusion flame, premixed and catalytic, are being investigated. The candidate combustion systems will be developed through component modeling studies specifically for syngas and hydrogen application; through subscale test programs to evaluate critical combustion and operational issues; and through validation testing that will include module testing and both reduced and full pressure basket testing using syngas, high hydrogen content and natural gas fuels. Two combustors will be down-selected at the end of Phase 1 for further development and testing in Phase 2.

Hydrogen is deemed the most challenging fuel being considered for this project, due to its high flame speed, propensity for flashback and higher dilution requirement for NOx emissions, flame speed and flashback abatement. University partners will continue to validate prediction methods for flame speed and ignition delay with hydrogen and syngas fuels.

Advanced turbine aerodynamic and cooling concepts will be further evaluated and developed to produce a turbine design with the lowest possible cooling air requirements, excellent mechanical integrity and high efficiency. To achieve this, novel aerodynamic design concepts, high effectiveness cooling schemes, high temperature low conductivity thermal barrier coating systems and advanced alloy castings will be incorporated into the turbine design. Preliminary 2D aerodynamic designs were completed on all turbine airfoils for use in cooling concept evaluations. Preliminary cooling concepts were also generated for all vanes and blades and heat transfer analyses carried out.

Models of selected cooling configurations will be fabricated, instrumented, implemented and tested to identify the most promising concepts and verify prediction methods. These concepts will be evaluated and down-selected for further development and eventual incorporation into the hydrogen turbine vanes and blades. The tests will be conducted at the University of Central Florida and Texas A&M University test facilities.

Special Recognitions & Awards/Patents Issued

1. More than 25 patent disclosures have been submitted on the new technologies being investigated in this program.

FY 2007 Publications/Presentations

1. Advanced Hydrogen Gas Turbine Development Program" ASME Paper GT2007-27869.

2. Customer Advisory Board Meeting, November 2006.

3. IGTI Conference Presentation, May 2007.

4. EPRI Hydrogen Combustion Workshop, March 2007.

5. DOE Quarterly Review Presentation, January 2007.

6. DOE Quarterly Review Presentation April 2007.

References

1. Bancalari, E., Chan P., Diakunchak, I. "Advanced Hydrogen Gas Turbine Development Program" ASME Paper GT2007-27869.

2. Bancalari E., Chan P., Diakunchak, I. 2006 "Advanced Hydrogen Turbine Development" 23rd International Pittsburg Coal Conference, Pittsburgh, PA.

3. E.L. Peterson et. al. "New Syngas/Air Ignition Data at Lower Temperature and Elevated Pressure and Comparison to Current Kinetics Models" Combust. Flame (2007), doi:10.1016/j.combustflame.2006.12.007.

II.3 Partial Oxidation Gas Turbine for Power and Hydrogen Co-Production from Coal-Derived Fuel in Industrial Applications

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Subcontractors:
- Siemens Power Generation, Orlando, FL
- Solar Turbines, San Diego, CA
- Oak Ridge National Laboratory (ORNL), Oak Ridge, TN
- Georgia Institute of Technology (Georgia Tech), Atlanta, GA

Objectives

- Develop a feasibility design for retrofitting a conventional gas turbine for partial oxidation duty in the integrated gasification combined cycle (IGGC) plant.
- Produce a conceptual IGCC plant design (systems study) that integrates the retrofitted turbine design.
- Conduct a preliminary market study that projects demand for the IGCC plant for industrial applications.

Accomplishments

- Four candidate turbines for a retrofit design study of conversion to partial oxidation gas turbines (POGT) have been selected: the SGT-800 and SGT-900 from Siemens and the Titan 130 and Mercury 50 from Solar; retrofit design approaches for the selected candidates have been developed: replacing the combustor with a partial oxidation reactor (POR), compressor downsizing for about 30-50% design flow rate, generator replacement with 60-90% power output increase, and overall unit integration.
- POR performance for the selected turbines including required range of fuel/oxidant/steam ratios, temperature and pressure, working fluid compositions have been calculated, and POR exit parameters (expander inlet parameters) have been defined; conceptual decisions were made regarding the number of PORs to be connected with the SGT-800 and SGT-900 expanders, the number of expander inlet segments will remain the same as in the conventional turbines.
- POGT performance for the four retrofitted turbines have been calculated. The more detailed calculations were performed for the SGT-800. With a POGT as the topping cycle for co-production of power and syngas/hydrogen, the power output from the turbine could be increased by about 90% compared to a conventional SGT-800 keeping hot section temperatures and pressures practically identical.
- A POGT-based advanced IGCC detailed scheme has been developed and major components have been identified.
- A fuel-flexible fluid bed gasifier with moderate (~1,800°F) product gas temperature and a novel POGT unit are the key components of the 100 MW IGCC plant for co-producing electricity, hydrogen and/or syngas.
- Gasifier performance for bituminous coal and both air-blown and oxygen-blown versions have been calculated. Product gas and clean syngas compositions as well as all required parameters have been defined.
- Materials study and evaluation for hot sections of a POGT have been initiated. Siemens and Solar have selected candidate materials for operation in the hot, reducing atmospheres of the POGT. ORNL and GTI have prepared a test plan for experimental study of the selected materials at the ORNL test facility.

Introduction

There are two main features that distinguish a POGT from a conventional gas turbine: the design arrangement and the thermodynamic processes used in operation. One feature is utilization of a non-catalytic POR in place of a typical combustor. An important secondary design distinction is that a much smaller compressor is required, one that typically supplies less than half of the air flow required in a conventional gas turbine. From a thermodynamic point of view, the turbine working fluid provided by the POR (a secondary fuel gas) has a higher specific heat than the complete combustion products. This allows higher energy per unit mass of fluid to be extracted by the POGT expander than in the conventional case. A POGT thus produces

two products: power and a secondary fuel that usually is a H_2-rich fuel gas.

GTI has been advancing the POGT concept since 1995. Siemens, with GTI's participation, has performed technical feasibility and cost analysis studies of the partial oxidation power cycle. GTI, Solar and Tritek have designed, built and successfully tested a 7 MW_{th} non-catalytic pressurized POR. The POR was integrated with the modified 200 kW gas turbine. The experimental study of the 200 kW POGT prototype is currently underway, and results of this study are being used for the development of a feasibility design to convert a conventional gas turbine to POGT duty.

This report was prepared by GTI with significant contribution from the Siemens team led by Mr. Dennis Horazak.

Approach

The project approach includes mostly analytical, modeling and design studies, and some experimental study of materials for hot sections of the turbine. The following steps are being taken: selection of gas turbine candidates for retrofit to POGT duty; evaluation of the POGT performance for the retrofitted turbines; identification of the IGCC schemes for industrial application; preparation of an Aspen-based model for POGT and IGCC studies; definition of specifications for retrofit design of the selected turbines to POGT; fulfillment of the feasibility retrofit design and required drawings; development of a conceptual design of a IGCC-POGT plant and selection the major equipment; and conducting performance and cost analysis to form the basis for decision making to construct POGT and new power plants offering a mix of multiple products (electricity, syngas and/or hydrogen) for industrial operations.

Results

Two systems of the IGCC-POGT plants with air-blown and oxygen-blown gasifiers have been developed and implemented in the Aspen-Plus program.
A simplified schematic of the oxygen-blown version of the IGCC-POGT plant is presented in Figure 1. Evaluation of the IGCC key components, gasifier and POGT, has been performed during the reporting period. Syngas recirculation was used for the oxygen-blown fluid-bed gasifier to maintain the required gasifier performance.

A preliminary selection of syngas recycle compressors that can accommodate syngas upstream from syngas cleaning and supply to the gasifier has been conducted. Schematics and equipment for the air separation unit (ASU) have been reviewed, and a cryogenic ASU has been selected for application in the IGCC-POGT plant.

Gasifier performance for bituminous coal and both air-blown and oxygen-blown versions have been calculated, and product gas and clean syngas compositions as well as all required parameters have been defined. Based on gas turbine standards for gaseous fuel contaminant levels, the impurity requirements have also been calculated to set the basis for the clean-up system evaluation. The POR has also been evaluated, and composition as well as other parameters of the POR exit which is the working fluid for the POGT, have been calculated for the selected fuel/air/steam ratios. Good matches between the POR outlet and POGT parameters and existing SGT-800 and SGT-900 expander parameters have been achieved. The results of calculations to date for an oxygen-blown gasifier and POGT are presented in Figure 2.

Evaluations of POGT performance for the retrofitted Siemens SGT-800 and SGT-900 continue; evaluations for the Solar Mercury 50, Titan 130 and Centaur 40 have been initiated. With a POGT as the topping cycle for co-production of power and syngas/hydrogen, the power output from the turbine could be increased by up to 90% compared to conventional engines.

The conceptual modification designs of gas expanders based on the SGT-800 and SGT-900 were

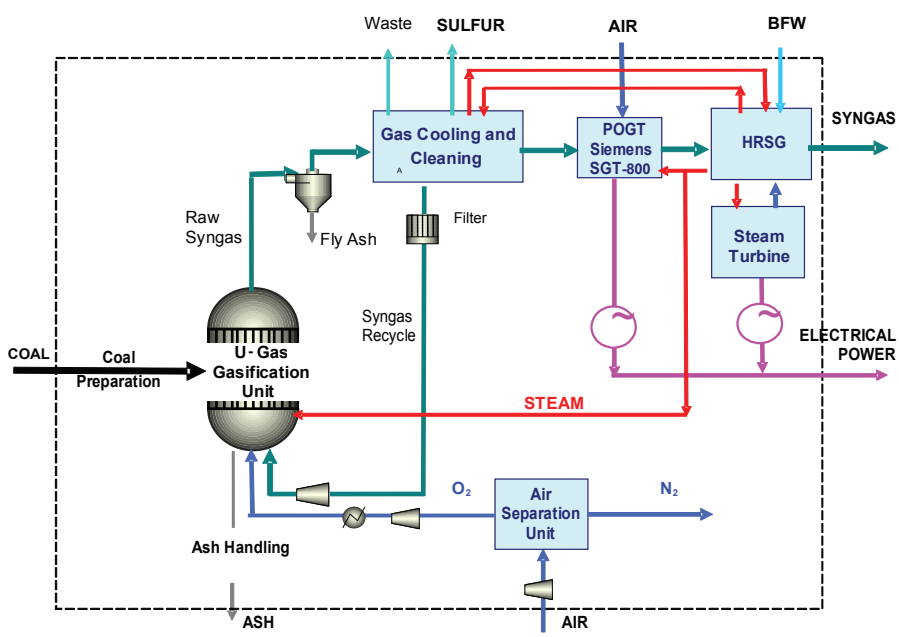

FIGURE 1. IGCC-POGT Plant Schematic with an Oxygen-Blown Gasifier

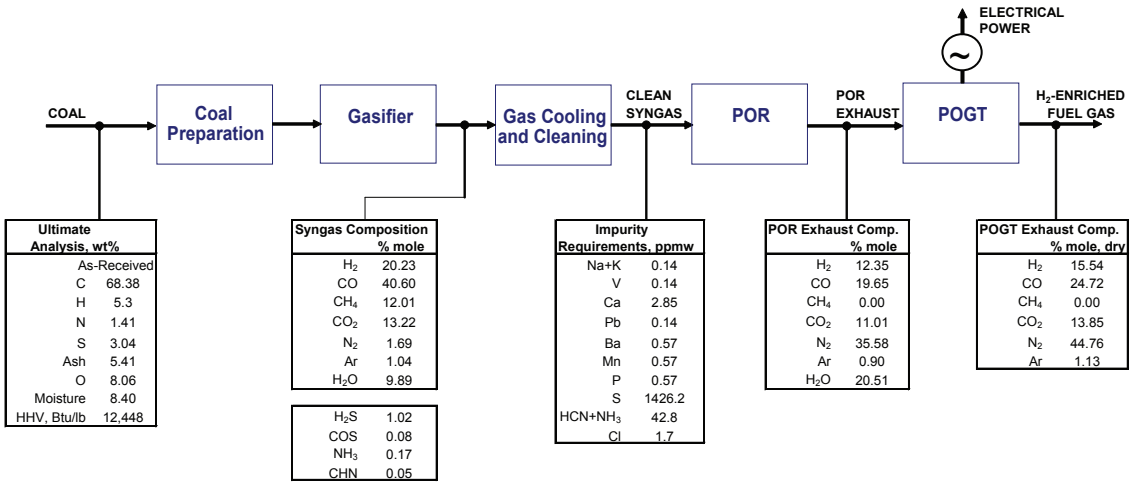

FIGURE 2. Compositions of Coal, Syngas, Impurities, and Turbine Working Fluid and Product Fuel Gas for the IGCC-POGT Plant with an Oxygen-Blown Gasifier

evaluated, with attention to the cooling requirements of the expanders. From a POGT perspective, the expander should produce the purest (least steam) partially-oxidized syngas without overheating the blades, vanes, or other expander parts. From a gas turbine perspective, the blade path temperatures should be about the same as in natural-gas-fueled versions of the same turbines, to minimize the need for design changes to the expanders. Siemens worked iteratively with GTI to define satisfactory steam cooling rates - for both blade path temperatures and cooling capacity - for the SGT-800 (GTX-100) POGT expander with both air-blown and oxygen-blown syngas, and the POGT SGT-900 (W251B) POGT expander with oxygen-blown syngas. Work on advanced cooling of the POR and expander for POGT will be continued.

GTI and Solar have conducted calculations of the POGT performance for the retrofitted Mercury 50, Titan 130 and Centaur 40. The results were compared to conventional engine performance firing natural gas.

Evaluation of the material requirements for hot sections of the POGT has been initiated and will be continued. Siemens identified candidate turbine materials for possible testing under reducing conditions at ORNL. The list of the Siemens candidate materials and samples for testing has been sent to ORNL. Solar has identified candidate materials and prepared a detailed report titled "Solar's Hot Gas Component Materials" which was sent to ORNL. Solar and ORNL have agreed on the list of materials for testing, and Solar will prepare the required samples. ORNL is investigating various turbine alloys and coatings designed to operate in hot, reducing atmospheres and preparing a plan to conduct laboratory testing of the samples sent by Siemens and Solar.

Combustion instabilities in a POGT have been evaluated by Georgia Tech. Modeling of the sensitivity of rich, premixed flames to oscillations at a given velocity and fuel/air ratio, and comparing these responses to lean, premixed flames has been conducted. The key conclusion that has been drawn to date is that rich, premixed systems are certainly not more susceptible to these instabilities than lean systems, and are possibly less prone to instability.

An initial market study has been conducted in the identified areas of industrial applications. GTI personally contacted oil/gas and steel companies and had meetings with high level company representatives. The company's representatives revealed a real interest in a POGT system for on-site co-production of electrical power and hydrogen/syngas at the refinery and the steel mill. Petrochemical and steel industries are the major potential areas of IGCC-POGT applications.

Conclusions and Future Directions

A POGT-based advanced IGCC process has been developed and major components have been identified. A fuel-flexible fluid bed gasifier with moderate (~1,800°F) product gas temperature and novel POGT unit are the key components of the IGCC plant for co-producing electricity, hydrogen and/or syngas.

A POGT could be retrofitted from a conventional gas turbine by replacing the combustor with a POR, compressor downsizing for about 30-50%, generator replacement with 50-90% power output increase, and overall unit integration. Four candidate turbines have been selected for a POGT retrofit conversion study: the SGT-800 and SGT-900 (Siemens), and Titan 130 and Mercury 50 (Solar), and a feasibility design is underway.

The IGCC-POGT system study is in progress. Gasifier and POGT performances have been calculated for two types of syngas from air- and oxygen-blown gasifiers. Their performance is used for the feasibility design of the retrofitted turbines.

Materials study and evaluation for hot sections of the POGT is underway and preparation for testing of the selected materials is in progress.

The major future direction is to continue the IGCC-POGT system study and complete performance and cost analyses to create the basis for construction of a commercial POGT prototype.

FY 2007 Publications/Presentations

1. Four Quarterly Progress Reports, DOENT 42649-3, 4, 5, 6.

2. J. Rabovitser, S. Nester, S. Wohadlo, M. Tartan, D. White, K. Smith, W. Nazeer "Partial Oxidation Gas Turbine for Power and Hydrogen/Syngas Co-Production" – Presentation at ICEPAG 2006.

3. J. Rabovitser, S. Nester, S. Wohadlo, D. White, K. Smith, W. Nazeer "Development of a Partial Oxidation Gas Turbine for Innovative Gas Turbine Systems" – Presentation and Paper at ASME Turbo Expo 2007.

II.4 Fuel Flexible Combustion System for Co-Production Plant Applications

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Subcontractors:
- Tim Lieuwen, Suresh Menon, Jerry Seitzman, Georgia Institute of Technology, Atlanta, GA
- GE Energy, Greenville, SC

Objectives

- Develop a multi-fuel low-emission combustor for co-production plant and gas turbine system applications.
- Demonstrate low-emission combustor performance on both syngas and natural gas.
- Quantify syngas flame speeds at gas turbine temperatures and pressure.
- Develop combustion modeling tools for low-Btu fuel compositions.
- Optimize co-production plant design.

Accomplishments

- Defined syngas fuel design space for various plant applications.
- Measured $H_2/CO/CO_2$ mixture laminar flame speeds as a function of strain and temperature.
- Evaluated 9- and 14-step reduced-order mechanism for syngas combustion which gave good agreement with measured $CO:H_2$ flame speeds for mixtures with up to 50% H_2.
- Evaluated multiple combustion technologies with respect to performance with natural gas and syngas. Technologies were evaluated based on cost of electricity, reliability, availability, maintainability, and emissions. Emission models were developed for each technology to examine the effects of fuel variability. Two concepts were selected for prototype evaluation based upon the scorecard results.
- Demonstrated 3 ppm NOx emissions and low CO at advanced gas turbine conditions using the novel trapped vortex combustor (TVC).
- Defined integrated gas turbine operating conditions for optimal performance.
- Integrated co-production plant models with NOx prediction models to determine operating conditions – including diluent usage – for meeting emission targets and maximizing plant efficiency.

Introduction

The aim of this project is the demonstration of a combustion technology that will overcome the limitations of current syngas gas turbine combustion systems and enable improved co-production plant designs. The abilities to handle low-heating value syngas, better use fossil fuels, reduce process waste, and produce clean and efficient power are the benefits of this type of system. Combustor development requires the development of improved modeling tools to capture the behavior of syngas at gas turbine conditions, and system modeling tools to validate improvements in plant efficiency.

Approach

The project characterized existing processes and resulting off-gas stream compositions to define fuel specifications from existing processes. Forecast improvements in plant design and their impact on fuel stream compositions were modeled. A system model of a co-production plant incorporating a fuel-flexible combustor concept will be produced at the end of the project.

Combustor development began with a characterization of the limitations of existing combustor design approaches. Flame extinction limits as a function of fuel composition were also measured to develop improved combustion models. Reduced-order sub-models for computational fluid dynamics design tools were evaluated. Two combustor prototypes incorporating appropriate emerging technologies were developed. The leading design will be evaluated against the needs of a fuel-flexible co-production production plant.

Results

A TVC prototype was evaluated at advanced syngas cycle conditions. The fuel composition was set to the targeted Early Entrance Co-Production Plant composition. The syngas has moderate levels of hydrogen. The firing temperature was far above current

syngas gas turbine firing temperatures and represented an advanced syngas machine.

The combustor demonstrated ultra-low NOx emissions at advanced firing temperature conditions. The combustor had good operability and low combustion dynamics. Table 1 shows the measured performance.

TABLE 1. TVC Combustor Performance

NOx @ 15%O_2	3.1 ppmvd
CO @ 15%O_2	18.7 ppmvd
Peak-Peak Dynamics	<0.5 psi

The low-emission performance with syngas at high firing temperatures is critical to increasing overall plant efficiency. The performance exceeded the emission goal of 9 ppm for the combustor at advanced conditions.

Fundamental syngas properties were studied for the development of advanced syngas combustion modeling tools. Experiments were carried out for lean mixtures over a range of reactant preheat temperatures from 300 to 700 K. As the unburned reactant temperature increases, the flame speed should increase due to increased chemical rates and thermal and mass diffusivities. This increase in flame speed requires the burners to be operated at higher average flow velocities. Fortunately, the increase in the unburned reactant temperature also increases the viscosity of the unburned mixture, which allows the flow to remain laminar even at the higher operating velocities. Hence, the same diameter burners used for the room temperature cases were used for the preheated cases.

Figure 1 reveals the influence of preheat temperature on flame speed for the 50% hydrogen content fuel (50:50 H_2:CO). The measured flame speeds increase rapidly with the unburned temperature for any given equivalence ratio and are in good agreement (within ~5%) with the Gas Research Institute (GRI) Mech 3.0 predictions, up to a preheat temperature of about 500 K. For further increases in preheat temperature, the discrepancy between the measured and GRI Mech 3.0 predictions increases. For the 600 K preheat temperature, the GRI predictions are higher than the measured flame speeds by roughly 10% throughout the equivalence ratio (Φ) range. For the highest preheat case (700 K), the simulations with GRI Mech 3.0 over-predict the measured flame speeds by as much as 15% near stoichiometric and 30% at the leanest conditions tested. The flame speeds predicted with the Davis et al H_2/CO mechanism are also shown in Figure 1. The H_2/CO mechanism predictions are very similar to those found with GRI Mech 3.0 except at the leanest Φ, where the H_2/CO mechanism predictions are higher than the GRI predictions by 5%. Thus the

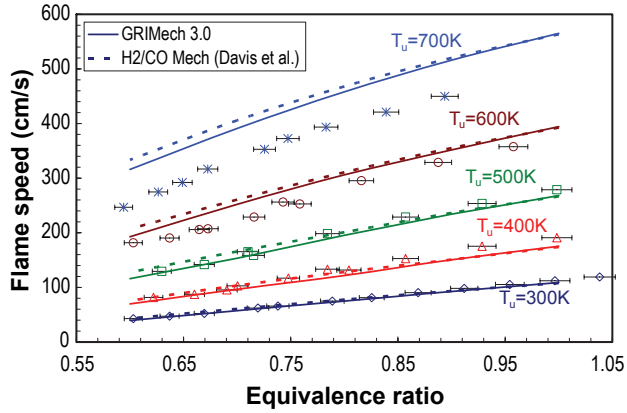

FIGURE 1. Laminar flame speed for fuels with 50:50 H_2:CO composition for various preheat temperatures; experimental data (symbols) and PREMIX predictions (lines).

H_2/CO mechanism has an even larger over-prediction for the undiluted, 50:50 H_2:CO mixture at 700 K preheat temperature.

Figure 2 shows the measured strained flame speeds for the same 50:50 H_2:CO composition at 700 K preheat temperature for 0.6 and 0.8 equivalence ratios. The measured strained flame speed increases with the imposed strain rate linearly for both equivalence ratios. It is important to note that the flame at 0.6 equivalence ratio is more strain sensitive than at Φ=0.8. Figure 2 also shows the OPPDIF predictions for Φ=0.6 and 0.8 in the same strain rate range as that of experiments for all four mechanisms. It can be observed from Figure 2 that the model results with all four mechanisms over-predict the measurements. The Chen 14-species mechanism is closest to the measurements, while the 9-species mechanism over-predicts the measurements by more

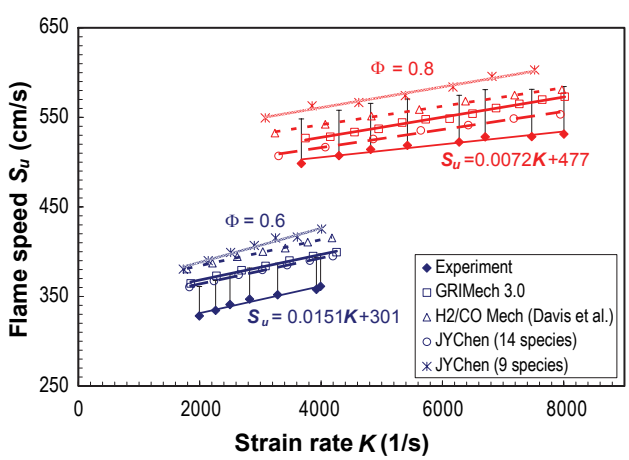

FIGURE 2. Flame speeds for a 50:50 H_2:CO composition at 700 K preheat temperature for two equivalence ratios. (The vertical bar on measurements indicate 10% deviation from the data. It is not the error in measurement).

than 10%. As the equivalence ratio is reduced to 0.6, the difference between the measurements and the model predictions increases. Predictions with GRI Mech 3.0 and the Chen 14-species mechanism are very similar, and they over-predict the measurements by 10%. However, the H_2/CO mechanism of Davis et al and the Chen 9-species mechanism over-predict the data by 15% and 20%, respectively.

The best reduced-order model, the 14-species mechanism by Chen, was applied to a large-eddy simulation (LES) model of the combustor. The LES model predicts unsteady flame behavior using these models. Temperature and species profiles in the combustion system are predicted as a result.

Conclusions and Future Directions

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

The 14-species Chen mechanism predictions at high temperature had reasonably good agreement with the measurements, within the accuracy of the more detailed models. Similarly, the discrepancy between the measurements and the Chen 9-species mechanism predictions were always the greatest. Therefore, the experiments suggest that the reduced 14-species mechanism by Chen is the superior choice for implementing into the LES code for the high-temperature reactant gas conditions expected in the gas turbine environment. In addition, with 10% or better agreement with the experiments, the mechanism should not require changes to make reasonably accurate predictions in the LES modeling.

The 14-species kinetics model used with the LES model provides some insight into the flame structure caused by both CO and H_2 reaction kinetics. As determined in this study, it is essential to include some detailed kinetics in order to properly capture the physics of syngas combustion in a turbulent environment. The current simulations and results have established a new simulation capability that could be used in the future to further study syngas combustion in complex combustor designs.

Special Recognitions & Awards/Patents Issued

1. Combustor nozzle for a fuel flexible combustion system (Patent pending).

FY 2007 Publications/Presentations

1. Joel Haynes, Matt Mosbacher, Tim Lieuwen, Suresh Menon, Jerry Seitzman, "Fuel-Flexible Combustion System for Co-Production Plant Applications," DOE Semi-Annual Report, January 2007.

II.5 Low-Swirl Injectors for Hydrogen Gas Turbines in FutureGen Power Plants

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Subcontractor:
Georgia Institute of Technology, Atlanta, GA

Objectives

- Adapt dry low NOx (DLN) combustion to the gas turbines in integrated gasification combined cycle (IGCC) clean coal power plants that burn coal-derived syngases and hydrogen.
- Develop an advanced near-zero emissions DLN method for syngases and hydrogen fuels based on a patented low-swirl combustion (LSC) technology from LBNL.
- Evaluate the effects of hydrogen fuels on the performance and emissions of the LSC at relevant gas turbine conditions.
- Establish scaling rules and engineering guidelines for the adaptation of LSC to the IGCC gas turbines
- Design low-swirl injectors (LSI) for the gas turbine combustors to utilize hydrogen and the high hydrogen content syngases.
- Demonstrate a LSI for large-frame gas turbines to meet the cost-effectiveness and performance targets of FurtureGen.

Accomplishments

- Developed an analytical model for the governing process of H_2 and syngas LSC flames.
- Designed and tested a fuel-flexible LSI prototype that operates with hydrocarbons, syngases and H_2.
- Demonstrated a low-swirl combustor injector capable of firing hydrogen at temperatures of interest with low single-digit NOx.

Introduction

This project is focused on developing a cost-effective and robust combustion system for the gas turbines in FutureGen IGCC power plants that burn hydrogen-rich syngases or pure hydrogen derived from coal gasification. FutureGen sets a very challenging near-zero emission goal of less than 2 ppm NOx for these turbines. The DLN combustion technologies developed for burning natural gas may not be readily adaptable to the fast burning and dynamic characteristics of hydrogen flames. Some manufacturers are considering reverting to more conventional combustion methods and mitigate the NOx emissions problem via catalytic treatment of the gas turbine exhaust or by diluting the H_2 fuel stream. These are relatively costly and complex remedies that can impact the system operation of the IGCC power plant. LBNL has developed a simple DLN combustion technology called low-swirl combustion that shows very good promise for resolving the combustion issues on burning H_2 in gas turbines.

All DLN methods involve lean premixed combustion where NOx can be controlled by diluting the premixture with excess air to lower the flame temperature. These premixed flames have characteristic wave-like behavior and they burn faster or slower according to the combustion properties of the fuel/air mixture, the initial temperature and pressure, and most importantly the turbulence intensity in the flow of the reactants. Conventional DLN methods are based on holding these fast moving flames within the combustion chamber of a gas turbine. The most common means to hold the flame is by the use of highly swirling flows to “anchor” the flame. Low-swirl combustion takes an opposite approach. It utilizes an aerodynamic flow feature called divergence to enable the premixed flame to burn and propel freely and producing a lifted flame that is the characteristic signature of the low-swirl combustion method (Figure 1). Matching the flow velocity to the turbulent flame speed is therefore the foundation of this combustion technology.

Approach

The LSC method was originally conceived for basic research on premixed turbulent combustion. Laboratory studies of LSC and subsequent analysis have provided a scientific foundation that has facilitated the transfer of this novel concept to industrial burners and to small natural gas fueled gas turbines. To advance this

FIGURE 1. A lifted self-propel flame is a characteristic feature of low-swirl combustion. Since the flame does not impart heat to the burner, the burner can be made of conventional materials. The burner shown in the photograph was made of PVC pipe sections to illustrate this unique feature.

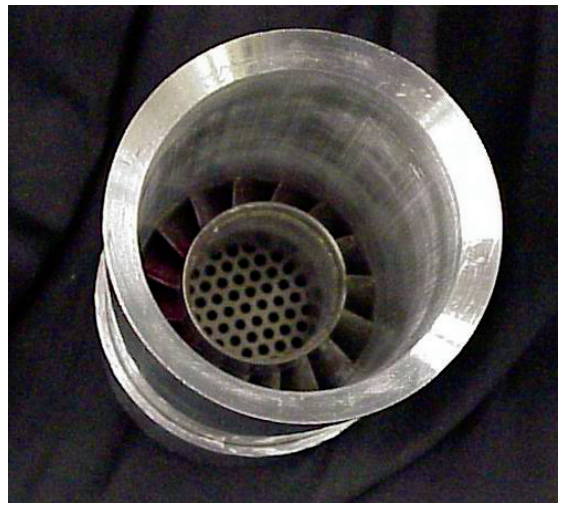

FIGURE 2. The LSI design is relatively simple. It consists of an annulus swirler fitted with curved swirl blade and a center-channel covered by a perforated plate. Flow through the center-channel promotes flow divergence that is the key fluid mechanical element for the low-swirl combustion concept.

technology for the large IGCC hydrogen turbines, the strategy is to adapt the design of a LSI developed for a 7 MW natural gas engine. The heart of the LSI is a patented swirler (Figure 2) that produces a divergent flow that supports stable lean premixed flames under a wide range of operating conditions. The divergence rate of the flowfield is an adjustable parameter that can be varied to accommodate the differences in the combustion properties of various fuels. This is achieved by altering the dimensions and configurations of the swirler components to change the swirl number of the LSI.

The development of a LSI for IGCC gas turbines starts with laboratory studies to optimize the configuration for burning the lean hydrogen flames whose NOx emissions are below 2 ppm. The experiments also provide turbulent flame speed data and quantitative information on the flowfields to support the development of an analytical model that can be used to design gas turbine hardware. Testing of the LSI at simulated gas turbine conditions verifies its operability and indicates improvement needs. Scaling of the LSI to large capacities and adaptation to different engine configurations require the development of new design tools. This is accomplished by detailed experimental and computational studies in collaboration with researchers from national laboratories, universities and original equipment manufacturers (OEMs). Joint developments of the analytical model for hydrogen flames and the state-of-the-art computational methods are the essential steps to resolve issues on combustion intensity, dynamics, emissions, flashback, blowoff and auto-ignition. The designs of the LSI for different engines are led by the OEMs to configure hardware that meets specific engine and system operation requirements.

Results

Laboratory experiments have been conducted to obtain the basic information to guide the adaptation of the LSI to burn syngases and hydrogen. To start, the lean blow-off limits for flames burning H_2 and H_2 diluted with N_2 were determined for a LSI with a swirl number $S = 0.54$. This LSI has been configured for natural gas but the results show that it also operates on very lean H_2 flames (equivalence ratio $\phi \approx 0.17$) and the lean blow-off limit is independent of velocity within the velocity range of $10 < U_0 < 20$ m/s. However, it cannot generate a lifted flame at higher stoichiometries due to the high diffusivity of H_2. This problem was addressed by a flame shaping method. Four additional LSIs with the flame shaping devices were evaluated. The best performance was provided by a LSI with $S = 0.51$. The results illustrate that the faster burning H_2 flames can be accommodated by a slight reduction of the swirl rate.

To quantify the effects of H_2 on LSI flowfield, extensive particle image velocimetry (PIV) experiments were performed to measure the turbulent velocity statistics and investigate changes in the flowfield with

increasing flow velocity and heat release. The data set consisted of 32 flames burning H_2 and nitrogen diluted H_2. Quantitative features extracted from the velocity data include the divergence rate, the virtual origin of the divergent flow, turbulence intensity, and the turbulent flame speed. The analysis showed that the overall flowfield features of the H_2 flames are not significantly different than those of the hydrocarbon flames. Most importantly, the magnitudes of the normalized divergence rates are the same and they do not vary with increasing velocity. This shows that the flowfields of the H_2 flames are self-similar and the basic LSC mechanism is unchanged despite the different properties of the hydrocarbons and H_2 flames.

The turbulent flame speeds of the H_2 flames deduced from the PIV data show a linearly increasing trend with turbulence intensity, u'. Though the linear trend is also found for the hydrocarbon flames, the turbulent flame speed correlation constant for H_2 flame is 50% higher (Figure 3) because H_2 burns faster than hydrocarbons. The difference, however, is less in the LSI than in other combustion systems. When applied to the analytical model, the higher flame speed correlation for H_2 flames implies an upstream shift of the flame brush closer to the exit of the LSI. The results of the laboratory studies provide an explanation to why that the LSI is amenable to burning hydrocarbon as well as H_2 fuels.

Knowledge gained from the laboratory studies was used to design a LSI for testing at the SimVal facility at the National Energy Technology Laboratory at Morgantown, WV. SimVal is developed for combustion research at realistic gas turbine conditions. It offers for the first time a direct observation of the LSI flames at high temperatures and pressures. The SimVal tests were conducted using natural gas, mixtures of natural gas and hydrogen and pure hydrogen. The experimental conditions varied from 30 to 50 m/s, pressures of 2 to 8 atms and temperatures of 600°F. SimVal tests showed that the LSI flame positions remain unchanged with velocity and confirmed the prediction of the analytical model. The most significant finding however is that LSI can meet the FurtureGen goals of firing with H_2 at combustion temperatures of 2,500 to 2,650°F and emit less then 2 ppm NOx (Figure 4). Experiments were also performed in a small facility at Georgia Institute of Technology to verify the operation of the LSI with syngases. Success in firing a reduced scale LSI at pressures of up to 4 atm, U = 30 m/s and T = 500°F verified that the LSI concept can also accept syngases of various compositions.

In parallel to the laboratory studies, discussions with OEMs were also carried out to seek their comments and feedbacks on the compatibility of the LSC concept for the IGCC turbines. These discussions have helped to identify the engineering issues and the research pathways to resolving them. Formal and informal

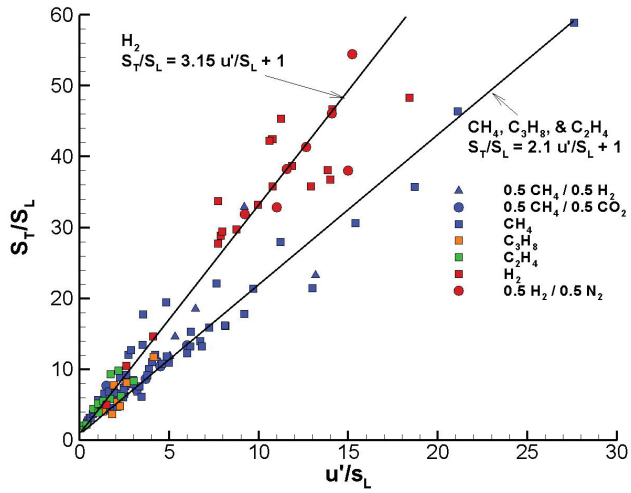

FIGURE 3. Turbulent flame speed, S_T has a linear dependency on the turbulence intensity, u,'. Data normalized by the laminar flame speed, S_L provide the correlation constants for the analytical model for LSI.

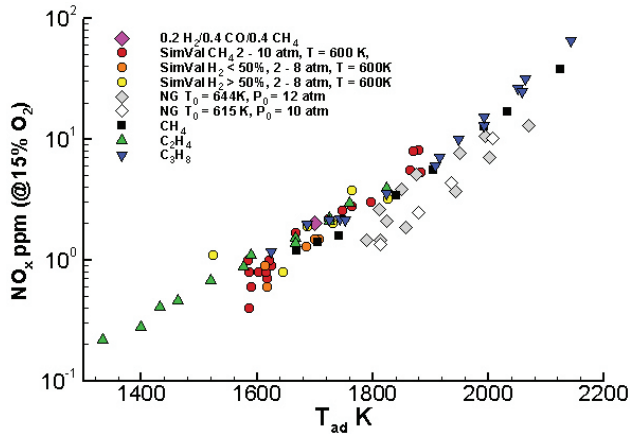

FIGURE 4. The NO_x emissions from laboratory experiments using a variety of fuels at atmospheric and simulated gas turbine conditions show a strong dependency on the adiabatic flame temperature, $T_{ad.}$. The FutureGen goal of <2 ppm can be achieved for flames with T_{ad}<1,700 K.

collaborations with the OEMs have been established to guide our laboratory studies to investigate and address issues on flame holding, premixing, staging, and scaling to the larger sizes and outputs of utility turbines. These are the steps leading to the OEMs' participations in joint developments of LSC hardware for FutureGen.

Conclusions and Future Directions

A DLN method developed at LBNL called low-swirl combustion is a promising technology for the H_2 and syngas fueled gas turbines in IGCC power plants. To adapt LSC for these faster burning fuels, laboratory studies have been conducted to gain the

basic information on the governing processes. The knowledge has been used to design a LSI prototype that has been tested on a simulated gas turbine to show the potential of the technology to meet the FutureGen goal of firing with pure H_2 at temperatures of 2,500 to 2,650°F while emitting less than 2 ppm NOx. Also initiated are collaborations with OEMs to identify and begin to address engine compatibility, scale-up and system integration issues. Future work is focused on verifying the analytical model for H_2 flames at gas turbine conditions and to develop computational design tools. Other studies include gaining insights into the H_2 specific combustion phenomena such as the thermal-diffusive effects, flashback, flame ejection, and auto-ignition to optimize the LSI and its components.

FY 2007 Publications/Presentations

1. Cheng, R. K. "Low-Swirl Combustion for Ultra-Low Emissions Gas Turbines and Its Potential for High-Hydrogen Fuels" Presentation to Siemens Power Generation, Orlando, Fl., October 5, 2006.

2. Cheng, R. K. "Low-Swirl Combustion – An Ultra-Low Emissions Combustion Technology for Industrial Heating & Gas Turbines, and Its Potential for Hydrogen Turbines," LBNL, DOE-FE & EPRI Webcast, November 8, 2006.

3. Cheng, R. K. "Fuel Flexible Low-Swirl Combustion for Ultra-Low Emissions Heating and Power Systems," Presentation to United Technology Research Center, East Hartford, CT, March 15, 2007.

4. Cheng, R. K. "Fundamental Issues of Lean Premixed H_2/Air Combustion for Gas Turbine Development," DOE/EPRI Workshop on H_2 Combustion in Gas Turbines, March 22, 2007.

5. Littlejohn, D., Cheng, R. K., Nazeer, W. and Smith, K. O. "Development of the Low-swirl Injector for Fuel-Flexible Gas Turbines," Paper H13, The 5th U.S. Combustion Meeting, March 25–28, 2007.

6. Cheng, R. K., & Littlejohn, D. "Laboratory Study of Premixed H_2-Air & H_2-N_2-Air in a Low-swirl Injector for Ultra-Low Emissions Gas Turbines," Paper GT2007-27512 ASME Turbo Expo 2007, Montreal, Canada, May 14–17, 2007. To appear in the Journal of Engineering for Gas Turbines and Power.

II.6 Combustion Systems for Hydrogen-Based Turbines

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Objectives

This work seeks to provide significant input to and support for the long range goal of developing turbine combustors capable of NOx performance of 2 ppm or less using coal syngas or H_2. In addition, this project supports the development of oxy-fuel combustors capable of near-zero CO_2 emissions.

Use of fuels with high H_2 contents in gas turbines raises a number of significant concerns, including flashback, combustion dynamics, flame blowoff, and NOx formation. This work plan addresses these critical needs through the following objectives:

- Identify and evaluate possible combustion alternatives for hydrogen turbine applications.
- Evaluate/test novel combustor designs, both premixed and non-premixed, for low NOx operation with high hydrogen fuels.
- Investigate methods, both passive and active, to extend the flashback stability limits in high-hydrogen fuels.
- Measure laminar flame speeds of gas mixtures appropriate for a variety of oxy-fuel combustion applications for gas turbines.
- Develop and test methods to stabilize combustion in practical applications.
- Identify the effects of fuel variability on combustion dynamics.

Accomplishments

- Completed draft whitepaper on hydrogen combustion alternatives and issues.
- Completed preliminary "proof-of-concept" testing of a N_2 diluted diffusion flame approach at elevated pressure and temperature.
- Completed "proof-of-concept" testing of novel hydrogen premixed (low-swirl injector) combustor at elevated pressure and temperature.
- Completed test series of flashback sensing and combustion diagnostics for high-hydrogen content fuels.

Introduction

A major driver of the DOE Turbine Program is the need for affordable, clean power-generation options that meet future environmental regulations. Integrated gasification combined cycle (IGCC) coal power plants can utilize domestically abundant coal supplies to generate power, chemical feedstock, or both. If an IGCC plant incorporates carbon-dioxide removal upstream of the gas turbine power island, a significant portion of the carbon in the fuel gas can be removed prior to combustion in the gas turbine. The remaining "carbon-free" syngas entering the turbine combustor is then significantly enriched in hydrogen.

The demands of improved efficiencies and near-zero emissions performance for coal-derived fuels such as syngas and hydrogen represent a significant challenge for the combustion section of the turbine. This work is directed toward developing turbine combustion technologies that can meet the targets of the DOE Turbines Program in the following general areas:

- Premixed combustors for hydrogen applications,
- Dilute diffusion hydrogen combustion concepts,
- Oxy-fuel combustion, and
- Combustion dynamics.

Approach

This work supports the long range goal of developing turbine combustors capable of NOx performance of 2 ppm at 15% oxygen using coal syngas or H_2 as well as supporting the development of oxy-fuel combustors capable of near-zero CO_2 emissions. The overall approach involves a variety of laboratory-scale [1,2], atmospheric pressure bench-scale, and high pressure larger-scale test rigs [3] to study a variety of possible combustion alternatives for hydrogen turbine applications. These facilities are used to evaluate and test novel combustor designs to assess their applicability for low NOx operation with high hydrogen fuels.

Combustion dynamics and flashback are also important phenomena that could limit the deployment of certain combustion approaches. Flashback stability margins in high-hydrogen fuels are being evaluated for some of these combustion approaches, and methods to extend stability regimes are being investigated. Computational fluid dynamics (CFD) simulation methods to reliably simulate or predict flashback behavior are being explored. A laboratory facility is being developed that is suitable for measuring laminar flame speeds of gas mixtures in high steam environments that are appropriate for oxy-fuel combustion applications for gas turbines. Following assembly and shake-down of this system, flame speed measurements of oxy-fuel systems will commence.

Results

Combustor performance (flashback, combustion dynamics, and emissions, especially NOx) is very sensitive to fuel properties. In particular, the presence of substantial concentrations of hydrogen in the coal-derived fuel of interest to DOE will substantially increase the burning velocity of the fuel compared to traditional hydrocarbon fuels such as natural gas. This large increase in burning velocity can lead to undesirable consequences including flashback and potential damage to combustion hardware.

NETL's high-pressure Simulation Validation (SimVal) combustor has been used to experimentally determine lean blowoff and flashback margin [4,5] for varying equivalence ratio, bulk gas velocity, operating pressure, and hydrogen fraction in natural gas/hydrogen blend fuels. Measurements of equivalence ratio and hydrogen concentration at flame flashback have been made at pressures ranging from 1 to 8 atmospheres, hydrogen concentration in the fuel of 60 to 100% and inlet velocities of 10, 20, 40 and 80 m/s. Results show that increasing the hydrogen concentration in the fuel significantly lowers the equivalence ratio at flashback. This is believed to be the result of the much higher flame speed for hydrogen compared to methane. An increase in the operating pressure also decreases the equivalence ratio at flashback. An increase in the inlet velocity increases the equivalence ratio at flashback.

These experimental data have been used for validation and development of CFD numerical simulation tools.

Figure 1 shows selected frames from the simulation of the flashback process. These numerical results agree qualitatively and, to a certain extent, quantitatively with experimental data. The pressure dependence on the equivalence ratio at flashback is also predicted by numerical simulations. An analysis of the numerical flow and species large eddy simulation (LES) field suggests that flashback is caused by the swirl as well as by the combustion-induced vortex breakdown.

Current state-of-the-art NOx emissions performance for industrial gas turbines fired on natural gas is typically achieved using lean premixed combustion technology. Premixing the fuel and air serves to eliminate fuel-rich regions which could produce excessive flame temperatures and, hence, elevated levels of thermally-produced NOx. However, the use of fuels with high levels of hydrogen can experience flashback in premixed combustors. The use of diffusion flame approaches can significantly reduce the potential for flashback problems. However, this combustion approach will produce NOx emissions that are substantially higher than the DOE Turbines Program goal of 2 ppm NOx at 15% O_2.

NETL researchers are investigating the potential of using flame strain with nitrogen diluted hydrogen fuel to achieve satisfactory NOx emission performance in a diffusion-style burner. Measurements of NOx emissions have been determined for a various jet diameters, nitrogen dilution, and jet velocities for turbulent hydrogen/nitrogen jets in an atmospheric pressure combustor. Figure 2 shows global NOx measurements plotted against jet exit velocity for different jet diameters and nitrogen diluent fractions. In addition to these atmospheric pressure studies, NOx measurements were also made in a high-pressure combustor at 2, 4 and 8 atm for N_2:H_2 ratios of 40:60 and 50:50 by volume. Figure 3 shows a plot of measured NOx versus jet velocity for the pressures and compositions that were examined. NOx was found to increase significantly with pressure, which was attributed to an increase in reaction rates as pressure was increased. The effect of

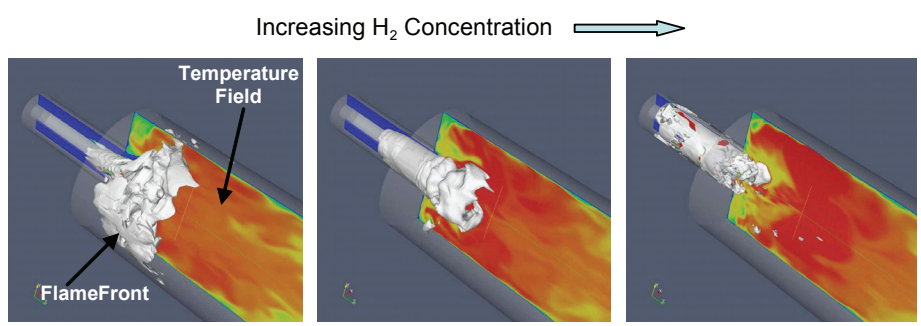

FIGURE 1. LES Simulation of a Flashback Event

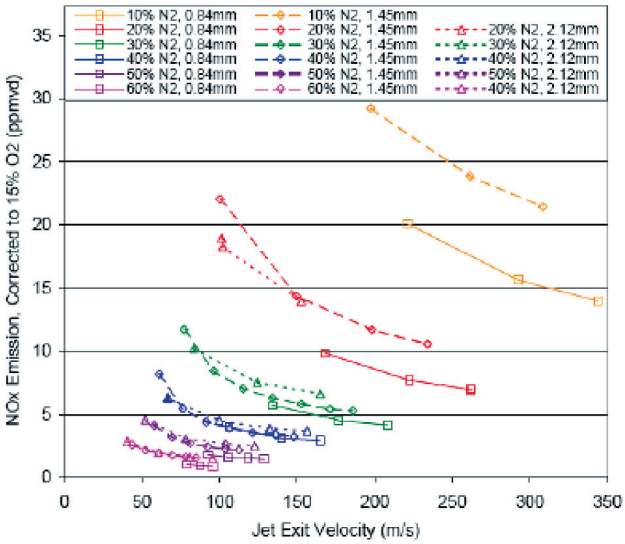

FIGURE 2. Corrected Global NOx Measurements vs. Jet Exit Velocity for All Jet Diameters and Nitrogen Diluent Fractions

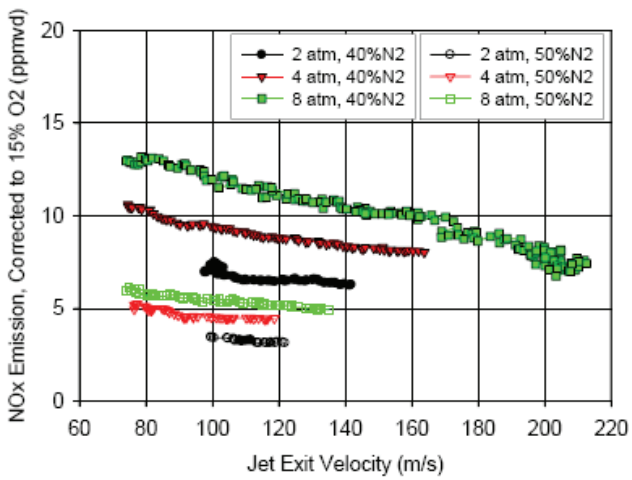

FIGURE 3. NOx Emissions vs. Jet Exit Velocity for High-Pressure Experiments; Jet dia. = 4.57 mm

pressure on NOx emissions was found to be dependent on nitrogen dilution in the fuel with a secondary dependence on jet velocity. Averaging over all velocities, NOx emission was found to scale with pressure to the 0.38 power for the 40% nitrogen dilution and pressure to the 0.32 power for the 50% nitrogen dilution. The dependence on pressure is expected to be a complex function of radical concentrations in the flame, especially O-atoms.

Conclusions and Future Directions

Flashback:

- The effects of hydrogen addition on a lean-premixed swirl-stabilized combustor operating on natural gas and air were studied both experimentally and numerically.
- Qualitative and semi-quantitative agreement between numerical simulations results and experimental data has been observed.
- An analysis of the numerical flow and species LES field suggests that flashback is caused by the swirl as well as by the combustion-induced vortex breakdown.

Hydrogen Dilute Diffusion:

- Compared to the range of parameters studied here, higher velocities and lower residence times would be required in order to achieve NOx levels in line with DOE program goals.
- Additional high-pressure work is planned that would use an array of small, low-residence time jets to achieve this.

FY 2007 Publications/Presentations

1. Weiland, N., and Strakey, P., "Global NOx Measurements in Turbulent Nitrogen-Diluted Hydrogen Jet Flames," Paper B22, 5th U.S. Combustion Meeting, San Diego, CA, March 25–28, 2007.

2. Weiland, N., and Strakey, P., "Stability Regimes of Turbulent Nitrogen-Diluted Hydrogen Jet Flames, Poster P56, 5th U.S. Combustion Meeting, San Diego, CA, March 25–28, 2007.

3. Thornton, J. D., Chorpening, B. T., Sidwell, T. G., Strakey, P. A., Huckaby, E. D., and Benson, K. J., "Flashback Detection Sensor For Hydrogen-Augmented Natural Gas Combustion," 2007 ASME TurboExpo, ASME Paper GT2007-27865.

4. Strakey, P., Sidwell, T., Ontko, J., "Investigation of the Effects of Hydrogen Addition on Lean Extinction in a Swirl Stabilized Combustor," Proceedings of the Combustion Institute, 31, 2007, 3173-3180.

5. Strakey, P. A., Woodruff, S. D., Williams, T. C., and Schefer, R. W., "OH-PLIF Measurement of High-Pressure, Hydrogen Augmented Premixed Flames in the SimVal Combustor," Paper AIAA 2007-0980, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 8–11, 2007.

6. Straub, D., Ferguson, D., Rohrssen, R., Perez, E., "Design Considerations for Remote High-Speed Pressure Measurement of Dynamic Combination Phenomena," Paper AIAA 2007-0561, AIAA 45th Aerospace Sciences Meeting and Exhibit, Reno, NV, January 8–11, 2007.

References

1. Weiland, N., and Strakey, P., "Global NOx Measurements in Turbulent Nitrogen-Diluted Hydrogen Jet Flames," Paper B22, 5th U.S. Combustion Meeting, San Diego, CA, March 25–28, 2007.

2. Ferguson, D., "Experimental Investigation of Oscillatory Heat Release Mechanisms and Stability Margin Analysis in Lean-Premixed Combustion", Ph.D. Dissertation, West Virginia University, https://eidr.wvu.edu/etd/documentdata.eTD?documentid=3854, 2005.

3. Sidwell, T., Richards, G., Casleton, K., Straub, D., Maloney, D., Strakey, P., Ferguson, D., Beer, S., and Woodruff, S., 2006, "Optically Accessible Pressurized Research Combustor for CFD Model Validation," AIAA Journal, 44(3), pp. 434-443.

4. Straub, D., Bedick, C., Sidwell, T., Strakey, P., and Casleton, K., "Flashback Studies in a Lean Premixed Combustor Operating on Hydrogen/Natural Gas Fuel Blends," Paper 06S-35, 2006 Spring Meeting of the Western States Section of the Combustion Institute, University of Idaho, Boise, ID, March 27–28, 2006.

5. Eggenspieler, G., Strakey, P.A., and Sidwell, T., "Experimental and Numerical Study of Flashback in the SimVal Combustion Chamber," (manuscript in preparation).

II.7 Micro-Mixing Lean Pre-Mixed System for Ultra-Low Emission Hydrogen/Syngas Combustion

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- University of California at Irvine, Irvine, CA
- Solar Turbines Incorporated, San Diego, CA

Objectives

- Develop and test a practical and scalable, high-performing multi-point injector module for hydrogen and syngas fuels, that is applicable across a wide spectrum of gas turbine engine sizes, and that achieves Department of Energy (DOE) program goals of NOx emissions of 3 ppm (2 ppm stretch goal) at full-power conditions.
- Demonstrate NOx emissions of less than 10 ppm for single-cup fuel-injector designs burning hydrogen, without auto-ignition or flashback, operating at 8 atm pressure and inlet temperature that is representative of practical full-scale engine operation (intermediate Phase II objective).
- Achieve NOx emissions of about 5 ppm or less without auto-ignition or flashback for at least one multi-cup design when burning hydrogen or syngas at 8 atm pressure and inlet temperature that is representative of practical full-scale engine operation (Phase II objective).
- Demonstrate stable combustion with NOx emissions at or below 3 ppm at full power conditions for full-scale (1 MW) injector operating on hydrogen or syngas.

Accomplishments

- Completed Phase I (April 30, 2007).
- Studied 24 micro-mixing cup geometries for hydrogen and syngas fuels using detailed computational fluid dynamics (CFD) numerical simulations.
- Selected for further development in Phase II the six best micro-mixing-cup concepts that numerical simulations show are most promising for achieving the program goals and the DOE goals of 2 ppm NOx emissions.
- Completed preliminary design of single-cup injector modules that are to be tested in Phase II.

Introduction

The utilization of hydrogen in a gas turbine combustion system presents a number of challenges, especially when constrained by a need to meet aggressive NOx emissions levels. Specifically, the high flammability and the high flame speed of hydrogen makes it a challenge to design combustion systems to produce flames that burn at the optimal ratio of fuel to air for low emissions and, at the same time, are stable and do not flashback into the fuel-air mixing devices. To achieve goals of ultra-low NOx emissions, the overall fuel-air mixture must be sufficiently lean, and peak combustion temperatures must be minimized. The reason is that the predominant chemical pathway for NOx formation is extremely sensitive to temperature, such that even localized pockets of fuel-rich, hot-burning mixture can increase harmful emissions. Thus, to minimize emissions, all modern combustion systems burn a fuel-air mixture that is lean (low fuel-air ratio) and uniformly-mixed. Conventionally, uniform mixing is achieved by using a *premixer* for the air and fuel, in which multiple small injection points are placed at a significant distance upstream of the exit of the premixer, allowing the fuel and air sufficient time and flow-distance (premixing length) to mix thoroughly before burning in the combustor. The premixer design must prevent spontaneous ignition of the fuel-air mixture in the premixer and flashback of flame into the premixer, both of which defeat the purpose of premixing and can cause severe damage to the combustion system. For hydrogen or hydrogen-rich fuels, the high speed at which flames propagate through a fuel-air mixture (4-10 times that of natural gas), the high rate of molecular diffusion of hydrogen, and the low amount of fuel required to sustain a flame may essentially eliminate conventional premixing approaches for achieving the mixing necessary to achieve the low NOx targets due to propensity for auto-ignition and flashback. This project proposes a new approach for achieving the necessary fuel-air mixing and stable combustion, in which the conventional large-scale injectors and premixers are replaced with a large

number of small premixers in a highly-integrated multi-point fuel injector, building on a proven technology for liquid fuel injection. The objective is to develop injectors that offer high performance in terms of emissions and flame stability, offer fuel-flexibility, and are scalable to all common engine sizes.

Approach

This project addresses the challenge of premixing hydrogen and air for stable low-emissions combustion by developing **micro-mixing multipoint-injection technologies** for gaseous fuels. The essential idea is to use multiple small premixers or "mixing cups" where fuel and air are allowed to mix at a much smaller spatial scale than in conventional premixers, thereby allowing fast and well controlled mixing. The proposed technology builds on multi-point injection schemes for liquid fuel, developed by Parker Hannifin, that have been proven to yield record-low NOx emissions (see Figure 1). Each mixing cup will be approximately ¼-inch to ½-inch in diameter and will contain four to eight fuel injection points. A full-scale injector will contain 30-60 closely-packed mixing cups for every megawatt of thermal power (see Figure 2). The multi-point injectors will be fabricated using Parker Hannifin's Macrolamination technology, in which the micro-mixing cups are created from layers of etched or machined metal plates that are stacked and diffusion bonded to create an integrated structure with passages that feed gaseous fuel and air into the mixing cup. While the project's deliverables are focused on hydrogen utilization in megawatt-scale turbines, the proposed technology is *scalable* and can be used across the whole *size spectrum* of gas turbine engines, both in *new equipment* and as *retrofits* to existing equipment.

Anticipated benefits of the new injector technology are as follows:

- The multi-point injection strategy will result in significant reduction in combustor length and thus engine weight and size will be reduced. With the new nozzle, complete combustion of the reactants will occur in small distributed flames within a distance of about one inch of the face of the nozzle.
- Liner cooling air requirements will be reduced as a result of the shorter combustor.
- Turbine inlet temperature pattern factor will be improved as a result of significant reduction in temperature gradients because of the small distributed flames.
- Cost effective fuel-injection technology for improved U.S. competitiveness – Macrolamination affords us increased complexity with reduced manufacturing costs.

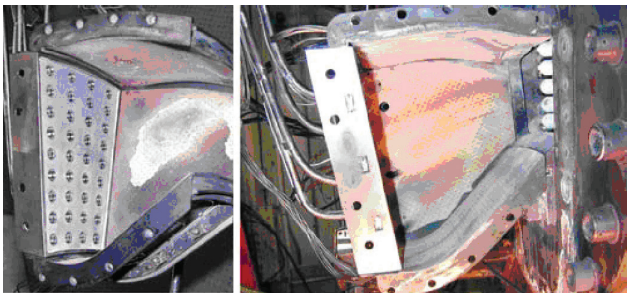

FIGURE 1. Photograph of 36 injection module installed in the NASA GRC facility that achieved NOx levels less than 30% of the ICAO standard [Tacina, et al. 2002]. The design shown received national awards for "Turning Goals into Reality" from the NASA Administrator in 2001.

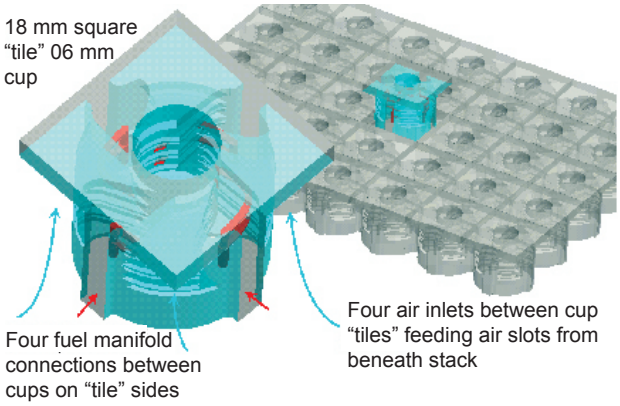

FIGURE 2. Micro-Mixing Cups Arranged in an Array, Demonstrating the Modularity of the Injector Concept, and Some Detail of a Single Cup

The research project consists of three phases: an analytical phase (Phase I), where multiple mixing-cup designs are generated and evaluated using numerical simulations; an experimental phase (Phase II), where the most promising mixing cup concepts will be tested and optimized; and a final validation phase (Phase III), where the performance of a full-scale injector will be demonstrated and evaluated.

Results

In Phase I, completed on April 30, 2007, 24 micro-mixing cup geometries for lean premixed combustion were generated, taking advantage of the versatility offered by Parker Hannifin's Macrolamination technology to arrive at compact, high-performance designs. The concepts were screened with respect to fuel-air mixing performance using detailed numerical simulations that predict the rate of mixing of fuel and air. Six mixing-cup concepts were then selected for further study and optimization in Phase II. A detailed research and development (R&D) implementation plan was created for Phases II and III, identifying advanced diagnostics to be used in experiments in Phases II

and III, and laying out a schedule of experiments and analysis that are needed to optimize the selected mixing cup concepts.

In addition to the design and analysis work done in Phase I, data were collected from the open literature and other sources on various aspects of hydrogen and syngas utilization for power generation. Component gases of typical syngas fuels were identified for the purpose of allowing the creation and use of representative mixtures in experiments planned for Phases II and III, and data on combustion characteristics of hydrogen and syngas fuels were collected for use in design and analysis. The findings of the study are detailed in a design specification report that has been delivered to DOE.

Conclusions and Future Directions

The objective of Phase I, of generating six micro-mixing cup concepts for hydrogen and syngas that show promise for stable, low-emission combustion of coal-derived fuels, was met. The design and analysis work done to date has led to injector designs that are compact and scalable. Phase II, just under way, will focus on testing multiple variants of the mixing cup concepts that were selected at the end of Phase I for further development and optimization. Taking advantage of the modularity of the mixing-cup concept, initial experiments will be conducted using only single-mixing-cup modules. This greatly reduces the required scale of each test and the total cost of experimental work, allowing a greater number of cups to be tested, and increases the likelihood of success. Following the initial single-cup experiments two mixing-cup concepts will be selected for multi-cup studies (four to nine cups) that will investigate the effects of interaction between neighboring mixing cup on fuel-air mixing, flame dynamics, and emissions. At the end of Phase II, a final design will be selected for use in a full-scale 1 MW injector that will be tested in Phase III.

FY 2007 Publications/Presentations

1. Design Specification Report, Submitted to DOE on May 4, 2007.

2. Test and Diagnostics Plan, Submitted to DOE on May 4, 2007.

3. R&D Implementation Plan, Submitted to DOE on May 4, 2007.

4. "Micro-Mixing Lean Premix System for Ultra-Low NOx Emission Hydrogen/Syngas Combustion – Phase I Summary Report," Parker Hannifin Engineering Report, ER MEN07-052, Gas Turbine Fuel Systems Division, April 30, 2007, Submitted to DOE on May 4, 2007.

References

1. Tacina, R, Wey, C, Laing, P, A. Mansour, "*Sector Test of A Low NOx, Lean Direct Injection Multipoint Integrated Module Combustor Concept",* Paper 2002-GT-30089, ASME: Turbo Expo 2002, Amsterdam, The Netherlands.

II.8 Catalytic Combustion for Ultra-Low NOx Hydrogen Turbines

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Objectives

- Four year program in collaboration with Solar Turbine, Inc.
- Demonstrate NOx <3 ppm, for megawatt-scale hydrogen gas turbine application.
- Same or lower pressure drop (4%) than existing gas turbine.
- Fuel: hydrogen and fuel flexible - natural gas, syngas.
- New and retrofit machines (sized to fit existing combustor envelope).
- Meet 24,000-hour life requirement.
- Allowance for single injector fabrication and testing by utility original equipment manufacturers (OEMs).

Accomplishments

- Solar Turbines, Inc. the world's largest manufacturer of mid-range industrial gas turbines (1-15 MW) is on-board. The Solar Taurus 70 (T70) engine has been down selected as the engine development platform in terms of RCL® (rich catalytic lean-burn) integration, lowest development cost, and engine efficiency among the Solar Turbines, Inc. engine family.
- Reactor Durability Testing: Three reactor catalyst/ substrate combinations have been selected for short term durability tests.
- Reactor Design: Gen. II design to represent engine hardware has been developed and fabricated as a subscale reactor to validate performance and robustness. Multiple tests have been performed on this subscale reactor design. Results of testing show high turndown and low NOx emissions.
- Preparation of research and development (R&D) implementation plan by both PCI and Solar Turbines, Inc. completed and submitted to the Department of Energy (DOE).
- Diluent selection study completed.

Introduction

The project will develop and achieve demonstration of an ultra-low NOx rich catalytic combustion system for fuel-flexible hydrogen combustors in megawatt-scale turbines. This will develop PCI's rich catalytic combustion technology for fuel flexible hydrogen application, in collaboration with Solar Turbines, Inc. and provide a roadmap to commercialization of the technology across all size ranges of power generation turbines. This technology, in a current DOE program, has demonstrated subscale ultra-low NOx emissions with syngas and with hydrogen diluted with nitrogen (low single digit NOx corrected to 15% O_2 with operation at integrated gasification combined cycle [IGCC] base load combustor temperatures and 10 atm rig pressure). The benefits include combustors capable of delivering near-zero NOx without costly post-combustion controls and without the requirement for added sulfur control. This advances DOE's objectives for achievement of low single digit NOx emissions, improvement in efficiency v/s post-combustion controls, fuel flexibility, a significant net reduction in IGCC system net capital and operating costs, and a route to commercialization across the power generation field.

The work plan is in three phases. Phase I (completed) involved the development of conceptual designs for catalytic combustion technology for hydrogen fuel and the production of a detailed R&D implementation plan. Phase II, Detailed Design and Validation Test Program, concentrates on development of multiple full-scale modules for validation testing including full pressure testing, and resolution of key issues. In Phase III, the full-scale design will be frozen, and a full combustor system (sector) with multiple catalytic combustor modules will be fabricated for initial rig testing.

Approach

To achieve project objectives, PCI, in close collaboration with Solar Turbine, Inc., is developing its catalytic combustion system for hydrogen fuel and for fuel-flexible operation in megawatt scale gas turbines. Conceptually, work centers around three primary system

functions (premixing, catalytic reaction, and gas phase reaction [combustion]), their integration with each other, and their integration in a gas turbine engine. These primary systems need to be integrated in a manner that resolves potential issues of flashback, autoignition, flameholding, and flame stabilization. Related scale-up issues must also be considered as the system is integrated into an engine. The overarching goal throughout the project is to achieve ultra-low NOx emissions below 3 ppm with good engine performance and operability using multiple fuels.

Results

For the combustion of natural gas, PCI has developed and demonstrated, in an engine, a RCL® combustion system capable of delivering NOx emissions lower than 2.0 ppm. The RCL® system is based on the concept of stabilizing combustion with catalytically-reacted fuel and air having a temperature below the instantaneous autoignition temperature [1]. The combustion air stream is split into two parts upstream of the catalyst. One part is mixed with all or the majority of the fuel and contacted with the catalyst, while the second part of air is used to backside cool the catalyst. The cooling air stream can also carry a small amount of fuel with flashback controlled by maintaining the fuel concentration below the flammability limit. At the exit of the reactor, the catalyzed fuel/air stream and the cooling flow are combined to finalize combustion. Using rich catalytic combustion has been shown to offer the same low NOx advantage for hydrogen fuel.

Subscale reactor/combustor 10 atm testing continues using the Gen. II reactor design, which more closely approximates engine hardware than the previous Gen. I reactor design. This new reactor shows good performance, achieving low single digit ppm NOx at F-class firing temperatures with good combustor stability and turndown. The reactor design is being optimized to produce greater catalytic conversion within the reactor which will improve performance further with promising initial results (Figure 1).

Based on results of Phase I, three catalyst/washcoat formulations were shown to have promise for achieving long term (25,000-hour) operation. One of the three candidates has completed limited short-term durability tests at simulated engine conditions with the remaining two being tested in the near future. The completed test shows stable performance both in catalytic wall temperature and catalytic conversion efficiency.

In discussions with Solar Turbine, Inc., an initial design envelope of the full-scale single injector hydrogen combustor is being finalized for T70 hydrogen application. Also, an initial reactor design is being

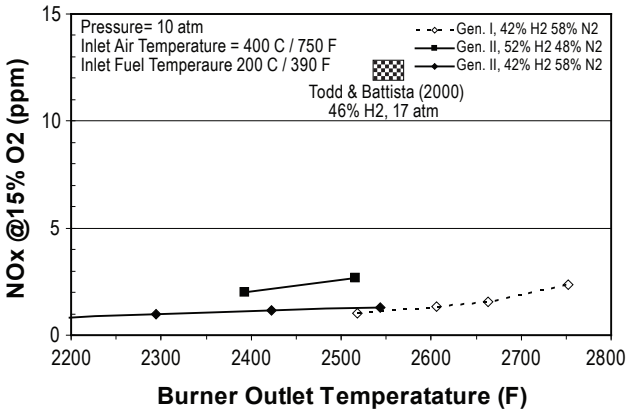

FIGURE 1. NOx Emissions Results of Hydrogen Reactor Designs

produced to be reviewed for engine fit and suitability for use in a T70 engine. Major progress is being made in upgrading the Solar Turbines, Inc. test facility for the large flow rates of hydrogen and diluent necessary for full-scale testing. The Solar high pressure test facility upgrades are expected to be completed in summer 2007.

Conclusions and Future Directions

- Successful sub-scale rich catalytic combustor operation with low NOx emissions demonstrated for hydrogen.
- Identified areas of improvement for robust engine operation.
- Target engine has been determined by Solar and PCI for further engine testing.
- Solar's 17 atm high pressure facility is being upgraded for hydrogen testing.
- Detailed drawings for full-scale catalytic injector, to be tested at Solar Turbine Inc.'s high pressure facility to be completed and fabrication to begin.

FY 2007 Publications/Presentations

1. "Catalytic Combustion for Ultra-low NOx Hydrogen Turbines", Technical presentation at the 23rd Annual International Pittsburgh Coal Conference, Pittsburgh, PA, Oct. 2006.

2. "Catalytic Combustion for Ultra-low NOx Hydrogen Turbines" Technical presentation at 7th Annual International Colloquium on Environmentally Preferred Advanced Power Generation, Irvine, CA, Sept. 2006.

3. Attended "Workshop on Hydrogen Combustion in Gas Turbines" held by EPRI, Washington, D.C., Mar. 2007.

References

1. Smith, L. L., Karim, H., Castaldi M. J., Etemad, S., Pfefferle, W. C., Khanna, V., Smith, K. O. (2005). Rich-Catalytic Lean-Burn Combustion for Low-Single-Digit NOx Gas Turbines", Journal of Engineering for Gas Turbines and Power, Vol. 127, pp. 27-35.

2. Todd, D. M., and Battista, R. A., (2000) "Demonstrated Applicability of Hydrogen Fuel for Gas Turbines", Proceedings of Gasification 4 the Future, Noordwijk, Netherlands.

II.9 Catalytic Combustion for Fuel-Flexible Turbine

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Objectives

- Develop a fuel-flexible catalytic combustion system capable of operation on natural gas, syngas and hydrogen containing fuels for a large scale industrial gas turbine such as the Siemens SGT6-5000F.
- Catalytic combustor design should be capable of operating at SGT6-5000F conditions with NOx emission of less than 2 ppm without the need for backend cleanup technology.
- Develop catalyst materials which are capable of operation on natural gas, syngas and hydrogen with acceptable light-off, fuel conversion and durability.

Accomplishments

- Module testing demonstrated NOx emissions less than 2 ppm at SGT6-5000F temperatures and 3 ppm at SGT6-6000G firing temperatures on natural gas.
- Module and basket design changes identified for syngas operation.
- Module testing demonstrated operation on syngas at SGT6-5000F. Further optimization required to meet emission targets.
- Alternative lower cost basket design developed for fuel flexible combustor. Initial testing performed on this design. Further optimization required.
- Coatings identified with acceptable light-off and fuel conversion capabilities on natural gas, syngas and high hydrogen fuels.
- Effects of sulfur poisoning evaluated for the most promising coatings.
- Durability testing performed for over 100 hours and 30 cycles on natural gas for multiple coating designs.
- Coating durability testing performed for the most promising coatings over 110 hours with syngas fuel from a small scale gasifier.

Introduction

The goal of this project is to develop a fuel-flexible catalytic combustor for integrated gasification combined cycle (IGCC) applications for a large industrial gas turbine which could meet 2 ppm NOx emissions without the need for backend cleanup such as selective catalytic reduction (SCR). Of all the available combustion technologies, the catalytic combustor shows the greatest potential for low emissions. Siemens has been investigating the rich catalytic lean burn (RCL™) technology for several years on natural gas fuel. Operation of the catalyst under rich conditions provides a robust design which can tolerate the changes in fuel compositions required for an IGCC plant. The goal of this project is to develop a fuel-flexible catalytic combustor by adapting the RCL™ technology to syngas and high hydrogen content fuels. The resulting combustion system designed in this project will be applicable to the Siemens SGT6-5000F engine.

Approach

The rich catalytic combustor concept can be seen schematically in Figure 1. In this design, the main air flow is split into two streams. A portion of the air is mixed with the fuel and flows through the catalyst region where it reacts under fuel rich conditions. The remaining air is used to cool the catalyst. Both streams are rapidly mixed at the exit of the catalyst section and the remaining fuel reacts in a homogeneous burnout zone.

The design of the catalytic combustor can be split into different tasks, catalytic coatings, catalytic reactor design, catalytic module design and full scale catalytic basket design. For the full basket design, a modular approach was employed where the combustor consists of a series of catalytic combustor modules surrounding a central pilot. The pilot is required only for operation at low loads; at base load the pilot is not fueled. With

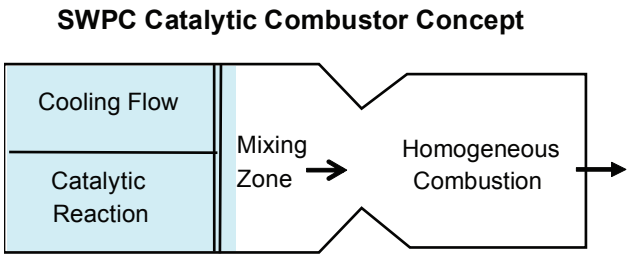

FIGURE 1. Rich Catalytic Combustor Concept

this modular design, it is possible to evaluate catalytic concepts at the subscale level. Catalytic coatings are evaluated in the Siemens single tube test facility. In this facility the catalytically coated elements are exposed to the same flow conditions typical of full scale SGT6-5000F operation. This facility can be fueled with, natural gas, syngas and hydrogen fuel. For each fuel, measurements are obtained for the critical properties, light-off temperature, fuel conversion, surface temperature and coating durability. The catalytic basket conceptual design was performed for several alternative module concepts. Validation of these basket concepts is performed through testing of subscale catalytic modules in the Siemens catalytic module test facility. This facility is capable of operation at full pressure conditions on natural gas, syngas and hydrogen. The down selected catalytic module will be utilized for the final full scale fuel flexible catalytic basket.

Results

Catalytic coating development was performed in the Siemens single tube facility. Catalytic coatings from five different suppliers were tested for light-off temperature, fuel conversion and durability. Precious metal catalysts (platinum, palladium, rhodium) were employed in this study. Based on these test, the two best catalysts were down selected for future testing. Testing was performed for natural gas, syngas and pure hydrogen. Catalyst activity is lowest for natural gas and increases with increasing hydrogen content in the fuel. Natural gas light-off temperatures are between 300-350°C, syngas between 250-300°C and hydrogen below 100°C. In addition to lower light-off temperatures, the fuel conversion in the catalyst also increases with hydrogen content. The higher fuel conversion means that the amount of air in the catalyst section must be reduced to keep the surface temperature of the catalyst in a range which will provide adequate catalyst life. Figure 2 shows the effect of the percent air in the catalyst region on catalyst temperature and fuel conversion for syngas. These test results indicate that for syngas, the optimal air split in the rich region is 10% compared to 15% for natural gas.

Catalyst durability testing was performed on both natural gas and syngas. Syngas testing was performed with and without a sorbent system for sulfur capture. With the sorbent system, the sulfur concentration in the fuel was less than 3 ppm, without it the sulfur concentration was 300 ppm. Figure 3 shows the gas temperature rise in the catalyst section for both cases. For the low sulfur tests the outlet temperature remained stable indicating that there was no degradation in catalyst performance. For the high sulfur tests, there was a decrease in outlet temperature during the initial portion of the test after which the output remained stable. This decrease in output was reversible when the catalyst was operated on natural gas.

Two approaches were pursued for the syngas capable catalyst combustor. The baseline design utilized a catalyst section composed of individual tubes, while the alternative design used a catalyst composed of corrugated concentric cylindrical plate sections. The initial basket design for the full scale engine was completed for both concepts and subscale modules were

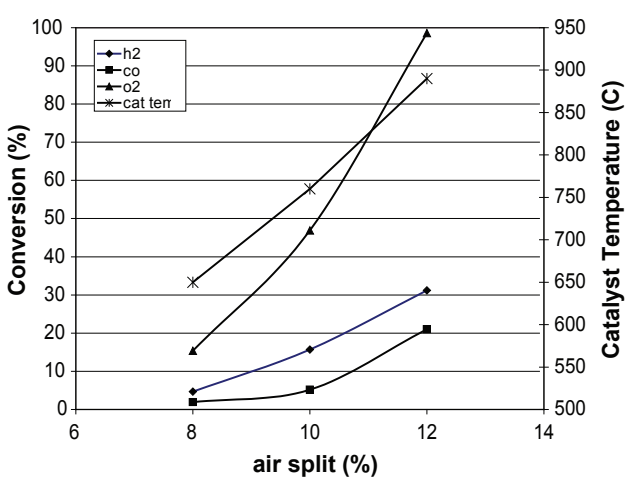

FIGURE 2. Effect for Air Split on Catalyst Activity for Syngas

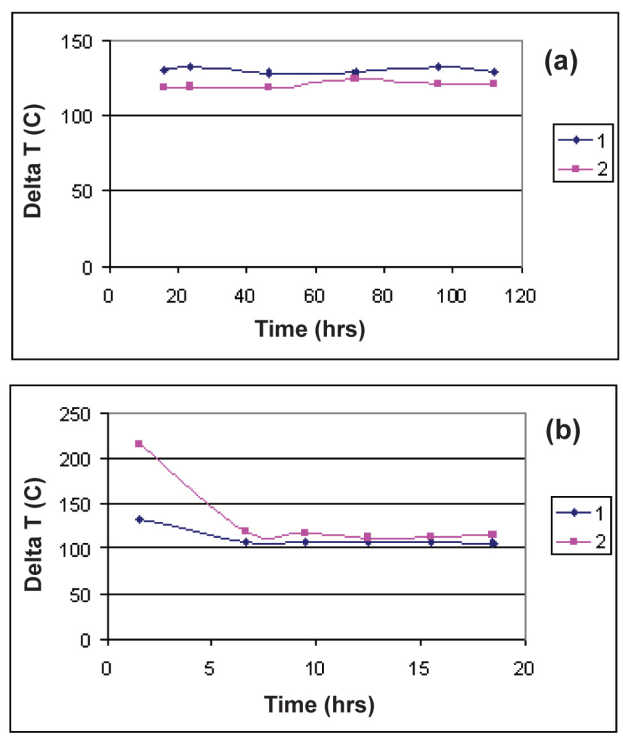

FIGURE 3. Syngas Durability Results for a) Low Sulfur and b) High Sulfur

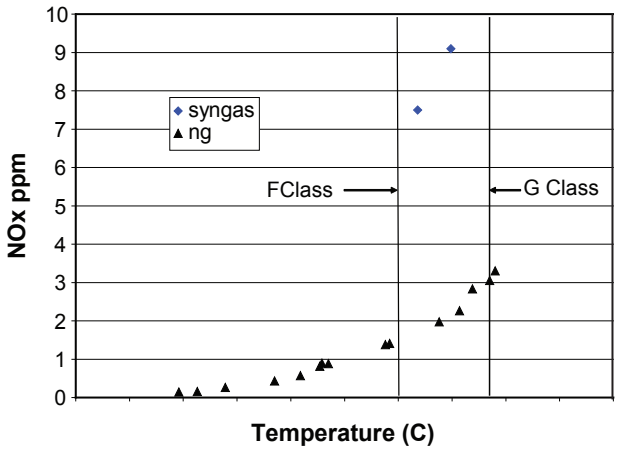

FIGURE 4. NOx Emissions from Module Testing

built for each concept. Figure 4 shows subscale module results for the baseline design for natural gas and syngas fuels. Operability of the design was confirmed on both natural gas and syngas. Higher emission numbers for syngas indicate that there is still some optimization work necessary for syngas operation. Testing of the alternative concept showed promise but again some additional design changes are necessary to optimize the design.

Conclusions and Future Directions

Based on this study the rich catalytic combustion approach shows potential for low emission operation on fuels typical of IGCC applications. Subscale module testing has been performed on both natural gas and syngas. Additional design work is necessary to optimize the design for application for syngas and hydrogen fuels. Additional testing needs to be performed at the subscale level on both syngas and hydrogen before this design is ready for application to a full scale basket. The alternative catalytic reactor design shows promise to significantly reduce the costs of the design.

FY 2007 Publications/Presentations

1. W. R. Laster, P. Nag, E. Anoshkina, B. C. Folkedahl, "Development of a Fuel Flexible Catalytic Combustor for IGCC Applications" 23rd International Pittsburgh Coal Conference, September 2006.

III. ADVANCED OXY-FUEL TURBINES

III.1 Zero Emissions Coal Syngas-Oxygen Turbo Machinery Development

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Subcontractor:
Although not a subcontractor to Siemens, Clean Energy Systems (CES), Inc. in Rancho Cordova, CA has a parallel project (DE-FC26-05NT42645) for developing a combustor to be used with the turbines developed by Siemens.

Objectives

This project involves a partnership with CES who is responsible for plant cycle modeling and optimizing the fluid conditions to maximize the cycle efficiency. The turbine development program by Siemens is planned in two phases. The objectives in each phase are as follows:

Phase I

- Working with CES, define the baseline, near-term and far-term temperature and pressure conditions for turbines in order to maximize the cycle efficiencies for each time frame. This will lead to cycle selection. Detailed turbine design for the selected cycle would follow in Phase II.
- Develop conceptual designs of turbines suitable for the three cycles (baseline, near- and far-term) up to a point where risk analysis can be performed to solidify future approach to detailed design that will minimize the technical risks.
- Review of available materials and processes to meet the design needs. Prepare a realistic assessment and a plan to bridge the gap between available materials and those needed to manufacture the turbines as designed.
- Perform cost estimates and feasibility studies. These would be used in economic analysis and risk analysis.
- Methods and tools development in areas that are most challenging due to their departure from the state-of-the-art technology of gas and steam turbines.

Phase II

- Develop detailed designs of the turbines for the selected cycle (near-term or far-term). These would be either steam/CO_2 turbines or 100% steam turbines depending on whether a turbine is in the "topping" cycle or in the "bottoming" cycle.
- Undertake tests to validate design concepts new to the turbine design, e.g. steam cooling effectiveness, heat transfer coefficients for steam/CO_2 mixture, airfoil cooling effectiveness, etc.
- Develop materials and processes such as higher temperature capable alloys, ceramic matrix composites, thermal barrier coatings and specialty coatings.
- Develop a database of physical and mechanical properties for materials and coatings for the use of design engineers.
- Perform manufacturing trials of critical components by working with vendors. Perform rig testing on selected components to validate design calculations.

Accomplishments

- Together with CES, selected the drive gas conditions and turbine arrangements to maximize cycle efficiency for near-term and far-term cycles. Selected far-term cycle for research and development (R&D).
- Completed conceptual designs of the high pressure (HP) and intermediate pressure (IP) turbines; held internal peer reviews and identified critical areas to develop ahead of the detailed design of turbines.
- Conducted a review of turbine conditions and identified shortcomings in available materials and coatings necessary to withstand the very aggressive operating conditions, particularly in the high temperature IP turbine.
- Performed a high level risk analysis based on the turbine designs and the expected stretch in turbine technology compared to the state-of-the-art.
- Completed an economic analysis and market demand simulation of power generation using oxy-fuel turbine technology. The simulation used the Energy Information Agency's National Energy Modeling System (NEMS) under an assumed CO_2 tax scenario.

Introduction

Advanced power systems that utilize nearly pure oxygen as the oxidant and coal-based gaseous fuels are an attractive approach to highly efficient, zero emissions coal-based systems that capture and sequester carbon dioxide. In these systems, the oxidant and fuel are combusted to create a working fluid composed mostly of steam and CO_2. This working fluid can be utilized in a Rankine cycle turbine to generate power while CO_2 can be captured after condensation of the drive gas mixture. In order to achieve high cycle efficiency, it is necessary to use the drive gas at temperatures comparable to or higher than those of today's gas turbines. Turbines using such a drive gas at high temperatures (1,750°C or higher) have not been developed.

Power generation using the oxy-fuel combustion process has been demonstrated by CES of Rancho Cordova, CA, albeit on a small scale. The advantages of developing turbines large enough for commercial power generation are as follows:

- Use of coal – the least expensive and most abundant domestic fuel.
- No NOx emissions since the oxidizer is pure oxygen instead of air.
- Greater than 99.5% of CO_2 captured.
- Materials and coatings development will benefit gas turbines used in combined cycle or peaking power generation applications.
- Steam cooling and other design technologies such as rim cavity sealing will also benefit gas turbine products.
- Technology will also apply to oxy-fuel turbines using natural gas (since the drive gas is the same) for near-term applications such as peaking power generation with enhanced oil recovery (EOR).

Approach

The project approaches turbine development for syngas-oxygen combustion products in a pragmatic way by evaluating the technology promise in the short-term as well as in the far-term. The strengths of Siemens Power Generation, Inc. and Clean Energy Systems, Inc. in commercial turbines and oxy-fuel combustion technology respectively, are utilized in this project to arrive at an arrangement of combustors, re-heaters and turbines that provide competitive plant cycle efficiency. In order to achieve high efficiency, it is necessary to use the drive gas at a very high temperature. For the far-term, the target value of the drive gas (steam, CO_2 mixture) in this project is 1,760°C (3,200°F) for the intermediate pressure turbine (IPT) and 760°C (1,400°F) for the high pressure turbine (HPT). These temperatures are significantly higher than those utilized in current day gas turbines or steam turbines. The project takes a phased approach to developing the technologies in the areas of turbine cooling systems, design methods, materials, thermal barrier coatings and component manufacturing. The high temperatures and new working fluid will require that both gas turbine and steam turbine technologies will need to be stretched beyond the current state-of-the-art.

Results

1. Drive Gas Conditions, Turbine Configuration and Cycle Efficiencies

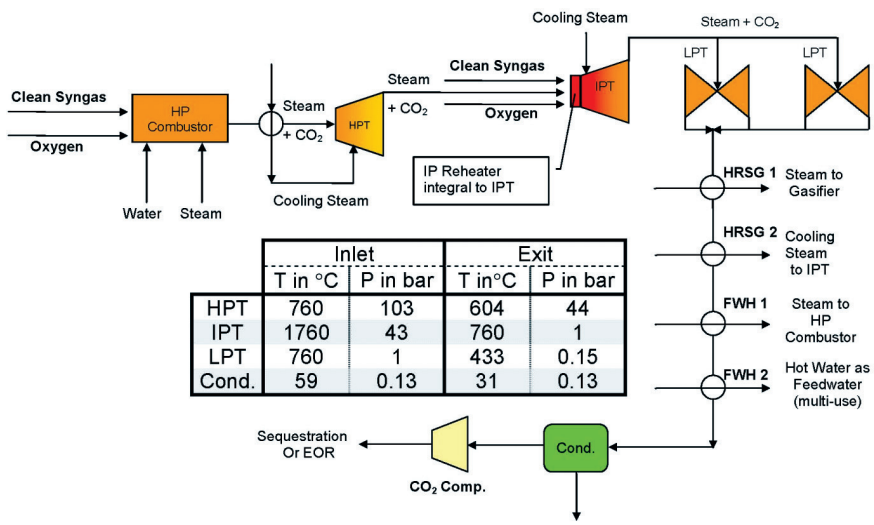
The cycle conditions for a time-phased design approach have been identified. The *baseline* case is a turbine arrangement that can be offered now for a zero CO_2 emissions oxy-fuel plant without much R&D. The *near-term* (~2010) and *far-term* (~2015) cases offer higher efficiency at the cost of increasingly aggressive technology development. Early in the project, maximum allowable operating conditions for the turbines were defined for these three cases. These are shown in Table 1 along with the rationale for each condition. CES has modeled the cycles using *Aspen* and the expected range of efficiency is shown in Table 2. It is clear from the results shown in Table 2 that the far-term turbine conditions offer the highest potential to meet the DOE goals for cycle efficiency. Therefore, the far-term cycle (and turbines for the associated drive gas conditions) has been selected for development. The drive gas conditions and the cycle are shown in Figure 1.

2. Conceptual Design of the High Temperature IPT

The IPT for the far-term cycle is conceptualized as a seven-stage steam/CO_2 turbine with a turbine inlet temperature (TIT) of 1,760°C. Seven stages are required to expand the drive gas from approximately 43 bar to atmospheric pressure. All stages of the IPT will be open-loop steam cooled with the exception of three vane stages. These stages are conceptualized as made of a ceramic matrix composite (CMC) that will require minimum cooling. The drive gas then expands to sub-atmospheric pressure of 0.15 bar in a separate un-cooled low pressure turbine (LPT). While a LPT for steam/CO_2 working fluid is a new concept and temperatures are expected to be higher (760°C inlet and 433°C exhaust) than a "standard" low pressure steam turbine, the design of such a turbine is not expected to pose major challenges. However, upgrade in materials may be required. The IPT, on the other hand, is the most challenging component in the turbo machinery. As such, most of the effort to date has been utilized on identifying the design challenges relative to the IPT. The highlights of the conceptual design of the IPT are shown

TABLE 1. Summary of Working Fluid Conditions Defined for Time-Phased Cases

	Max. Inlet Temp. °C (°F)	Max. Inlet Pressure Bar (psia)	Rational for Working Fluid Temperature and Pressure
Baseline Case			
High pressure 100% steam turbine downstream of a HRSG.	593 (1,100)	350 (5,075)	Use of current steam turbine technology without additional R&D. Isolate CO_2 from turbine.
Near-Term Case			
Intermediate pressure "steam/CO_2" turbine	1,450 (2,642)	43 (624)	Allows sufficient time to incorporate current gas turbine materials technology to a new working fluid without exceeding the inlet temperature
High pressure 100% steam turbine	620 (1,148)	350 (5,075)	Allows a stretch of approx. 25°C in inlet temperature from current technology without significant changes in materials of construction
Long-Term Case			
Intermediate pressure "steam/CO_2" turbine	1,760 (3,200)	43 (624)	Efficiency gain is the primary focus. Significantly higher temperatures may help in this regard
High pressure "steam/CO_2" turbine	760 (1,400)	350 (5,075)	Current U.S. DOE program on ultra-supercritical steam turbine materials technology targets this temperature



	Inlet		Exit	
	T in °C	P in bar	T in°C	P in bar
HPT	760	103	604	44
IPT	1760	43	760	1
LPT	760	1	433	0.15
Cond.	59	0.13	31	0.13

FIGURE 1. Zero CO_2 Emissions Oxy-Syngas Far-Term Cycle Conditions

TABLE 2. Expected Plant Efficiency Range from Modeling Studies

	Turbine Arrangement	Working Fluid	Expected Efficiency ***
Baseline	"Indirect"	Pure steam	13% -15%
Near-Term	Direct	Steam/CO_2 for IPT, Pure steam for HPT	25% - 30%
Far-Term	Direct	Steam/CO_2 for all turbines	31% - 35%

*** Coal-to-grid, HHV including CO_2 compression to 152 bar

in Figure 2. Preliminary work has been performed on blade design for high heat flux cooling, advanced rim sealing concepts and balancing of the rotor system thrust loading.

3. Conceptual Design of the HPT

The HPT design takes off from the design platform of a conventional (100% steam) high pressure turbine. The target inlet temperature is 760°C (1,400°F) which is about 150°C higher than currently used in commercial steam turbines. Therefore, an upgrade in materials (from ferritic to nickel-based alloys) for the rotating and stationary blades is expected along with the material for the rotor.

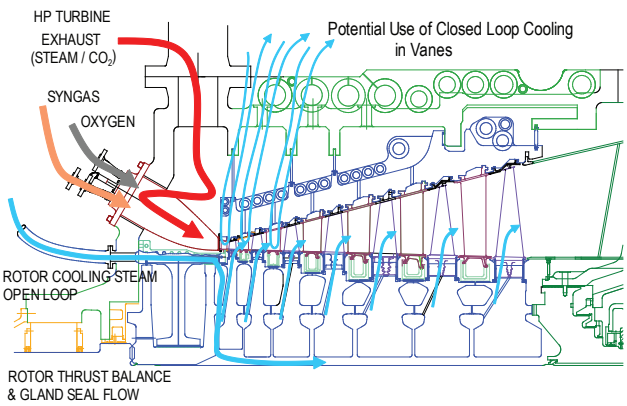


FIGURE 2. IPT Cross Section Showing the Primary Flow Path and Steam Cooling Scheme

4. Materials and Coatings for the IPT

A complete review of the currently available materials and thermal barrier coatings has been conducted to assess their applicability to the design needs of the IPT. Steam/CO_2 effects at high temperatures are major concerns on materials life. Single crystal and directionally solidified gas turbine alloys have been identified as reference alloys for cooled blades and vanes. In addition, a ceramic matrix composite material has been identified as the reference material for three sets of vanes to minimize the cooling requirements of the turbine. The rotor, exhaust casing and ring segments may also need to be upgraded from the materials used in conventional gas turbines.

5. Risk Analysis and Economic Analysis

A systematic approach has been applied to evaluate high level risks associated with the turbine conceptual designs and interfaces with the rest of the plant machinery. A risk portfolio has been developed and mitigation measures have been established. These will be used to plan future R&D effort. In addition, a study was subcontracted to Science Applications International Corp. (SAIC) to evaluate the commercial attractiveness of power generation using the oxy-syngas turbine cycle. SAIC utilized the NEMS to evaluate the competitiveness of this technology. The simulation indicated that under a reasonable carbon tax scenario starting in 2012, the oxy-syngas power generation is competitive with other carbon limiting technologies that use either pre-combustion or post-combustion CO_2 removal methods.

Conclusions and Future Directions

Phase I work performed in FY 2007 has indicated that in a carbon-constrained world, provided the expected efficiency can be achieved in the far-term cycle, power generation using syngas-oxygen combustion process is economically viable in the time frame 2015-2030. It can compete successfully with other carbon limiting fossil fuel based technologies including integrated gasification combined cycle (IGCC). The capture and sequestration of CO_2 is relatively easier since it is isolated at the end of the expansion cycle of the drive gas. There are major technical hurdles that need to be overcome in steam cooling technology, heat transfer, blade design, materials, thermal barrier coatings and manufacturing methods during basic and detailed turbine design effort

The future direction will involve optimization of the plant cycle, basic turbine design, evaluation of the required materials and development of suitable thermal barrier coatings. A database of mechanical properties of the most suitable materials and coatings under steam/CO_2 mixtures will need to be developed along with manufacturing trials of critical subcomponents such as blades.

References

1. Hebbar, M., Dinkar, S., Gutierrez, J., Downs, J., "Development of Turbo Machinery for a Zero CO_2 Emissions Oxy-Fuel Cycle", *Proceedings of the Pittsburgh Coal Conference,* September 25–28, 2006.

III.2 Coal-Based Oxy-Fuel System Evaluation and Combustor Development

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Objectives

- Develop a detailed design of a 50 MW_{th} CES oxy-syngas combustor.
- Fabricate the oxygen/syngas/water injector – the core component of the combustor.
- Prepare a validation test plan to support testing of the oxy-syngas combustor. Identify possible test sites, methods, schedules, and test matrices for the demonstration of the 50 MW_{th} combustor on coal-derived syngas. Develop a detailed validation test plan.
- Provide a preliminary design concept for an oxy-syngas reheat combustor. The reheat combustor offers significantly improved plant efficiency in longer-term oxy-fuel cycles.

Accomplishments

- Determined that the long-term (2015) CES oxy-syngas cycle can attain coal-to-grid higher heating value (HHV) cycle efficiencies of 35%, with >99% CO_2 capture. Verified by the Advanced Power and Energy Program (APEP) group at UC Irvine.
- Completed most drawings of the 50 MW_{th} oxy-syngas combustor and its components.
- Prepared a piping and instrumentation diagram (P&ID) of the combustor skid assembly and a detailed listing of valve specifications, piping and tubing specifications, and a complete instrumentation specification.
- As part of the control system design, prepared diagrams that will be used to describe and document control strategies and systems designed for industrial and utility applications.

Introduction

CES has a developed a novel oxy-fuel power generation concept that uses proven aerospace technology to enable near zero-emission power generation from fossil fuels. The core of the technology is a high-pressure oxy-combustor that burns gaseous fuels with oxygen in the presence of water to produce a steam/CO_2 working fluid for steam turbines or modified gas turbines. The CES oxy-combustor has been demonstrated mainly on natural gas at CES's 20 MW_{th} Kimberlina Power Plant (KPP) outside Bakersfield, CA, where it was used to produce electricity for export to the grid.

Under this Department of Energy (DOE) award (DE-FC26-05NT42645), CES is developing its oxy-combustion technology for coal-based power plants that utilize synthesis gas as the fuel. It is closely associated with DOE award DE-FC26-05NT42646 to Siemens Power Generation to develop high-temperature turbines that would be powered by steam/CO_2 working fluid from the oxy-combustor [1]. The combination of the two technologies represents an attractive approach to highly efficient, zero-emissions coal-based systems that capture and sequester carbon dioxide.

The overall objective of the project is the design and demonstration of a pre-commercial oxy-syngas combustor that will enable the commercialization of a high-efficiency coal-based power generation process with >99% CO_2 capture by 2015. The combustor development project was planned in three one-year phases, coincident with DOE fiscal years 2006, 2007, and 2008.

Approach

In Phase I of the project (FY 2006), CES performed the following tasks: (i) conducted systems studies of long-term oxy-syngas power plants that will be deployable by 2015, (ii) fabricated a pilot-scale oxy-syngas injector that was installed in CES's Kimberlina Power Plant, and (iii) tested the combustor with simulated syngas and H_2-depleted syngas at power levels of up to 5 MW_{th}.

In Phase II (FY 2007), CES is preparing a detailed design of a 50 MW_{th} pre-commercial syngas combustor. This design effort relies on data collected from the Phase I tests, as well as information from a parallel CES activity in which a similar-sized combustor is being designed for natural gas applications. Once the design is complete, CES will then fabricate the combustor injector, which serves to inject oxygen, syngas, and water into the

combustion chamber. CES will also identify possible locations that would permit testing of the 50 MW_{th} combustor in Phase III (scheduled for FY 2008). These sites include pilot-scale and commercial-scale gasifiers that can operate in O_2-blown mode at pressure. CES will prepare a validation test plan that includes test methods, schedules, and test matrices.

Results

In Phase I, CES performed systems studies on the long-term (2015) oxy-syngas cycle using AspenPlus® process modeling software. Process information was provided by Siemens Power Generation (Turbines), Siemens Fuel Gasification (Gasifier), Air Products (Air Separation Unit), and other subcontractors. CES concluded that coal-to-grid HHV cycle efficiencies of 35% could be attained with >99% CO_2 capture. In Phase II, CES contracted with the APEP at UC Irvine to perform an independent verification of the cycle performance. They verified CES results, and concluded that cycle efficiencies of 35% are attainable.

Detailed design work on the pre-commercial oxy-syngas combustor began in early October 2006. Design progress has been accelerated by parallel activities in a natural gas (NG)-fired CES combustor development project. Common features between these projects include combustor chamber size (12-inch inside diameter), oxygen and water manifolding, cool-down chambers, valve and instrumentation layout, compact skid design, and control system design. Although the firing rate of equivalent NG-fired combustors is higher than that for syngas, the process mechanics proved to be very similar. Specific activities include:

Combustor: A drawing tree was prepared listing all drawings required for manufacturing and assembly of the main injector, combustion chamber, cool-down chambers, and water diluent injectors. A total of 34 drawing sets constitute the complete package required to manufacture and assemble the unit. Since October 2, 2006, 26 drawings sets have been completed and approved (ready for fabrication). Of the remaining eight drawing sets, only two comprise major assemblies. The most significant detailed design drawing remaining to be accomplished is the syngas main injector. Main injector design efforts were placed lower in the design queue to take advantage of parallel design efforts already in progress for commercial-scale NG-fueled main injectors. As a direct result of these NG design efforts and lessons-learned in Kimberlina operations, the syngas main injector design will incorporate a more corrosion-resistant material in the outer platelet layer, improving overall main injector durability.

Combustor Skid Assembly: The first step in detailed skid assembly design was taken with creation of a P&ID in October, 2006. The P&ID incorporates all piping, valves, and instrumentation, including piping sizes, valve types and design, valve failure modes, and wiring layout. CES plans to use "intelligent" control valves utilizing Foundation Fieldbus control networks. Design of a detailed piping and skid layout reflecting the latest P&ID is approximately 90 percent complete. The assembly shows detailed piping and valve layouts, and will incorporate line drawings for tubing and instrumentation. The assembly drawings also specify enclosure dimensions and relative support equipment placement. CES has also prepared a detailed listing of valve specifications, piping and tubing specifications, and a complete instrumentation specification. A vendor will eventually use the assembly drawings, P&IDs, and equipment specifications to fabricate the piping and tubing, install the valves and instrumentation, and construct the enclosure for the assembly.

Combustor Control System: CES' control system approach utilizes "smart" valves and reporting protocols to take advantage of their internal diagnostics capabilities and reduced wiring requirements. "Hard-wired" controls will be avoided except where valve response time is critical. In the latter case, direct-wired 4-20 ma signals will be used. The control system logic is being documented via Scientific Apparatus Makers Association (SAMA) symbols and diagramming conventions. These functional control diagrams are commonly used in the power industry to represent control logic that includes continuous, binary logic, and sequential functions. SAMA diagrams are used to describe and document control strategies and systems designed for industrial and utility applications. Approximately 95 percent of the roughly 60 sheets in the SAMA diagrams are complete. Once finished, a completed SAMA diagram can be given to virtually any PLC programmer and the PLC successfully programmed from the diagrams.

Conclusions and Future Directions

Results from Phase I of the project demonstrated the feasibility of operating the CES oxy-combustor with coal-derived syngas as the fuel, and concluded that attractive coal-to-grid cycle efficiencies may be attained with >99% CO_2 capture in CES oxy-syngas plants deployable by 2015.

CES is currently developing a detailed design of a 50 MW_{th} oxy-syngas combustor, including the skid assembly and control system, and plans to fabricate the most complex assembly of the combustor, the oxygen-syngas-water injector. In Phase II, CES will develop a test validation plan and identify possible sites for testing of the 50 MW_{th} combustor, and will develop a conceptual design for an oxy-syngas reheat combustor.

In Phase III, CES will fabricate the remaining oxy-syngas combustor components, and will conduct tests of the assembled combustor at a test site, preferably one with an operating gasifier.

FY 2007 Publications/Presentations

1. MacAdam, S., Anderson, R., Viteri, F., and Pronske, K., "Kimberlina - A Zero-Emission Multi Fuel Power Plant and Demonstration Facility", Presented at 23rd International Pittsburgh Coal Conference, Pittsburgh, PA, September 25–28, 2006. Accepted for publication in conference proceedings.

2. Pronske, K., Devanna, L., MacAdam, S., and Anderson, R., "Coal-Based Oxy-Fuel System Evaluation and Combustor Development", Presented at 6th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 7–10, 2007.

3. MacAdam, S., Biebuyck, C., Anderson, R., and Pronske, K., "Coal-Based Oxy-Fuel System Evaluation and Combustor Development", Poster presentation at Second Annual Freiberg Conference on IGCC and XtL Technologies, Freiberg, Germany, May 8–12, 2007. Accepted for publication in conference proceedings.

4. MacAdam, S., Anderson, R., Viteri, F., and Pronske, K., "Coal-Based Oxy-Fuel System Evaluation and Combustor Development", Presented at 32nd International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, FL, June 10–15, 2007. Accepted for publication in conference proceedings.

References

1. Hebbar, M.A. et al: Development of Turbo Machinery for a Zero CO_2 Emissions Oxy-Fuel Cycle, Proceedings of 23rd International Pittsburgh Coal Conference, Pittsburgh, PA. September 25–28, 2006.

IV. ADVANCED RESEARCH

IV.1 Analysis of Gas Turbine Thermal Performance

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Objectives

- Develop and evaluate an analysis tool that can be used to examine and explore heat transfer design issues in turbine components to support the development of turbine technologies for advanced FutureGen-type coal-based power systems.
- Apply the analysis tool to explore heat transfer design issues in turbine components to support the development of turbine technologies for advanced FutureGen-type coal-based power systems.

Accomplishments

- Organized a literature review of research on turbine cooling, seals, erosion/deposition, superalloys, and thermal-barrier coatings with focus on performance and durability. This work is documented in a special section on "Turbine Science and Technology" in the *AIAA Journal of Propulsion and Power*, Vol. 22, No. 2, March-April 2006, pp. 225-396.
- Evaluated analysis tools for predicting conjugate heat transfer.
- Developed and evaluated a method to estimate grid-induced errors in solutions generated by computational-fluid-dynamics-based analysis tools.
- Applied the analysis tool to study the conduction heat transfer in a superalloy plate with and without a layer of thermal-barrier coating that is cooled by film cooling on the hot-gas side and by internal cooling on the other side.
- Applied the analysis tool to study the flow and heat transfer in an L-shaped internal cooling passage lined with pin fins under rotating and non-rotating conditions.

Introduction

Developing efficient and long service life turbine technologies to operate on coal-derived synthesis gas (syngas) and hydrogen fuels is critical to the development of advanced power generation technologies such as integrated gasification combined cycle (IGCC) and the deployment of FutureGen-type power plants that can lead to the capture and separation of carbon dioxide (CO_2). For turbines, high efficiency demands high temperatures at the turbine inlet, and long service life demands effective cooling to ensure material temperatures do not exceed maximum allowable for strength and durability. The 2010 goal on turbine efficiency demands the turbine inlet temperature to be 2,500°F for syngas turbines and 2,600°F for hydrogen turbines – temperatures that far exceed the maximum allowable temperatures of the best superalloys even with thermal-barrier coatings. Thus, developing efficient and effective cooling strategies is a critical component in achieving the 2010 goal on turbine efficiency and service life.

The objective of this project is to develop an analysis tool that can be used to examine and explore heat transfer design issues in turbine components to support the development of turbine technologies for advanced IGCC and FutureGen-type coal-based power systems. The tool will consider additional complications to heat transfer that arise from burning syngas and hydrogen, including heat transfer from the hot gases to the thermal-barrier-coating (TBC) system and the superalloy as a function of the cooling strategy, fuel used (e.g., natural gas, syngas, hydrogen fuels, and oxy-fuels), amount of and the nature diluents used to control combustion and formation of nitric oxides, mass flow rate, firing temperature and turbine inlet temperature, and the thermodynamic cycle (e.g., coal-based oxy-fuel Rankine cycles or advanced Brayton cycles).

Approach

A comprehensive design and analysis tool for turbine performance based on an integral approach is being developed at the Oak Ridge National Laboratory. However, models based on the integral approach require inputs on the details of the three-dimensional flow and heat transfer in the gas phase and the conduction heat transfer in the solid material. There are two ways to provide the detailed information needed; they are experimental and computational. The computational approach based on computational fluid dynamics (CFD) analysis is adopted here. CFD analyses are based on the

conservation/balance equations of species, continuity, momentum, and energy that govern the details of the three-dimensional flow and heat transfer processes in the gas phase and the Fourier law in the solid phase.

The following effects will be examined by CFD: (1) fuel used [e.g., natural gas, syngas (including different ratio of CO/H_2), H_2 ….], (2) firing temperature, (3) amount of diluents and diluents used (e.g., N_2 or steam to control NO_x formation), (4) amount of steam and different ratios of CO_2/H_2O in the working fluid, (5) mass flow rate, (6) different cooling strategies with and without thermal barrier coating, and (7) different thermo cycles (e.g., coal-based oxy-fuel Rankine cycles and advanced Brayton cycles).

Results

Analysis that accounts for conjugate heat transfer was found to be critical in revealing the effectiveness of film and internal cooling in ensuring material temperature is kept below critical values for long service life. In particular, conduction heat transfer in the superalloy was found to smooth out the adverse effects of hot-gas entrainment by film-cooling jets, whereas conduction heat transfer was found to intensify the adverse effects of separated regions in internal cooling passages in creating hot spots. Also, the temperature distribution around film-cooling holes was found to be highly three-dimensional when the thermal conductivity of the material is low. This may affect the accuracy of experimental measurements that utilize one-dimensional conduction equations to extract information on surface adiabatic effectiveness and heat transfer coefficients in the region about film-cooling holes.

The accuracy of CFD in predicting heat transfer hinges not just on the modeling of turbulence but also on the grid system used to resolve the geometry and enable the numerical method of solution to resolve the key physical phenomena driving the heat transfer. A method based on the discrete-error transport equation (DETE) was developed to assess and to correct for errors in CFD solutions induced by the grid system – structured or unstructured. Results obtained show that if the residual in the DETE is modeled correctly, then grid-induced errors can be assessed perfectly. However, the modeling of the residual is not trivial. Two classes of models were devised for the residual. One class involves generating one or two solutions on the same grid, and the other involves generating additional solutions on finer grids. Of the single-grid methods, one is based on using the leading terms of the truncation error in the modified equation. With this method, no new solutions need to be generated in estimating and correcting for errors in a CFD solution. The other single-grid method requires the generation of one additional solution on the same grid but by using a higher-order scheme. For the multiple-grid method, truncated Taylor series were used to construct the residual from the solutions generated on the multiple grids. Preliminary results show these methods to be promising, but their range of usefulness still needs to be quantified.

Conclusions and Future Directions

Since advanced turbines are designed to operate at the upper limit of allowable material temperature, validated analysis tools with known error bounds are critical in the exploration of efficient, effective, and reliable cooling strategies and in the analysis of designs that utilize these strategies. Such a validated analysis tool must be able to account for the details of the conjugate heat transfer and the coupling between internal and film cooling across the turbine material. Future directions include studying the effects of different hot-gas constituents in the turbine hot-gas path due to combustion of different fuels such as syngas and hydrogen and the associated complexities such the type and amount of diluents used to control nitric oxides emission and the differences in the mass flow rates to achieve maximum power. Other physics that need to be included in the analysis tool include the ability to account for thermal stress and gas radiation. Also, additional efforts are needed to ensure that the CFD solutions generated are meaningful from a grid-independence perspective, which can be quite challenging for realistic configurations that invariably involve a very large number of grid points or cells.

FY 2007 Publications/Presentations

1. Na, S., Zhu, B., Bryden, M., and Shih, T.I-P., "CFD Analysis of Film Cooling," AIAA Paper 2006-0022, Aerospace Sciences Meeting, Reno, Nevada, January 2006.

2. Yoon, S., Na, S., Wang, Z.J., Bons, J.,P., and Shih, T.I-P., "Flow and Heat Transfer over Rough Surfaces: Usefulness of 2-D Roughness-Resolved Simulations," AIAA Paper 2006-0025, Aerospace Sciences Meeting, Reno, Nevada, January 2006.

3. Qin, Y., Chi, X., and Shih, T.I-P., "Modeling the Residual in the Error-Transport Equation for Estimating Grid-Induced Errors in CFD Solutions," AIAA Paper 2006–892, Aerospace Sciences Meeting, Reno, Nevada, January 2006.

4. Shih, T.I-P. and Chyu, M., Guest Editors, "Turbine Science and Technology," *AIAA Journal of Propulsion and Power,* Vol. 22, No. 2, March-April 2006.

5. Shih, T.I-P., "Error Estimation in CFD Solutions," invited keynote, 13th National CFD Conference, Taiwan, August 14, 2006. Proceedings of the 13th National Conference on Computational Fluid Dynamics, August 2006, pp. 1–14.

6. Shih, T.I-P., "Enhancing the Effectiveness of Film Cooling," invited keynote, 1st International Symposium on Jet Propulsion and Power Generation, Kunming, China, 20 September 2006. *Proceedings of the 1st International*

Symposium on Jet Propulsion and Power Generation, Vol. 1, 2006, pp. 28–34.

7. Na, S. and Shih, T. I-P., "Enhancing Film-Cooling Effectiveness via an Upstream Ramp," *ASME Journal of Heat Transfer*, Vol. 129, No. 4, April 2007, pp. 464–471.

8. Zhu, B., Chi, X., Dennis, R.A., Chyu, M.K., Bryden, K.M., and Shih, T. I-P., "Internal Cooling inside an L-Shaped Duct with Pin-Fin Turbulators under Rotating and Non-Rotating Conditions with and without Sand Particles," ASME IGTI Paper GT-2007-27598, IGTI Conference and Expo, Montreal, Canada, May 14–17, 2007.

9. Na, S., Williams, B., Dennis, R.A., Bryden, K.M., and Shih, T. I-P., "Internal and Film Cooling of a Flat Plate with Conjugate Heat Transfer," ASME IGTI Paper GT-2007-27599, IGTI Conference and Expo, Montreal, Canada, May 14–17, 2007.

10. Shih, T. I-P. and Na, S., "Enhancing the Effectiveness of Film Cooling," *Journal of Aerospace Power*, accepted (to appear in 2007).

IV.2 Development of Comprehensive Detailed and Reduced Reaction Mechanisms for Syngas and Hydrogen Combustion

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Subcontractors:
- Hai Wang, University of Southern California
- Angela Violi, University of Michigan

Objectives

- Generate a detailed experimental database of coal-derived synthesis-gas (syngas) and hydrogen (SGH) combustion at integrated gasification combined cycle (IGCC)-like conditions.
- Investigate the fundamental chemical kinetics of $H_2/CO/O_2/N_2/H_2O/CO_2$ at pressures, temperatures, and concentrations typical of SGH combustion in gas turbines.
- Develop detailed and reduced chemical mechanisms based on this database, capable of predicting NOx formation during SGH combustion.

Accomplishments

- Obtained extensive experimental data for autoignition of dry syngas mixtures at elevated pressures in a rapid compression machine and assessed the performance of existing kinetic mechanisms.
- Assessed the kinetics of syngas combustion at elevated pressures using global uncertainty analysis methods.
- Investigated the reaction kinetics of $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$ by *ab initio* calculations and master equation modeling, and derived a rate expression for this reaction.
- Obtained preliminary experimental data for autoignition of moist syngas mixtures.
- Obtained preliminary experimental data for flame propagation of moist syngas mixtures.

Introduction

This project aims to provide comprehensive and computationally efficient chemical kinetic mechanisms for facilitating the design of future SGH fueled combustion turbines through computational fluid dynamic (CFD) simulations. Benchmark experimental data are obtained for combustion characteristics, such as laminar flame speeds and ignition delays of syngas mixtures. This critical database is needed for validation of chemical kinetics of syngas combustion and is used in conjunction with computation methods, such as global uncertainty analysis, to assess the performance of the literature kinetic mechanisms. The present assessment revealed discrepancies in the existing value of a key reaction, $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$. Reaction kinetics of this reaction was investigated theoretically and a new rate expression was suggested which corrected the noted disagreement in predictions of the existing mechanisms for syngas combustion. More extensive studies are being conducted to acquire experimental data which will be used to develop reliable chemical kinetic mechanisms for combustion simulation in syngas-based IGCC plants.

Approach

In order to obtain extensive experimental data for validation of chemical kinetic mechanisms over a wide range of physical conditions, experiments are carried out in a rapid compression machine (RCM) and a counterflow burner apparatus. RCM allows access to the low-to-intermediate temperature chemistry at elevated pressures, whereas a counterflow burner allows experimentation with flames under conditions related to high temperature kinetics. In conjunction with experimental data, quantum chemical calculations are conducted to determine the rate constants of critical reactions.

Results

An experimental and numerical study using uncertainty analysis of the most important parameters was conducted to evaluate the mechanisms for the combustion of $CO + H_2$ mixtures at high pressures in the range 15-50 bar and temperatures from 950-1,100 K. Experiments were performed in an RCM. Autoignition delays were measured for stoichiometric compositions of $CO + H_2$, with varying proportion of $R_{CO} = [CO]/([CO]+[H_2])$, while keeping the combined

[CO]+[H_2] constant, where brackets indicate molar concentrations of respective species. The experimental results showed an unequivocal monotonic increase in ignition delay as the proportion of CO in the mixture was raised, whereas simulations using the reaction mechanisms of references [1–3] show a qualitatively different behaviour of almost no sensitivity to R_{CO} till it reaches 0.8, as shown in Figure 1. Global uncertainty analyses, including Morris and Monte Carlo Analyses, were then applied to the kinetic model of Davis et al. [1] in order to trace the origins of this discrepancy. The analyses took into account the uncertainties in all rate parameters in the model, which is a prerequisite for evaluation against ignition delay data. Morris analyses identified the reaction, $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$, as the most important reaction which leads to largest absolute mean perturbation and standard deviation in predicted ignition delay when rate parameters for all other reactions are varied within their uncertainty range. Figure 2 shows a scatter plot from Monte Carlo analysis which reflects the values for ignition delay that are predicted within the ranges of uncertainties of all other pre-exponential factors when log A of the reaction, $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$, takes set values over the range $-12 < \log A < -10$. With a commonly used value of log A, experimentally observed ignition delay is predicted in very few cases. This suggests that the accepted value of log A is incorrect. Log $A < -11$ would fix it but the present analysis based on ignition delay measurements does not permit us to do more than indicate that the overall reaction rate is too fast. This constraint arises from the uncertainty in other rate parameters that gives the scatter in the predicted ignition delays – which is a problem for any model validation using ignition delay data. Corrected parameters cannot be generated for this reaction solely from ignition delay evaluations. Direct experimental or theoretical approaches are therefore required to determine the rate parameters.

The reaction kinetics of $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$ were subsequently studied using the single-reference CCSD(T) method with Dunning's cc-PVTZ and cc-PVQZ basis sets and multireference CASPT2 (complete active space second order perturbation theory) methods. It was found that the classical energy barriers are about 18 and 19 kcal/mol for $CO+HO_2\bullet$ in addition following the *trans* and *cis* paths, as shown in Figure 3. Figure 3 also demonstrates that the HOOC•H adduct has a well defined local energy minimum in the *trans* configuration, but the *cis*-conformer is either a very shallow minimum or an inflection point on the potential energy surface. This observation led us to treat the *cis*-pathway by the classical transition state theory and the *trans*-pathway by a Master Equation analysis. The computation showed that the overall rate is independent of pressure up to

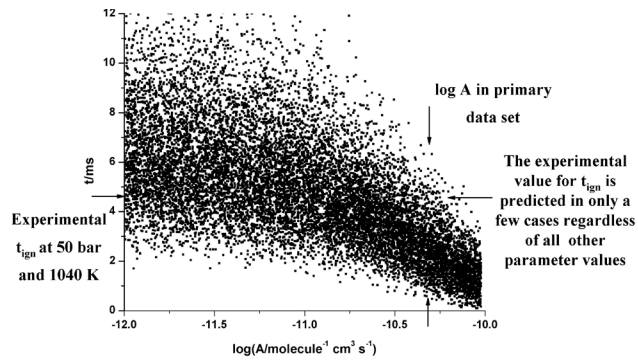

FIGURE 2. Monte Carlo analysis from 13,000 simulations for variation of the pre-exponential factor for $CO+HO_2\bullet \rightarrow CO_2 + \bullet OH$ over the range $-12 < \log A < -10$. Pre-exponential terms for the remaining reactions in the scheme were varied within the estimated uncertainty. In the primary data set log (A/ cm^3 molecule^{-1} s^{-1}) = -10.3, as marked (vertical arrows). The experimentally measured ignition delay is 4.6 ms (horizontal arrows).

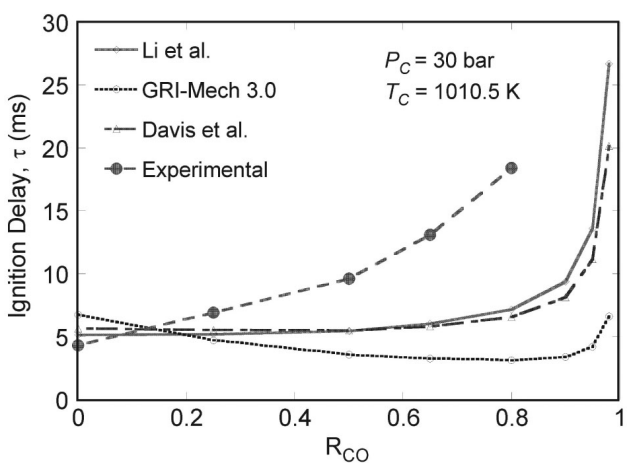

FIGURE 1. Comparison of experimental and computed results, showing the effect of CO addition on ignition delay. Molar composition: (H_2+CO)/O_2/N_2/Ar = 12.5/6.25/18.125/63.125. Conditions at TDC: P_c = 30 bar and T_c = 1,010.5 K.

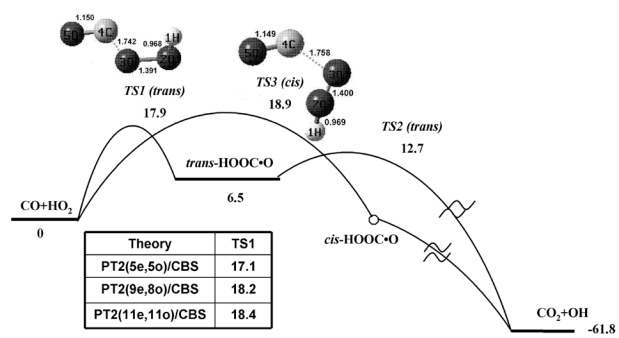

FIGURE 3. Potential energy diagram for $CO + HO_2\bullet \rightarrow CO_2 + \bullet OH$. The energy values are determined using the CCSD(T)/CBS method, and include zero-point energy corrections.

500 atm. Upon a careful treatment of the hindered internal rotations in the HOOC•H adduct and relevant transition states, the rate coefficient expression for this reaction was obtained as:

$$k\ (\mathrm{cm^3/mol.s}) = 1.6 \times 10^5\, T^{2.18} e^{-9030/T}$$

for $300 \le T \le 2{,}500$ K. Lastly, we examined the accuracy of the previously proposed Davis et al. [1] model by updating only three rate coefficients: k_1 based on the current study, the rate coefficient of CO + •OH → CO_2 + H• from Joshi and Wang [4], and the rate coefficient for HO_2• + OH → H_2O + O_2 evaluated in Sivaramakrishnan et al. [5]. Figure 4 shows the comparison of experimental and computed ignition delays for RCM experiments at 30 bar, before and after these updates. It is seen that the updates just discussed led to drastic improvement of the predictions, as expected. The improvement was brought almost entirely from the revision of the rate coefficient of CO+HO_2• → CO_2 + •OH [6].

Preliminary experiments were also conducted to determine the effect of water addition on ignition characteristics of H_2/CO mixtures in a rapid compression machine while keeping the total [H_2]+[CO] mole fraction constant. It was noted that the small amount of water addition does not alter the ignition delay of the mixtures investigated. In contrast, the kinetic models showed a relatively stronger retardation of ignition due to the small amount of water addition.

The high pressure oxidation of dilute CO mixtures doped with 150-200 ppm of H_2 reflecting shock waves up to 600 atm was also examined. The experimental data was collected in the University of Illinois at Chicago high pressure single pulse shock tube. Simulations using a previously published reaction model showed that within experimental error, the kinetic model is able to capture the experimental trends for the lower pressure data sets (average nominal pressures of 24 and 43 bars). However, the model under-predicts the CO and O_2 decay and subsequent CO_2 formation for the higher pressure data sets (average nominal pressures of 256 and 450 bars). With updated rate parameters for HO_2+OH=H_2O+O_2 the model was found to reconcile the elevated pressure data sets.

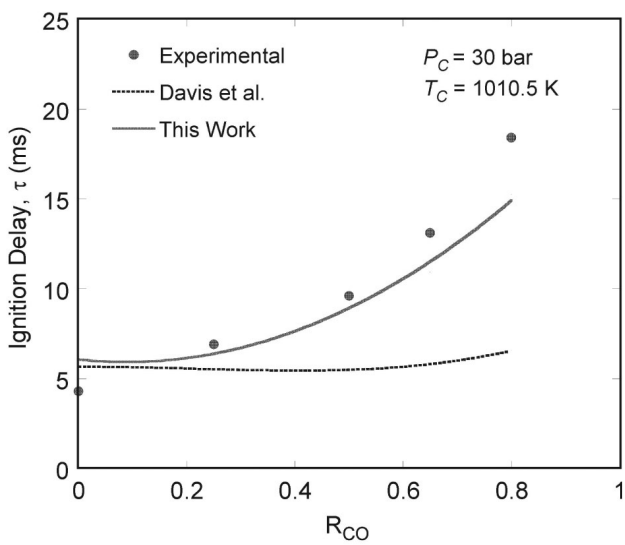

FIGURE 4. Prediction of RCM ignition delay times at P_c = 30 bar and T_c around 1,010.5 K. Molar composition: (H_2+CO)/O_2/N_2/Ar = 12.5/6.25/18.125/63.125. Solid lines: updated model of Davis et al. [1]; dashed line: original model of Davis et al. [1].

In addition, the counterflow burner apparatus has been adequately adapted and characterized for investigations of combustion characteristics, such as laminar flame speeds and extinction stretch rates, of SGH mixtures. Preliminary results on flame speed measurements indicate that the effect of water addition can lead to an increase or decrease of flame speed depending upon mixture composition.

Conclusions and Future Directions

- Significant discrepancies exist in the literature chemical kinetic models of syngas combustion.
- An extensive experimental database is needed for mechanism validation, particularly under conditions of elevated pressures and with addition of water.
- Theoretical calculations for a key reaction, CO+HO_2• → CO_2 + •OH, resolved some discrepancies of the existing mechanisms at elevated pressures.
- Future work will focus on the following aspects:
  - Obtain detailed experimental data in RCM and counterflow burners on the effects of CO_2 and H_2O addition on ignition delays, laminar flame speeds, and stretch induced extinction limits.
  - Conduct *ab initio* quantum chemistry calculations and master equation modeling for certain key reactions, including HO_2 + HO_2 → H_2O_2 + O_2 and HO_2 + OH → H_2O + O_2.

FY 2007 Publications/Presentations

1. G. Mittal, C.J. Sung, M. Fairweather, A.S. Tomlin, J.F. Griffiths, and K.J. Hughes, "Significance of the HO_2+CO Reaction during the Combustion of CO+H_2 Mixtures at High Pressures," *Proceedings of the Combustion Institute*, 2007, Vol. 31, 419-427.

2. R. Sivaramakrishnan, A. Comandini, R.S. Tranter, K. Brezinsky, S.G. Davis, and H. Wang, "Combustion of CO/H_2 Mixture at Elevated Pressures," *Proceedings of the Combustion Institute*, 2007, Vol. 31, 429-437.

3. X. You, E. Goos, C.J. Sung, and H. Wang, "Reaction Kinetics of $CO+HO_2 \rightarrow CO_2+OH$ ab initio Study and Master Equation Modeling," work-in-progress poster, 31st International Symposium on Combustion, Heidelberg, Germany, August 2006.

4. G. Mittal and C.J. Sung "Ignition of Moist Syngas in a Rapid Compression Machine", 5th U.S. Combustion Meeting, San Diego, March 2007.

5. X. You, H. Wang, E. Goos, C.J. Sung, and S. J. Klippenstein "Reaction Kinetics of $CO+HO_2 \rightarrow$ Products: ab initio Study and Master Equation Modeling," 5th U.S. Combustion Meeting, San Diego, March 2007.

6. X. You, H. Wang, E. Goos, C.J. Sung, and S. J. Klippenstein "Reaction Kinetics of $CO+HO_2 \rightarrow$ Products: ab initio Study and Master Equation Modeling," *Journal of Physical Chemistry A*, 2007, Vol. 111, 4031-4042.

7. C.J. Sung and C.K. Law "Fundamental Combustion Properties of H_2/CO Mixtures: Ignition and Flame Propagation at Elevated Pressures," *Combustion Science and Technology*, submitted.

References

1. Davis, S.G.; Joshi, A.V.; Wang, H., Proc. Combust. Inst., 2005, 30, 1283-1292.

2. Smith, G.P.; Golden, D.M.; Frenklach, M.; Moriarty, N.W.; Eiteneer, B.; Goldenberg, M.; Bowman, C.T.; Hanson, R.K.; Song, S.; Gardiner, W.C.; Lissianski, V.V.; Qin, Z. http://www.me.berkeley.edu/gri_mech.

3. Li, J.; Zhao, Z.; Kazakov, A.; Dryer, F.L., 30th International Symposium on Combustion, Chicago, 2004, 1F1-04 WIP Poster.

4. Joshi, A.V.; Wang, H., Int. J. Chem. Kinet. 2006, 38, 57-73.

5. Sivaramakrishnan, R.; Comandini, A.; Tranter, R.S.; Brezinsky, K.; Davis, S.G.; Wang, H., Proc. Combust. Inst., 2007, 31, 429-437.

6. You, X.; Wang, H; Goos, E.; Sung, C.J.; Klippenstein, S.J., Journal of Physical Chemistry A, 2007, Vol. 111, 4031-4042.

IV.3 Development of Electrically Mediated Electrophoretic Deposition for Thermal Barrier Coating Systems

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Objectives

- Optimization and validation of the *Faradayic* electrophoretic deposition (EPD) process for deposition of thermal barrier coatings with the appropriate microstructures to prevent coating failure during standard and accelerated turbine engine operation in natural and syngas environments.
- Development and validation of a post deposition thermal treatment for the EPD coatings to preserve the necessary microstructure to maintain coating durability and reliability during operation.
- Selection of appropriate tests of merit, e.g. thermal stability, thermal cycling, thermal conductivity, etc., to qualify coating durability and reliability.

Accomplishments to Date

- Task 1a – Procurement of Haynes® 230® alloy coupons for deposition experiments.
- Faraday visit by Lee Flowers, Market Manager and Metallurgist for Haynes International.
- Task 1a – Discussions with Allister James of Siemens Power Generation regarding sample procurement of turbine alloys for deposition experiments.
- Task 1a – Discussions with David Helmick of GE Energy regarding sample procurement of turbine alloys for deposition experiments.
- Task 1b – Bath formulation of stable suspensions for deposition experiments.
- Task 2 – Modification to existing bench top EPD cell for entire coupon coating.
- Task 3a – DC EPD experiments.
- Task 4 – Thermal post processing of thermal barrier coatings following EPD.
- Task 5c – Thermal conductivity of a Phase I sample.
- Task 5d – Scanning electron microscopy (SEM) of EPD thermal barrier coatings.
- Poster presentation at the American Ceramic Society's 31st International Cocoa Beach Conference and Exposition on Advanced Ceramics and Composites.
- Project update meeting at DOE's National Energy Technology Laboratory in Morgantown, WV.

Introduction

The design and manufacturing of gas turbine engines is challenging from both an engineering and material science standpoint due to the engine's high rotational speeds and high operating temperatures. Component failure stems from several sources including corrosion due to hot gases contaminated with chloride and sulfate, oxidation in an enriched oxygen environment, and mechanical wear and erosion. Additionally, the components experience extreme temperatures, constant thermal cycling and thermal shock. Turbine blades are especially susceptible to damage, requiring routine maintenance for repairs, refurbishing or replacement. Thermal barrier coatings (TBC) are employed to protect the turbine engine components. These coating systems provide thermal, oxidation and mechanical protection, reduce thermal gradients and lower the metal substrate surface temperature, extending the life of the engine components.

Approach

Electrophoretic Deposition

EPD is the migration of small, suspended particles or large molecules in a liquid driven by an electrical potential difference, and offers a promising alternative to conventional deposition methods for deposition of thermal barrier systems. The process has found applications ranging from nanoparticle composites to large colloidal molecules, including deposition of paint primers onto steel, phosphors in the manufacturing of screens for information displays, solid oxide fuel cell components and functionally graded materials. EPD allows for the deposition of fine particles on irregular or curved surfaces, making the technique ideal for blades, cylinder liners and exhaust valves. The advantages of EPD include [1,2,3]:

- Fast deposition rates (several seconds to a few hours).
- Control of deposit thickness and uniformity of the deposition even for complex shapes.
- Reduction of waste encountered by dipping and spraying techniques.
- Low levels of contamination.
- Simple deposition equipment and continuous processing.
- Low cost.

EPD is similar to electrolytic deposition except that the deposited particles do not undergo a valence change during deposition. The EPD process can be divided into three fundamental steps: (1) charging of the particles in suspensions, (2) migration of the particles toward an oppositely charged substrate in the presence of an electric field, and (3) deposition and adherence of the particles onto the substrate. Figure 1 shows the basic principles of the EPD process. Two electrodes are suspended in solution. In the case of the positively charged particles shown in Figure 1, the cathode is the workpiece and the anode is the counter-electrode. The deposition bath consists of a stable colloidal suspension of the deposition material. When the voltage is applied, the charged particles in the suspension migrate towards the cathode under the influence of the electric field, and are deposited on the cathode where they coagulate into a dense mass. Post treatment, such as sintering of ceramic coatings, is required to convert the coating into its final form. In this example the particles are positively charged and deposit on the cathode; however, it is possible for particles to be negatively charged and deposit on the anode.

Typically EPD is accomplished using constant voltage or current conditions. It has been shown [4] that during EPD a constant voltage controls the drift velocity of spherical particles in suspension. This is expressed in Equation (1) [5]:

$$V = \frac{2}{3}\varepsilon_0 \varepsilon_r \zeta \eta^{-1} (df/dx) \qquad (1)$$

where ε_0 is the permittivity of vacuum, ε_r is the relative permittivity of the solvent, ζ is the zeta potential of the particle, η is the viscosity of the solvent and *df/dx* represents the strength of the applied electric field.

Equation (1) suggests that the drift velocity of the spherical particles in the suspension is a function of the applied electric field during the EPD process. This implies that the homogeneity of the electric field (i.e., the "current distribution") is important for the preparation of dense coatings of uniform thickness. Typically, during a constant voltage or current process, some areas of the substrate are exposed to higher current densities than others and are coated preferentially, resulting in a non-uniform coating (i.e. poor throwing power). By utilizing electrically mediated voltages, i.e. reversing the polarity of the electrodes during the EPD process, the coating is preferentially removed from areas exposed to higher current densities, improving the throwing power and producing fully dense coatings of uniform thickness.

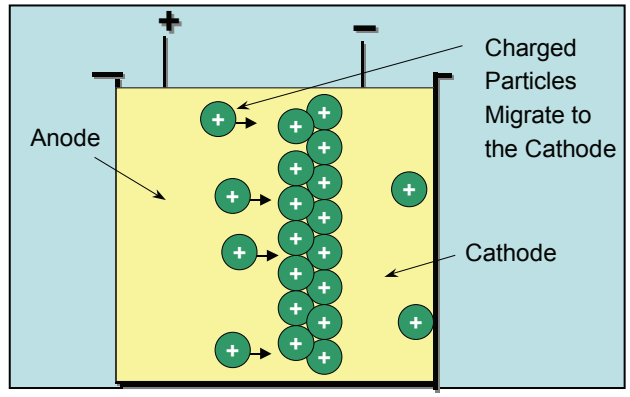

FIGURE 1. Principles of EPD

Electrically Mediated Waveforms Applied to EPD

An electrically mediated waveform (Figure 2) is an interrupted, asymmetric waveform characterized by a cathodic period followed by an anodic period and an off time. The waveform parameters are: (1) the anodic pulse current density, i_a, (2) the anodic on time, t_a, (3) the cathodic pulse current density, i_c, (4) the cathodic on time, t_c, and (5) the off-time, t_o. The sum of the anodic and cathodic on times and the off time is the period, T, of the modulation. The inverse of the period is the frequency, f, of the modulation. The anodic, γ_a, and cathodic, γ_c, duty cycles are the ratios of the respective on times to the modulation period. For a cathodic process, the average current density (i_{aver}) or net deposition rate is given by:

$$i_{aver} = i_c\gamma_c - i_a\gamma_a \qquad (2)$$

Just as there are infinite combinations of height, width, and length to obtain a given volume, in electrically mediated processes there are unlimited combinations of peak current densities, duty cycles, and frequencies to obtain a given deposition rate. These parameters provide the potential for much greater process/product control compared to DC electrophoretic deposition. With improvements in the output, control and accuracy of available power supplies, electrically mediated electroplating has been widely investigated and is currently used in some production facilities [6]. These same principles bring similar advantages in electrophoretic deposition.

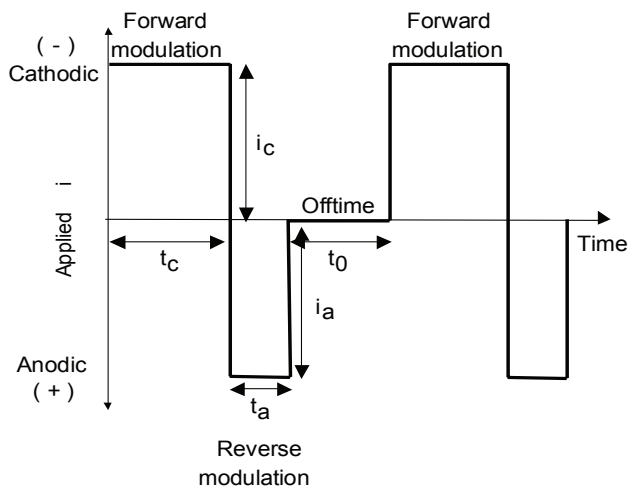

FIGURE 2. An Electrically Mediated Waveform

Results to Date

According to Hamker's Law [7], during the EPD process the deposit mass is linearly proportional to the deposition time. In order to determine the deposition rate, four experiments were conducted on 2" x 2" copper substrates. Copper was chosen because it is a soft metal, enabling simplistic cross sectioning and mounting techniques. DC EPD was conducted at a constant potential of 50 volts for 15, 30, 60 and 120 seconds from a suspension containing 6.5% (w/v) submicron yttria-stabilized zirconia (YSZ) powder, the dispersant PDDA cationic polymer and polyvinyl alcohol binder in 90% ethanol. A distance of 10 mm was maintained between the deposition coupon and counter electrodes. Coupons were massed before and after EPD experiments in order to obtain the green coating deposit mass. Figure 3 provides optical micrographs of coating cross sections and a graph showing that the deposition rate is linearly proportional to the deposit mass.

Figure 4 shows a cross-section of the YSZ coating on a coupon subsequent to laser assisted sintering. The microstructure of the coating appears to be more of a laminar microstructure, similar to what is achieved when thermal barrier coatings are deposited via the plasma spray process. This type of microstructure will likely minimize the thermal conductivity, protecting the substrate from the extreme temperatures experienced by the turbine engine components during normal engine operation.

Conclusions and Future Directions

- EPD can achieve uniform coatings.
- EPD can achieve fast deposition rates.
- EPD is not limited to line-of-sight applications.

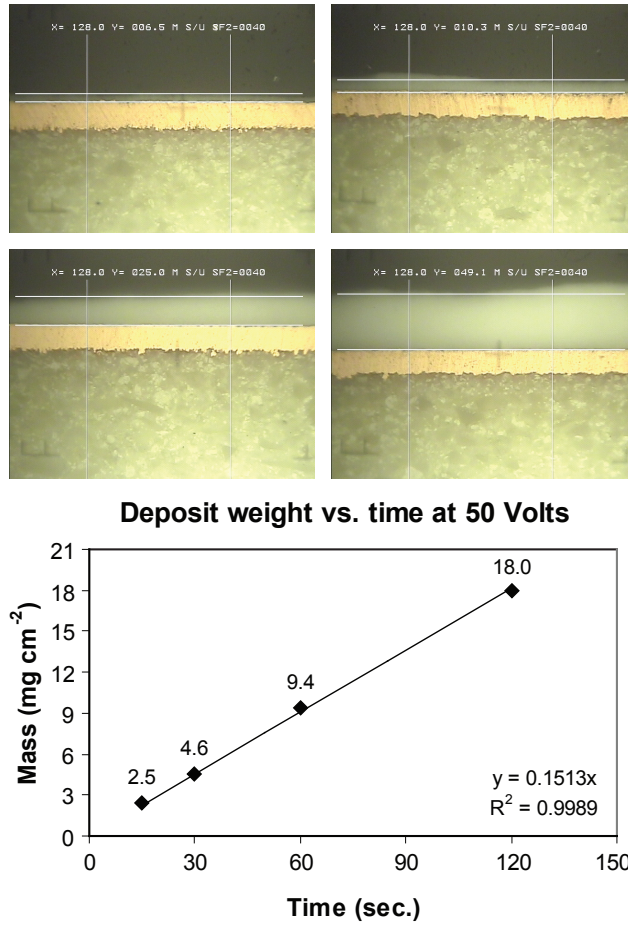

FIGURE 3. Optical Micrographs for Cross-Sections of Thermal Barrier Coatings (top) and Mass vs. Time Plot Illustrating the Linear Relationship Between Coating Mass and Deposition Time (bottom) During EPD

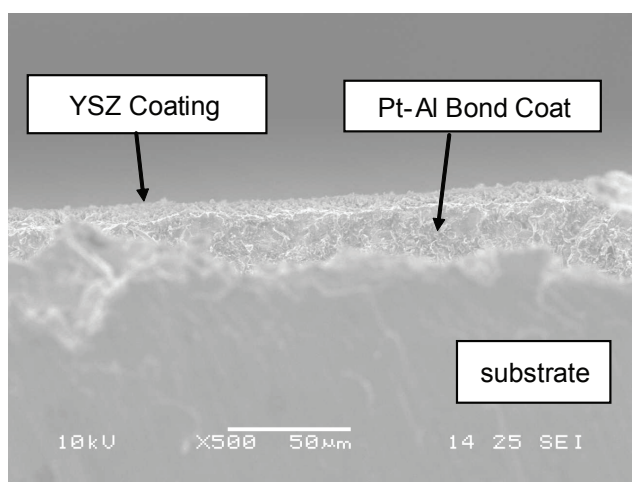

FIGURE 4. Cross-Section of Inconel 718 Coupon Coated with a Pt-Al Bondcoat and an YSZ Thermal Barrier Coat

Future work includes: 1) improving adherence during post processing, 2) exploring additional post processing techniques including microwave sintering, 3) optimizing the electrically mediated electric field process control, and 4) controlling microstructure of the coating.

FY 2007 Publications/Presentations

1. "Faradayic Process for Electrophoretic Deposition of Thermal Barrier Coatings", 31st Annual Cocoa Beach Conference & Exhibition on Advanced Ceramics & Composites – American Ceramics Society, Daytona Beach, FL, January 2007.

2. "Development of Electrically Mediated Electrophoretic Deposition for Thermal Barrier Coatings", Project Status Report, National Energy Technology Laboratory (NETL), Morgantown, WV, April 2007.

References

1. G. Chiodelli, A Magistris, M. Scaliotti & F Parmagiani, Electrical Properties of Plasma-Sprayed Yttria-Stabilized Zirconia Films, *J Mater. Sci.*, 23 {4} 1159-63 (1988).

2. Z. Ogumi, Y Uchimoto, Y. Tsuji & Z Takerhara, Electrodeposition of Thin Yttria-Stabalized Zirconia Layers using Glow Discharged Plasma, *J. Appl. Phys.*, 72, 1577 (1994).

3. J. Zhang, B.I. Lee, Electrophoretic Deposition and Characterization of Micrometer Scale $BaTiO_3$ Based X7R Dielectric Thick Films, *J. of the Cer. Soc.*, 10, 2417-22 (2000).

4. Y. Hirata, A. Nishimoto, and Y. Ishihara, "Forming of Alumina Powder by Electrophoretic Deposition", Seramikusu Kyukai Ronbunshi, **99**, 108 (1991).

5. H. Tamura Y. Matsuda, Gendai Denki Kagaku, 92 (1987).

6. E. J. Taylor, *et al.*, Electrically Mediated Plating of Semiconductor Substrates, Chip Packages and High Density Interconnect PWBs, *Plating and Surf. Fin.*, **89**, 88 (May 2002).

7. Hamaker, H.C., Trans. Faraday Soc. **36**, 279 (1940).

IV.4 High Temperature Capability and Innovative Cooling with Spar and Shell Turbine Blade

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Objectives

- Define the mechanical arrangement of an optimized turbine blade based on spar and shell construction.
- Identify materials best optimized to the spar and shell turbine blade for use in specific environments.
- Define cooling system features required to produce high thermal efficiency.
- Identify manufacturing and fabrication requirements.
- Evaluate benefits and costs of this system.
- Produce a design concept to carry forward into a Phase II development project.

Accomplishments

- At the time of writing of this report, this project had been awarded but had not yet been kicked-off/started. Therefore, this report is submitted to express the research need and project plan only.

Introduction

The use of cooling in the turbine, although permitting turbine components to operate within an environment of high temperature and pressure, causes an efficiency debit to the turbine subsystem and overall power plant. Current gas turbine systems already operate at temperature and pressure levels that are sufficiently high to require the use of advanced material systems and cooling of the turbine components. Technology advances within the turbine systems therefore represent an excellent avenue for improving the overall power plant efficiency. In particular, technologies that permit turbines to operate at increased temperatures and pressures are desired to achieve the specific performance goals. Advances of both the materials and cooling systems are clearly required to extend the envelope for improved performance and efficiency in the future systems.

To meet future power generation needs, Florida Turbine Technologies, Inc. (FTT) has proposed the development of an innovative design approach to provide highly durable turbine components that increase efficiency by requiring the lowest cooling flow possible. The proposed gas turbine blade design is constructed of an internal structurally supporting member (spar) and a separate external shell to provide the aerodynamic envelope. The so-called spar and shell system enables the use of advanced, high temperature materials that are not available based on current design philosophies and manufacturing approaches. In addition to providing higher temperature capabilities, features of this system resolve the well-known technical barrier, thermal-mechanical-fatigue (TMF). This barrier limits heat flux levels and cyclic life of today's turbine components, particularly at the interface between the main airfoil body and the platform/attachment structure. Further, this architecture facilitates the cooling system to be optimized to the smallest possible cooling flow required by enabling the use of practical and robust near-wall cooling features while minimizing the plugging risk of systems such as those associated with effusion and other porous hole schemes. With this proposal, FTT has laid out a comprehensive plan for the design and development of this concept. Further, FTT has the full support and backing of a primary original equipment manufacturer (OEM), namely Siemens Power Generation (SPG), with the expressed commitment to evaluate the design within the SPG design review process. Further, upon successful completion of these reviews, SPG proposes to install development hardware in an engine to permit validation test data to be acquired.

Approach

FTT has proposed the development of a spar and shell turbine component system to realize the future turbine system goals of reduced cooling flow consumption and increased efficiency. Development of the proposed spar and shell turbine component system offers several advantages relative to the current state-of-the-art. To realize these goals, several objectives, as delineated in the following paragraphs, must be pursued.

The concept of a spar and shell turbine component is not new. FTT recognizes the limitations of current

material and cooling systems and has been actively investigating alternatives to resolve the major issues. As a result, development of the spar and shell system has proceeded to the point where detailed analytical and empirical verification is now required as a prerequisite to ultimate verification of the design concept in a test engine. One example of such a component is described in U.S. patent #7080971, "Cooled Turbine Spar Shell Blade Construction" by Wilson and Brown. Although development of the spar and shell system has proceeded beyond this patent, namely with respect to attachment features and shell loading, the art reproduced in Figure 1 illustrates the basic concepts of this design approach. As shown, this design approach utilizes an internal spar which is surrounded by an external shell. This fabrication approach has several advantages relative to the current state-of-the-art monolithic cast structures. First, the internal spar represents the primary framework of this concept. Since this member is thermally protected by the shell from the hot working fluid passing around the airfoil, it can be maintained

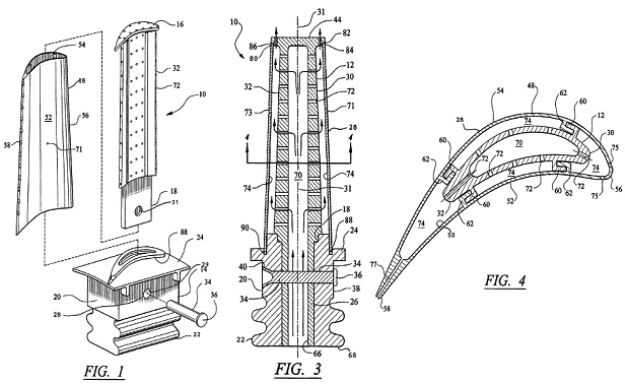

FIGURE 1. U.S. Patent #7080971, "Cooled Turbine Spar Shell Blade Construction"

at a relatively low temperature very near that of the coolant. The spar material can therefore be optimized for very high strength at a moderate temperature level. Second, since the shell is structurally isolated from the spar, its material can be selected on the basis of high temperature capability. Thermally induced stresses are a primary driver and limiter of existing cooled turbine components. This design approach serves to mitigate the associated effects on low cycle fatigue (LCF) and TMF distress through both thermal and mechanical isolation of the spar and shell. Further, other desirable thermal attributes, such as the ability to support high temperature and heat flux, can be considered as primary drivers in the shell material selection.

Results

This project has not yet started.

Conclusions and Future Directions

Under this Phase I Small Business Innovation Research (SBIR) project, FTT proposes to develop a high efficiency, cooled spar and shell turbine component system from its inception through a concept design review. This requires the development of a mechanical design configuration with sufficient analytical heat transfer, flow and structural computations to support the feasibility of the concept and to verify the design. Further, a comprehensive plan will be defined in sufficient detail to support the manufacturing and cost feasibility of the proposed concept.

In future plans, a detailed design of the concept developed under this Phase I SBIR will be performed as Phase II. The detailed design will focus on development of a demonstration test article that could be evaluated in a test engine during Phase III.

IV.5 Flashback Characteristics of Syngas-Type Fuels Under Steady and Pulsating Conditions

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Objectives

- Remove most critical barrier to usage of high hydrogen fuels in low emissions turbines by improved understanding of flashback phenomenon.
- Determine mechanisms of flashback in high hydrogen combustors.
- Perform parametric studies that determine flashback studies at realistic conditions over a range of fuel compositions and operating conditions.
- Perform complementary modeling to predict flashback as function of fuel composition.

Accomplishments

- Demonstrated that multiple flashback mechanisms exist at conditions of interest to gas turbine combustors.
- Obtained data quantifying flashback boundaries over a wide range of operating pressure, temperature, and fuel composition.
- Obtained high speed visualizations of flashback phenomenon.
- Developed model predicting influence of flame on upstream flow field, a key process influencing flashback.
- Performed kinetic calculations to correlate flashback data obtained during experiments.
- Transitioned knowledge to industry through seminars at several gas turbine original equipment manufacturers (OEMs) and publications.

Introduction

This project is motivated by the fact that the inherent variability in composition and heating value of coal-derived, high hydrogen fuels provides one of the largest barriers towards their usage. This fuel composition variability is of concern because low emission combustion systems are generally optimized to operate with fuels that meet tight specifications. The objective of this proposed project is to improve the state-of-the-art in understanding and modeling flashback, an issue that will be of acute significance in realization of low emissions, fuel-flexible gas turbines that burn hydrogen-containing fuels. The term "flashback" refers to flame propagation upstream of the combustion chamber into the fuel/air mixing passages, which causes severe damage to parts. Flashback occurrences in modern gas turbines occur occasionally and can easily cost millions of dollars in replacing damaged parts and lost revenue.

Approach

This project is investigating this problem with a three pronged approach: experiments at realistic conditions, computational kinetic calculations, and analytic modeling. The experiments are performed at the Georgia Tech gas turbine combustor simulator, which can operate at the conditions encountered in gas turbine combustors. This state-of-the-art facility is unique in its full optical access, allowing for usage of modern laser based diagnostic techniques to interrogate the critical internal flow and flame characteristics. A photograph of this facility is shown in Figure 1.

In parallel, computations of the flame speeds, strain sensitivities, Lewis numbers, and other key combustion properties are performed using state-of-the-art numerical tools and kinetic mechanisms. These tools allow for predictions of key combustion parameters that are not directly observable. Finally, analytic investigations of flame/flow investigations are performed using advanced theoretical approaches that have allowed us to understand how the flame interacts with the approach flow field.

Results

The objective of this proposed project is to improve the state-of-the-art in understanding and modeling flashback, which is known to be the most significant

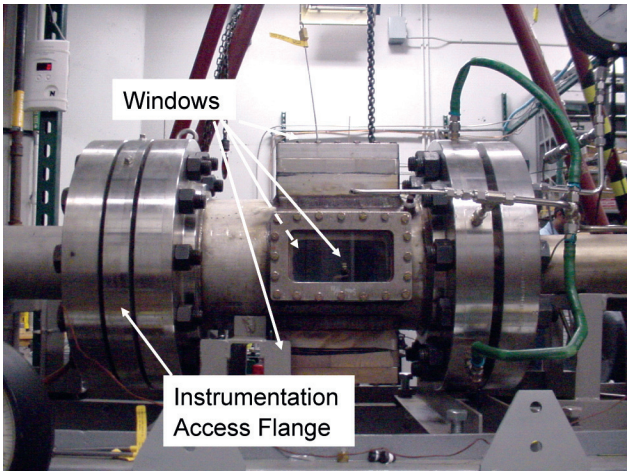

FIGURE 1. Georgia Tech Gas Turbine Combustor Simulator

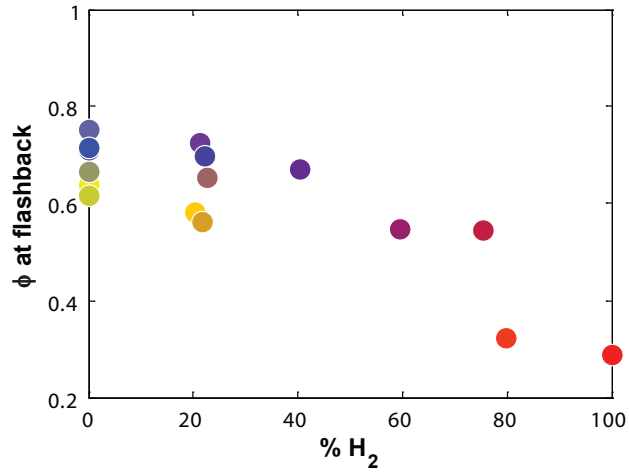

FIGURE 2. ϕ at Flashback versus $\%H_2$ at Nozzle Velocity of 40 m/s, $T_0 = 458$ K and $P = 4.4$ atm

issue in low emissions combustors containing high levels of hydrogen.

One of the key complexities associated with this problem is the multitude of flashback mechanisms present. In a non-swirling flow, the flame can flashback either in the core flow or through the boundary layer, if the flame speed exceeds the flow speed. In a swirling flow an additional, recently proposed mechanism also is present, termed combustion induced vortex breakdown.

By obtaining data over a range of hydrogen levels, pressures, temperatures, and nozzle velocities, we have been able to confirm that two distinct mechanisms of flashback occur. Most significantly, we have found that the flashback mechanism changes substantially between high and low/intermediate hydrogen levels. The former case is apparently associated with fast flame propagation through the boundary layer or in the core flow. The latter mechanism is a gradual flame movement that appears to scale with temperature ratio across the flame, and not the flame speed. Typical data showing the dependence of the flashback fuel/air ratio as a function of the fraction of hydrogen in the fuel are shown in Figure 2. This data illustrates that high hydrogen mixtures are extremely prone to flashback.

More recently, we have obtained high speed visualizations through an optically accessible nozzle section of the flashback phenomenon, showing the flame propagation upstream in a helical fashion. A typical image set showing this is shown in Figure 3.

Throughout the project we have maintained close communication with technical personnel at two Department of Energy labs, National Energy Technology Laboratory and Sandia. We have also maintained our interactions with several gas turbine manufacturers with whom we have closely worked in prior and ongoing programs.

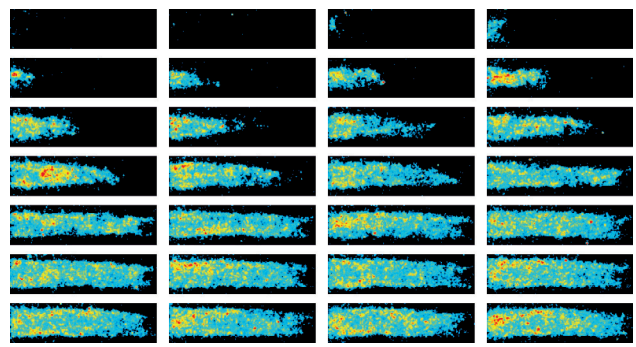

FIGURE 3. 80% CH_4, 20% H_2 flashback at 359 K, 1 atm, and nozzle velocity of 49 m/s. Shows the flame propagation sequence zoomed in on the quartz tube. Images are 0.5 ms apart.

Conclusions and Future Directions

A key conclusion of this work is that several distinct flashback mechanisms exist, each with different parametric sensitivities on combustor parameters. For example, the combustion induced vortex breakdown mechanism is apparently critically controlled by temperature ratio across the flame, as well as flame speed. Key future work is further translating this improved qualitative understanding of the phenomenon into quantitative prediction capabilities.

Publications

1. Zhang, Q., Noble, B., Meyers, A., Xu, K., Lieuwen, T., "Characterization of Fuel Composition Effects in $H_2/CO/CH_4$ Mixtures upon Blowout", *J. Engineering Gas Turbines and Power*, to appear.

2. Lieuwen, T., McDonell, V., Petersen, E., Santavicca, D., "Fuel Flexibility Influences on Premixed Combustor Blowout, Flashback, Autoignition, and Stability", *J. Engineering Gas Turbines and Power*, to appear.

3. Noble, D., Zhang, Q., Lieuwen, T., "Hydrogen Effects Upon Flashback and Blowout", Proceedings of the International Colloquium on Environmentally Preferred Advanced Power Generation, ICEPAG 2006–24012.

4. Noble, D., Zhang, Q., Lieuwen, T., "Syngas Fuel Composition Sensitivities of Combustor Flashback and Blowout", Proc. of the 23rd International Pittsburgh Coal Conference, 2006.

5. Lieuwen, T., McDonell, V., Petersen, E., Santavicca, D., "Fuel Flexibility Influences on Premixed Combustor Blowout, Flashback, Autoignition, and Stability", ASME paper #2006-90770, Presented at the ASME-IGTI Turbo Expo, 2006.

6. Noble, D., Zhang, Q., Shareef, A., Tootle, J., Meyers, A., Lieuwen, T. "Syngas Mixture Composition Effects Upon Flashback and Blowout", ASME paper #2006-90470, Presented at the ASME-IGTI Turbo Expo, 2006.

7. Lieuwen, T., Richards, G., "Burning Questions: Combustion Research prepares for the More Complex Fuel Supply of the Near Future", Mechanical Engineering, March, 2006.

8. Zhang, Q., Noble, D.R., Lieuwen, T., "Blowout Measurements in a Syngas-Fired Gas Turbine Combustor", Proc. of the 22nd Annual International Pittsburgh Coal Conference, 2005.

IV.6 Prediction of Combustion Stability and Flashback in Turbines with High-Hydrogen Fuel

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Objectives

- Remove critical barriers to usage of high hydrogen fuels in low emissions turbines by developing predictive capabilities for flashback and combustion instability.
- Develop computational simulation capabilities to predict the conditions under which detrimental flashback and combustion instabilities occur.
- Perform validating experiments of conditions under which flashback and instabilities occur.
- Distill knowledge gained from simulations and experiments into a reduced order model which can be used as a design tool.

Accomplishments

- Project just initiated.
- Kickoff meeting between university participants held to clarify responsibilities and research emphases.
- Advised industry partners on project and obtained input on key problems and approaches of most interest.

Introduction

This project is motivated by the fact that the inherent variability in composition and heating value of coal-derived, high hydrogen fuels provides one of the largest barriers towards their usage. This fuel composition variability is of concern because low emissions combustion systems are generally optimized to operate with fuels that meet tight specifications. The objective of this proposed project is to improve the state-of-the-art in understanding and modeling combustion instabilities and flashback, probably the two most critical issues associated with burning high hydrogen fuels in low emissions turbines. The term "flashback" refers to flame propagation upstream of the combustion chamber into the fuel/air mixing passages, which causes severe damage to parts. "Combustion instabilities" refers to damaging pressure oscillations excited by the combustion process. The damage due to these oscillations and flashback cause hundreds of millions of dollars of damage in low emissions turbines every year, through forced outages and broken parts.

Approach

This project is investigating this problem with a three pronged approach: experiments, computational kinetic calculations, and analytic modeling. It consists of a collaborative effort involving two universities, both with strong expertise in dynamical combustion phenomenon, and two gas turbine manufacturers. In addition, the proposed research will be structured to provide significant student involvement (including high school teachers, undergraduate students, and graduate students) and therefore will make an important contribution to the future science and technology base of our nation. Its focus upon high fidelity simulations, coupled with validating measurements, and development of reduced order models will significantly improve understanding of these phenomenon and capabilities for predicting their occurrence.

IV.7 Embedded Sensors in Turbine Systems by Direct Write Thermal Spray Technology

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Subcontractors:
- HiTec Products, Inc., Ayer, MA
- Stony Brook University, Stony Brook, NY

Objectives

1. Design and optimize the location of sensors with respect to component geometry.
2. Optimize strain gauge and thermocouple (TC) sensor materials to meet required component sensing needs that both perform as needed and are also amicable to thermal spray.
3. Optimize direct-write thermal spray processes to achieve high quality, reliable, reproducible materials with requisite sensor performance.
4. Reduce line width and line thickness of embedded thermocouples to be as non-intrusive as possible on the component platform while providing a sufficient signal for easy monitoring.
5. Investigate the impact of embedded sensor(s) on the life and performance of thermal barrier coatings. Assess role of materials, sensor dimensions, location and microstructure on the coating and sensor lifetime.
6. Examine sensor and coating degradation issues through static furnace, cyclic furnace and burner rig tests.
7. Quantify electrical properties of sensor materials deposited by direct write thermal spray.
8. Optimize processing conditions for the deposition of embedded thermocouples and strain gages in thermal barrier coatings.
9. Demonstrate long term survival and stability of direct write thermal spray embedded sensors at elevated temperatures in oxidizing atmospheres.

Accomplishments

- Demonstration of a functional thermocouple element embedded within a thermal barrier coating (TBC).
- Demonstration of a functional strain gauge element within a ceramic coating.
- High quality functionality of the embedded thermocouple (no hysteresis, reliable, repeatable).
- High temperature functionality of the embedded thermocouple (up to 1,200°C).
- Demonstrated functionality during both cyclic and isothermal long duration burner rig test (~300 hours at a 1,200°C surface temperature).
- No premature failure of sensor or the TBC top coat during these tests.
- Demonstration of capability for conformal direct write on a blade.
- Demonstration of thermocouple wire-welding onto sensors for signal extraction.
- Engaged a major turbine original equipment manufacturer for future technology insertion.
- Developed a heat flux sensor for harsh environments that functions with a TBC surface temperature of 1,200°C.
- Demonstrated the type N thermocouples prepared by Direct Write thermal spray (DWTS) have significantly longer life than type K thermocouples in oxidizing environments at high temperatures greater than 1,000°C.

Introduction

The goal of the project is to create a technology that will enable low cost, robust, reliable, embedded harsh environment sensors fabricated directly onto heat engine components. This will represent a paradigm change from the current passive or reactive mode of operating and maintaining turbine engines based on a predetermined set of rules, to a proactive method based on 'state awareness' and knowledge of operating components *in situ*. This will not only improve the operating conditions of advanced turbine engines, which will increase reliability, reduce fuel costs and decrease down time, but also provide a unique new means of condition monitoring and machinery prognostics.

MesoScribe's ultimate goal is to integrate embedded sensors into critical components of turbines and other heat engines during manufacturing so that expensive, alloy systems and coated components can be closely monitored and their performance optimized while in service to maximize their utility and provide overall cost savings.

Approach

MesoScribe Technologies, Inc., a spin-off company from Stony Brook University, is commercializing its Direct Write process to fabricate embedded temperature and strain sensors for high-temperature environments. MesoScribe has partnered with Hitec Products, Inc., a supplier of specialized sensors to the high-temperature turbine industry, and Siemens Power Generation to provide sensor specifications and an understanding of gas turbine component operation. This partnership between MesoScribe and Hitec along with the R&D capabilities at Stony Brook and the insertion capabilities of Siemens will assure rapid deployment of this new technology to the advanced turbine engine marketplace.

Embedded sensors within coatings based on thick films offer a unique method for intelligent assessment of harsh environment components. Coatings offer the best platform for semi-intrusive interrogation of the system because they can be used in a non-prime reliant fashion in this technology test bed. Thermocouples and strain gauges based on metallic alloys can be integrated into turbine components, if appropriately chosen. Their integration through system-level design offers a convenient method for instrumenting the turbine system.

Results

MesoScribe has fabricated Type K and Type N thermocouples using the company's Direct Write MesoPlasma™ process. Figure 1 shows a pair of Direct Write Type N thermocouples deposited onto a 1" x 6" Hastelloy X substrate and overcoated with a TBC.

Sensors have been deposited onto coupons and gas turbine engine components and tested using furnaces, burner rigs and high heat flux lasers to 1,200°C. Examples are shown in Figure 2. Actual instrumented components are not shown due to proprietary restrictions.

Type N thermocouples were furnace tested in a long-term soak at 1,010°C. The specimens were arranged in a 2" tube furnace with 5.5" of the 12" bar extending outward from the tube. This enforces the maximum temperature difference between the two thermocouple junctions. In this way, the direct-write section of the circuit contributes the bulk of the electromotive force (EMF). The extension leads that join the 'cold end' of the bar to the instrumentation contribute almost none. The Type N thermal output is shown in Figure 3. The Direct Write Type N TCs held within 2% of the reference thermocouple output and survived 160 hours before failure (Figure 3). NASA-Glenn has conducted cyclic testing using high heat flux lasers and the Direct Write sensors have survived over 300 hours of cyclic testing to 1,000°C using 1 hour heat soaks.

Since nickel-based alloys are susceptible to oxidation either during processing or during operation at elevated temperatures, new TCs are being developed from precious metals and ceramic materials.

MesoScribe has been developing resistive gages that can accurately measure dynamic and static strain. Resistive gages are made by depositing patches of strain gage material (e.g., NiCr) using the company's MesoPlasma™ process, followed by a laser micro-

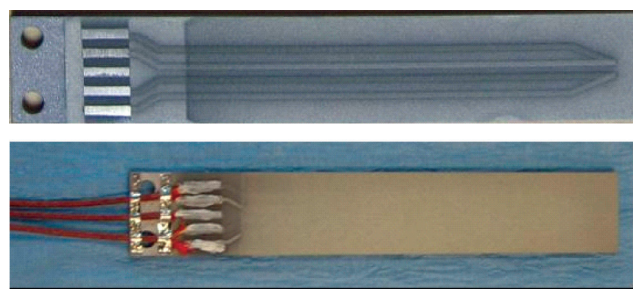


FIGURE 1. Direct Write thermocouple before and after TBC topcoat. Lead-wires are micro-welded to each TC element and cemented for added durability.

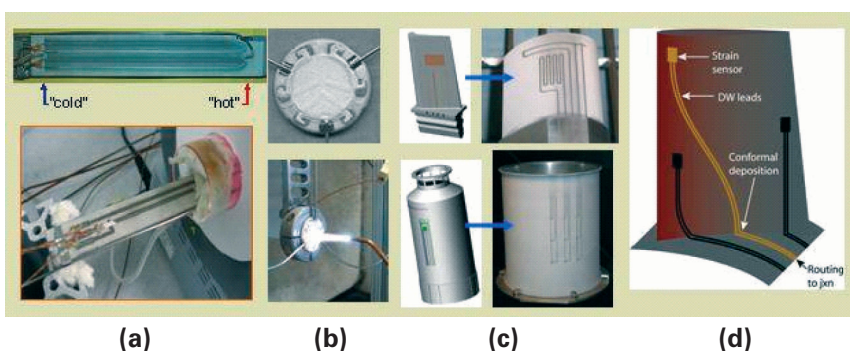


FIGURE 2. Examples of DWTS thermocouples: (a) planar DWTS thermocouple (two on sample + wire reference for testing) along with furnace test photo; (b) multilayered heat flux sensor based on three vertically spaced thermocouples with photo of flame impingement test; (c) DWTS thermocouples on mock turbines blades and mock combustors; (d) schematic of a DWTS sensor array on a turbine blade.

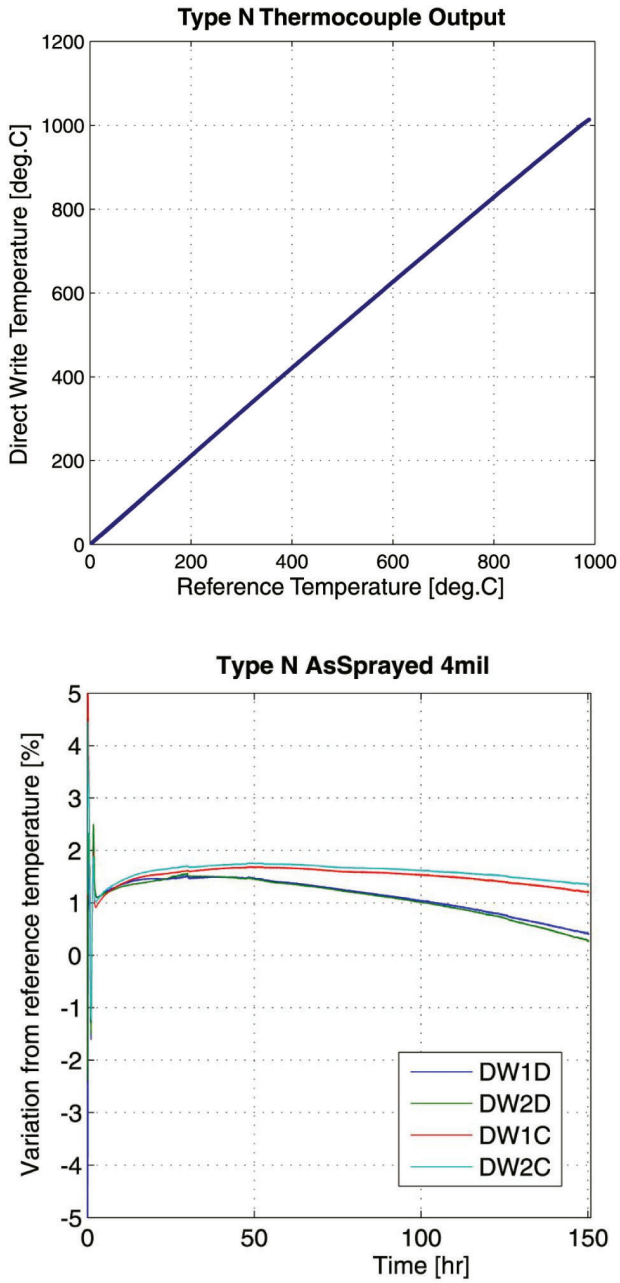


FIGURE 3. (top) Direct Write Type N Temperature Output as a Function of Reference Temperature and (bottom) Variation from Reference during a 150 Hour Durability Test at 1,010°C

machining process, and overcoated with a protective coating as shown in Figure 4. Feasibility in fabricating capacitive gages that can be passively interrogated by radio frequency excitation has also been demonstrated.

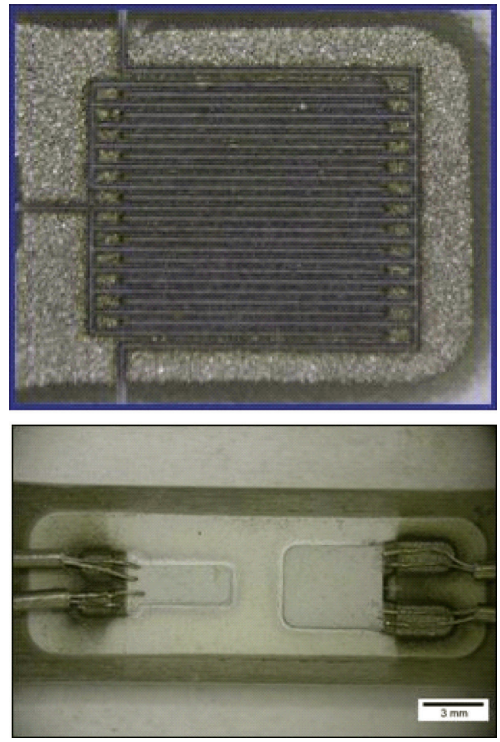


FIGURE 4. Examples of a 3 mm x 3 mm Resistive Strain Gage (top) and Overcoated Gages (bottom)

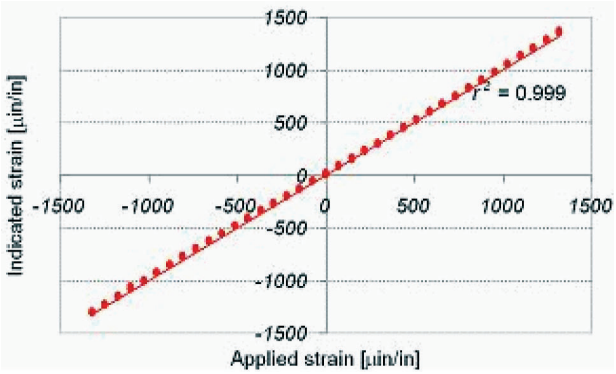
The strategy is to fabricate these sensors in critical locations to obtain the following information:

- Strain history (magnitude and orientation of strains; occurrence of overloads) under cyclic loading.
- Dynamic strain response (creep; stress-relaxation; vibration) under monotonic and/or cyclic loading.
- Appraisal of fatigue damage via static change.

Strain gages were deposited onto constant strain cantilever beams and deflected in tension and compression in an automated fashion. The strain gages exhibit a very linear strain response when compared to reference foil gages (Figure 5).

MesoScribe's dynamic laser-cut strain gages now achieve:

- Linear strain reporting (correlation with reference r2>0.99)
- Repeatable performance over time (steady-state gage factor = 1.3)
- Consistent peak-to-peak (insensitive to temperature, zero drift)
- Consistent batch performance



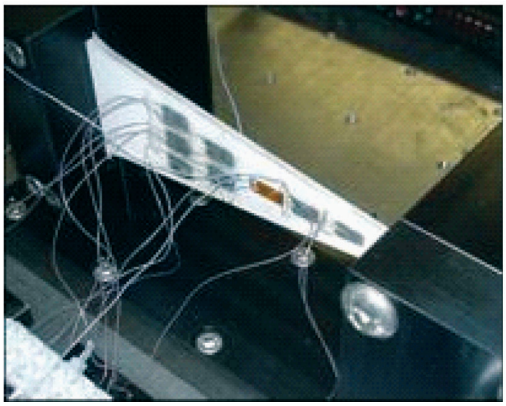


FIGURE 5. Accurate Linear Strain Response When Tested in an Automated Cantilever Bending Apparatus

Conclusions and Future Directions

Direct Write thermal spray technology has demonstrated the capability to fabricate thermocouples, heat flux sensors, thermopiles and strain gages within TBCs for use at high temperature. This technology offers new opportunities for structural health monitoring within gas turbine engines to enable real-time performance evaluations and proactive maintenance scheduling for power generation and aircraft/spacecraft propulsion. Prototype sensors are being tested at our customer's facilities and have demonstrated high performance and durability at temperatures up to 1,100°C.

Future effort is focused on the following activities:

- Development of high temperature dielectric coatings to provide greater electrical insulation at high temperature and that are compatible with conventional TBCs.
- Development of precious metal and ceramic sensors to provide greater durability at high temperature than nickel-based alloys (to be conducted under an Air Force contract).
- Improving Direct Write hardware and processing to increase efficiency and decrease sensor manufacturing costs.

Special Recognitions & Awards/Patents Issued

1. MesoScribe Technologies and Siemens Power Generation signed a joint venture agreement and were awarded a $5.4 million Advanced Technology Program award through the National Institute of Standards and Technology to develop "high temperature, wireless smart turbine components".

Patents Pending:

1. Thermocouples, Assignee: MesoScribe Technologies, Inc., Inventors: R. J. Gambino, J. P. Longtin, J. A. Brogan, J. S. Gutleber and R. J. Greenlaw.

FY 2007 Publications/Presentations

Publications

1. C. Gouldstone, J. Brogan, R. Greenlaw, R. Gambino, J. Gutleber, S. Sampath, J. Longtin., "Embedded resistive strain sensors for harsh environments," in *2006 IEEE Aerospace Conference Proceedings*, Big Sky, MT, March 4–11, 2006.

2. J. Gutleber, J. Brogan, R. Gambino, C. Gouldstone, R. Greenlaw, S. Sampath, J. Longtin, D. Zhu., "Embedded temperature and heat flux sensors for advanced health monitoring of turbine engine components," in *2006 IEEE Aerospace Conference Proceedings*, Big Sky, MT, March 4–11, 2006.

Presentations

1. J. Brogan, "*Direct Write Sensors for Turbine Engine Applications,*" AEROMAT 2007, Baltimore, MD.

IV.8 Materials and Component Development for Advanced Turbine Systems

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Subcontractors:
- Coatings for Industry, Souderton, PA
- University of Pittsburgh, Pittsburgh, PA
- Carnegie Mellon University, Pittsburgh, PA
- West Virginia University, Morgantown, WV

Objectives

- Initiate development and assess the extended long-term response (stability or degradation) of an alternate, novel, projected lower cost, NETL-bond coat system for use in advanced turbine hydrogen-fired and oxy-fuel applications.
- Initiate and demonstrate the use of confocal laser scanning microscopy analysis, micro-indention measurements, and non-linear acousto-ultrasonic diagnostic techniques to define the stability or degradation of the thermal barrier coating (TBC), bond coat, or underlying metal substrate system.
- Expand NETL's turbine aero-thermal 3D computational modeling capabilities, initiate modeling of stress-strain characteristics within the turbine airfoil and hot gas interfaces, and develop cumulative creep and fatigue damage models for lifing predictions.

Introduction

Increasing the power efficiency of stationary land-based industrial gas turbines to meet Fossil Energy's contribution to DOE's Advanced Power Systems 2010-2020 goals will require future turbine inlet temperatures to increase to >1,400°C (Table 1). Cooling air will simultaneously need to be controlled to avoid an increase in NO_x emissions. The concept of ultra-low or "zero" emission power generation has focused on an oxy-fuel combustion process in which nitrogen is removed in the combustion air, and replaced with steam, thereby preventing the formation of nitrogen oxides. The exhaust stream of the oxy-fuel process is separated into concentrated CO_2 and water. Alternately, hydrogen-fired turbine systems are conceptually based on a complex cycle composed of a closed Brayton cycle and a Rankine cycle. Hydrogen turbines are expected to be a key part of near-term integrated gasification combined cycle (IGCC) plants that can sequester carbon dioxide, such as FutureGen. Hydrogen and oxygen are supplied as the fuel and oxidant respectively to a compressor, and burned in steam. The pressurized steam feed enters a high temperature turbine at 1,700°C for stator blades, and 1,570°C for rotor blades. Since these elevated temperatures are typically higher than the melting temperatures of alloys used in the construction of the hot gas structural components, the components are cooled by air extracted from the turbine compressor and directed through the cooling passages designed into the component.

TABLE 1. Projected Advanced Turbine Operating Parameters

	Syngas Turbine 2010	Hydrogen Turbine 2015-2020	Oxy-Fuel Turbine 2010	Oxy-Fuel Turbine 2015-2020
Combustor Exhaust Temp, °F (°C)	~+2,700 (~+1,480)	~+2,700 (~+1,480)		
Turbine Inlet Temp, °F (°C)	~2,500 (~1,370)	~2,600 (~1,425)	~1,150 (~620)	~1,400 (~760) (HP) ~3,200 (~1,760) (IP)
Turbine Exhaust Temp, °F (°C)	~1,100 (~595)	~1,100 (~595)		
Turbine Inlet Pressure, psig	~265	~300	~450	~1,500 (HP) ~625 (IP)
Combustor Exhaust Composition, %	CO_2 (9.27) H_2O (8.5) N_2 (72.8) Ar (0.8) O_2 (8.6)	CO_2 (1.4) H_2O (17.3) N_2 (72.2) Ar (0.9) O_2 (8.2)	H_2O (82) CO_2 (17) O_2 (0.1) N_2 (1.1) Ar (1)	H_2O (75-90) CO_2 (25-10) O_2, N_2, Ar (1.7)

Oxidation and hot corrosion of industrial land-based power generation gas turbines are principal concerns, particularly in view of long-term operation (30,000 hrs), as well operation with advanced combustion cycles that potentially target turbine inlet temperatures of >1,500°C. Current structural materials as nickel and cobalt-based superalloys cannot withstand temperatures of >950°C. Although single crystal substrates as René N5, increase the durable operating temperature for the structural airfoil support, operation in the advanced combustion

cycles will require development and application of stable TBCs with better insulation properties, as well as implementation of acceptable internal component cooling techniques, in order to achieve extended operational life of oxy-fuel and hydrogen fired land-based turbines. Should the applied TBC and internal cooling be inadequate to sustain the life of the turbine blade and vane materials, development of advanced, high temperature stability substrates will be required.

Approach

The approach of the NETL-University Collaborative Research (UCR) program is to combine the expertise of NETL, University of Pittsburgh, Carnegie Mellon University (CMU), and West Virginia University (WVU) researchers, working in conjunction with commercial metal and coating suppliers as Howmet International and Coatings for Industry (CFI), and test facilities as Westinghouse Plasma Corporation (WPC) and Praxair to develop advanced material and aerothermal technologies for use in future hydrogen-fired and oxy-fuel turbine applications.

Results & Accomplishments

Current NETL-Bond Coat Development, Bench-Scale Testing, Materials Assessment, and Modeling

- The initial, projected lower cost, NETL-bond coat was manufactured by a commercial coating supplier – Coatings for Industry, and applied to Howmet International René N5 and Haynes 230 coupons (Figure 1).
- Preliminary bench-scale testing indicated adherence of the NETL-bond coat after:
  - 24 hrs of static air exposure at 800°C
  - 10 severe thermal cycles (room temperature to 1,000°C in 10 minutes (100°C/minute), followed by an 8 hour dwell at 1,000°C, and subsequent rapid cooling to room temperature)
  - 500 hours of static air testing at 1,000°C
- Based on state-of-the-art assessment criteria where weight change and base metal oxide scale formation were determined, the initial NETL-bond coat:

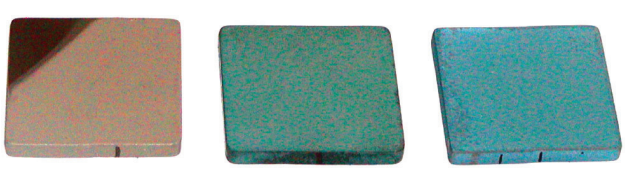

FIGURE 1. NETL-Bond Coated Test Coupons

  - At 900°C did not spall under thermal cyclic and isothermal conditions, but oxygen penetrated and oxidized the coating, as well as the René N5 and Haynes 230 substrates.
  - At 1,100°C the coating spalls under thermal cyclic and isothermal conditions, and the underlying René N5 and Haynes 230 substrates oxidize.
- The presence of water vapor did not affect the response of the NETL-bond coat during extended cyclic oxidation testing.
- Modifications to the initial NETL-bond coat are necessary, and are being made, to improve the oxidation protection that the coating may provide to the underlying René N5 and/or Haynes 230 substrate.

Non-Destructive Evaluation/Diagnostics

Confocal Scanning Laser Microscopy (CSLM)

- Current as-manufactured surface roughness of the NETL-bond coat limits the use of CSLM for demonstrating morphology/phase changes as a function of time at high temperature under various single and/or mixed gas phase environments.
- Initiated visualization of the high temperature transient and stable oxide formations along the surface of René N5. Current efforts to be extended to ODS alloys as PM2000, and Al-Ti-Nb (IMPRESS) matrices.

Micro-Indention Testing

- A new micro-indentation methodology was developed for determining room temperature mechanical properties (i.e., Young's modulus; surface stiffness) of non-smooth bond coats or complete TBC systems using an automated multiple loading/unloading indentation testing sequence.
- The technique confirmed reported Young's modulus for nickel-based Haynes 230.
- The technique demonstrated the ability to detect change in the surface stiffness properties (Figure 2; reduction of the NETL-bond coated René N5 and Haynes 230 coupon surface stiffness after exposure to 200 high temperature thermal cycles (room temperature ↔ 1,100°C)). Correlation with microstructural and weight changes is being initiated.
- This technology has the potential to develop a hand-held portable device for *in situ* non-destructive testing that may indicate where possible spallation areas of the top coat and/or bond coat may occur during/after field service operation.

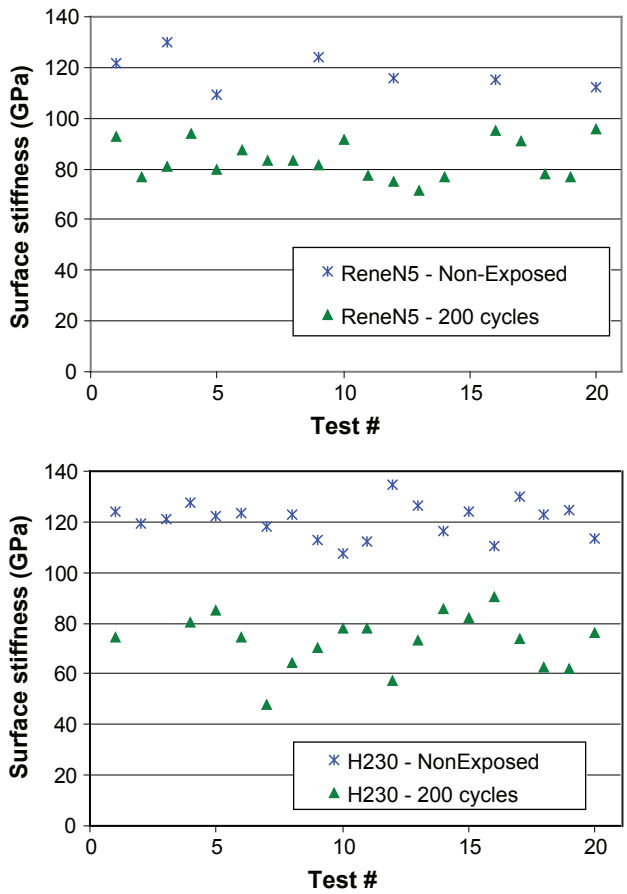

FIGURE 2. Comparison of the Measured Surface Stiffness Data at Multiple Locations on the As-Manufactured NETL-Bond Coat, and the Bond Coat after 200 Thermal Cycles

Non-Linear Acousto-Ultrasonic Diagnostics

- Non-destructive proof-of-concept testing using an acousto-ultrasonic technique was accomplished.
  - For this effort, testing is required to be non-destructive without liquids being deposited on the surface of the coupons.
  - A test set-up was developed and shows successful detection using a latex interface membrane (dry contact) with miniature piezoelectric sensors.
- The results successfully demonstrated that changes in the properties of a 40 μm bond coat can be detected using the proposed ultrasonic methods without the use of a contact agent (or coupling liquid) being applied to the surface of the coupons.
- The time histories of the surface displacements from finite element analyses are comparable to the theoretical Lamb's solution. The finite element methods (FEM) were then used to analyze a combination of more complicated material properties and geometry boundaries. The peak amplitudes and their corresponding arrival times are seen to be clearly influenced by the bond coat properties when the coating's Young's modulus and mass density were varied ± 20% from the substrate's properties. A comparison between experimental measurement and finite element simulation were used to estimate the material properties of the coatings and the substrate. A nonlinear wave modulation technique was also applied, and preliminary results show that the demodulated frequency with a sideband of one low frequency has high sensitivity toward the surface and boundary changes of the sample coupon.

Aerothermal Modeling

- Preliminary 3D flow simulations for next generation hydrogen-fired turbines were completed. Results are presented in terms of heat transfer coefficient contours and local distributions over a generic E^3 airfoil (Figure 3).
- Preliminary stress, strain and displacement field simulations were completed over the E^3 airfoil design. Maximum stress was identified at the trailing edge of the airfoil where it is attached to the firtree (root).
- Methodology is being developed for thermal-mechanical life predictions.

Conclusions and Future Directions

- Based on the NETL-bond coat bench-scale test performance results, modifications will be made to improve the protection that this coating provides to the René N5 and Haynes 230 substrates.

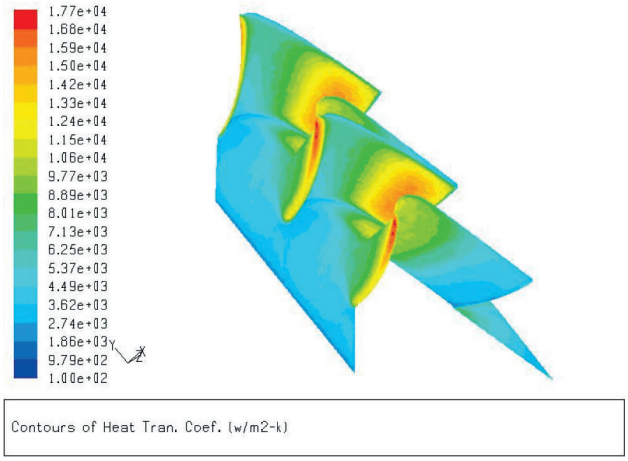

FIGURE 3. Heat Transfer Coefficient Contours over 3D Blade

Additional single crystal coupons will be coated with the modified coating systems, and bench-scale laboratory testing will be conducted to evaluate their stability during extended high temperature, cyclic oxidation exposure in laboratory air and/or in air containing water vapor at 0.1 atm.

- Thermal flux testing is being initiated at the Westinghouse Plasma Corporation in Madison, Pennsylvania, evaluating the stability of various bond coats and full TBC systems that are applied to cylindrical tube coupons. Additionally, high temperature corrosion and erosion testing using simulated, projected, oxy-fuel and hydrogen-fired, turbine inlet gas chemistries is being initiated using similar coating systems.
- Based on our initial stiffness results which illustrate change in the NETL-bond coat material properties with extended thermal cycling, plans are to correlate the materials characterization data/trends with the non-destructive micro-indentation technique data, and construct and demonstrate the use of a portable micro-indentation system for field service operation.
- Continued effort will be directed to generation of computer-based models that project the 3D thermal and stress induced within the advanced airfoil concepts. Projections will address feasibility for use of materials selection and/or aerothermal cooling concepts. Laboratory testing will be defined and implemented to validate the 3D computer-based models.
- Should the applied TBC and internal cooling be inadequate to sustain the life of the turbine blade and vane materials, development of advanced, high temperature stability substrates will be required. Plans currently are to establish candidate next-generation, higher temperature, airfoil substrate materials; initiate processing and manufacturing; define material properties and potential projected performance.

FY 2007 Publications/Presentations

1. D. Mazzotta, M. K. Chyu, M. A. Alvin, "Aero-Thermal Characterization of Hydrogen Turbines," ASME Turbo Expo 2007, Land, Sea and Air, Montreal, Canada, May 14–17, 2007 (GT2007–28296).

2. M. A. Alvin, *Thermal Barrier Coatings,* Patent application filed May 31, 2007.

3. C. Feng, M. A. Alvin, B. S-J. Kang, "A Micro-Indentation Method for Assessment of TBC Bond Coat Systems," MS&T 2007 Conference, Detroit, MI, September 2007 (Paper 351171).

4. M. A. Alvin, D. Alman, B. Covino, J. Tylczak, F. Pettit, G. Meier, N. Yanar, M. Chyu, D.Mazzotta, W.Slaughter, V.Karaivanov, S.Seetharaman, B.Kang, C.Feng, R.Chen, T-C.Fu, "Materials and Component Development for Advanced Turbine Systems," 5th International Conference on Advances in Materials Technology for Fossil Power Plants, FL, October 3–5, 2007.

IV.9 Advanced Power Systems Sensors and Controls Development

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Research and Development Solutions (RDS)

Objectives

- Provide *in situ* monitoring of combustion parameters to enable sustained ultra-low emission performance of modern and future gas turbine systems.
- Investigate capacitance measurements with 100% H_2 flames in lab burner.
- Refine advanced flame ionization measurement system and test in pressurized combustor (Simulation and Validation/Dynamic Gas Turbine Combustor [SimVal/DGTC]).
- Support technology transfer and further development of combustion control and diagnostics sensor (CCADS) through cooperative research and development agreement (CRADA).
- Compare the results of multi-dimensional simulations to planned laboratory burner experiments, atmospheric and pressurized experiments completed in previous years and planned SimVal experiments.

Accomplishments

- Patent application developed for intelligent CCADS electronics (ICE) system.
- Advanced flame ionization measurement system (ICE) refined to provide real time monitoring of flame resistance and capacitance. System operation tested with industrial scale combustor operating at 5 atm.
- Flashback detection by CCADS with fuel blends from 30%-80% hydrogen demonstrated in SimVal combustor, which is an industrial scale lean premixed combustor with optical access. Flashback detection with CCADS demonstrated to be much faster than with a thermocouple.
- Preparations made for lab scale testing for 100% hydrogen flames in lab burner.

Introduction

To meet the goals of DOE's Advanced Power Systems Program, gas turbines are being developed to operate on syngas, and eventually pure hydrogen. The Turbine Program goals for the new class of turbines require incremental improvements in efficiency and NOx emissions (2 ppm NOx @15% O_2). Like natural gas fired turbines, syngas turbines will require precise fuel delivery to achieve fuel-lean homogenous mixing of the fuel and air in each local combustion zone, for operation at the required ultra-low emission levels. Even with elaborate control schemes, state-of-the-art gas turbines must maintain a wide operating margin away from the lean blowout limit. Turbine manufacturer's reluctance to minimize this stability margin stems from a lack of durable *in situ* combustion monitoring, and the many factors that can change the lean blowout limit during operations including component wear, daily environmental changes, and variations in fuel quality. This issue is further complicated by component size variations due to manufacturing tolerances, which can result in each local combustor having a different apparent lean blowout limit. As a result, finely tuned control of local combustion is required to maintain flame stability without compromising performance in advanced turbines. Responsive fuel quality monitoring, local fuel control hardware, and *in situ* monitoring of local combustion can be employed to achieve local combustion control, and improve gas turbine performance.

Approach

This project is focused on the development of a CCADS for *in situ* monitoring in gas turbine combustors. CCADS is a flame ionization sensor that utilizes two electrically isolated electrodes installed in the fuel nozzle, as shown in Figure 1. The electrode closest to the combustion zone is called the "guard" electrode, and the upstream electrode is called the "sense" electrode. When an equal voltage is applied to both electrodes, this novel arrangement facilitates current flow from the guard electrode through the flame. As a result, the guard electrode signal can provide a wealth of important information about the combustion process. On the other hand, a significant ionization

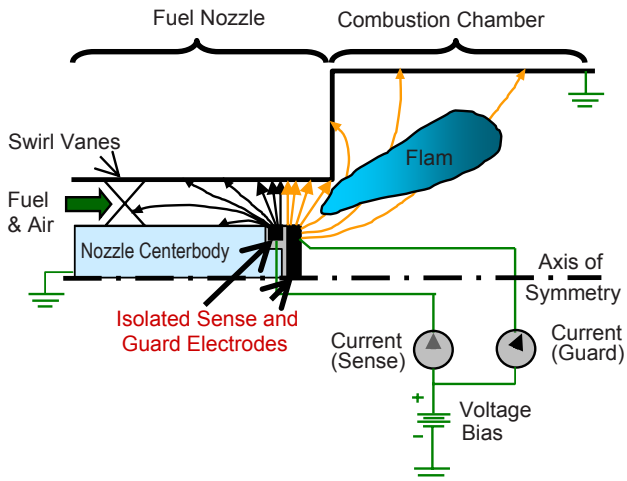

FIGURE 1. Schematic of CCADS Electrodes on the End of a Premixing Fuel Injector Center-Body, and a Representative Electrical Circuit for Flame Ionization Current Measurements

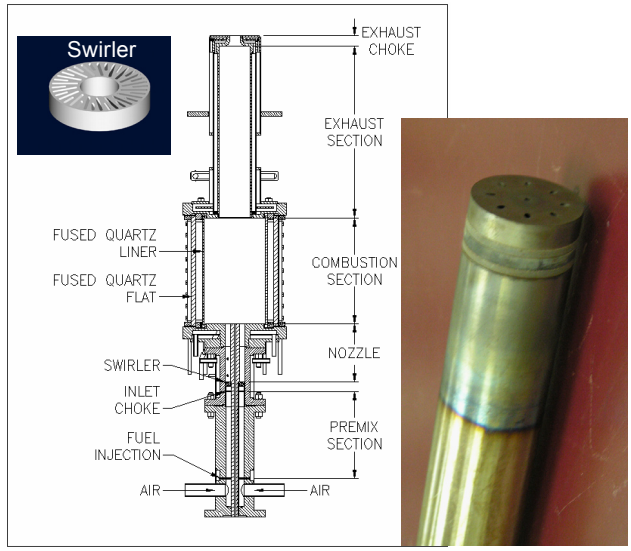

FIGURE 2. SimVal Combustor (left) and CCADS Center-Body Built by Woodward for Testing in SimVal as Part of CRADA

current from the sense electrode is produced only when the flame enters the upstream region of the fuel nozzle (i.e., during auto-ignition and/or flashback). The electrodes are incorporated onto the center-body of a gas turbine fuel nozzle and manufactured from the same material for durability.

Although CCADS has proven useful for monitoring natural gas fired turbine combustion, due to the low ionization potential of hydrogen, assessing CCADS performance with hydrogen fuel blends up to 99% hydrogen is necessary. The coal gasification process produces varying concentrations of hydrogen, and small concentrations of methane which will not be removed. Assessing the signal levels with laboratory tests with small concentrations of methane, and assessing flame impedance of hydrogen flames will provide the necessary assessment of the sensor technology for hydrogen turbine applications. In addition, fundamental laboratory and CFD model development supports the CCADS project by providing physical insight into the fundamental flame ionization and ion transport processes. Assessing CCADS performance in full engine testing, for natural gas and syngas applications, is essential for eventual implementation in fielded turbines. This is ongoing through a CRADA partnership with Woodward Industrial Controls.

Results

Tests have been conducted in NETL's SimVal combustion rig at 0.2-0.6 MPa (2-6 atm), demonstrating flashback detection with fuel compositions up to 80% hydrogen (by volume) mixed with natural gas. NETL's SimVal combustor offers full optical access to pressurized combustion during these tests. Figure 2 shows a schematic of the SimVal rig and a picture of

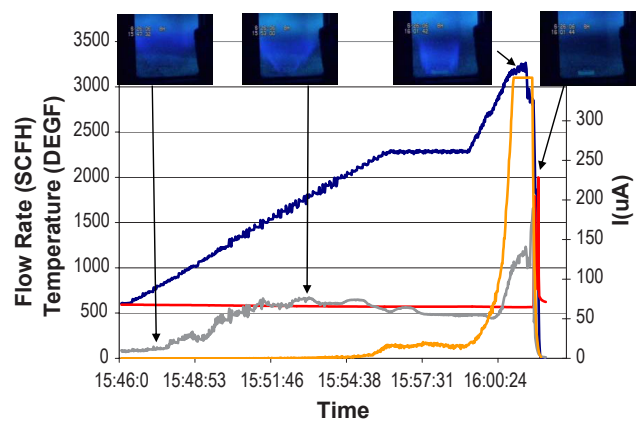

FIGURE 3. Flashback detection with hydrogen content increasing from 30 to 80%, in testing in SimVal. Sense electrode detects flashback much earlier than thermocouple.

the CCADS center-body designed and manufacturered by Woodward, NETL's CRADA partner. The data (see Figure 3) and high-speed video show the reaction zone moves upstream into the nozzle as the hydrogen fuel concentration increases, as is expected with the increased flame speed of the mixture. The CCADS data and video also demonstrate the opportunity for using CCADS to provide the necessary *in situ* monitor to control flashback and lean blowoff in hydrogen augmented combustion applications.

As part of this effort, combustion models are being developed which include the interaction between the electric field and the transport processes of the charged species. The primary combustion process is computed using a flame wrinkling model developed by Weller et al.

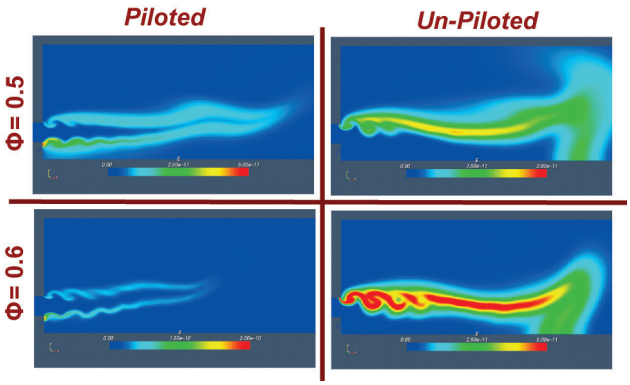

FIGURE 4. Simulation Results for Electron Concentrations from 2D CFD with 1-step Flame Model and Ionization

(1998). A sub-model for the transport of charged species is attached to this model. The formulation of the charged-species model is similar to that applied by Penderson and Brown (1993) for the simulation of laminar flames. Using the above procedure, numerical simulations are performed and the results are compared with experimental current measurements. Quantitative agreement with experiment was not obtained, however the model does display similar sensitivity to flow and operating conditions as observed in experiments. Figure 4 shows the numeric simulation results of electron concentration at the flame front.

A unique sensor interface system, named ICE (shown in Figure 5), has been developed to apply time-varying voltage to the CCADS electrodes for measuring both the flame resistance and capacitance. The resulting impedance measurements facilitate more information from the sensor for improved correlation to combustion operating conditions. This unique system was developed because all commercially available systems require full-loop connections or reference ground current measurements, which are different than the electrode current measurement used for CCADS. The system has been tested with laboratory flames, and at representative turbine conditions in NETL's DTGC. The data in Figure 6 shows the resistance and capacitance measurements from the ICE system at the respective operating equivalence ratio. Detailed evaluation of the data is ongoing. The system will also be used to conduct planned laboratory testing with pure hydrogen and hydrogen blends containing very low concentrations of methane to accurately assess the sensor potential in integrated gasification combined cycle (IGCC) applications.

Conclusions and Future Directions

The CCADS has been successfully tested at 80% hydrogen concentration (by volume) and shows excellent flashback detection capability. A unique

FIGURE 5. Intelligent CCADS Electronics System Refined for Measurement of Flame Resistance and Capacitance in Real Time (<1 Second Measurement Time)

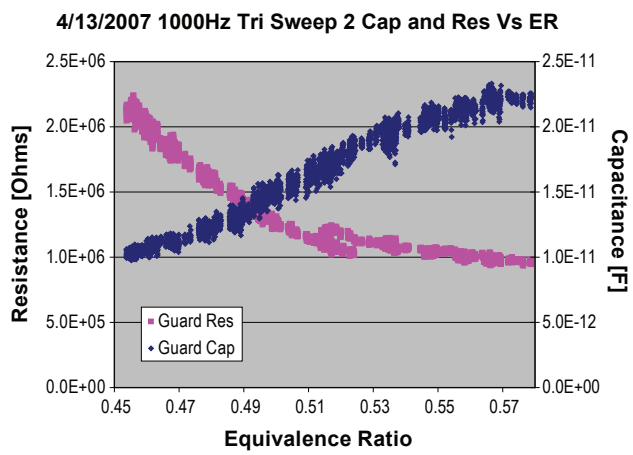

FIGURE 6. Results of Testing of ICE System in Industrial-Scale Lean Premixed Combustor at 5 atm

electronic interface for CCADS has been developed for analyzing the flame impedance properties of pure hydrogen combustion. A multidimensional model has been developed to better understand the physical relationship between the combustion operating conditions and the sensor measurements.

Further development of the multi-dimensional model is required to achieve better comparison with experimental data. The development includes the addition of the hydrogen combustion kinetics, and time-varying electric field.

Experimentally assessing the CCADS performance with pure hydrogen, and hydrogen with very small concentrations of methane are needed to fully assess the potential of CCADS for *in situ* hydrogen combustion monitoring. The development of local combustion control methods and algorithms for using CCADS to control local flame stability is essential part of closing the loop for local combustion control to provide fuel flexibility, improve efficiency, and reduce emissions for advanced gas turbines in IGCC configuration.

Special Recognitions & Awards/Patents Issued

1. US Patent 7,197,880 issued April 2007, Lean blowoff detection sensor, J. D. Thornton, B. T. Chorpening, D. L. Straub, E. D. Huckaby.

2. US Patent 7,096,722 issued Aug. 2006, Method and apparatus for detecting combustion instability in continuous combustion systems (jointly held with Woodward).

FY 2007 Publications/Presentations

1. B. T. Chorpening, J. D. Thornton, E. D. Huckaby, and K. J. Benson, "Combustion oscillation monitoring using flame ionization in a turbulent premixed combustor," Journal of Engineering for Gas Turbines and Power, v.129, n.2, pp. 352-357.

2. B. T. Chorpening, M. G. Dukes, P. Pich, and J. D. Thornton, "Combustion control and diagnostics sensor testing in a thermal barrier coated combustor," ASME Paper GT2007-27556, Proceedings of Turbo Expo 2007, Montreal, May 14–17.

3. J.D. Thornton, B. T. Chorpening, T. Sidwell, P. Strakey, E. D. Huckaby "Flashback detection sensor for hydrogen augmented natural gas combustion," ASME Paper GT2007-27865, Proceedings of Turbo Expo 2007, Montreal, Canada, May 14–17.

4. E. D. Huckaby, B. T. Chorpening, J. D. Thornton, "Computational fluid dynamics modeling of the operation of a flame ionization sensor," 5th U.S. Combustion Meeting, March 25–28, 2007, San Diego, CA.

5. Lilly, J., "One-Dimensional Computer Modeling of Electrical Conductivity through Methane and Synthesis Gas Flames", M.S. Thesis, West Virginia University, December 2006.

IV.10 Develop Data for Thermophysical Properties of Humid Gases in Power Cycles

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Objectives

- Use results of first-principles quantum mechanics to develop description of thermodynamics of humid gases in power cycles.
- Validate thermodynamic description by high-accuracy density measurements at high temperatures.
- Measure thermal conductivity of key water/gas mixtures at conditions relevant to power cycles.

Accomplishments

- Completed basic design of high-temperature densimetry system.

Introduction

Innovative power cycles (such as integrated gasification combined cycle [IGCC] and oxyfuel) are being developed for production of electric power with higher efficiency and reduced environmental impact, including the possibility of CO_2 sequestration. For optimizing the design of these systems, it is important to have accurate values of the thermophysical properties (density, heat capacity, thermal conductivity, etc.) of the fluid mixtures in the turbines and other parts of these cycles. These mixtures have a large water content, along with other gases such as nitrogen and carbon dioxide; they are at high temperatures where thermodynamic data are scarce, but the pressures are only moderately high. Typical approaches such as ideal-gas thermodynamics or common engineering equations of state are inaccurate for such systems, primarily due to the presence of water. Therefore, it is necessary to develop alternative modeling approaches, supplemented by selected high-temperature experimental measurements.

Approach

The description of the thermodynamic properties is developed at the level of the second virial coefficient, which is the first-order correction to the ideal-gas law. The key parameters are the "cross" second virial coefficients representing interactions between one water molecule and one gas molecule. Our approach is to use computational quantum mechanics to develop accurate surfaces describing the potential energy between the molecules, from which the virial coefficients can be calculated with high accuracy.

In order to validate our theoretical results, we will perform high-accuracy density measurements on the key water-nitrogen and water-CO_2 systems at high temperatures. The high temperatures are necessary because adsorption renders the measurements nearly impossible below about 500 K, but few laboratories have the capability for precision densimetry at high temperatures. We are developing such capability in conjunction with this work. The instrument is known as a "single-sinker magnetic-suspension densimeter." It operates on the Archimedes or buoyancy principle. By knowing the sinker volume and comparing the apparent weight while it is immersed in the gas mixture to the known mass of the sinker, the density is determined. This is an absolute method, meaning that no calibration fluids are required. The key elements of the instrument are the sinker (which is the actual sensing element), a magnetic suspension coupling which transmits the weight of the sinker to the balance and isolates the balance from the extreme conditions of the fluid, and the balance (which provides the quantitative measurement).

We are developing parallel capability for measuring the thermal conductivities of these mixtures at high temperatures; in this case the measurements are essential because no good theoretical approach is available for this property. The measurements will use the transient hot-wire method, which has become the method of choice for high-accuracy thermal conductivity measurements. Because water's electrical conductivity is likely to hamper the traditional DC implementation of this technique, an AC version of the apparatus is being designed.

Results

As a preliminary to this work (not funded by this project), we have produced potential-energy surfaces for the water-nitrogen and water-oxygen molecular pairs and used them to calculate second virial coefficients in a large temperature range with uncertainties better than all but the most precise experimental data. This work has been described in two publications [1,2]. The comparison of our calculated results to the available experimental data for water with nitrogen is shown in Figure 1.

For the high-temperature densimetry apparatus being constructed by NIST that will be used in this project, the basic design of the system has been completed; all essential elements of the apparatus have been decided, but final working drawings have not yet been produced. A design review was held November 17, 2006. In the design review, six members of the NIST technical staff met to review the design, offer suggestions, and brainstorm solutions to problems. This review considered the densimeter, thermostat, pressure system, and sample handling system.

The design of the densimeter itself has been worked out with Rubotherm GmbH (Bochum, Germany). They will provide a custom version of their high-temperature, high-pressure magnetic suspension coupling. The major custom items will be a silicon sinker (versus the standard titanium sinker) and a higher-resolution balance. These will provide an order of magnitude increase in the density resolution and a reduction in the density uncertainty of at least a factor of two compared to their standard system. This system has been ordered and delivery is expected early in Fiscal 2008.

A schematic of the actual densimeter or "measuring cell" is shown as Figure 2. The silicon sinker is just below the center of the cell. The thermal expansion of silicon is known to very high accuracy, and thus the volume of the sinker as a function of temperature can be computed accurately. The magnetic suspension coupling is at the top of the cell. The measuring cell is designed for pressures up to 50 MPa. Clamped to the measuring cell is a two-part copper sleeve. This reduces temperature gradients across the cell. Surrounding the cell is the "inner shield" of the thermostat, which provides an isothermal environment for the cell and further reduces temperature gradients.

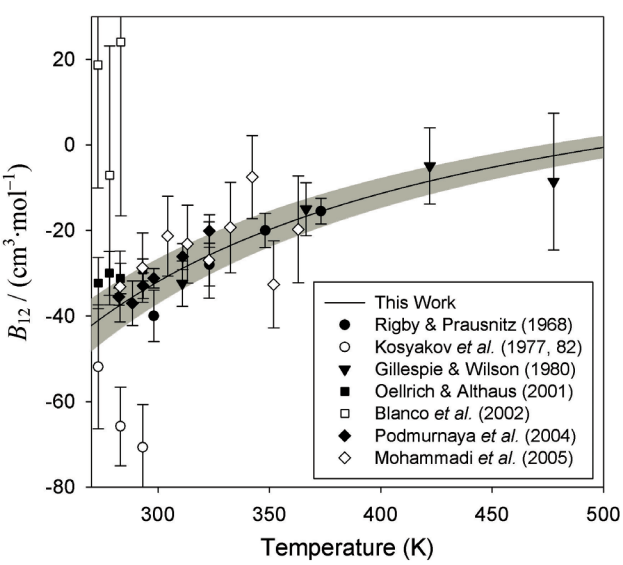

FIGURE 1. Theoretical calculations of second virial coefficient of nitrogen with water, compared with available experimental data. Shading represents uncertainty (95% confidence interval) in calculated results.

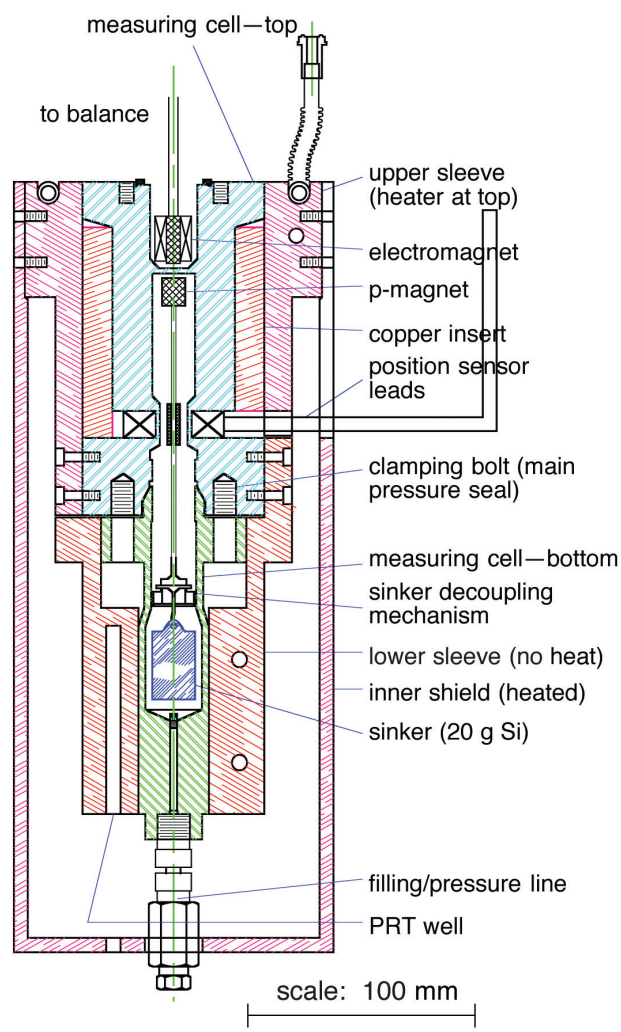

FIGURE 2. Design of Densimeter

An overall schematic of the densimeter is shown as Figure 3. The actual densimeter is at the center; it is surrounded by a multi-layer thermostat to provide very accurate temperature control. The thermostat is a vacuum-furnace-type design. Also indicated are some of the auxiliary systems–pressure transducer, sample system, vacuum system, instrumentation lines, etc.

Other key aspects of the design include the weighing process and the sample handling system. A weighing procedure has been worked out that will achieve the necessary high accuracy and that will correct to first order for any drift in the balance. The sample handling system will involve metering the water with a syringe pump and transferring the gas from a bottle that is carefully weighed. This will allow the composition of the mixture to be known with sufficiently high accuracy to derive the required thermodynamic quantities.

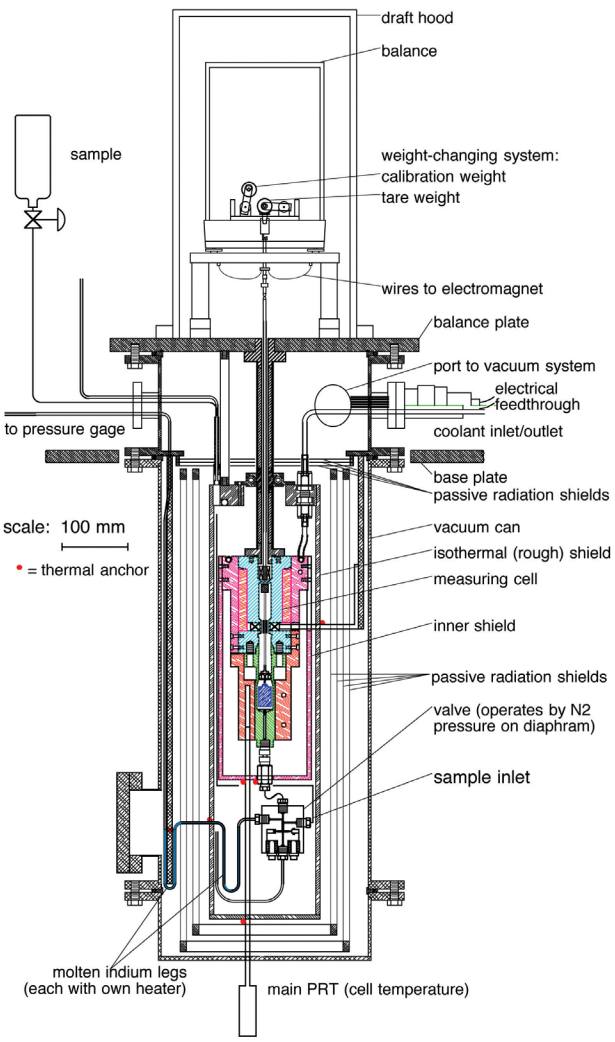

FIGURE 3. Overall Schematic of Densimetry Apparatus

Conclusions and Future Directions

This initial year of the project was mainly devoted to preparatory modeling work and to design of the experimental apparatus. In the following, we describe the future direction of the work.

For the modeling part of the work in Fiscal 2008, a potential-energy surface will be developed for the interaction between water and carbon dioxide. The thermodynamic quantities (second virial coefficients) derived from this surface will be combined with previous results to provide a complete description of the gas-phase thermodynamics of the main components of combustion gases. Work will begin to integrate these results into a mixture equation-of-state model.

On the experimental side, we anticipate that assembly and testing of the new densimeter will be completed in Fiscal 2008. Results for the H_2O/N_2 and H_2O/CO_2 systems will be obtained in the first half of Fiscal 2009. The modifications to the thermal conductivity apparatus will also be completed in Fiscal 2008, with results for the same two binary mixtures obtained in late Fiscal 2008 or early Fiscal 2009.

While this will complete the present project, there are related areas of need that could be considered as extensions to this work. These would include:

- Extension of the thermodynamic framework to allow prediction of condensation of water and of vapor-liquid equilibria more generally.
- Experimental measurements of the sound speed and/or the viscosity for gaseous H_2O/N_2 and H_2O/CO_2 mixtures.

References

1. A.S. Tulegenov, R.J. Wheatley, M.P. Hodges, and A.H. Harvey, "Intermolecular potential and second virial coefficient of the water–nitrogen complex," *Journal of Chemical Physics*, 126, 094305 (2007).

2. R.J. Wheatley and A.H. Harvey, "The water-oxygen dimer: first-principles calculation of an extrapolated potential energy surface and second virial coefficients," *Journal of Chemical Physics*, in press (2007).

IV.11 Materials Issues in Coal-Derived Synthesis Gas/Hydrogen-Fired Turbines

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Objective

Maximize the service lifetime of bond coatings in thermal barrier coatings (TBCs) by applying mechanistic understanding of the factors that contribute to their degradation in the environments expected in syngas/hydrogen-fired gas turbines.

Accomplishments

- Completed a critical review of the materials issues to be faced in developing advanced land-based gas turbines capable of the U.S. Department of Energy (DOE) performance goals, and of implications from burning syngas and hydrogen as fuels.
- Quantified the influence of water vapor on the oxidation behavior of bond coating alloys during thermal cycling exposures in air at 1,100°C; while an aluminide (NiAl+Hf) was essentially unaffected, a NiCrAlYHf composition showed a tendency for increased scale spallation with increased water vapor content.
- Demonstrated that for two-phase γ-γ' Ni-22 at%Al (all compositions are in at%) coating alloys, precious metal additions significantly decrease the formation of undesirable Ni-rich spinel oxides.
- Showed that in air oxidation at 1,000°C, Ir was as effective as Pt (which has been found to have the disadvantage of diffusing into the superalloy substrate at long times).
- Prepared samples of model alloys and coatings for exposure in original equipment manufacturer (OEM) baseline tests.
- Assembled and tested a preliminary mathematical model of thermodynamics and heat transfer in a gas turbine which produced useful guidance.
- Developed and tested computational thermochemistry methodology for predicting corrosive environment along the turbine hot gas path.

Introduction

The high turbine entry temperatures (TETs) required in the state-of-the-art natural gas-fired turbines necessitate reliable cooling of some components, since the temperature of the combustion gas is higher than the melting temperature of the available hot gas path alloys. The result is that the strongest alloys available (typically single-crystal Ni-based superalloys) are used for the blades and vanes in at least the first stage of the turbine, and operate essentially at their temperature limits. These components are cooled by air flow through complex internal cooling passages and the application of TBCs to the affected surfaces to maintain the desired metal temperatures, but it is necessary to minimize the air use to maximize engine efficiency. Increasingly, the full functioning of the TBC is essential, so that an unprecedented level of materials reliability and consistency of performance is required. Consequently, a major effort is ongoing worldwide to understand the failure mechanisms of TBCs, with the aim of achieving the degree of predictability needed and enabling non-destructive monitoring of the condition of the coatings.

A TBC consists of a thin, metallic bond coating applied to the superalloy substrate, and a layer of ceramic applied on top of the bond coating as the thermal barrier. The purpose of the bond coating is: (1) to anchor the ceramic layer to the superalloy; and (2) to protect against oxidation, and other forms of corrosion (gas-phase oxidation-sulfidation or molten salt attack) from the presence of impurities in the combustion gas. It is considered that the oxidation properties of the bond coating are one of the key issues to maximizing the performance of hot gas path components, and which is amenable to being addressed independently of the OEM efforts.

The requirements for an optimized bond coating are:

1. Rapid and reliable formation of a continuous alumina scale, specifically α-Al_2O_3, which is the

most thermodynamically stable and slowest-growing oxide that can be formed practically *in situ*.

2. Prevention of the formation of an external layer of base metal oxides, which are thermodynamically unstable and result in weak bonding with the ceramic, thermal barrier layer.
3. Good match with the coefficient of thermal expansion (CTE) of the superalloy to minimize the accumulation of stress-strain during thermal cycling, and maximize the adherence of the ceramic layer.
4. Minimized drop in Al content by interdiffusion with the superalloy, for increased bond coating life, as well as to minimize degradation of the strength properties if the superalloy due to the precipitation of unwanted phases.

Approach

Studies as part of the U.S. DOE's Advance Turbine Systems (ATS) program [1] demonstrated that aluminide coatings (β-NiAl) are superior to MCrAlY-type compositions in providing requirements (1) and (2), and form a slower-growing oxide scale that is reliable to higher temperatures. Issues with β-NiAl-type bond coatings are that, as Al is consumed to form and maintain the protective scale (and is lost by interdiffusion with the superalloy [2]), they can undergo phase transformations (involving volume changes) during thermal cycling that, possibly coupled with CTE differences with the superalloy, can disrupt the adherence of the ceramic thermal barrier layer. Two-phase γ-γ' NiPtAl-type aluminide coatings, which match the γ-γ' structure of superalloy substrates, were shown to minimize the problem of Al loss due to interdiffusion. An important issue is that these coatings have a lower Al level than does β-NiAl, so that their ability to reliably form a scale solely of α-Al_2O_3 must be augmented by appropriate platinum group metal (PGM) alloying.

The approach used in this project to investigate coating modifications is initially to use cast versions of the coating compositions to enable better control of composition (eliminates changes due to interdiffusion during processing or testing), and then to prepare the most promising compositions as coatings on superalloy coupons, using in-house processing (to ensure quality control). The issues addressed in coating alloy development were:

1. The effects of reduced levels of PGM additions (Pt, Pd, Ir) on the oxidation behavior Ni-22Al alloys. PGM additions suppress the formation of Ni-rich spinel oxides which weaken the bond between the alumina scale and the outer zirconia thermal barrier layer in a TBC. Loss of Pt due to interdiffusion was identified in previous ORNL work as a degradation mechanism for extended service times; also, the cost of the PGM additions is a concern.
2. Changes in Hf levels; a controlled level of Hf is key to controlling the microstructure and rate of growth of α-Al_2O_3 scales. To be effective, the Hf must be in solid solution in the coating, and its solubility changes with the level of each specific PGM.
3. Role of water vapor on oxidation behavior of coatings and cast alloys (increased water vapor contents are a feature of combusted syngas, and water vapor can interfere with the ability to form the desired protective scales).

To date, the ability of the alloys and coatings to meet the required goals has been assessed from kinetic measurements in cyclic oxidation tests in dry air (for direct comparison to baseline data for standard materials); in air-water vapor mixtures; and from subsequent characterization of the oxide scales formed. Of particular interest was information concerning the minimum Al level needed, and the influence of minor alloying changes.

Two efforts in support of the coating development are aimed at defining the corrosive environment and temperature regimes to be encountered by such bond coatings in actual turbine operation, as a function of fuel type. While it is understood that these conditions will be somewhat different from those in natural gas firing (for which the currently-used coatings were designed), it is necessary to define these differences as accurately as possible to provide realistic performance targets for the coatings. Further, while hydrogen firing is an unknown quantity, the U.S. DOE has set efficiency targets, and the realistic achievement of these is central to the overall strategic effort of the Fossil Energy Turbine Program, so that some kind of reality check is essential.

Results

Figure 1 shows the effect of PGM and Hf additions on the total mass gain of two-phase γ-γ' Ni-22Al alloys after a 500-hour isothermal exposure at 1,000°C in laboratory air. Without a PGM addition, the mass gains were higher, primarily due to the formation of Ni-rich spinel oxides. The lowest mass gains occurred for alloys that formed the desired α-Al_2O_3 scale, such as the single-phase, baseline aluminide (Hf-doped β-Ni-48Al) which also exhibited minimal Hf internal oxidation. Similar mass gains were achieved with only 22%Al and 15-30%Pt.

Higher Hf contents tended to lead to higher mass gains at lower PGM levels, due to Hf internal oxidation. Both Pt and Ir showed similar benefits at the 5% levels. Higher levels of Pd (which is significantly less expensive) were less effective. Also, the co-addition of 5%Cr had little effect with ~10%Pt (but high levels of Y+Hf present in this alloy may have resulted in additional internal oxidation that increased the mass gain). One reason for

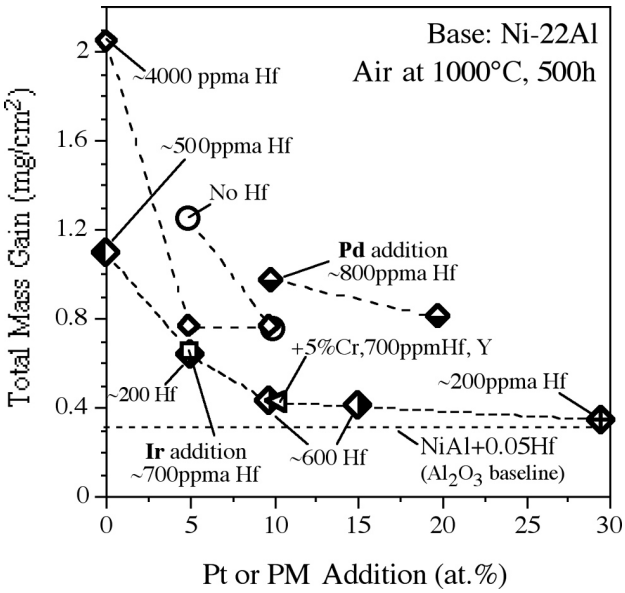

FIGURE 1. Total Mass Gain for Various PGM and Hf Additions to γ-γ′ Ni-22Al Coating Alloys after 500 Hours Isothermal Exposures at 1,000°C in Laboratory Air

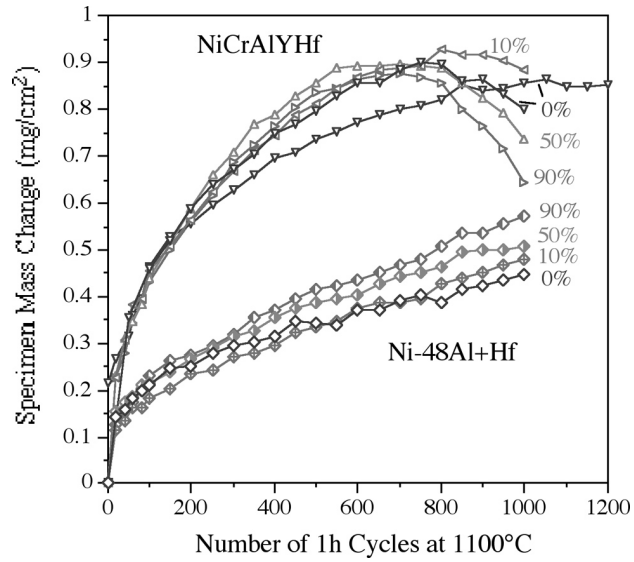

FIGURE 2. Comparison of Specimen Mass Gain for Cast MCrAl Alloy (Ni-20Cr-10Al+Y, Hf), and β-NiAl (Ni-48Al-0.05Hf) Specimens Exposed to 1 Hour Cycles at 1,100°C in Dry O_2 or Air with Various vol.% of H_2O (from 10-90%)

adding Cr was to increase the sulfidation resistance of the coating alloy.

Increased water vapor contents are a feature of combusted syngas. The role of water vapor on the oxidation behavior (specimen mass gains) at 1,100°C of two cast materials that represent the major classes of bond coatings, NiCrAlYHf and aluminides, is shown in Figure 2. The alumina scale on Hf-doped β-NiAl was relatively unaffected by increasing water vapor content, whereas the overall higher mass gain for cast NiCrAlYHf reflected faster scale formation. After ~800 cycles, some scale spallation from the NiCrAlYHf was noted by the loss in mass. This spallation tended to increase with water vapor content, suggesting such bond coatings will experience earlier TBC failure as the water vapor content increases. Initial results for γ-γ' compositions in water vapor suggest a negative effect on selective oxidation.

Figure 3 illustrates the two-phase structure of a γ-γ' NiPtAl coating fabricated at ORNL by diffusion of Al on a Pt-plated René N5 superalloy substrate. Some results of comparative oxidation tests of simple γ-γ' coatings (on various René N5 and 142 substrates with different levels of Hf and S) to modified γ-γ' coatings are shown in Figure 4. The 'modified' γ-γ' coatings were subjected to a pulsed-chemical vapor deposition (CVD) process to increase their Al contents. The modified two-phase coatings showed very good oxide adherence and a much lower rate of oxidation than the simple γ-γ' coatings, with performance in this 1 hour cyclic oxidation test that was similar to that of a coating of the standard β-aluminide on Y-containing superalloy René N5.

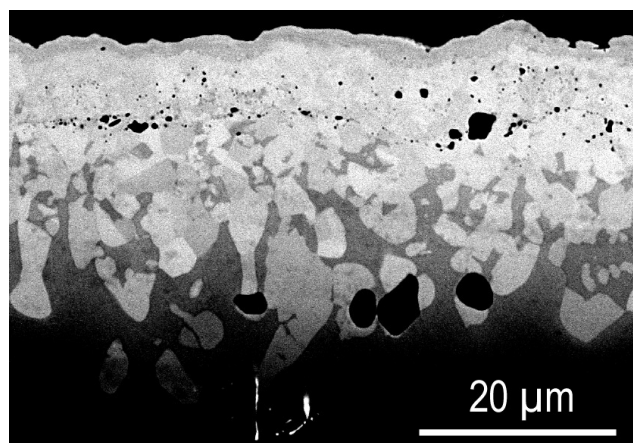

FIGURE 3. Back-scattered electron image of a cross section of a γ-γ′ coating on René N5. The contrast in this image depends on the atomic number of the elements; high-Z elements appear brightest.

The potential for significant deposition, erosion, or corrosion in syngas-fueled turbine systems is being examined by surveying reported observations, and through computational thermochemistry using published analyses of syngas compositions. This modeling approach has been exercised using "clean" syngas compositions, to which were added selected impurities, and showed that typical syngas compositions without added impurities are not expected to form any condensed phases along the turbine hot gas path, but that water vapor contents of the order of 10 mole%, and sulfur activities (mostly as SO_2) of approximately 10^{-7} at 1,050°C can be expected. When 100 ppm Na was added

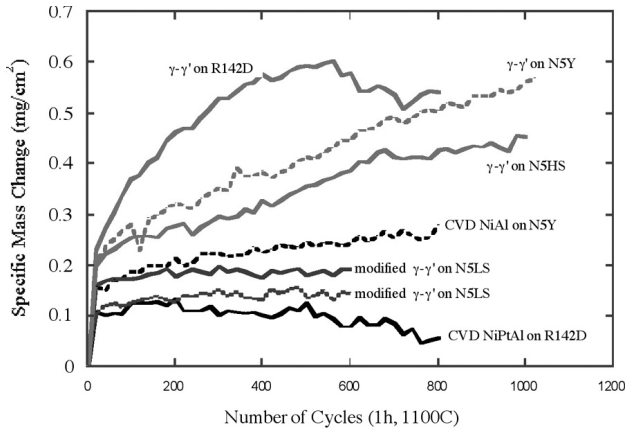

FIGURE 4. Cyclic Oxidation of γ-γ' NiPtAl Coatings on Various Substrates in Air at 1,100°C

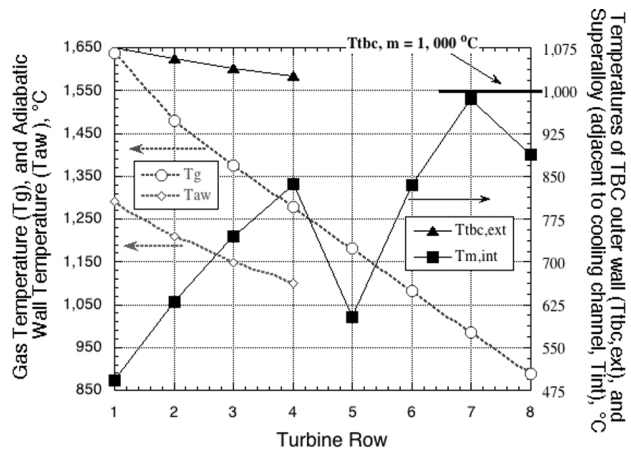

FIGURE 5. Calculated Hot Gas and Component Temperatures along the Turbine When Firing Syngas

to the syngas, condensation was predicted, starting at approximately 900°C at 1 atm pressure. Calculations involving additions of Fe to the syngas (following observations of metallic iron deposits on some samples of spalled TBC [3]) indicated no tendency for Fe condensation from syngas, suggesting that the source of the Fe may have been the TBC spray coating process, rather than the fuel.

Preliminary modeling of thermodynamics and heat transfer in a gas turbine provided useful information concerning the gas and component temperatures along the hot gas path of a generic four-stage turbine. The first two turbine stages were assumed to have film cooling and a TBC, and the last two stages to have internal convection cooling and no TBC. Initial calculations involved natural gas as fuel, and determined the combustion temperature corresponding to a given air/fuel ratio and total air flow, as well as the distribution of cooling air flow (to maintain a maximum temperature of 1,000°C at the interface between the bond coating and superalloy on the first stage blade), hence the gas and metal temperatures along the hot gas path. The same conditions were then used with syngas, with the exception that the amount and distribution of cooling air was allowed to vary; the results are summarized in Figure 5. The calculated temperatures appeared to be reasonable, but in all cases the temperatures for the syngas case were higher. Interestingly, the maximum superalloy temperature (adjacent to the internal cooling passage) was found to occur on the fourth stage vane in both cases, and was calculated to be 951°C for natural gas, but 987°C for syngas, close to the not-to-exceed temperature threshold.

Conclusions and Future Directions

- The high-temperature oxidation behavior of aluminide coating alloys is less affected than that of NiCrAlYHf by gas water vapor content.
- The formation of detrimental Ni-based transient oxides on two-phase γ-γ' NiAl-type coatings is significantly reduced by precious metal and Hf additions.
- Ir appeared to have a similar effect to Pt on oxidation behavior; Pd was less effective.
- Two-phase γ-γ' PtNiAl-type coatings can be successfully and reproducibly formed on superalloy substrates using laboratory processing techniques.
- The computational approaches for defining the temperatures and environments along the hot gas path are capable of providing valuable guidance.

The coatings that exhibit satisfactory performance in the oxidation environments incorporating water vapor will be candidates for testing under conditions intended to simulate the sulfidizing environment reportedly encountered in turbines in integrated gasification combined cycle (IGCC) operation. The detailed conditions for this test will be derived from consultation with the OEMs participating in the Office of Fossil Energy Turbine Program, and from the conditions projected by thermochemical modeling of the expected local environments in syngas-fired turbines. Depending on the specific conditions and cycle chosen, a test apparatus will be assembled and qualified using standard alloys (materials for which baseline performance data are available), before being used routinely in the research project.

FY 2007 Publications/Presentations

1. B.A. Pint, S.A. Speakman, Y. Zhang and I.G. Wright, "The Effect of Hf Content on the Phase Content, Oxidation Behavior and Phase-Transformation-Induced Deformation of Two Phase Ni-Al and Ni-Pt-Al Alloys," presentation at *TMS Annual Meeting 2007*, February 2007, Orlando, FL.

2. A.S. Sabau and I.G. Wright, "Numerical simulations of the effects of changing fuel for turbines fired by natural gas and syngas," paper No. GT2007-27530, presented at the *ASME Turbo Expo 2007: Power for Land, Sea and Air*, Montreal, Canada, May 14–17, 2007.

3. I.G. Wright and T.B Gibbons, "Recent developments in gas turbine materials and technology and implications for syngas firing," *Intl. J. of Hydrogen Energy* (2007), in press.

4. T.B. Gibbons and I.G. Wright, "A Review of Materials For Gas Turbines Firing Syngas Fuels," *ORNL Technical Report*, ORNL/TM-2007/086, in press.

References

1. W.P. Parks, Jr., P. Hoffman, M.A. Karnitz, and I.G. Wright, "The Advanced Turbine Systems Program in the U.S.A.," pp. 1789-1805 in Materials for Advanced Power Engineering 1998, J. Lecomte-Beckers, F. Schubert, and P.J. Ennis, Eds., Forschungszentrum Julich (1998).

2. W.S. Walston, J.C. Schaeffer, and W.H. Murphy, pp. 9–18 in *Superalloys 1996*, TMS, Warrendale, PA (1996).

3. R.A. Wenglarz and J.E. Oakey, "Gas turbine issues in advanced gasification systems," pp. 233-243 in *Materials for Advanced Power Engineering 2006*, J. Lecomte-Beckers, M. Carton, F. Schubert, and P. J. Ennis, Eds., Schriften des Forschungszentrums Jülich (2006).

IV.12 Chemical Kinetics in Support of Syngas Turbine Combustion

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Objectives

- Determine experimentally the third body efficiencies of CO_2 and H_2O in reaction (R1); see Table 1.
- Generate new experimental validation targets for H_2-CO-O_2-N_2 reaction kinetics in the presence of significant diluent fractions of CO_2 and/or H_2O, at temperatures near 900 K.
- Use new published data to refine a detailed mechanism for syngas/O_2/diluent kinetics.
- Analyze and demonstrate issues controlling NOx formation in syngas combustion.

TABLE 1. Elementary Kinetic Reactions and Nomenclature

$H+O_2 + M = HO_2 + M$	(R1)
$H+O_2 = OH + O$	(R2)
$H + OH + M = H_2O + M$	(R3)
$H_2+OH = H_2O+H$	(R4)
$HO_2 + OH = H_2O + O_2$	(R5)
$HO_2 + H = OH + OH$	(R6)
$HO_2+H = H_2+O_2$	(R7)
$HO_2+H_2 = H_2O_2 + H$	(R8)
$H_2O_2+M = OH+OH+M$	(R9)
$CO + OH = CO_2 + H$	(R10)
$CO + O + M = CO_2 + M$	(R11)
$CO + HO_2 = CO_2 + OH$	(R12)
$HCO + M = H + CO + M$	(R13)
$HCO + O_2 = HO_2 + CO$	(R14)
$NO + HO_2 = NO_2 + OH$	(R15)
$NO_2 + H = NO + OH$	(R16)

Accomplishments

- Confirmed that linear combinations of pressure fall-off descriptions are accurate for predictions of syngas combustion involving water and carbon dioxide as diluents.
- Validated C_1 mechanism against new high pressure syngas oxidation data.
- Demonstrated that $CO + HO_2 = CO_2 + OH$ (R12), is important to chemical reaction induction processes in syngas combustion, but not to post induction (heat release/flame) chemistry.
- Demonstrated the importance of NOx in modifying syngas chemical kinetic oxidation rates at gas turbine conditions through its catalytic conversion of HO_2 to OH radicals.
- Showed that syngas ignition properties in the mild ignition regime are controlled by the formation of HO_2 and H_2O_2, and the decomposition of H_2O_2, and are subject to significant perturbations by fluid dynamic, mixing, and catalytic effects.
- Showed that the presence of iron carbonyl, often found in CO compressed gas stored in steel cylinders, may affect burning velocities in fuel-rich regimes and ignition delays under gas turbine conditions.

Introduction

The present research aims to further extend our prior work in developing and validating kinetic models for the CO/hydrogen/oxygen system to be applied under gas turbine operating conditions. Experimental and numerical analysis methods developed and applied in prior and this work are utilized in these tasks. Contaminants such as small hydrocarbons, NOx, and metal carbonyls can have significant influence on kinetic behavior. The effects of small local amounts of NOx and iron pentacarbonyl on kinetics relevant to ignition and combustion phenomena are investigated.

Approach

The collision efficiencies of water and carbon dioxide in (R1) differ significantly from N_2 and O_2. Thus, dilution typically utilized to reduce combustion temperatures and NOx formation can influence the overall rate of (R1). The measurement of $k_{1,0}$ (the low pressure limit reaction rate constant) at combustion temperatures is indirect and complicated by competition between $H + O_2 = OH + O$ (R2) and (R1). Small

quantities of NO greatly modify the kinetic behavior from that of the pure system by providing an alternate consumption route for HO_2 radicals via $NO + HO_2 = NO_2 + OH$ (R15), followed by $NO_2 + H = NO + OH$ (R16) to give back NO. The catalytic cycle, consisting of reactions (R1), (R15), (R16), and $H_2 + OH = H_2O + H$ (R4), consumes H_2 at temperatures well below the explosion limits of the unperturbed system. For appropriate NOx concentrations (R16) competes effectively with reaction (R2) for H atoms, and it is found that $[NO_2]_{SS} = k_{1,eff}\,[O_2]/k_{16}$. Reaction (R16) is very well-characterized [1]. We have used this relationship previously [1] to determine the collision efficiencies of N_2 and Ar through variable pressure flow reactor experiments on the H_2/O_2 system perturbed with a small amount of NO. In the present work, we are using nitrogen as the principal carrier gas and perturbing the collision characteristics of the system by addition of up to 10% carbon dioxide or a few percent water vapor to determine the third body collision efficiencies of the N_2/CO_2 and N_2/H_2O mixtures and extract the collision efficiencies for H_2O and CO_2.

Kinetic analyses of these and other data in the literature are performed to further validate and extend a C_1 mechanism [3], and to investigate the perturbing presence of small amounts of NOx and iron pentacarbonyl on shock tube, flow reactor, stirred reactor, laminar burning rate, and stagnation flame observations.

Results

Reference [3] develops and validates a C_1 mechanism for modeling the oxidation reactions of hydrogen, carbon monoxide, formaldehyde, and methanol over a wide range of conditions. We have compared our model predictions against new data obtained at high pressures in a rapid compression machine [4], a high pressure shock tube [5] and in high pressure experiments to obtain laminar burning rates [6,7]. We found that reactions (R5) and (R12) appear to have, separately, distinct impacts on the predictions on measured ignition delays. At shock tube pressures and temperatures, the predictions are unchanged by variations of as much as a factor of five in the rate of reaction (R12). In contrast, changes in reaction (R5) yield little effect at rapid compression machine (RCM) conditions. On the other hand reaction (R12) strongly influence ignition in RCM studies [4]. It is further noted that using the same higher concentrations of fuel and oxidizer as those studied in RCM investigations, reaction (R12) affects high pressure shock tube ignition delay predictions; dilution, thus, plays a role in the relative importance of specific reactions for these different investigations. We note, however, that reactions (R11) and (R12) affect ignition delay predictions only by affecting chemical induction times and are of little significance to predicting heat release rates and laminar burning rates of syngas/air mixtures at high pressure. Substitution of new, recently reported rate parameters [8] for (R12) in the C_1 mechanism results in very good agreement of predictions with all experimental data. Finally, it should be noted that all predictions are strongly influenced by (R1), confirming that refinements in collision efficiencies of diluents to be utilized in gas turbines (CO_2, H_2O) is warranted.

More recently, data on ignition delay for syngas/air mixtures in a high pressure shock tube, a flow reactor and a RCM have been reported [9] that are in substantial disagreement with homogenous chemical kinetic predictions at conditions of direct interest to industrial gas turbine operation. The disparity is evident in a wide range of experiments, cannot be attributed to differences in criteria used to determine the observations, and is observed for a wide range of alternative choices in modeling assumptions, inferring that missing gas phase kinetic paths or uncertainties in kinetic/thermo-chemical parameters may account for the discrepancies. The experiments were performed at lean conditions ($\phi \sim 0.5$) and for pressure/temperature ranges of 16-29 atm/940-1,150 K (shock tube) and 5 atm/760-785 K (flow reactor). These new data were summarized in an Arrhenius-type plot (Figure 1) along with other recently published data from the rapid compression studies of Walton et al [10] and from an earlier high pressure flow reactor study, all normalized to conditions of 20 atm pressure. For reaction temperatures lower

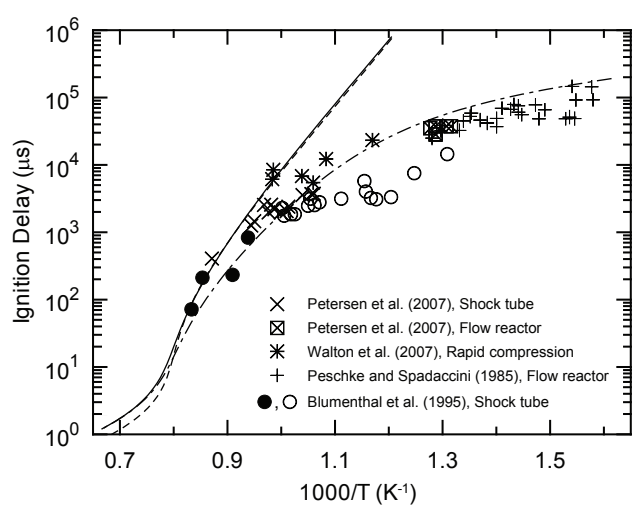

FIGURE 1. Comparison of Ignition delay times for syngas/air reported in [9] with hydrogen-air data [16]. Filled and open circles correspond to strong and weak ignition events [16]. Data scaled by P^{-1} to 20 atm pressure. Lines: ignition delay calculations using [3] for syngas mixture (solid line) and hydrogen oxygen (dashed line). Dash-dot line: predictions for syngas ignition with catalyzed-enhanced reactions for formation and decomposition of H_2O_2 (R8 and R9).

than about 1,050 K, experimental observations of ignition delay begin to substantially depart from zero-dimensional, homogeneous gas phase predictions utilizing any of the recently published H_2/CO kinetic models including that from [3]. Petersen et al. [9] indicate that the disagreement "may not be surprising, since few data have existed at the temperature and pressure ranges of the present study to which the (previously) published models could be calibrated."

In further analyses of these results [11,12,13] and considering other measurements in the literature, we observe that the noted discrepancies bear strong similarity to those known to exist for pure hydrogen oxygen ignition delay measurements, some noted as early as the 1960s. Our analyses provide strong support that the disparities result from the fact that in each of the experimental sources referenced, the relevant homogenous gas phase kinetics are not only dominated by those of the hydrogen-oxygen system at reaction temperatures between the extended second and third explosion limits (frequently referred to in the literature as the "mild ignition regime"), but that key limiting processes are perturbed by one or more phenomena that significantly enhance the overall rate of reaction typical of pure homogenous gas phase chemistry. The source(s) of these aberrations are multi-dimensional, compressible fluid dynamics, reactant mixing phenomena, and catalytic surface reactions on surfaces that stimulate the decomposition of hydrogen peroxide formed as an intermediate during the chemical induction reactions, leading to significant reductions in overall ignition delay times.

Finally, iron pentacarbonyl, $Fe(CO)_5$, is known to be a potential contaminant present in compressed carbon monoxide sources stored in steel compressed cylinders [14], and it is known that this material can influence combustion kinetics through its ability to enhance removal of reactive species, principally H atoms, from the radical pool [15]. We have shown numerically [13] by modifying the C_1 mechanism with detailed iron pentacarbonyl kinetics [15] that levels of 100-200 ppm in the compressed fuel source can significantly depress laminar burning rates of fuel/air mixtures at fuel-rich conditions (Figure 2). Such effects may be responsible for the present experimental scatter in fuel-rich burning rates for syngas/air mixtures. Using these data to adjust/validate syngas kinetic models may lead to incorrect modifications [6] that degrade prediction of other burning rate data (Figure 3). Similarly, ignition of premixed mixtures can be inhibited by the presence of carbonyl, while there appears to be little effect on combustion properties under non-premixed stagnation flame conditions. Experiments are planned to corroborate these numerical predictions [13] regarding the influence of metal carbonyls on burning rates.

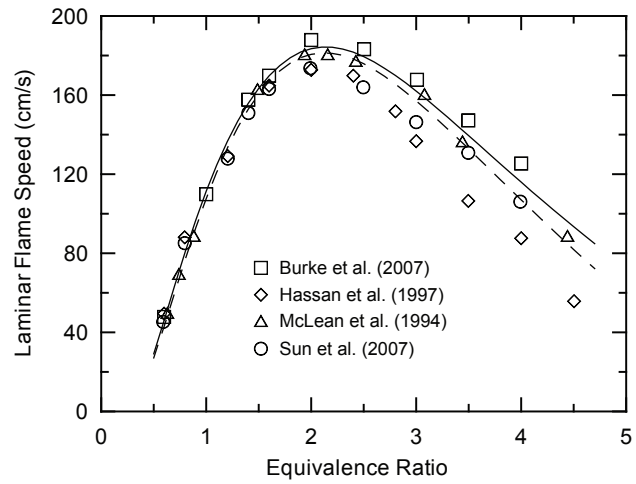

FIGURE 2. Laminar burning velocities of H_2:CO mixtures (1:1) in air at 1 atm. Symbols: experimental measurements. Solid line: predictions using [3]. Dashed line: predictions using [3] and kinetic subset for iron pentacarbonyl [15] with $Fe(CO)_5$ content of 200 ppm in the CO.

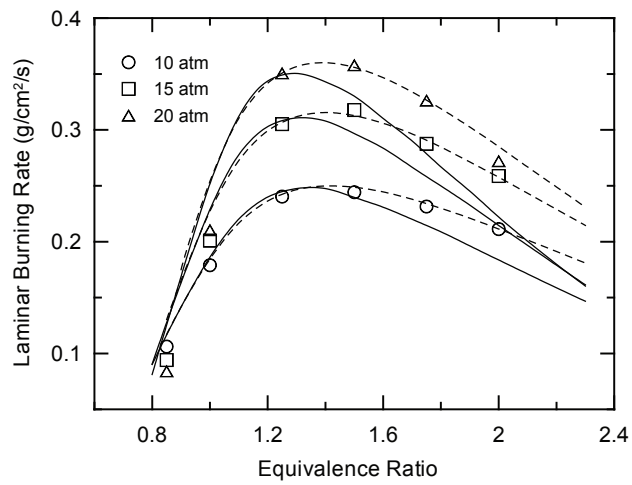

FIGURE 3. Measured and calculated unstretched laminar mass burning rates for H_2 + (O_2:He – 1:11.5) flames at 10, 15, and 20 atm. Symbols: experimental data [17]; solid lines: predictions using [6] developed to predict data in Figure 2; dashed lines: predictions using [3].

Future Directions

This project will be concluded July 31, 2007, and the final report will present the experimental analyses and results on the collision efficiency measurements of CO_2 and H_2O in reaction (R1).

FY 2007 Publications/Presentations

1. J. Li, Z. Zhao, A. Kazakov, . Chaos, and F.L. Dryer, "A Comprehensive Kinetic Mechanism for CO, CH_2O, CH_3OH Combustion", *Int. J. Chem. Kin.*, **39**, 109-136 (2007).

2. F.L. Dryer and M. Chaos, "Ignition of Hydrogen/Air and Syngas/Air Mixtures: Experimental Data Interpretation and Kinetic Modeling Implications", Workshop on Hydrogen Combustion in Gas Turbines, EPRI, Washington, D.C., March 22, 2007.

3. F.L. Dryer and M. Chaos, "Ignition of Syngas/Air and Hydrogen/Air mixtures at Low Temperatures and High Pressures: Experimental Data Interpretation and Kinetic Modeling Implications", *Combust. Flame* (2007). Submitted.

4. M. Chaos and F.L. Dryer, "Syngas Combustion Kinetics and Applications", in Syngas Combustion, (V. Yang and T. Lieuwen, eds.), *Combust. Sci. Tech.* Special Issue (2007). To Appear.

References

1. N.K. Srinivasan, M-C. Su, J.W. Sutherland, J.V. Michael, and B. Ruscic, *J. Phys. Chem. A*, **110**, 6602 (2006).

2. M.A. Mueller, R.A. Yetter and F.L. Dryer, *Proc. Combust. Inst.*, **27**, 177 (1998).

3. J. Li, Z. Zhao, A. Kazakov, M. Chaos, and F.L. Dryer, *Int. J. Chem. Kin.* **39**, 109 (2007).

4. G. Mittal, C-J. Sung, and R.A. Yetter, *Int. J. Chem. Kinet* 38, 516 (2006).

5. R. Sivaramakrishnan, A. Comandini, R.S. Tranter, K. Brezinsky, S.G. Davis, and H. Wang, *Proc. Combust. Inst.* **31**, 429 (2007).

6. H. Sun, S.I.Yang, G. Jomaas, and C.K. Law, *Proc. Combust. Inst.*, **31**, 439 (2007).

7. M.P. Burke, X. Qin, Y. Ju, and F.L. Dryer, Measurements of Hydrogen Syngas Flame Speeds at Elevated Pressures. Proceedings of the Fifth U.S. Combustion Meeting, San Diego, CA (2007). Paper A16.

8. X. You, H. Wang, E. Goos, C.J. Sung, and S.J. Klippenstein, *J. Phys. Chem. A*, **111**, 4031 (2007).

9. E.L. Petersen, D.M. Kalitan, A.B. Barrett, S.C. Reehal, J.D. Mertens, D.J. Beerer, R.L. Hack, V.G. McDonell, *Combust. Flame*, **142**, 244 (2007).

10. S.M. Walton, X. He, B.T. Zigler, and M.S. Wooldridge, *Proc. Combust. Inst.*, 31, 3147 (2007).

11. F.L. Dryer and M. Chaos, "Ignition of Hydrogen/Air and Syngas/Air Mixtures: Experimental Data Interpretation and Kinetic Modeling Implications", Workshop on Hydrogen Combustion in Gas Turbines, EPRI, Washington, D.C., March 22, 2007.

12. F.L. Dryer and M. Chaos, "Ignition of Syngas/Air and Hydrogen/Air mixtures at Low Temperatures and High Pressures: Experimental Data Interpretation and Kinetic Modeling Implications", *Combust. Flame* (2007). Submitted.

13. M. Chaos and F.L. Dryer, "Syngas Combustion Kinetics and Applications", in Syngas Combustion, (V. Yang and T. Lieuwen, eds.), *Combust. Sci. Tech.* Special Issue (2007). To Appear.

14. T.C. Williams and C. R. Shaddix, *Combust. Sci. Tech.*, **175**, 1225 (2007).

15. M.D. Rumminger, D. Reinelt, V. Babushok, and G.T. Linteris, *Combust. Flame*, **116**, 207 (1999).

16. R. Blumenthal, K. Fieweger, K.H. Komp, G. Adomeit, and B.E. Gelfand, *Proc. of the 20th Int. Symp. on Shock Waves*, 935 (1995).

17. S.D. Tse, D.L. Zhu, and C.K. Law, *Proc. Combust. Inst.*, **28**, 1793 (2000).

IV.13 Reduced and Validated Kinetic Mechanisms for Hydrogen-CO-Air Combustion in Gas Turbines

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Objectives

- Develop an accurate experimental method for flame speed measurement at high pressures by using outward propagating spherical flames.
- Measure the flame speeds and flammability limits of syngas at normal and high pressures.
- Develop an accurate radiation model for CO_2 and H_2O diluted syngas combustion.
- Develop a validated detailed mechanism for hydrogen-CO-H_2O mixtures.
- Develop a reduced mechanism for syngas combustion.

Accomplishments

- Developed a rigorous method to include the effects of flow compression, non-spherical flow field, and flame stretch to measure the flame speeds at high pressures more accurately. The present approach formed a solid base for the future validation and development of the reduced kinetic mechanism for syngas mixtures.
- Measured the flame speeds of syngas-CO_2 mixtures at 1, 10, and 20 atm.
- Developed a fitted statistical narrow band correlated-k (FSNB-CK) radiation model to simulate the effect of radiation reabsorption on flame speed and NOx emissions in H_2O, CO, and CO_2 diluted syngas combustion.
- Demonstrated analytically that the combined effect of transport and radiation of syngas will extend the flammability limit dramatically.
- Designed new counterflow flame burners to measure the syngas flame speeds with high H_2O dilution at high temperatures.

Introduction

Coal-based syngas and hydrogen production with CO_2 storage will play a dominant role in producing clean and efficient energy sources in the future. The high concentrations of CO and hydrogen in combustion systems along with the likelihood of dilution with H_2O will significantly affect burning properties due to the high diffusivity of hydrogen, enhanced third-body effects of recombination reactions, and spectral radiation properties at high pressures. New kinetic, radiation, and transport models are important to developing robust computational design codes for gas turbine applications. However, few fundamental experimental data and models are available for the burning properties of syngas and hydrogen, particularly for high dilution and pressure conditions for the development and validation of the needed models.

In this research, a rigorous experimental method for an accurate measurement of flame speeds at broader pressure and stretch conditions and a robust FSNB-CK radiation model were developed to measure and model the burning properties of hydrogen syngas with CO, CO_2, and H_2O dilutions. Flame speeds of syngas mixtures were measured up to 20 atm. The obtained models and experimental data at high pressures provided a solid base to establish and validate a reduced mechanism for hydrogen syngas combustion at gas turbine conditions.

Approach

In order to achieve high pressure flame speed measurements, a magnetically controlled dual-chamber cylindrical bomb was designed to achieve near-constant pressure combustion. A potential flow theory was developed to take account for the effect of non-spherical flow field on burning velocity. To include the flow compression and stretch effects on the measured burning velocity, analytical formulations for burned gas velocity and flame stretch effects were obtained. The measured flame speeds were corrected by using these analytical models.

In the thermal radiation analysis of CO, H_2O, and CO_2, a FSNB-CK model was developed to model radiation for spherical flame propagation. This model was also integrated with detailed chemistry to validate the kinetic mechanism.

Results

Effect of flow compression and stretch on flame speed measurements: Pressure waves produced in the experiments of flame speed measurement using a spherical bomb will induce an inward flow velocity in the burned gas region. This inward burned gas velocity will affect the measured flame speeds. Discussions of the compression effects on flame speed measurement were either missing or neglected in the previous studies [1-3]. Figure 1 shows the dependence of the measured flame speed of a stoichiometric hydrogen-air mixture on the range of flame radii used in the experiments. Due to the flow compression effect, the error of the measured flame speeds could be larger than 15% depending on range of flame radii chosen in the experiment. The correction of the flow compression effect by using an analytical expression [4] significantly improved the accuracy of the flame speed measurements (less than 5%). To measure the flame speed at both high pressure and high temperature, a constant volume spherical flame bomb has been used. In this approach, the transient flame propagation speed was used directly as the flame speed of the mixture and the effect of flame stretch on the flame speed was neglected. Figure 2 shows the comparison of the computed planar flame speed with the flame speeds predicted from the constant spherical bomb with and without considering the effect of flame stretch. It is seen that as the flame propagates outward, the flame speed obtained without flame stretch correction does not agree with the unstretched planar flame speed until the flame radius is larger than 60% of the chamber size. However, by considering the flame stretch effect [4], the agreement between the flame speeds computed from the planar flame and the spherical flame was improved significantly in a broader range of pressure and flame radius.

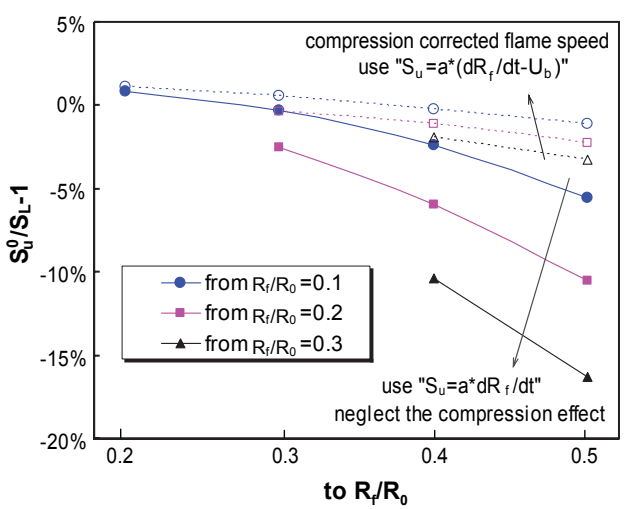

FIGURE 1. Accuracy of the Unstretched Flame Speed With and Without Compression Correction Using Different Flame Radii Ranges for a Stoichiometric H_2/Air Flame

Effect of non-spherical flow field on flame speed measurements: In addition to the compression and stretch effects, the non-spherical flow field in the cylindrical bomb also produced errors of flame speed measurement. An analytical relation to correct for the flow field effect in the cylindrical bomb was derived by using the potential flow analysis [5]. The flame speeds of hydrogen/CO-air mixtures were measured at 1, 10, and 20 atm. The measured flame speeds were compared to the existing data and model predictions. Figure 3 shows the comparison of the measured flame speeds with other experimental data and numerical predictions [6-8]. It is seen that the data reported in the literature are much lower than the present results. The comparison also shows that the present data agree well with the modeled results using the hydrogen-CO mechanism developed

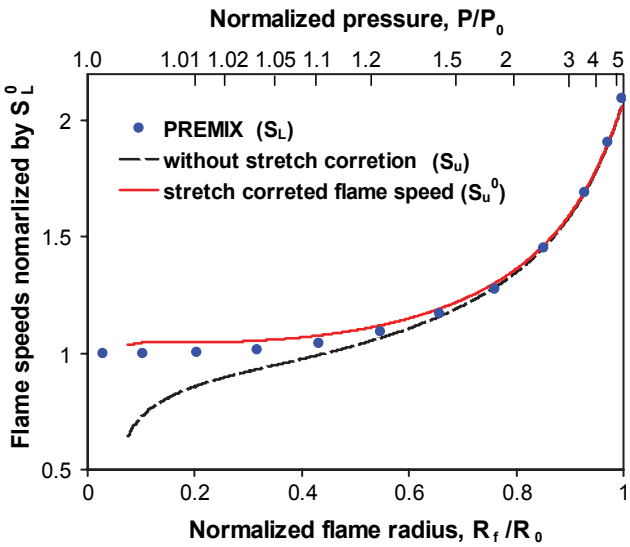

FIGURE 2. Flame Speeds of a Rich Hydrogen/Air Mixture at Equivalence Ratio of Four With and Without Stretch Correction as a Function of Normalized Flame Radius and Pressure in a Spherical Chamber

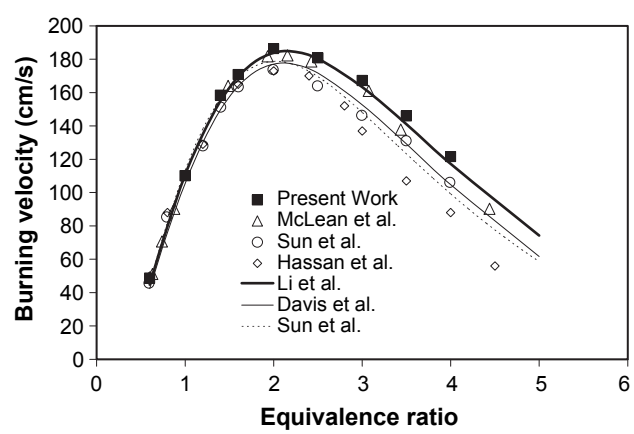

FIGURE 3. Comparisons of Measured Hydrogen Syngas Flame Speed for an H_2-CO (50:50) Syngas Mixture in Air at 1 atm

by Li et al. [7]. The results clearly demonstrate that the experimental accuracy of flame speed is a key issue for the validation of the kinetic mechanism.

Effect of flame radiation on flame speeds: The appearance of CO, H_2O, and CO_2 in coal-derived syngas will significantly increase the spectral dependent radiation heat transfer, which consequently changes the flame temperature, burning velocity, and NOx emissions. Therefore, an accurate radiation model is needed to model the radiation of syngas and to validate the kinetic mechanism for fuel oxidation and NOx emission in syngas combustion. In this research, a FSNB-CK model is developed to account for the spectral dependent radiation from CO, H_2O, and CO_2 in syngas and natural gas combustion [9]. Figure 4 shows the comparison of the measured flame speed with those predicted by using the optically thin model, statistical narrow band (SNB) model, and the FSNB-CK model. The results show that radiation plays an important role in affecting the flame speed and burning limit. In addition, the FSNB-CK model gives a good prediction of flame speed.

Conclusions and Future Directions

- Compression waves and non-symmetrical flow field produced by outward propagating flames significantly affect the accuracy of the measured flame speeds. Models to correct the effects of compression waves, non-symmetrical flow field, and flame stretch on flame speed in the spherical bomb experiments were derived and validated. These models yielded a considerable improvement in the accuracy of the flame speed measurements.

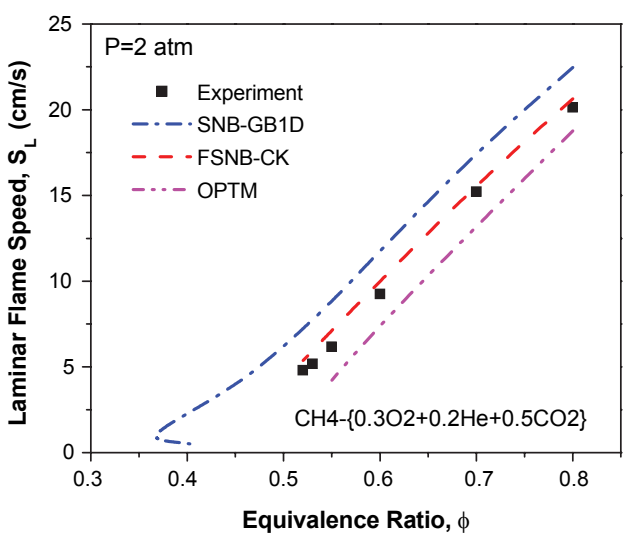

FIGURE 4. Effect of Flame Radiation on the Flame Speed of CH_4-($0.3O_2$+0.2He+$0.5CO_2$) Mixtures

- A near-constant pressure spherical bomb for flame speed measurement at high pressures and temperatures was developed. The flame speeds of hydrogen/CO-air mixtures were measured in a range from 1 atm to 20 atm. It was found that the appearance of non-symmetrical flow field led to lower flame speeds.
- Radiation from CO, H_2O, and CO_2 in syngas combustion needs to be considered to predict and correct the measured flame speeds and burning limits. An accurate FSNB-CK radiation model was developed for syngas combustion.
- Flame speeds data at high temperatures and high H_2O and CO_2 dilutions need to be obtained to validate kinetic mechanism for syngas combustion in gas turbines.

FY 2007 Publications/Presentations

1. Z. Chen, X. Qin, B. Xu, Y. Ju, F. Liu, "Studies of radiation absorption on flame speed and flammability limit of CO_2 diluted methane flames at elevated pressures", *Proceedings of the Combustion Institute* (2007) 31: 2693-2700.

2. 1. Chen, Z.L., Ju, Y. "On the Accurate Determination of Flame Speeds at Normal and Elevated Pressures by Using a Spherical Bomb: the Effects of Compression and Stretch." AIAA 2007-378 45th AIAA Aerospace Sciences Meeting and Exhibit. 8–11 January 2007, Reno, Nevada.

3. Burke, M.P., Ju, Y., Dryer F.L. "Measurements of Hydrogen Syngas Flame Speeds at Elevated Pressures." Proceedings of the 5th US Combustion Meeting organized by the Western States Section of the Combustion Institute, March 17–19, 2007, San Diego, USA.

4. Zheng Chen and Yiguang Ju, "On the accurate determination of flame speeds at normal and elevated pressures by using a spherical bomb: the effects of compression and flame stretch," Combustion and Flame, Submitted, 2007.

5. Z. Chen, X. Qin, Y. Ju, "Burning properties of dimethyl ether/methane/air mixtures at normal and elevated pressures," 18th International Symposium on Transport Phenomena, Daejeon, Korea, August 2007.

6. Z. Chen, Y. Ju, "On the accurate determination of flame speeds at normal and elevated pressures by using a spherical bomb: the effect of compression and stretch (detailed chemistry)", 6th Asian-Pacific Conference on Combustion (ASPACC07), Nagoya, Japan, May 2007.

References

1. M.I. Hassan, K.T. Aung, G.M. Faeth, *Journal of Propulsion and Power* 13 (1997) 239-245.

2. H. Y. Sun, S. I. Yang, G. Jomaas, C. K. Law, *Proceedings of the Combustion Institute* 31 (2007) 439-446.

3. X Qin, Y. Ju, *Proceedings of the Combustion Institute 30* (2005) 233-240.

4. Zheng Chen and Yiguang Ju, "On the accurate determination of flame speeds at normal and elevated pressures by using a spherical bomb: the effects of compression and flame stretch," *Combustion and Flame*, Submitted, 2007.

5. Burke, M.P., Ju, Y., Dryer F.L. "Measurements of Hydrogen Syngas Flame Speeds at Elevated Pressures." *Proceedings of the 5th US Combustion Meeting* organized by the Western States Section of the Combustion Institute, March 17-19, 2007, San Diego, USA.

6. I.C. McLean, D.B. Smith and S.C. Taylor, *Proceeding of Combustion Symposium* 25 (1994) 749-757.

7. J. Li, A. Kazakov, Z. Zhao, M. Chaos, F.L. Dryer, J.J. Scire, *International Journal of Chemical Kinetics* 39 (2007) 109-136.

8. S.G. Davis, A. Joshi, H. Wang, and F.N. Egolfopoulos, *Proceedings of the Combustion Institute* 30 (2005) 1283-1292.

9. Z. Chen, X. Qin, B. Xu, Y. Ju, F. Liu, "Studies of radiation absorption on flame speed and flammability limit of CO_2 diluted methane flames at elevated pressures", *Proceedings of the Combustion Institute* (2007) 31: 2693-2700.

IV.14 CO_2 Compression Using Supersonic Shockwave Technology

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Objectives

- Demonstrate a single stage high pressure ratio supersonic shock compression rotor (Rampressor™) and show feasibility of shock compression technology for stationary devices.
- Complete the research and development (R&D) plan and a conceptual design for CO_2 compression using the Rampressor™.
- Demonstrate a low emissions Advanced Vortex Combustor (AVC) at realistic gas turbine operating conditions.

Approach

- Validate the design and analysis tools for a high pressure ratio shock wave compression device using the test results from the compression rig.
- Analyze performance data from the compression rig test to anchor analysis tools at high Mach number.
- Perform the "gap" analysis between the test results and CO_2 compression requirements and develop a technology development plan to meet the requirements.
- Perform a combustion experiment and measure emissions while independently varying the main equivalence ratio, cavity equivalence ratio, reference velocity and cavity loading at realistic gas turbine conditions.

Accomplishments

- Design and test of a high pressure ratio supersonic shock compression rotor demonstrated several important milestones:
  - Shock structures were established in all three rotor inlets.
  - The rig operated at a pressure ratio of approximately 7.9:1 and a mass flow of approximately 2.43 lbm/s without the optimization of the geometry, boundary layer techniques and tip clearance, etc.
  - The technical design and analysis tools have been validated for a range of Mach 2.4 to 2.7 designs.
  - Improved computational fluid dynamic (CFD) analysis tools and techniques, whose methodology has been reviewed and validated by a Department of Energy (DOE)-appointed independent third party.
  - Identified and addressed the mechanical structure and system challenges of high compression ratios over a single stage device e.g. rotordynamics, bearing life, high rotational stresses and high secondary flow temperatures.
- Design and test of the AVC combustor at the National Energy Technology Laboratory (NETL) yielded the following:
  - NOx emissions below 3 ppmv (at 15 percent oxygen) were achieved, and combustion efficiency was in excess of 99.5%. The measured emission levels were within +/- 1.2 ppmv based on a 95% confidence level.
  - No significant root mean square (RMS) pressure levels were observed during this testing. This is a crucial finding because it indicates a very stable combustion system.
  - The combustor pressure drop for the AVC is significantly lower than that of a comparable conventional gas turbine combustor, which could result in significant increases in the power and efficiency levels of a gas turbine engine.

Future Directions

- Design the CO_2 compression test rig to run at higher pressure ratio:
  - Design and test subcomponent tests in parallel to achieve target subcomponent performance levels.
- Achieve higher efficiency through optimization of the tip clearance and rotor geometry.
- Investigate key technology challenges to successfully incorporate the superior compression technology into a commercially viable compressor product:
  - Aerodynamic optimization
  - Tip leakage mitigation
  - Rotor mechanical design optimization
  - Diffuser pressure loss mitigation
  - Thrust load mitigation

- Apply the technical knowledge gained to compress high volumes of CO_2 in support of Clean Coal, FutureGen and Carbon Capture & Storage programs.
- Demonstrate the emissions and stability characteristics of the AVC with liquid, syngas, hydrogen fuels, etc.
- Achieve higher efficiency through optimization of the AVC design.
- Design and demonstrate the AVC for gas turbine engines.

Introduction

Since the sound barrier was broken in the late 1940s, ramjet engines have been widely used as a means to propel aerospace vehicles at supersonic speeds. Ramgen Power System's ("Ramgen") primary innovation has been to apply the well understood supersonic shock wave compression techniques (applied in ramjet engine concepts) in a stationary "shock" compressor. The principal advantage of shock compression is that it can achieve exceptionally high compression efficiency, at very high compression ratios. The importance of a breakthrough in compression and combustion technology cannot be overstated as it is becoming increasingly evident that gas compression, particularly CO_2 compression, along with gas combustion at low emission levels are pivotal to the clean generation of power from coal.

Approach

The technology development path for the Rampressor technology started with our Rampressor-1 rotor test rig at a relatively low pressure ratio and performance, which was followed by a higher pressure ratio and performance rotor test rig - the Rampressor-2 test rig. This test helped anchor our design and analysis tools at high pressure conditions. Successful rotor test results are now allowing us to design a compressor package targeted toward the CO_2 compression market. The bridge between successful rotor testing and a compressor package demonstration will be crossed by investigating the design requirements and options for an industrial drive, rotor manufacturing, controls, tip clearance system, self contained supporting systems, etc. The next test rig will be a CO_2 compressor demonstrator including all the major components of a functional compressor package. This rig will first be tested and optimized in a test cell, then field demonstrated.

The technology development path for AVC technology started with a test of the first generation AVC design at the General Applied Sciences Laboratory (GASL) facility followed by a testing of the second generation hardware at the DOE NETL facility. These tests, which were conducted at realistic gas turbine engine operating conditions, helped anchor our design and analysis tools and additional testing activities are planned to understand the technological benefits offered by AVC. Implementation of this technology into a single combustor can and demonstration in a gas turbine engine package are expected to be the next evolutionary steps for this technology.

Results

During FY 2007, Ramgen succeeded in completing testing of the Rampressor-2 compressor test rig (see Figure 1). Testing was run at the Boeing Nozzle Test Facility in Seattle, Washington. The test was successful in many ways.

One of the testing accomplishments achieved by Ramgen was to successfully "start" the inlet, at significantly higher Mach numbers than Rampressor-1. Inlet starting is a critical step in achieving an efficient operation of a supersonic inlet design.

During the test many different test conditions were run to create a compressor map for the Rampressor rotor, which indicated very benign surge characteristics in spite of the high stage pressure ratio. 3-D viscous CFD simulations indicate that the test results are close to analysis predictions. A key preliminary conclusion from our testing is that our performance prediction tools matched the experimental results (see Figure 2). The confidence in these tools will help in designing the next generation test rig for CO_2 compression. Ramgen's CFD methodology have been reviewed and approved by a DOE analyst.

The results from the AVC test rig (see Figure 3) show that this technology is capable of achieving less than 3 ppm NOx levels at combustion efficiencies in excess of 99.5% (see Figure 4). These results were

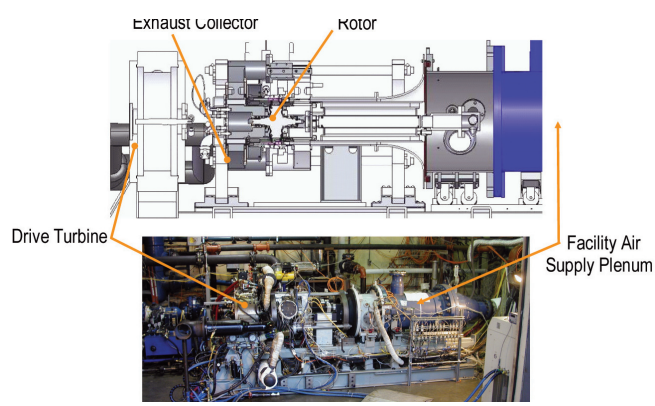

FIGURE 1. Rampressor-2 Test Rig

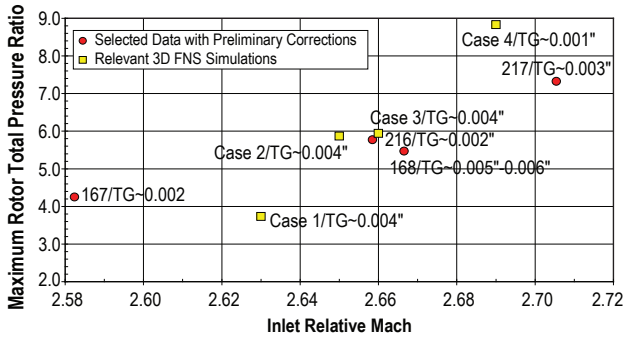

FIGURE 2. Preliminary Results from Rampressor-2 Tests

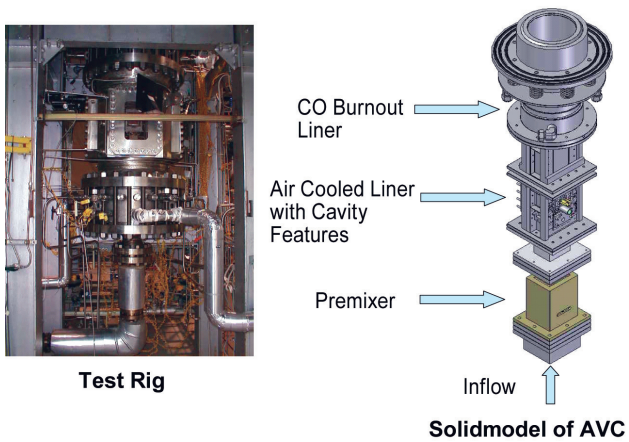

FIGURE 3. AVC Test Rig

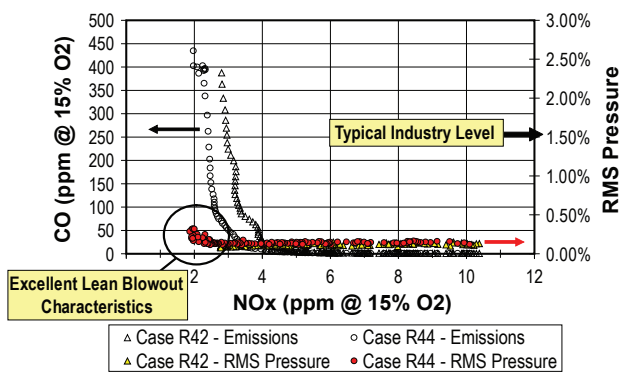

FIGURE 4. Final Results from AVC Tests

achieved at realistic gas turbine operating conditions, i.e., 147 psia and 625°F air.

In addition to the excellent emissions performance, the measured pressure loss across the AVC is lower than that of a swirl stabilized combustor design. Combining these technological benefits along with the lack of combustion oscillation issues makes this an attractive technology for implementation in advanced gas turbine engines.

Conclusions

Ramgen Power Systems, Inc. has completed a series of tests that validate the technological base for a compressor and combustor product for a gas turbine to generate electricity. Past compressor and combustor tests have successfully demonstrated a number of the fundamental technical requirements that are critical to achieving high efficiency compression and combustion. Ramgen will continue to validate the engineering design and analysis tools needed to move towards successful products. These products are expected to leapfrog existing technology by achieving higher efficiency, reduced cost and lower emissions.

FY 2007 Publications/Presentations

1. Paper for ASME 2007 Turbo Expo on RANS Prediction of Transonic Compressive Rotor Performance Near Stall.

2. Paper for ASME 2007 Turbo Expo on Advanced Supersonic Component Engine For Military Applications.

3. Presentation on Supersonic Component Technology For Military Applications at Army Science Conference, November 2006.

4. Presentation on Benefits to IGCC Gas Turbines of Advanced Vortex Combustion at Pittsburgh Coal Conference, September 2006.

IV.15 Systems Analyses of Advanced Brayton Cycles for High Efficiency Zero Emission Plants

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Objectives

- Main objective is to identify and assess advanced improvements to the Brayton cycle that will lead to significant performance improvements in coal-based near zero emission gasification plants (approximately an 8% reduction in heat rate over an integrated gasification combined cycle [IGCC] plant utilizing the H class steam cooled gas turbine).
- Second objective is to quantify any performance improvements that may be gained by incorporating advanced CO_2 shock compression concepts being developed by Ramgen.
- Third objective is to identify the basis for design of turbo-machinery for use in a fuel cell gas turbine power block integrated with a gasification plant.

Accomplishments

- Developed the performance of an H class gas turbine-based IGCC to serve as the baseline case. The corresponding efficiency of the plant was 35% (higher heating value [HHV] basis) for a Pittsburgh No. 8 coal feed at ISO (International Organization for Standardization) conditions.
- Completed the screening analysis of advanced Brayton cycle concepts to identify those worthy of detailed analysis.
- The ongoing detailed analysis has shown that a Brayton cycle with rotor inlet temperature (RIT) of 1,734°C is required to realize the 8% improvement in heat rate over the baseline case. Corresponding pressure ratio for the gas turbine to take full advantage of the higher RIT is 50.
- It was shown that incorporation of spray intercooling into the above advanced RIT Brayton cycle has an insignificant affect on the plant heat rate but reduces the NOx emissions while decreasing the temperatures within the compressor and increasing the engine specific power output.
- It was also shown that incorporation of reheat into the Brayton cycle reduced the required RIT to 1,592°C.
- Completed assessment of utilizing Ramgen compression technologies in IGCC plants. The intercooled Ramgen compressor can reduce the CO_2 compression load (subject to verification of compressor efficiencies) but the non-intercooled Ramgen compressor coupled with compressor discharge heat recovery decreased the net plant output.
- Stand-alone dynamic ejector model that solves for pressure, temperature and Mach number at each section of ejector geometry has been completed. Model output agrees well with ejector performance described in the literature. Integration of the model into dynamic solid oxide fuel cell/gas turbine (SOFC/GT) power block model has been accomplished.

Introduction

The goal is the conceptualization of near zero emission (including CO_2 capture) integrated gasification power plants producing electricity as the principle product. This assessment is being conducted in the context of conceptual design studies (systems studies) that advance state-of-art Brayton cycles and result in coal-based efficiencies equivalent to 65%+ on natural gas basis (lower heating value [LHV]), or approximately an 8% reduction in heat rate of an IGCC plant utilizing the H class steam cooled gas turbine. Examples for the advanced improvements to the Brayton cycle include higher RIT, higher pressure ratio, intercooling, reheat, fuel or combustion air augmentation, blade cooling schemes as well as improvements to the bottoming cycle.

Also included in this project are performance evaluations of other advanced technologies such as advanced compression concepts and a fuel cell-based combined cycle.

Approach

Since a total systems solution is critical to establishing a plant configuration worthy of significant market interest, a baseline IGCC plant scheme is developed and used to study how alternative process

schemes and power cycles might be used and integrated to achieve higher system efficiency. To achieve these design results, the total systems approach taken requires creative integration of the various process units within the plant. The studies are being sufficiently detailed and documented so that third parties will be able to quickly validate portions or all of the studies. Steady-state simulation software consists of Aspen Plus for the gasification island and Thermoflex for the power block.

In the case of the integrated gasification fuel cell task, a steady-state simulation of the entire plant is developed and then using dynamic simulations of the hybrid SOFC/GT sub-system the turbo-machinery performance is investigated. From these investigations the desired performance characteristics and a basis for design of turbo-machinery for use in a fuel cell gas turbine power block are developed.

Results

Baseline Case. The selected plant scheme for the baseline case consists of a cryogenic air separation unit (ASU) supplying 95% purity O_2 to GE-type high pressure (HP) total quench gasifiers (see Figure 1). The raw gas after scrubbing is treated in a sour shift unit to react the CO with H_2O vapor to form H_2 and CO_2. The gas is further treated to remove Hg in a sulfided activated carbon bed. The syngas is desulfurized and decarbonized in a Selexol acid gas removal unit and the decarbonized syngas after humidification and preheat is fired in a GE 7H type steam cooled gas turbine. Pressurized N_2 from the ASU is also supplied to the combustors of the gas turbines as additional diluent for NOx control. A portion of the air required by the ASU is extracted from the gas turbines.

Screening Analysis. Table 1 lists the advanced Brayton cycle concepts identified for screening analysis. Among these various concepts screened, increased firing and blade surface temperatures, as well as reheat and pressure gain combustion showed promise of significant efficiency improvement.

TABLE 1. Advanced Cycles Considered for Screening Analysis

1. Increased RIT / Blade Surface Temperature	7. Oxy Combustion Gas Turbine including the Partial Oxidation Gas Turbine
2. Intercooled Gas Turbine	8. HAT Cycle
3. Intercooled and Reheat Gas Turbine	9. Supercritical Rankine Bottoming Cycle
4. Humid Air Cooling of Gas Turbine Blades	10. Chemical Recuperation
5. Pressure Gain Combustor	11. Inlet Air Fogging
6. High Efficiency Exhaust Diffuser	12. Inverse Cycle

Detailed Analysis of Simple Cycle Gas Turbine based IGCC with Increased RIT. The gas turbine has a simple cycle configuration as in the baseline case (without intercooling or reheat). The gas turbine RIT required to realize the 8% improvement in heat rate over the baseline case is 1,734°C (342°C above the baseline case) while increasing the blade surface temperatures by about the same amount over the baseline case. The

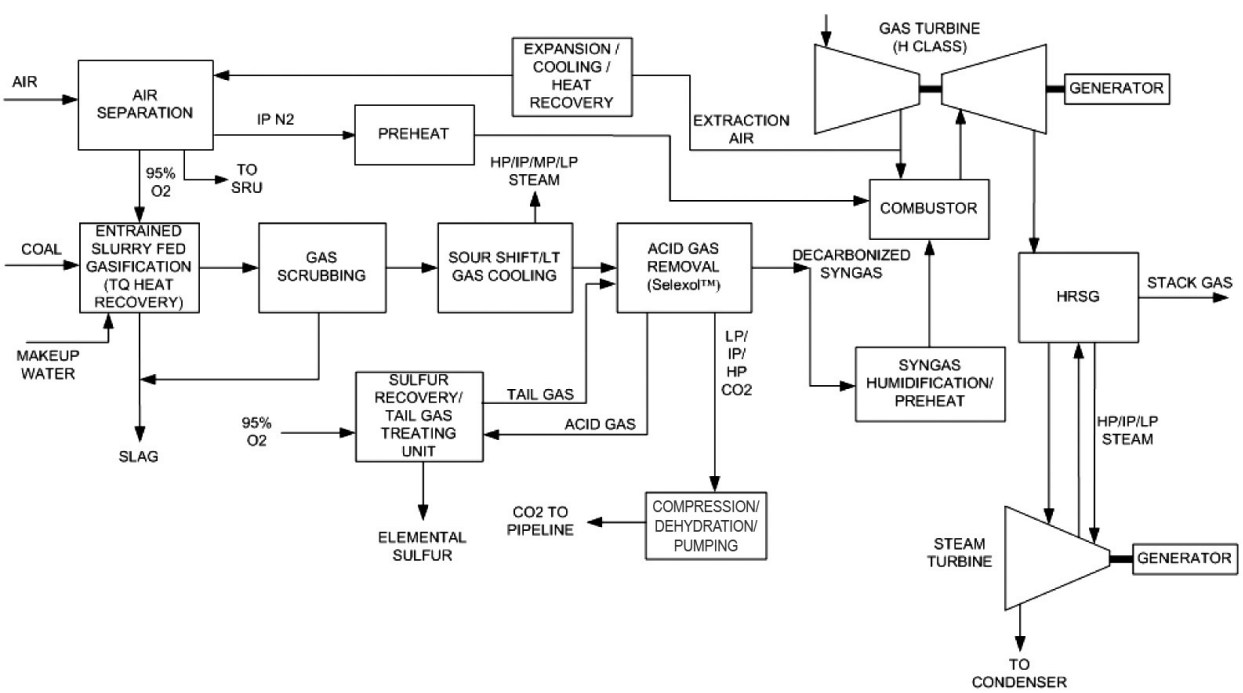

FIGURE 1. Overall Block Flow Diagram – Baseline Case IGCC with CO_2 Capture

corresponding pressure ratio of the gas turbine while maintaining an exhaust temperature of about 650°C[1] is 50. This pressure ratio is significantly higher than currently demonstrated but such a high pressure ratio has been proposed by Pratt & Whitney for Boeing's 7E7 transport plane. Maximum pressure ratio for a commercial gas turbine without intercooling is 36 (Rolls-Royce's Trent 60 with water injection). A lower pressure ratio case is thus also investigated (a pressure ratio of 37 which is close to that of the Trent 60) while letting the turbine exhaust temperature rise significantly above the 650°C constraint. Significantly higher steam superheat and reheat temperatures are required than those in the 50 pressure ratio case in order to limit the irreversibility in heat transfer.

Detailed Analysis of Intercooled Gas Turbine based IGCC with Increased RIT. Advantages of intercooling are (1) lower compressor discharge temperature resulting in savings in materials of construction and lower NOx and (2) higher specific power output because of reduced compressor work. More complex turbomachinery (multi-spool engine) is required, however. There are two choices for the type of intercooler: (1) shell and tube and (2) spray-type (as used in the GE LM6000 SPRINT engine). An evaluation of the two types of intercoolers along with its location in the compressor from a cycle thermal efficiency standpoint was made (see Figure 2). Advantages of the spray-type intercooler over the shell and tube type, in addition to having an efficiency advantage, are (1) lower equipment cost, (2) lower equipment footprint, and (3) spray adds motive fluid for expansion in the turbine and thermal diluent for reducing NOx. The spray intercooler does need high quality spray water and the spray system needs to be carefully designed to minimize any large droplet carryover into the high pressure compressor in order to avoid impingement and erosion of compressor blades. Compression pressure ratio (i.e., that of the low pressure compressor) chosen for locating this intercooler is 2.75. The thermal efficiency is increased but only slightly as this pressure ratio is decreased below 2.75 but the other advantages of spray intercooling listed above are compromised. The overall plant heat rate for this intercooled case is similar to that of the previous non-intercooled case. A substantial decrease in compressor discharge temperature of 136°C is realized for the intercooled case.

Intercooled-Reheat Gas Turbine based IGCC with Increased RIT. The RIT required to realize the target improvement goal in heat rate over the baseline case is 1,592°C (which is 142°C lower than the previous increased RIT cases).

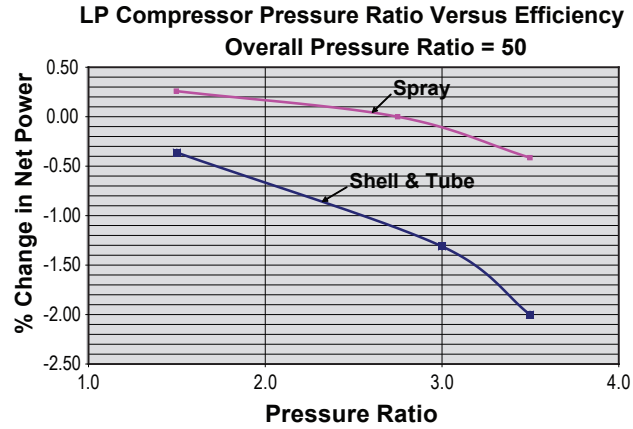

FIGURE 2. Spray vs. Shell and Tube Intercooler

Gas Turbine for SOFC Integration. After the SOFC/GT design and baseline operating conditions were established, the dynamic SOFC-GT power block model was exercised by perturbing power demand and fuel composition. Compressor dynamics were investigated and found to respond to some power and fuel composition perturbations by going into a surge condition, as shown for example in Figure 3.

Conclusions and Future Directions

Aero-engine designs are required for these high RIT and pressure ratio gas turbines. The resulting high combustion air temperatures pose additional challenges for low NOx decarbonized syngas combustor design. More extraction air is required (used in the air separation unit) for these high RIT gas turbines if the gas turbine is designed for dual applications, i.e., natural gas and then operated in off-design mode for IGCC applications. Less air is then available for combustor liner cooling. Spray intercooling is advantageous in lowering the compressor discharge temperature while adding moisture to the combustion air. The corresponding NOx emissions are reduced by more that 20% while the engine specific power output is increased by 17%. Reheat lowers the required RIT and also the NOx but a gas turbine with a pressure ratio of 70 is required. NOx emissions as estimated by modeling the primary and dilution zones of the combustor as perfectly stirred reactors in series [1] while utilizing the Konnov model [2] for the reaction mechanism and kinetics varied from a low of 42 ppmVd for the case with an intercooled-reheat gas turbine to a high of 251 ppmVd (15% O_2 basis) for the simple cycle gas turbine (non-intercooled) with advanced RIT. It was found that NOx continued to form at a significant rate in the

[1] Such that strength in the roots of the long and uncooled last stage blades is maintained. Furthermore, use of advanced superheat and reheat steam temperatures of 613°C for the bottoming cycle is facilitated without having very large temperature differences between the gas turbine exhaust and the steam such that the irreversibility in heat transfer is maintained similar to that in the baseline case.

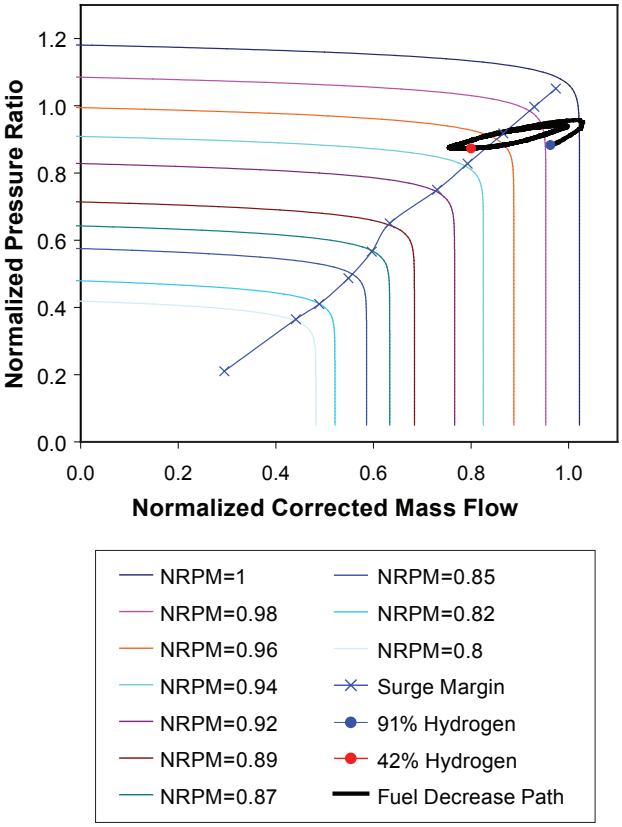

FIGURE 3. Gas Turbine Compressor Dynamic Response to Fuel H_2 Mole Fraction Decrease of 54% from 91% (Blue) to 42% (Red)

dilution zone of the combustor because of the very high RITs required by these cycles. Residence time in the dilution zone of these advanced gas turbine combustors should be limited by constructing a short combustor in order to limit the NOx generation. By reducing the residence time from 30 ms to 5 ms in this zone, the NOx was reduced by about 70% for the increased RIT cases while the burnout of the H_2, and the small amounts of CO and CH_4, were not affected significantly for this decarbonized syngas. It appears that selective catalytic reduction (SCR) would still be required for these cases to achieve the 2 ppmVd target.

The next steps for this study to be completed in September 2007 are:

- Complete detailed analysis of additional advanced cycles and select most promising cycle(s).
- For selected cycle(s), investigate low NOx strategies: increasing diluent addition and adding SCR. Assess sensitivity to higher gas turbine component efficiencies. Finally, define research and development (R&D) needs, costs and relative (differential) economics of the advanced Brayton cycle over an H Class gas turbine-based IGCC will be defined.
- Complete definition of gas turbine requirements for integration with the SOFC.

References

1. Touchton, G. L., "An Experimentally Verified NOx Prediction Algorithm Incorporating the Effects of Steam Injection," *Journal of Engineering for Gas Turbines and Power*, 1984, Vol. 106, 833-840.

2. Konnov, A. A., "Detailed Reaction Mechanism for Small Hydrocarbons Combustion," Release 0.5, http://homepages.vub.ac.be/~akonnov/, 2000.

IV.16 Novel Concepts for the Compression of Large Volumes of Carbon Dioxide

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Objectives

- Reduce the compression power penalty associated with carbon capture in integrated gasification combined cycle (IGCC) and oxy-fuel power plants.
- Develop improved methods to compress CO_2.
- Develop concepts that liquefy the CO_2 and boost pressure through cryogenic pumping.

Accomplishments

- Identified an optimum compression concept that provides a 25% power savings.
- Identified an alternative pumping arrangement that provides a 30% power savings.
- Combining the two concepts permits up to 35% total power savings.

Introduction

One effort being pursued to reduce the release of carbon dioxide (CO_2) greenhouse gases to the atmosphere is sequestration of CO_2 from IGCC and oxy-fuel power plants. This approach, however, requires significant compression power to boost the pressure to typical pipeline levels. The penalty can be as high as 8% to 12% for a typical IGCC plant. For a project funded by the National Energy Technology Laboratory (NETL) within the Department of Energy (DOE) and with co-funding provided by Dresser-Rand, Southwest Research Institute (SwRI) has investigated novel methods to minimize this penalty through novel compression concepts.

For gaseous compression, the project seeks to develop improved methods to compress CO_2 while removing the heat of compression internal to the compressor. The high pressure ratio compression of CO_2 results in significant heat of compression. Because less energy is required to boost the pressure of a cool gas, both upstream and inter-stage cooling are desirable. This project has determined the optimum compressor configuration and has developed technology for internal heat removal. Other concepts that liquefy the CO_2 and boost pressure through cryogenic pumping have been explored as well.

Approach

This project is divided into three phases. Phase I, to develop the most promising concepts that meet the efficiency goals and integrate them into the IGCC environment, has been completed. Phase II involves detail design of the optimum solution and prototype development testing. Phase III will provide a full-scale compression solution to an existing or proposed IGCC plant.

Results

Table 1 lists the CO_2 streams of a sample 700 MW IGCC plant using a Selexol separation process. The expected discharge pressure for pipeline transmission was assumed to be 2,215 psia at 70°F, which is a supercritical state. The higher pressure streams provide additional volume flow that helps offset most of the large volume reduction that naturally occurs when compressing CO_2 at a high pressure ratio.

TABLE 1. CO_2 Streams from Selexol Separation Process

CO_2 Gas Streams	LP	MP	HP 1	HP 2
Pressure (psia)	21.9	160.0	250.0	299.0
Temperature (°F)	51.0	68.0	90.0	75.0
Density (lbm/ft^3)	0.177	1.30	1.87	2.088
Flow Rate (acfm)	33,257	2,158	3,374	1,073

The initial analysis of horsepower was conducted for a conventional approach to compressing the CO_2, using multiple stages of centrifugal compression. The low pressure stream is compressed and blended with the medium pressure stream (which enters the compressor

as a side stream). The discharge from the low pressure (LP) compressor is blended with the two higher pressure streams to compress the carbon dioxide to its final delivery pressure of 2,215 psia in the high pressure (HP) body. The compressor train consists of two parallel trains with a LP and a HP compressor driven by either a steam turbine or electric motor. Because each compressor is a back-to-back design, inter-cooling is used with each body as well as for the flow exiting the LP compressor totaling three inter-cooling steps. This process is shown schematically on a pressure-enthalpy diagram in Figure 1. The compression and inter-cooling steps are also shown. Option A provides a baseline to compare to alternative compression technologies. A second option (B) with lower inter-cooling temperatures is also shown.

Because less energy is required to compress a cool gas, the concept of isothermal compression is explored next. In Option C, the inlet-cooling concept is applied to each stage, using the same inter-stage pressures as Options A and B. An ideal isothermal compression process was analyzed in Option C.1 for an isothermal compression temperature of 70°F. To gauge the effect of the choice of isothermal temperature (and the required cooling power), Option C.2 was analyzed as an isothermal compression with a constant temperature of 100°F. In reality, an isothermal compression process is difficult to achieve. A typical compression process uses an increasing number of finer steps with inter-stage cooling in between each compression stage, so the actual compression process begins to approach isothermal compression. To analyze the practical realization of the isothermal process, Option C.3 uses many small compression steps with inter-stage cooling between each stage to achieve a semi-isothermal process. An illustration of the thermodynamic path taken by Options C.1 and C.3 is shown in Figure 2 to illustrate the semi-isothermal process. Figure 3 plots the compression power versus the number of inter-cooling steps and demonstrates that isothermal compression can be achieved if inter-cooling is used between each stage for the 17 total stages in the baseline selection.

Option D utilizes a high-ratio compression process, where extremely high pressure ratios (up to 10:1) are assumed. The process allows the gas to be compressed in only two stages between 22 and 2,215 psia. However, only one cooling step is performed in between the two stages. Without the added cooling between smaller stages of compression, Option D requires significantly more horsepower than Option A. Also, high-ratio stages typically possess limited flow range, which may require cycle during part-load power plant operation.

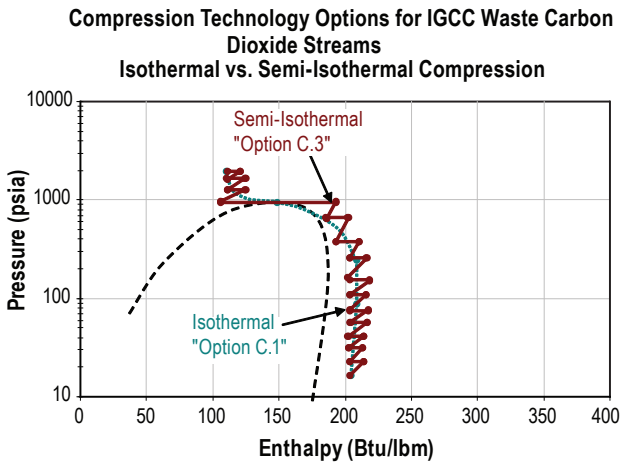

FIGURE 2. Comparison of Isothermal and Semi-Isothermal Compression Paths

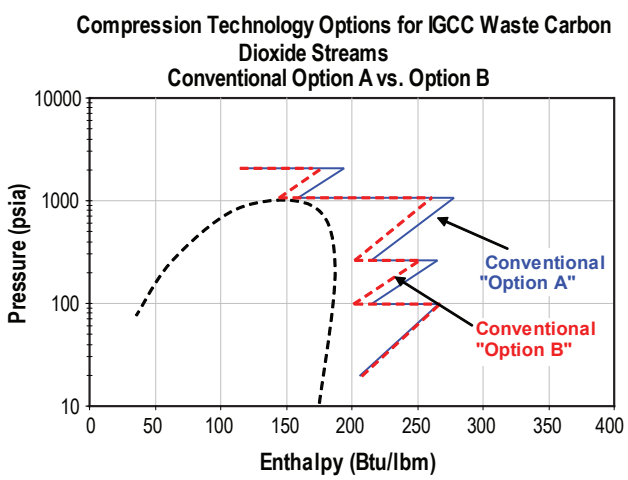

FIGURE 1. Comparison of Thermodynamic Paths for Baseline Case

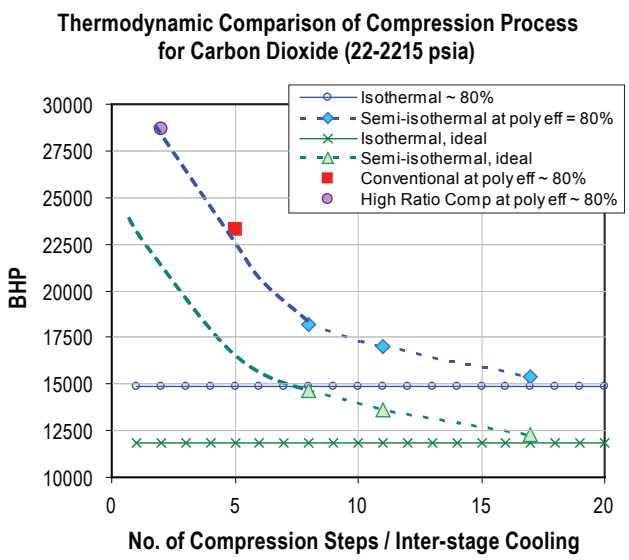

FIGURE 3. Brake Horsepower vs. Number of Intercooling Steps

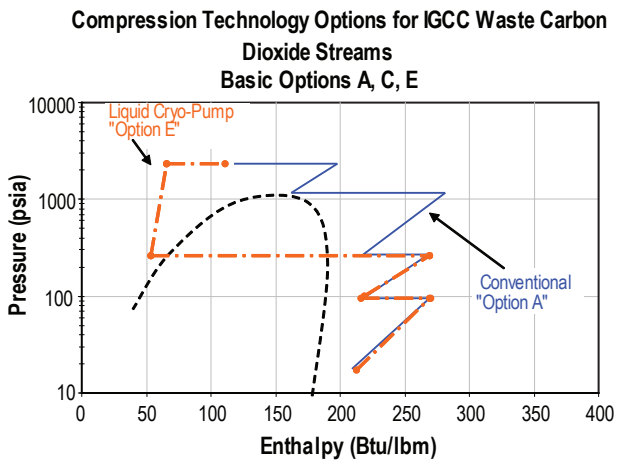

FIGURE 4. Comparison of Option E for Liquid Cryogenic Pump to Centrifugal Compression in Option A

The final option (Option E) pumps the carbon dioxide in a liquid state. To achieve cryogenic temperatures without forming solid carbon dioxide, it is necessary to compress the low and medium pressure streams to 250 psia. These can be joined with the high pressure stream to undergo a refrigeration process. Normal air cooling can be used to reduce the temperature of the carbon dioxide from 255°F to 100°F or lower. Refrigeration units (typically an ammonia absorption cycle) must be used to reduce the temperature to -25°F because of the significant heat transfer required to overcome the latent heat in the gas. At -25°F and 250 psia, the carbon dioxide will be 100% liquid and can be pumped at a relatively low power to 2,215 psia. Figure 4 illustrates Option E and the reduction in temperature required to clear the gas-liquid dome.

Table 2 summarizes these compression calculations listing the power required for each thermodynamic process. The Option A conventional compression technology requires a total horsepower of 23,251 BHP. As the results show, the amount of horsepower required by each compression option varies significantly according to the thermodynamic path. Option B provides a small improvement in compression power but requires that cold nitrogen be delivered from the air separation units. While this provides some savings to the CO_2 compression, it will reduce the efficiency of the air separation units and thus was discounted.

The Option C concepts show that near isothermal conditions can be achieved and result in significant power savings over the baseline case. Semi-isothermal compression can be achieved by an integral geared centrifugal compressor with intercoolers between each stage. While this is a commercially viable approach today, these machines introduce greater size and more complexity than the two-body, in-line barrel compressor described in Option A.

Because of the high molecular weight of CO_2, very high pressure ratios are possible in a single stage resulting in a compact compression solution. However, Option D shows this approach results in significantly

TABLE 2. Summary of Compression Technology Options – Power and Cooling Requirements

Option	Compression Technology	Power Requirements	% Diff from Option A	Cooling Technology
A	Conventional Dresser-Rand Centrifugal 10-stage Compression	23,251 BHP	0.0%	Air-cool streams between separate stages
B	Conventional Dresser-Rand Centrifugal 10-stage Compression with additional cooling	21,522 BHP	-7.4%	Air-cool streams between separate stages using ASU cool N_2 stream
C.1	Isothermal compression at 70°F and 80% efficiency	14,840 BHP	-36.2%	Tc = 70°F inlet temp throughout
C.4	Semi-isothermal compression at 70°F, Pressure Ratio ~ 1.55	17,025 BHP (Required Cooling Power TBD)	-26.8%	Tc = 70°F in between each stage
C.7	Semi-isothermal compression at 100°F, Pressure Ratio ~ 1.55	17,979 BHP (Required Cooling Power TBD)	-22.7%	Tc = 100°F in between each stage
D.3	High ratio compression at 90% efficiency – no inter-stage cooling	34,192 BHP	47.1%	Air cool at 2215 psia only
D.4	High ratio compression at 90% efficiency – intercooling on final compression stage	24,730 BHP	6.4%	Air cool at 220 and 2215 psia
E.1	Centrifugal compression to 250 psia, Liquid cryo-pump from 250-2215 psia	16,198 BHP (Includes 7,814 BHP for Refrigeration)	-30.3%	Air cool up to 250 psia Refrigeration to reduce CO_2 to -25°F to liquefy
E.2	Centrifugal compression to 250 psia with semi-isothermal cooling at 100°F, Liquid cryo-pump from 250-2215 psia	15,146 BHP (Includes 7,814 BHP for Refrigeration)	-34.9%	Air cool up to 250 psia between centrifugal stages, Refrigeration to reduce CO_2 to -25°F to liquefy.

greater power requirements especially if no inter-cooling is used.

Finally, Option E.1 utilizes part compression followed by liquefaction and pumping. The pump requires only 1,400 BHP, but the refrigeration system requires almost 8,000 BHP. Nevertheless, significant power savings can be achieved with this approach. Option E.2 combines semi-isothermal compression with liquefaction and results in a 35% reduction in compression power. Obviously capital expenditure will be greater because of to the additional refrigeration system, but some of this cost will be offset by the elimination of two coolers and a lower cost of the pump compared to the HP compressor.

Conclusions and Future Directions

Because of the environmental pressures to reduce greenhouse gas emissions, the U.S. government and utilities are developing technologies to separate CO_2 both pre- and post-combustion. However, the total penalty for CO_2 sequestration because of compression power requirements is on the order of 10% of a power plant's output. The additional capital and operational expenses can increase the cost of electricity between 20 and 80%. This power and cost requirement is significant and is deterring many power producers from implementing carbon capture projects. Reducing this power requirement will improve overall plant efficiencies and encourage sequestration of CO_2 on both existing and future power plants. The results of this study indicate that a 25% reduction in compression power requirements is possible with pure compression using an isothermal process. A second approach that partially liquefies the CO_2 can achieve as much as a 30% reduction. A third option combines the two approaches and can achieve more than a 35% reduction compared to currently available technology. These concepts will be further refined and tested in Phase II of this project, currently under way.

FY 2007 Publications/Presentations

1. CO_2 Compression Panel Session, ASME Turbo Expo, International Gas Turbine Institute, Montreal, Canada, May 14-18, 2007.

2. Presentation at CO_2 Compression, Injection Technology–Performance and Economics, The Economics and Impacts of Carbon Capture, Transport & Sequestration, Denver, CO, November 13, 2006.

IV.17 Solid Oxide Fuel Cell Turbine Subsystem Performance, Test Program for High Efficiency Gas Turbine Exhaust Diffuser

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Objectives

Evaluate turbine exhaust diffuser aerodynamic strutlets for more power and efficiency.

Accomplishments

Project work has not begun at the time of this writing.

Introduction

Phase I seeks to demonstrate technical viability of a new, more aerodynamically efficient strut system in a turbine exhaust. Struts are located in the turbine exhaust diffuser, usually just downstream of the turbine wheel. More efficient flow around struts would incrementally increase turbine efficiency and power. The result is really just a low back-pressure exhaust for the turbine engine, analogous to a low back-pressure exhaust header on a "hot rod" race car engine. Application would be to any large turbine with struts, new or existing.

Approach

The approach is to measure efficiency of flow around a standard and modified strut using a physical scale model. Poor strut flow is a leading cause of inefficiency in turbine diffusers.

The model will include components, called "strutlets" that guide flow into the strut more directly, so that sideways flow is reduced. Aerodynamically speaking, the strut angle of attack to incident flow is, in effect, reduced. The effect is similar to a "slat" at the leading edge of an airplane wing. One or more strutlets are placed next to and just ahead of the main strut. We will measure the backpressure of the diffuser with and without these strutlets, and also look at flow patterns around the struts. Success would be indicated by lower back-pressure and smooth flow around the main struts. An unfavorable result would be characterized by aerodynamic stalls, including zones of reversed or stagnant flow, large eddies, and little back-pressure reduction.

In Phase I, we will test for flow efficiency, as stated, in a large scale model. Later project phases would install first in a model, and then in an operating turbine the strutlets and other components, and evaluate turbine back-pressure performance and efficiency.

Results

Premature, work has not yet begun. However, we anticipate a positive result, that is, turbine efficiency will be improved. For operating large turbines, a successful result would, for the same power, reduce fuel consumption on average an anticipated 0.5 percent.

Even less than one percent is very significant, financially. Using Energy Information Administration data, in 2005, natural gas alone accounted for $52.3 billion of power plant fuel purchases. A half percent savings would be $261 million annually, for gas. For 50 percent market penetration, this would be $130 million saved annually, or over ten years, $1.3 billion.

The benefit to solid oxide fuel cell power plants depends on the specific mass flow through the exhaust diffuser, that is, the kilograms of mass flow per megawatt-hour. We cannot predict this at this time, but the benefit varies with flow, and for now, we could only speculate if solid oxide fuel cell flows will be greatly different than in today's best gas turbines.

Conclusions and Future Directions

Premature, it is too early to state conclusions.

V. UNIVERSITY TURBINE SYSTEMS RESEARCH

V.1 University Turbine Systems Research (UTSR) Program

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Subcontractors:

Active research subcontracts during FY 2007

- Brigham Young University, Provo, UT
- Clemson University, Clemson, SC
- Cleveland State University, Cleveland, OH
- Georgia Institute of Technology, Atlanta, GA
- Louisiana State University, Baton Rouge, LA
- Massachusetts Institute of Technology, Cambridge, MA
- Pennsylvania State University, University Park, PA (2)
- University of California, Santa Barbara, CA
- University of Central Florida, Orlando, FL (3)
- University of Colorado, Boulder, CO
- University of Connecticut, Storrs, CT
- University of North Dakota, Grand Forks, ND
- University of Pittsburgh, Pittsburgh, PA (3)
- University of Texas, Austin, TX
- University of Wisconsin, Madison, WI
- Texas A&M, College Station, TX
- Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA (4)

*Numbers in parentheses indicate total number of subcontracts awarded

Objectives

Develop and transition technologies to the gas turbine industry in the areas of aerodynamics/heat transfer, combustion and materials needed to achieve the following Department of Energy (DOE) Turbine Program goals for syngas/high hydrogen fuel turbines:

- Improve combined cycle efficiency 2-3 percentage points by 2010 and 3-5 percentage points (total) by 2015.
- Reduce capital cost by 20-30%.
- Reduce combustor emissions to 2 ppm NOx (at 15% O_2) or less.

Accomplishments

Technology results from 19 ongoing university projects (and six new awards in 2007) have been compiled and provided quarterly to the DOE Turbine Program and U.S. gas turbine industry. Key results from these research efforts include:

- Fundamental understanding has been obtained of operating conditions and design parameters that affect performance, emissions, and the dynamic and static instability of low NOx gas turbine combustors.
- Combustion modeling approaches for combustor design have been advanced such as ignition time delay and chemical kinetics models for syngas fuels containing high levels of hydrogen.
- Fuel composition and variability effects on operating parameters such as autoignition, ignition delay, dynamic instability and blowout have been characterized for high hydrogen fuels derived from syngas.
- Effects of deposition due to fuel impurities on film cooling of turbine components has been evaluated and cooling approaches that alleviate deposition effects on turbine efficiency have been identified.
- Advanced and lower cost computational methods for the design of internal cooling passages of turbine airfoils have been developed which should aid in improving the efficiency of turbines that operate with syngas derived and conventional fuels.
- Experiments have identified effects of ash particle size distribution and turbine flow path temperature on deposition from fuel impurities.
- Fiber-optic sensing approaches have been advanced for measurement of turbine gas and component temperatures.
- Deposition and corrosion of turbine components from syngas turbines have been analyzed. Alloys and coatings have been evaluated and compared for improved performance in turbines operating with impurities from syngas derived fuels.
- A thermal barrier coating application process to increase insulation thickness and reduce spallation resulting from deposition has been verified. Commercialization would reduce turbine cooling requirements and improve engine efficiency.

Introduction

The DOE Turbine Program is focused on the time-phased development of coal-based power systems with increased efficiency and emissions performance and decreased capital cost per kW output. These advancements involve a transition from turbines operating on syngas with current integrated gasification

combined cycle (IGCC) plant properties, to very high hydrogen fuels derived from syngas, to syngas burned in nearly pure oxygen using steam to control temperatures (oxy-fuel systems). The transition requires the development of low-emission turbine combustion technologies for this variety of fuels; improved turbine hot section flow path aero/heat transfer methods to accommodate expansion gases that are not only increasingly hotter but also contain higher levels of water vapor and particulates; and durable, low-cost materials for this stressing environment.

The UTSR Program is focused on obtaining the fundamental technical information needed for gas turbines to support the turbine program objectives. The emphasis is on understanding the underlying factors affecting combustion, aero/heat transfer and materials for current IGCC syngas turbines and using that knowledge to design and conduct the research needed to transition to nearly pure hydrogen fuels derived from coal syngas and to syngas burned in oxygen. Through activities coordinated by SCIES, the goals of the DOE Turbine Program are advanced by the UTSR consortium, which consists of 111 performing member universities from 42 states, a 14 member Industrial Review Board (IRB) composed of major turbine manufacturers and operators, and an Academic Advisory Board (AAB) composed of leading turbine researchers from the member universities.

Approach

In the UTSR Program, inputs from the DOE, the IRB, and the AAB are used to identify research topics for yearly request for proposals (RFPs) issued by SCIES to the performing member universities that advance the DOE Turbine Program goals and meet the needs of the U.S. energy industry. Technical experts from the IRB companies review the proposals and recommend projects for award, subject to DOE approval and available funding. SCIES awards subcontracts to the selected performing member universities, who conduct the research. The activities of the UTSR consortium are coordinated and managed by SCIES. Research results are disseminated to the IRB members by SCIES via quarterly progress reports, yearly peer review workshops, and a final report for each research subcontract.

Results

Selected results from three of the 19 on-going university projects presented at the most recent UTSR Workshop (Reference 1) are described below:

Superior Thermal Barrier Coatings for Industrial Gas Turbine Engines, Professor Eric Jordan, University of Connecticut (UConn) and Professor Nitin Padture, Ohio State University (OSU).

Thermal barrier coatings (TBCs) provide insulation to turbine parts which reduces cooling requirements and resulting penalties on turbine power and efficiency. However, the degree of insulation has been limited by a maximum TBC thickness on the order of a few hundred microns. TBCs of greater thicknesses have tended to spall off, especially under thermal cycle conditions of turbine startup and shutdown. Spallation is aggravated by the presence of deposits on the TBCs, as has been experienced by syngas turbines.

The UTSR project at UConn and OSU has evaluated a new small particle plasma spray (SPPS) process for producing ultra-thick TBCs with improved durability and greater potential for resistance to spallation under deposition conditions. The laboratory thermal cycle test results of Figure 1 indicate an improvement of 2.6x in cycles to failure for an SPPS TBC compared to a conventional air plasma sprayed (APS) TBC with the same 250 micron thickness. An ultra-thick 3.3-mm SPPS TBC is shown to have over 20x improvement in cycles to failure over a 3.3-mm APS TBC and more than 2x improvement over the APS coating with the conventional 250 micron thickness. The project also demonstrated the feasibility of using the SPPS process to produce TBCs resistant to spallation due to deposits.

The research in this UTSR project provides a foundation for not only contributing to the efficiency goals of the DOE Turbine Program but also alleviating the degrading effects of deposits on TBCs which have been experienced at IGCC plants.

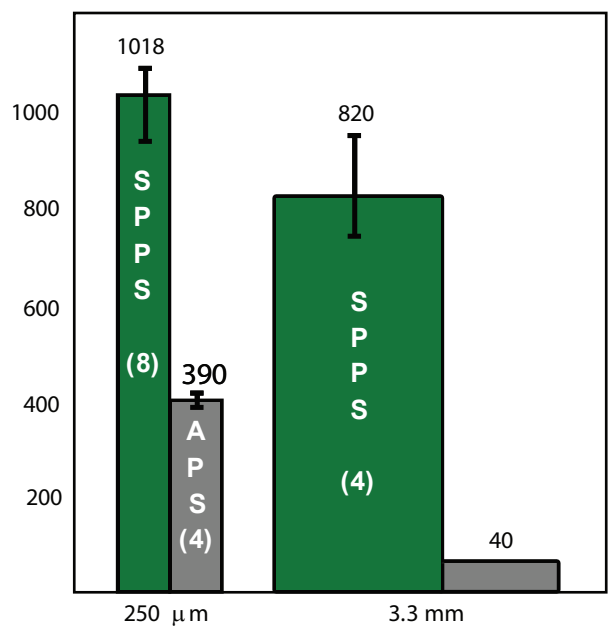

FIGURE 1. Number of 1-hour Cycles to Failure

Combustion Characterization and Modeling of Fuel Blends for Power Generation Gas Turbines, Professor Eric Petersen, University of Central Florida (UCF).

The design of low NOx turbine combustors requires information on the fuel dependent ignition delay in the lean pre-mixer section. Ignition delay information for conventional fuels has been determined. However, for high hydrogen fuels at turbine combustor conditions, only limited data have been available and ignition delay models for combustor design have been deficient.

The UTSR project at UCF not only expanded the data base for ignition delay but also developed an improved ignition delay model for high hydrogen fuels. As shown in Figure 2, the model predictions are vastly superior to those of a previous model and agree well with data for a high hydrogen (39%) fuel mixture at high pressures (20 atmospheres) representative of turbines. These results have been made available to the gas turbine industry for the design of low NOx combustors for operation with high hydrogen fuels derived from syngas.

Enhanced Prediction Techniques Based on Time-Accurate Simulations for Turbine Blade Internal Cooling, Professor Danesh Tafti, Virginia Tech.

The design of the complex internal cooling passages needed to efficiently cool turbine components has been hindered by inaccuracy of computer simulation methods, long computer run times and corresponding costs of the simulations, and the very high costs of testing candidate cooling passage designs. The UTSR project at Virginia Tech is the first to apply detached eddy simulations to predict heat transfer in ribbed cooling passages and the project showed favorable comparisons with previous simulation methods but at an order of magnitude lower computation times and corresponding reduced costs (see Figure 3).

Advancements in this UTSR project have brought closer the day that computer simulations can replace much of the very expensive rig testing needed by turbine manufacturers to verify cooling designs for turbine airfoils. Project results will also enable more efficient cooling designs for turbines, thereby facilitating DOE Turbine Program by reducing cooling penalties on engine efficiency.

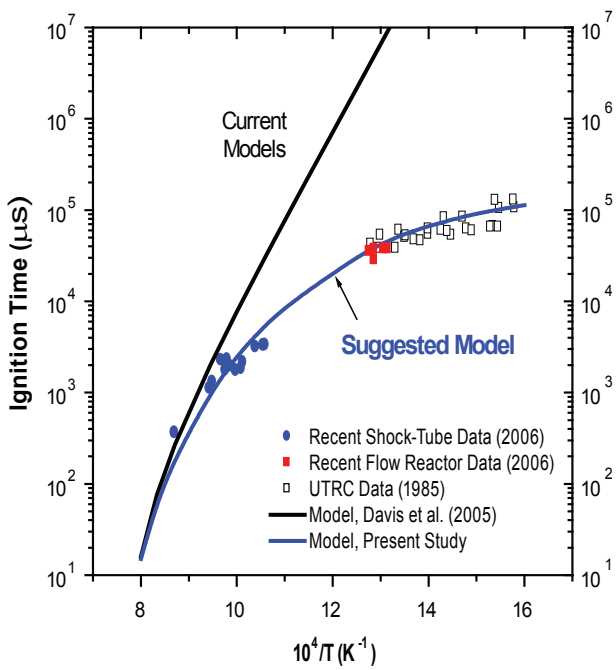

FIGURE 2. Improved Ignition Time Model for High Hydrogen Fuels

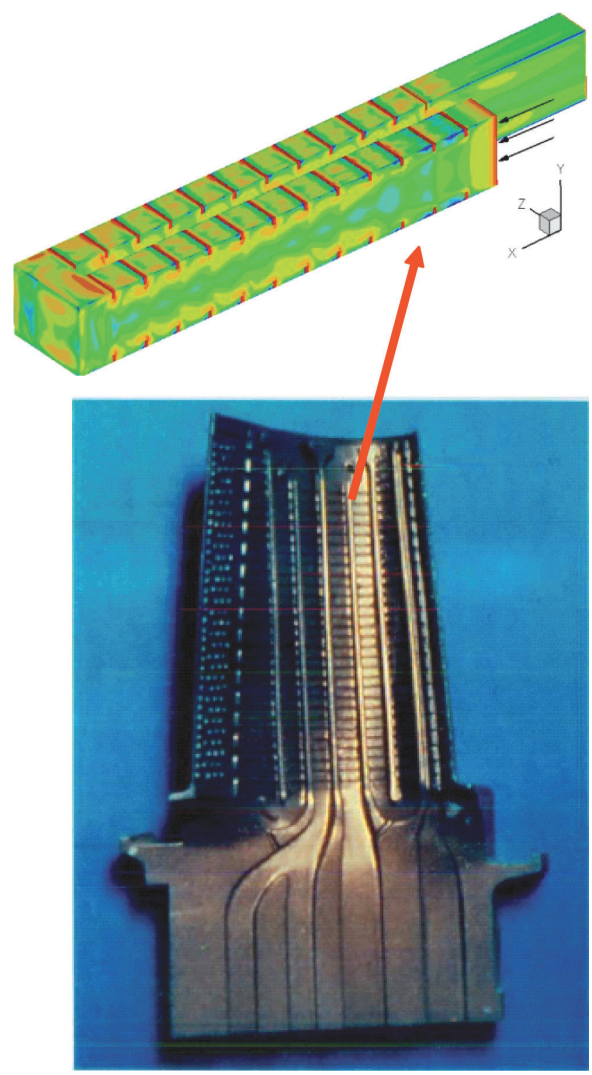

FIGURE 3. Computer Simulation of Turbine Airfoil Cooling Passages

Conclusions and Future Directions

Supporting the DOE Turbine Program goals, UTSR university research has provided fundamental data and analyses to address key turbine combustion, emissions, efficiency, and life issues specific to the composition, variability, and impurities for syngas and high hydrogen fuels derived from coal syngas. Although progress has been substantial, the following additional research is needed and will be the subject of future UTSR solicitations:

- Complete the kinetics data base for the full range of compositions and representative turbine operating conditions associated with combustion of high hydrogen fuels.
- Improve kinetics models for lower cost design of low NOx combustors.
- Identify and verify novel lean-premixed combustion enhancements needed to achieve DOE emissions goals.
- Determine turbine flow path features that enable cooling or aero designs with performance less sensitive to deposition, erosion and corrosion (DEC) or alleviate DEC.
- Better define the thermal-chemical DEC environments in flow paths of turbines operating with syngas and high hydrogen fuels derived form syngas.
- Determine critical mechanisms/coal impurities that have caused materials degradation in syngas turbines. Use that knowledge for experiments to identify best materials for higher temperature future turbines operating with high hydrogen fuels derived from syngas.
- Conduct experiments to define acceptable bounds of water vapor and gaseous sulfur species for turbine materials operating in oxy-fuel turbines.

FY 2007 Publications/Presentations

Over 115 papers have been published in journals and conference proceedings from the nearly 40 UTSR projects. In addition, each UTSR project provides semi-annual reports and the results of ongoing projects are presented at the annual UTSR Peer Review Workshop last held in October 2006.

The following selected papers were produced during FY 2007:

1. Simulation of Flow and Heat Transfer in the Developing Flow Region of a Rotating Gas Turbine Blade Internal Cooling Duct with Coriolis and Buoyancy Forces - ASME J. of Turbomachinery, 2007.

2. Accelerated Cyclic Oxidation Testing Protocols for Thermal Barrier Coatings and Alumina-Forming Alloys and Coatings – Journal of Materials and Corrosion, 2007.

3. Effects of Deposits on Film Cooling of a Vane Endwall Along the Pressure Side - ASME Turbo Expo, Montreal, Canada, 2007.

4. Effects of Surface Deposition, Hole Blockage, and TBC Spallation on Vane Endwall Film Cooling - Accepted to the Journal of Turbomachinery, publication pending for 2007.

5. Effects of Regular and Random Roughness on the Heat Transfer and Skin friction Coefficient on the Suction Side of a Gas Turbine Vane - ASME Turbo Expo, Montreal, Canada, 2007.

6. Impacts of Hydrogen Addition on Near-Lean Blowout Dynamics in a Swirling Combustor - Proceedings of the ASME Turbo Expo, Montreal, Canada, 2007.

7. Effects of Particle Size, Gas Temperature, and Metal Temperature on High Pressure Turbine Disposition in Land Based Gas Turbines from Various Synfuels - Journal Publication pending for 2007.

References

1. Proceedings of the UTSR Workshop IV, October 17–19, 2006, South Carolina Institute for Energy Studies, Clemson, SC.

V. UNIVERSITY TURBINE SYSTEMS RESEARCH

A. Aero-Heat Transfer

V.A.1 Deposition of Alternative (Syngas) Fuels on Turbine Blades with Film Cooling

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Objectives

- Characterize deposition on turbine hardware from the combustion of synfuels that are or could be used in the power generation industry, including effects of fuel type, temperature, particle size, and backside cooling.
- Evaluate the influence of these deposits on turbine blade cooling.
- Determine the effects of these deposits on spallation of thermal barrier coatings (TBCs).

Accomplishments

Three series of experimental deposition tests were conducted during the last fiscal year:

1. Deposition from four different particle sizes of subbituminous coal flyash, with mass mean diameters ranging from 3 to 16 μm (at 1,183°C).
2. Deposition from subbituminous coal flyash at five different gas temperatures, ranging from 860 to 1,183°C.
3. Deposition on coupons with backside impingement cooling, including five tests with subbituminous coal flyash and three tests with petcoke ash.

In addition, an optical technique was implemented to map the surface temperature of coupons in the Turbine Accelerated Deposition Facility (TADF) using the red, blue, and green (RGB) signals from a digital camera.

Introduction

Turbine inlet temperatures for large power generation gas turbines have been steadily increasing over the last several decades due to significant advances in materials and cooling technologies. By incorporating these critical advancements, the H-class combined cycle machines are expected to operate at up to 1,425°C. While this higher combustor exit temperature translates directly to higher cycle efficiency, it does not bode well for the severe operating environment of turbine materials. At the same time, political and economic pressures are pushing utilities to consider fuel flexibility. Intermediate goals of the Department of Energy (DOE) FutureGen and DOE Turbine Program focus on coal syngas as a turbine fuel in an effort to reduce dependency on foreign supplies of natural gas. Petroleum coke and biomass fuels are also being considered. Compared to "clean" burning natural gas, these alternative fuels have higher concentrations of trace elements and ash that present significant corrosion challenges to turbine operation.

Although filters are installed in gas turbine systems to remove flyash from synfuels, small concentrations of fine particles pass through the filters and reach the turbine surfaces, even if the filters are well maintained. Deposits build up over a year or two of operation and cause operational problems. This project is a study of synfuel flyash deposition on representative turbine blade surfaces that include thermal barrier coatings, with the goal of determining the magnitude of deposition, erosion, and corrosion for the application of alternative fuels in modern gas turbines.

Approach

A TADF was originally built in 2004 (Figure 1), consisting of a partially premixed natural gas fired combustor capable of operating at an exit Mach number of 0.3 and an exit temperature of 1,183°C, thus simulating the conditions at the entrance of a typical first stage nozzle guide vane for an F-class power generation turbine. Coupons are obtained from turbine blade manufacturers that include the TBC. These coupons are placed at the exit of the combustor, and flyash particles are fed through the combustor to cause deposition on the coupon. Tests at atmospheric pressure have shown that deposits formed in 4 hours in the TADF are similar to deposits generated in 8,000 hours of turbine operation [1].

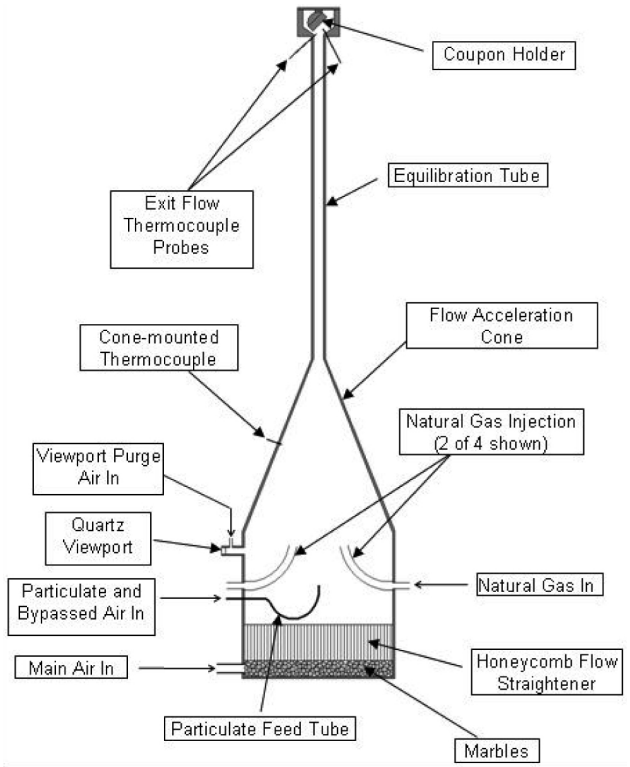

FIGURE 1. Schematic of the BYU Turbine Accelerated Deposition Facility (TADF)

Deposits formed in the TADF are photographed *in situ*, and then the coupon is removed for further analysis. Surface roughness characteristics are analyzed using a profilometer. Environmental scanning electron microscope (ESEM) analysis is used to take photos of the surface and perform X-ray elemental analysis. Coupons are then encased in epoxy, sliced in half, and the cross section is analyzed by ESEM.

Results

A. Particle Size Series. Deposition tests were conducted with four different sizes of flyash from a subbituminous coal. The coupon was not cooled, so the coupon surface temperature was the same as the gas temperature (1,183°C). The amount of deposit increased monotonically with particle size. The net capture efficiency was calculated by dividing the deposition rate of particulate (mg/hr) by the corresponding mass flow of particulate (mg/hr). Figure 2 shows the effect of particle size on net capture efficiency. Capture efficiency increases asymptotically with particle size, increasing more than 50% as particle size increased from 3 μm to 16 μm. These results suggest that with filter degradation, as larger particles pass through the filter, deposition problems as well as turbine hardware damage are likely to increase considerably. Additionally, it is important to

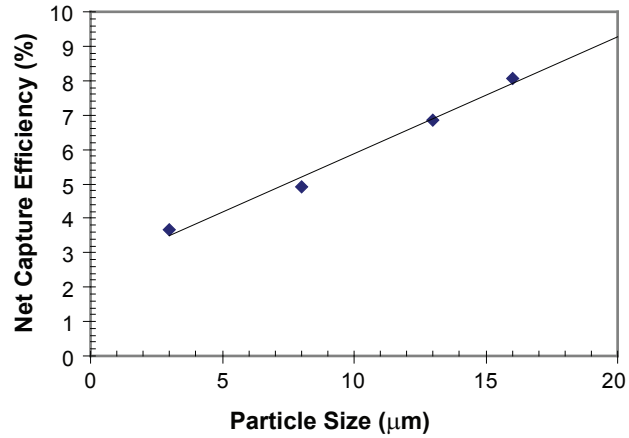

FIGURE 2. Effect of Particle Size on Net Capture Efficiency

note that even the smallest size particles tested showed significant deposition.

In some cases, the deposit was very fragile and much of it flaked off following the test as it cooled. The mass of the separated deposit was monitored as well as the attached deposit. Some samples exhibited significant spallation of the TBC layer, where the mass of the separated deposit (plus TBC) weighed more than the net specimen mass gain. Spallation seemed to occur at the leading edge of the coupon. The percentage of separated deposit increased with increasing particle size, indicating that TBC is more prone to spall with larger deposit formations.

B. Gas Temperature Series. A series of tests was conducted to determine how gas temperature affects the amount of deposition. Subbituminous coal flyash with a mass mean diameter of 3 μm was used in these tests. No cooling of the coupon was used, so that the coupon surface temperature was the same as the gas temperature. Figure 3 shows the net capture efficiency as a function of gas temperature. The same flaking

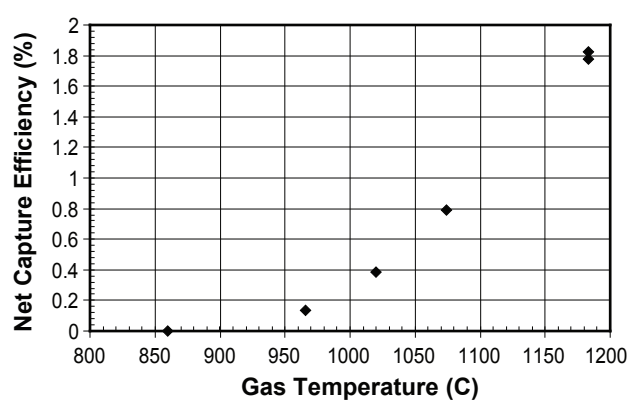

FIGURE 3. Effect of Gas Temperature on Net Capture Efficiency

was observed for the tests run at 1,183°C, but very little flaking was noticed at lower temperatures. At 860°C no deposit formed indicating a gas temperature threshold for deposition around 960°C for this study. This compares well with studies performed previously by Wenglarz and Fox [2] using coal-derived fuel, Kim et al. [3] using volcanic ash, Jensen et al. [1] using airborne dust. The strong dependency of deposition rate on gas (and particle) temperature has important implications for modern turbine blade rows where the gas temperature can drop by 150-250°C per stage. If the turbine inlet temperature is high enough so that particles are molten or sinter readily, they may collect primarily near the leading edge – since with falling temperatures through the vane passage, sintering may no longer be possible. If however, the gas temperature at the vane inlet is so high that corrosive elements in the vapor phase may not deposit until the temperature drops, perhaps in the subsequent blade row.

C. Impingement Cooling Series. The third test series was performed to study the effects of impingement cooling on deposition. The insulation was removed from the interior of the cooling fixture, and two K-type thermocouples were welded to the backside of each sample to measure the backside temperature. This test series used the same set of samples as in the particle size series. Four tests were run at varying mass flows of coolant and compared with the insulated case. The same coal ash was used as in the base case (3 μm diameter, 1,183°C, Mach No. = 0.25). Trends in net capture efficiency are shown in Figure 4. For this series, spallation occurred, but was limited to very small portions of the edge at the base of the sample. The amount of visible spallation decreased slightly with increased coolant mass flow.

Figure 5 shows the level of spallation which occurred at the leading edge as a result of deposit penetration. Similar spallation was seen in the particle size test series. Wammack et al [4] observed a similar deposit penetration effect although with a different

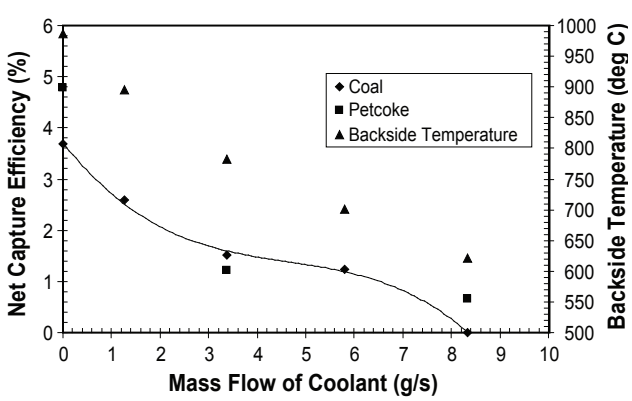

FIGURE 4. Effect of Impingement Cooling on Net Capture Efficiency

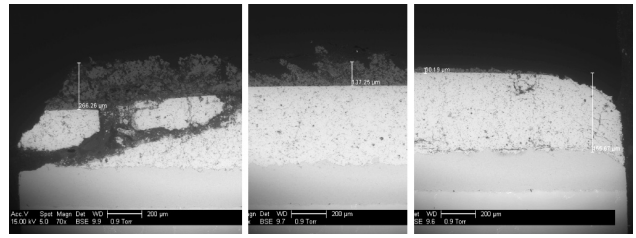

FIGURE 5. Typical Image Series of Bottom (left), Middle, and Top (right) Portions of 5.81 g/s Coolant Test Sample

TBC material system. With the exception of the highest cooling case, all other tests in this series had varying amounts of spallation damage caused by penetration of the deposit along the cross section.

Conclusions and Future Directions

- Increasing the flyash particle size from 3 to 16 μm more than doubled the deposition rate at 1,183°C.
- Particle deposition rate was found to decrease with decreasing gas temperature, with a threshold gas temperature for deposition of approximately 960°C.
- Deposition rates decreased with increasing mass flow of impingement cooling air, as expected.
- Deposits caused spallation of the TBC in some tests, particularly at the leading edge of the coupon.
- Post exposure analyses (scanning electron microscopy and X-ray spectroscopy) of the impingement cooling test series show decreasing TBC damage with increased cooling levels.
- Future experiments with film cooling through cylindrical and shaped holes in coupons are planned during the coming year.
- Roughness maps of deposits from film cooling experiments will be used to make scaled plexiglass models for wind tunnel testing. These tests will determine how deposits between cooling holes affect flow and heat transfer.

Special Recognitions & Awards/Patents Issued

Best paper awards from the ASME International Gas Turbine Institute Heat Transfer Division for two papers presented in 2006:

1. Wammack, J. E., J. Crosby, D. Fletcher, J. P. Bons, T. H. Fletcher, "Evolution of Surface Deposits on a High Pressure Turbine Blade, Part I: Physical Characteristics," Paper GT2006-91246, ASME Turbo Expo Meeting, Barcelona, Spain (May 8-11, 2006); accepted by *ASME Journal for Gas Turbines and Power* (2006).

2. Bons, J. P., J. E. Wammack, J. Crosby, D. Fletcher, T. H. Fletcher, "Evolution of Surface Deposits on a High Pressure Turbine Blade, Part II: Convective Heat Transfer,"

Paper GT2006-91257, ASME Turbo Expo Meeting, Barcelona, Spain (May 8-11, 2006); accepted by *ASME Journal for Gas Turbines and Power* (2006).

FY 2007 Publications/Presentations

1. Bons, J. P., J. Crosby, J. E. Wammack, B. I. Bentley, and T. H. Fletcher, "High pressure Turbine Deposition in Land Based Gas Turbines from Various Synfuels," *ASME Journal for Gas Turbines and Power*, **129**, 135–143 (2007).

2. Crosby, J. M., S. Lewis, J. P. Bons, W. Ai, and T. H. Fletcher, "Effects of Particle Size, Gas Temperature, and Metal Temperature on High Pressure Turbine Deposition in Land Based Gas Turbines from Various Synfuels," Paper GT2007–27531, presented at the ASME Turbo Expo Meeting, Montreal, Canada (May, 2007).

3. Crosby, J. M., "Particle Size, Gas Temperature, and Impingement Cooling Effects on High Pressure Turbine Deposition in Land-Based Gas Turbines from Various Synfuels," M.S. Thesis, Mechanical Engineering Department, Brigham Young University, April, 2007.

References

1. Jensen, J.W., Squire, S.W., Bons, J.P., and Fletcher, T.H., 2004, "Simulated Land-Based Turbine Deposits Generated in an Accelerated Deposition Facility," presented at IGTI 2004 in Vienna, June 2004. Paper #GT2004–53324.

2. Wenglarz, R.A., and Wright, I.G., "Alternate Fuels for Land-Based Turbines," published in proceedings of the "Workshop on Materials and Practices to Improve Resistance to Fuel Derived Environmental Damage in Land- and Sea-Based Turbines," October 22–24, 2002, Colorado School of Mines, Golden, CO.

3. Kim, J., Dunn, M.G., and Baran, A.J. et al, 1993, "Deposition of Volcanic Materials in the Hot Sections of Two Gas Turbine Engines," J. Engr. Gas Turbines & Power vol. 115, July 1993, pp. 641–651.

4. Wammack, J.E., Crosby, J., Fletcher, D., Bons, J.P., and Fletcher, T.H., 2006, "Evolution of Surface Deposits on a High Pressure Turbine Blade, Part I: Physical Characteristics," presented at IGTI 2006 in Barcelona, Spain, May 2006, #GT2006–91246.

V.A.2 Aero Losses, Heat Transfer, Discharge Coefficients for Different Vane Trailing Edge Cooling Technologies for Syngas Fired Turbines

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Objectives

- Develop four relevant trailing edge cooling concepts: gill slot, letterbox, covered trailing edge (TE), and pressure side holes.
- Develop three internal cooling geometries consistent with the trailing edge concepts.
- Characterize internal heat transfer and discharge pressure drop.
- Characterize external heat transfer and aerodynamics.
- Investigate the impact of syngas derived roughness on performance of cooling geometries.

Accomplishments

- Developed and tested gill slot and letterbox trailing edge cooling configurations.
- Designed and fabricated both standard and high solidity pin fin arrays.
- Characterized internal heat transfer and discharge pressure drop in standard solidity pin fin array with and without letterbox partitions.
- Characterized downstream heat transfer and adiabatic effectiveness for gill slot.
- Characterized letterbox partition heat transfer and adiabatic effectiveness.
- Acquired exit survey loss measurements for both gill slot and letterbox vanes over a wide range of Reynolds numbers, turbulence conditions, and blowing rates.
- Acquired representative roughness surface from Brigham Young's accelerated roughness rig.

Introduction

One of the most difficult regions of a gas turbine to cool is the trailing edge of a vane or blade. Aerodynamic considerations require the trailing edge to smoothly narrow to a small radius, while controlling the diffusion of boundary layers. Heat transfer challenges include cooling a surface with a high heat load far downstream from where film cooling protection is optimum in a region with little area for the flow of cooling air. At the same time, strong market forces are pushing the power industry toward the use of coal-derived syngas in gas turbine systems. However, even the cleanest syngas will contain small amounts of sulfur and particulate contamination, which can be expected to roughen turbine surfaces due to deposition and corrosion. Surfaces roughened from deposition and corrosion will produce higher surface heat transfer coefficients, higher aerodynamic losses, reduced film coverage, and reduced effective throat area. Turbine systems fueled by syngas will need designs tolerant of these effects. Consequently, the trailing edge region of vane and blades will be even more difficult to design.

Approach

The measurements for this study have been conducted using a "fully" or conventionally loaded vane. The large-scale, low-speed cascade facility at the University of North Dakota is being engaged to conduct these experiments. The UND cascade runs at low Mach numbers (0.05 – 0.2) and requires a special vane geometry to achieve a fully loaded pressure profile similar to the midspan pressure distribution of the engine nozzle guide vane. The large-scale low-speed cascade has been run at steady-state allowing for detailed 3-D exit surveys and good detail in internal pressure drop and external heat transfer and pressure distribution. The low Mach number geometry has a higher axial chord to true chord ratio and more surface curvature than the compressible vane. However, the dimensionless loading profile shown in Figure 1 is very consistent with a compressible vane with a fully loaded profile. (The incompressible and compressible vane geometries were graciously provided by the turbine aero-dynamics and heat transfer group at Rolls Royce.) The resulting calculated compressible (Mach = 0.8) and incompressible (Mach = 0.2) pressure profiles are compared in Figure 1 showing closely agreeing loading distributions. Figure 1 also shows a comparison between the measured and predicted pressure distributions

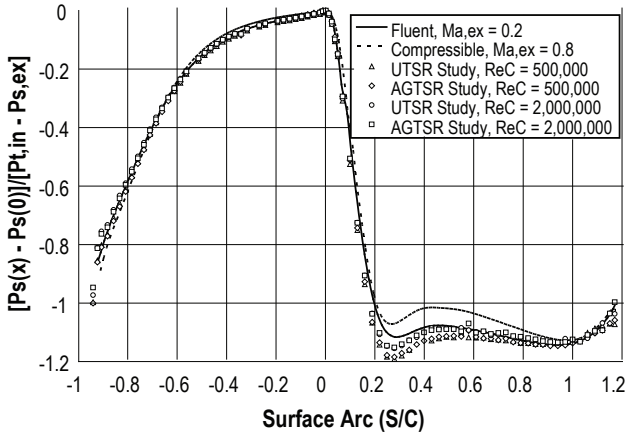

FIGURE 1. Measured Solid Vane Pressure Distribution Compared with Calculated Pressure Distributions for Incompressible and Compressible

for the incompressible vane, at Mach numbers of about 0.05 and 0.2. The comparison shows the very close agreement between the experimental base vane pressure distribution and the Fluent calculation. This close agreement provides confidence that the midline aerodynamics developed by the linear cascade are consistent with the 2-D blade to blade aerodynamics.

The initial geometry investigated was the gill slot. This geometry has been developed in the envelope of the base vane configuration. The letter box geometry is similar to the gill slot geometry but has the addition of partitions at the exit of gill slot vane. The letterbox geometry for UND's incompressible base vane is shown in Figure 2 along with the static pressure instrumentation. The scaling for UND's vane is 11 times. The locations of the pressure taps are displayed in the figure along with the locations of the five row pin fin array and the letterbox partitions which engage the gill slot and extend to the trailing edge. The locations of the pressure taps and thermocouples on the letterbox vane are consistent with the gill slot vane.

The converging pin fin array heat transfer levels were determined in a bench scale rig shown schematically in Figure 3. The bench scale rig consists of a small (2 kW) pressure blower controlled by a variable speed drive. The blower discharges into a plenum which directs the air through a heat exchanger and into a 15 cm diameter polyvinyl chloride (PVC) pipe used as an orifice tube. The PVC pipe then directs the air into the flow conditioning section of the bench scale pin fin rig. The flow conditioning section consists of a diffuser, a series of screens, and a converging section to the pin fin array. The converging section has three rows of wooden pins prior to the entrance of the aluminum pin fin array. The converging section, fabricated from 3.81 cm thick polystyrene insulation, the pin fin array,

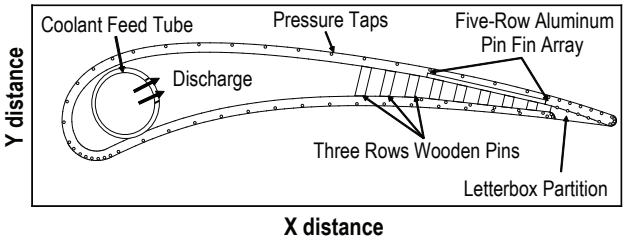

FIGURE 2. Letterbox Cane Geometry Showing Pressure Taps, Pin Fin Array and Partition Locations

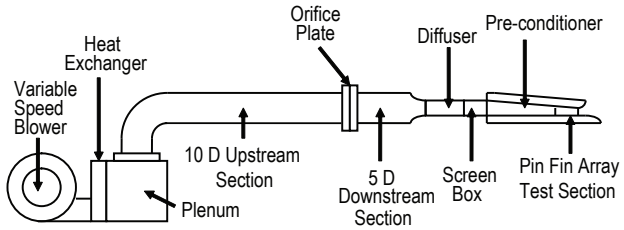

FIGURE 3. Schematic of Converging Channel Pin Fin Array Bench Scale Test Rig

and the polystyrene trailing edge contours are shown schematically in Figure 3.

Results

Our research on trailing edge heat transfer and aerodynamics provides quantitative information to designers allowing them to make choices between competing cooling designs. This information includes results that document vane exit losses and turning angle including effects of cooling flow, Reynolds number, and turbulence condition. We have also investigated heat transfer rates and adiabatic effectiveness levels downstream from pressure side coolant discharge. This comprehensive database is expected to allow heat transfer and aerodynamic performance comparisons between the different trailing edge cooling schemes. These cooling schemes include the common gill slot (sometimes called a cutback), a trailing edge with letterbox partitions, the covered trailing edge and a vane with pressure side hole ejection. We believe that this comprehensive information will allow designers to make more informed choices when selecting a cooling configuration.

Our exit loss measurements include a full exit survey taken over a four to one range in Reynolds number and at three separate turbulence conditions. Additionally, these measurements have been taken over a range of cooling flows. Figure 4 presents exit survey loss and secondary flow data for the letterbox vane with grid generated turbulence. This figure is an example of

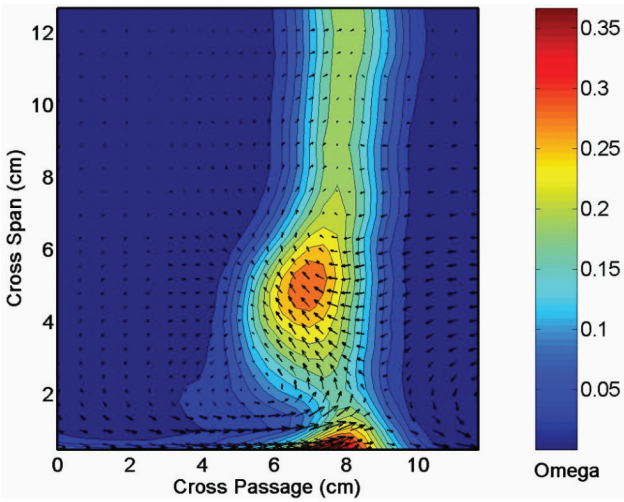

FIGURE 4. Total Pressure Loss Contours Ω (Omega) with Secondary Velocity Cectors for the Letterbox Vane at ¼ Axial Chord Location under Grid Turbulence at a Chord Exit Reynolds Number of 1,000,000 and Design Flow Rate Discharge

the exit loss surveys being taken during this research investigation.

Our heat transfer and adiabatic measurements have focused on determining how trailing edge geometries affect heat transfer and adiabatic effectiveness of surfaces downstream of cooling ejection. Additionally, we have also documented internal heat transfer for one standard pin fin array and are currently working on two high solidity internal cooling channels. Detailed heat transfer and adiabatic effectiveness distributions are critical input for designers charged with developing reliable and efficient cooling schemes for the trailing edges of turbine vanes and blades. An example of some of the adiabatic effectiveness measurements is shown in Figure 5. Figure 5 presents adiabatic effectiveness distributions for the side surfaces and for the top surface of the letterbox partitions as a function of local blowing ratio. The data are shown for a range of blowing ratios and for a four to one range in vane exit chord Reynolds numbers. Generally, the data are representative for all three turbulence conditions so this figure provides a comprehensive and useful look at partition film cooling levels. Partition film cooling effectiveness was found to be largely insensitive to both the external turbulence condition and the chord Reynolds number.

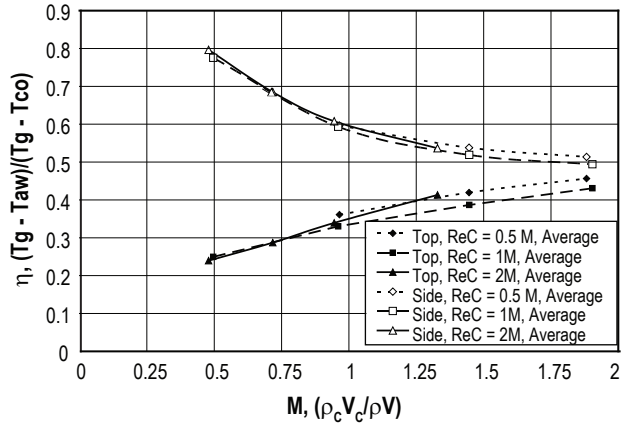

FIGURE 5. Adiabatic Film Cooling Effectiveness for Letterbox Partition Showing Effect of Local Blowing Ratio on Partition Side and Top Surfaces, Various Reynolds Numbers and Turbulence Conditions

Conclusion and Future Directions

Our comprehensive database for trailing edge cooling configurations is beginning to provide concrete information regarding the aerodynamic penalty associated with a cooling scheme at a given Reynolds number and cooling flow. We are currently beginning measurements related to the covered trailing edge geometry heat transfer and aerodynamic performance. In the near future we will begin developing our methodology to assess the influence of syngas roughened surfaces on surface heat transfer and aerodynamic penalties.

FY 2007 Publications/Presentations

1. Ames, F.E., Johnson, J.D., and Fiala, N.J., 2007, "Gill Slot Trailing Edge Aerodynamics– Effects of Blowing Rate, Reynolds Number, and External Turbulence on Aerodynamics Losses and Pressure Distribution," ASME Paper No. GT2007-27399. (Recommended for publication in the Journal of Turbomachinery and presented and published at Turbo Expo 2007, Montreal, Canada.)

2. Ames, F.E., Fiala, N.J., and Johnson, J.D., 2007, "Gill Slot Trailing Edge Heat Transfer – Effects of Blowing Rate, Reynolds Number, and External Turbulence on Heat Transfer and Film Cooling Effectiveness, ASME Paper No. GT2007-27397. (Presented and published at Turbo Expo 2007, Montreal, Canada.)

V.A.3 Effects of Coating Blockage and Deposits on Film Cooling Effectiveness and Heat Transfer

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Objectives

- To explore the transport phenomena related to the effects of blockage and surface deposits around film cooling holes in advanced gas turbines.
- To develop advanced concepts incorporating modifications in hole shape and surface profile for more effective film cooling.
- To quantify new film cooling concepts with a combined approach of detailed experimental measurements and computational simulations.
- To provide the turbine manufacturers with fundamental insight that can impact the future designs of turbine cooling systems.

Accomplishments

- Performed detailed measurements of both film effectiveness and heat transfer coefficient for 30-degree inclined film cooling holes with a transverse trench.
- Quantified the effects of the trench on improved film effectiveness; the improvement is about 30-100% for low blowing ratio M<0.5, and more than 150% for relatively high blowing ratio, say M>1.
- Revealed the insensitivity of the heat transfer coefficient to the presence of the trench, especially sufficiently far away from the injection hole, say X/D>8.
- Developed a new film cooling concept with W-shaped holes to alleviate coolant lift-off.
- Demonstrated computationally the film effectiveness of W-shaped holes up to 100% higher than the corresponding baseline case with straight circular holes.

Introduction

The primary goal of this university turbine research project is to provide the turbine industry with fundamental insight that can impact the future design of film cooling. The initial phase of the project is to characterize the effects of blockage and surface deposits on the film cooling performance. This will be followed by a systematic approach to explore innovative means to further improve the film cooling performance under realistic turbine conditions. Validation of computational models will use the heat transfer and flow data obtained from the experimental aspect of the project. On the other hand, information gained from the computation will provide the experiment with more detailed insight in data interpretation. A significant portion of the project is to incorporate the change in surface profile, due possibly to unavoidable deposits or intentional modification of the thermal barrier coating (TBC) for more effective cooling film protection. Several innovative concepts have been developed and fully characterized in this project. This will eventually aid the selection of optimal test geometry and parameters.

Approach

The project is a combined effort of experiment and numerical computation for studying the transport phenomena associated with the effects of surface profiles and hole shapes on the performance of film cooling. The research team consists of participants from two universities: University of Pittsburgh (Pitt) and Iowa State University (ISU). The Pitt portion of the combined project is an experimental investigation of the film cooling performance affected by surface features and hole geometry. The specific tasks conducted at Pitt include detailed measurements of surface heat transfer coefficient and film effectiveness. The research focus at ISU is to perform computational fluid dynamic (CFD) simulation of transport phenomena and providing guidelines for improved designs in film cooling. Validation of computational models use the heat transfer

and flow data obtained from the experimental aspect of the project. On the other hand, information gained from the computation provides the experiment with more detailed insight in data interpretation. This experiment-simulation combined approach has been demonstrated to be very effective for exploring complex aerothermal issues in advanced turbine systems.

Results

A discrete film cooling hole is typically cylindrical or diffusion fan-shaped with 30°-35° inclination relative to the protected surface along the streamwise direction. Full coverage thermal protection can only prevail when coolant flow keeps attaching onto the protected surface and never penetrates and dissipates into the hot mainstream. However, this desirable condition has never been achieved based on the current cooling technology, as the coolant will always lift-off from the surface because of the interaction between the mainstream and injected coolant. Figure 1 illustrates such a phenomenon with complex vortex structures.

To address the coolant lift-off issue, there have been numerous studies via either altering vortices structure or varying the geometry of the film cooling hole or both combined. In the earlier phase of this project, two advanced concepts with a placement of (1) upstream ramp, and (2) downstream aligned blocks, were explored. The results have been reported in the earlier annual report. As one of the main tasks in this year's project, the third approach with film cooling embedded in a two-dimensional trench developed earlier by Bunker [1] was further examined. While the trench concept is known to be working, the intent here is to obtain more detailed performance data, so a systematic comparison with other enhancement concepts can be made under the same platform and operating conditions. This will provide a viable guideline for down-selecting the optimal approaches for advanced film cooling technology.

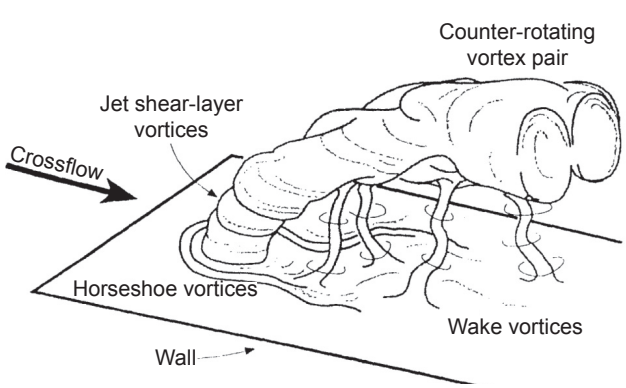

FIGURE 1. Schematic of Vortex Structure Associated with a Jet in Cross Flow

Figure 2 shows the actual test plate where three 30-degree inclined film cooling holes are embedded in a transverse shallow trench.

With the detailed data of both the local film effectiveness and heat transfer coefficient obtained from the experiments at Pitt, the ratio of heat flux, q/q_o, with film cooling injection to that without film cooling can be determined. While such a heat flux ratio is a viable indication of the overall film cooling performance, a lower ratio represents better film protection. Figure 3 shows the distribution of spanwise-averaged q/q_o. The baseline data represents the case of film cooling without a trench. Clearly the trench reduces the values of q/q_o for blowing ratios M>0.57. This is especially effective in the near hole region, say X/D<2, where the value of q/q_o is zero, signifying a perfect film protection. The improvement by the presence of the trench is nearly 100% compared to the corresponding baseline cases without a trench.

While a trench modifies the injected coolant for more lateral spreading before reaching the protected surface, shaped holes increase cooling effectiveness by expanding the cross-sectional area near the exit to augment lateral spreading. Also explored in this year's

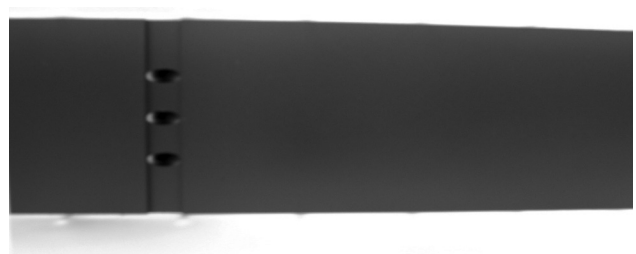

FIGURE 2. Photo of Test Plate with Film Cooling Holes Embedded in a Trench

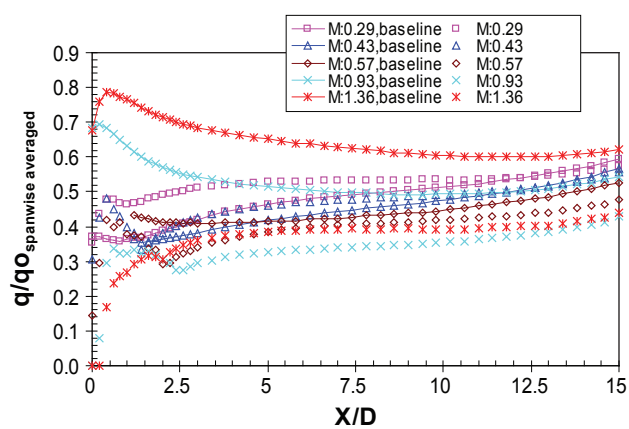

FIGURE 3. Streamwise Distribution of Spanwise Averaged Heat Flux Ratio

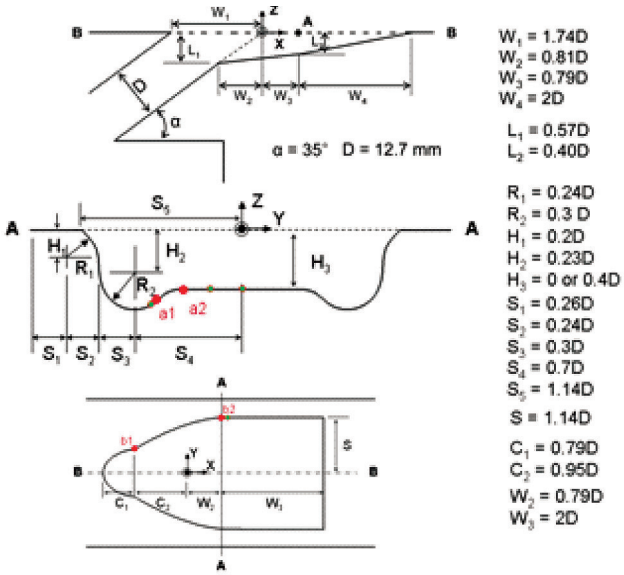

FIGURE 4. Schematic of W-Shaped Hole Design Concept

TABLE 1. Summary of Simulations

Case No.	Hole Geometry	H_3 (Fig. 3)	M
1	straight	N.A.	0.49
2	TSH*	N.A.	0.49
3	W-shaped	0.4D	0.49
4	W-shaped	0.0	0.49
5	W-shaped w/ trench	0.4D	0.49
6	W-shaped w/ trench	0.0	0.49
7	W-shaped w/ trench	0.0	0.31
8	W-shaped w/ trench	0.0	0.97
9	W-shaped w/ trench	0.0	1.40

*TSH = traditional shaped hole with the W shape

project is a new concept involving a W-shaped cross-sectional area in which the middle part of the W-shape protrudes and widens as the W-shaped hole widens. To examine the usefulness of the design concepts, CFD analyses were performed for a traditional shaped hole and two W-shaped holes. Figure 4 shows the W-shaped configuration studied, and Table 1 summarizes the cases studied.

The simulated results, as shown in Figure 5, reveal that the traditional shaped hole (case 2) is better than the straight hole (case 1), which is expected from previous studies on shaped holes. When the W-shaped hole with $H_3 = 0.4D$ (case 3) is compared with the

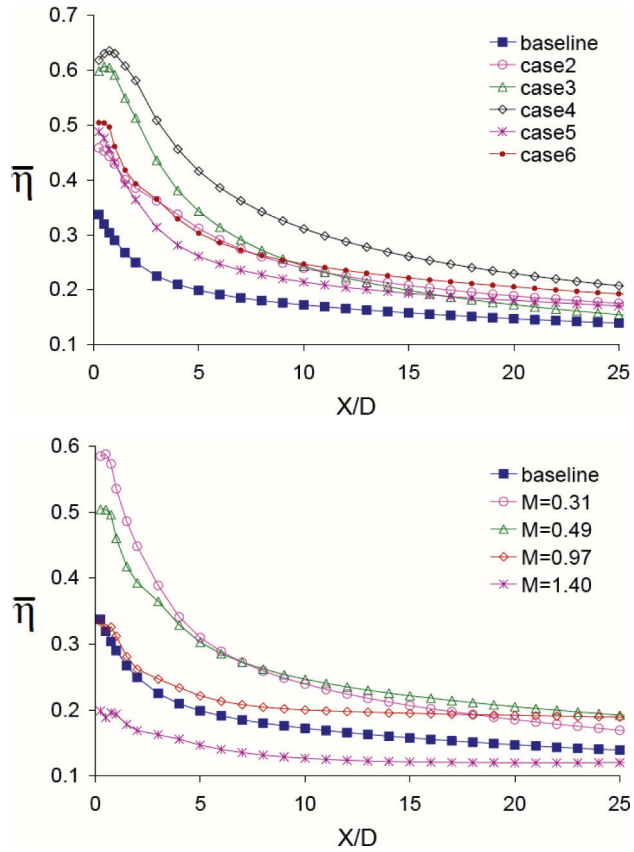

FIGURE 5. Predicted Laterally Averaged Adiabatic Effectiveness (baseline is case 1)

traditional shaped hole, it was found to perform better for X/D up to 11 or 12. Beyond X/D = 11 or 12, the traditional shaped hole performed better. However, for the W-shaped hole with $H_3 = 0$ (case 4) which has the highest protrusion (a protrusion that is flush with the flat plate), it did perform better than the traditional shaped hole for all X/D studied.

Conclusions and Future Directions

- Built on the accomplishments made in the first two years, reasonable progress in both experimental and computational fronts has been made in Year 3. As a continuing pursuit of optimizing film cooling performance with advanced concepts, the experimental effort during this phase of study is to characterize a recently identified approach with injection holes embedded in a two-dimensional trench. The experimental results show that a trench has a profound influence on reducing the heat flux imposing on the surface when the blowing ratio is higher than approximately 0.5. This effect is particularly significant in the region immediately downstream to the trench, with an impressive 180% increase. The reason of this is that the trench

helps the coolant to spread laterally, which reduces the momentum of injection coolant and better coverage toward downstream. Therefore, the trench configuration is especially effective for film cooling when the blowing ratio is sufficiently high.

- On the computational front, a new W-shaped-hole design concept was developed and evaluated. The protrusion in the middle of the W-shape cross-section is an added parameter to control the acceleration and momentum of the cooling jet for increased downstream and lateral coverage. Results obtained show the W-shaped holes to significantly improve film-cooling effectiveness when compared to a straight hole with the same angle of inclination and a shaped hole identical to the W-shaped hole except without the protrusion in the middle. Results obtained also show that a W-shaped hole with a trench performs well only with low blowing ratios, but pressure disruption is greatly minimized.
- The project is on schedule and no modification in work statement is needed.

Special Recognitions & Awards/Patents Issued

Patent Disclosures:

1. Preventing Hot-Gas Ingestion by Film-Cooling Jets Via Flow-Aligned Blockers (Application No.: 60/829,734; Filing Date: 10/17/06).

2. MOMENTUM PRESERVING FILM-COOLING SHAPED HOLES (Application No.: 60/829,712; Filing Date: 10/17/06).

3. INCREASING ADIABATIC FILM-COOLING EFFECTIVENESS BY USING AN UPSTREAM RAMP (Application No.: 60/829,737; Filing Date: 10/17/06).

FY 2007 Publications/Presentations

1. Li, Y., Zhou, Y., Shock, R., Staroselsky, Chen, H., and Shih, T.I-P., "Simulation of Film Cooling Flow from one Row of Inclined Cylindrical Jets by Using the Lattice-Boltzmann Method, AIAA Paper 2007-0127, Aerospace Science Meeting, Reno, January 2007.

2. Zhu, B., Chi, X., Dennis, R.A., Chyu, M.K., Bryden, K.M., and Shih, T. I-P., "Internal Cooling inside an L-Shaped Duct with Pin-Fin Turbulators under Rotating and Non-Rotating Conditions with and without Sand Particles," ASME IGTI Paper GT-2007-27598, IGTI Conference and Expo, Montreal, Canada, May 14–17, 2007.

3. Shih, T.I-P. and Na, S., "Momentum-Preserving Shaped Holes for Film Cooling," ASME IGTI Paper GT-2007-27600, IGTI Conference and Expo, Montreal, Canada, May 14–17, 2007.

4. Chen, S.P., Chyu, M.K., and Shih, T.I-P., "Effects of Upstream Ramp on the Performance of Film Cooling," ASME Paper GT2007-28137, Montreal, Canada, May 14–17, 2007.

5. Na, S. and Shih, T. I-P., "Enhancing Film-Cooling Effectiveness via an Upstream Ramp," ASME Journal of Heat Transfer, Vol. 129, No. 4, April 2007, pp. 464-471.

6. Shih, T. I-P. and Na, S., "Enhancing the Effectiveness of Film Cooling," Journal of Aerospace Power, accepted.

References

1. Bunker, R. S., 2002, "Film Cooling Effectiveness Due to Discrete Holes Within a Transverse Surface Slot," Paper GT-2002-30178, IGTI Turbine Expo, Amsterdam, Netherlands.

2. Na, S. and Shih, T.I-P., "Increasing Film-Cooling Adiabatic Effectiveness by Using an Upstream Ramp," ASME Paper GT-2006-91163, IGTI Conference and Expo, Barcelona, Spain, May 8–11, 2006.

3. Na, S. and Shih, T. I-P., "Enhancing Film-Cooling Effectiveness via an Upstream Ramp," *ASME Journal of Heat Transfer*, Vol. 129, No. 4, April 2007, pp. 464-471.

4. Shih, T.I-P. and Na, S., "Momentum-Preserving Shaped Holes for Film Cooling," ASME IGTI Paper GT-2007-27600, IGTI Conference and Expo, Montreal, Canada, May 14–17, 2007.

5. Shih, T.I-P., Na, S., and Chyu, M.K., "Prevent Hot-Gas Entrainment by Film-Cooling Jets via Flow-Aligned Blockers," ASME Paper GT-2006-91161, IGTI Conference and Expo, Barcelona, Spain, May 8–11, 2006.

V.A.4 Simulating Particle Deposition and Mitigating Deposition Degradation Effects in Film Cooled Turbine Sections

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Objectives

- Develop a methodology for simulating depositions of contaminant in a laboratory test facility that duplicates depositions in operating engines.
- Determine degradation caused by particle depositions for a film-cooled vane with coolant holes embedded in shallow trenches.
- Design improved shallow trench film cooling configurations that will have minimum degradation due to deposited contaminants.
- Evaluate the degradation of film cooling due to deposited contaminants along the endwall of a first vane passage.
- Optimize the film cooling configuration and endwall contour to alleviate and mitigate particle deposition effects on the cooling of an endwall.

Accomplishments

The project is due to begin August 1, 2007.

Introduction

A major concern for the next generation power generation gas turbines is the capability to operate with greater efficiency while using new coal-derived high hydrogen fuels. A major factor when using these fuels is the effects of contaminants on engine operation, particularly the hot section of the gas turbine. In general contaminants in the main flow can affect the turbine section by causing erosion, corrosion, or deposition to turbine airfoil and endwall surfaces. For higher temperature operation, which is the goal of for future designs, the primary degradation effect of contaminants occurs from deposition on turbine surfaces. This results in much rougher surfaces and partial blockage of film cooling holes which seriously degrade the cooling performance. Performing full engine tests to determine where these contaminants deposit and how to mitigate that deposition is cost prohibitive and often results in a lack of detailed information needed to understand the underlying physics of the deposition process. Methods need to be developed whereby accurate deposition simulations can take place in a facility that allows for the underlying physical effects on airfoil heat transfer and aerodynamics to be understood. A major objective of our proposed work is to determine a reliable methodology for simulating contaminant deposition in a low speed wind tunnel facility where testing is considerably less costly.

This project will develop new cooling designs for turbine components that will minimize the depositions of contaminant particles on turbine components and maintain good film-cooling performance even when surface conditions deteriorate. This will involve new film cooling designs on turbine airfoils and endwalls, and new endwall contouring. The focus of the new film cooling designs will be the use of coolant holes embedded in shallow trenches. Recent results from our laboratories, shown in Figures 1 and 2, demonstrate that this new "trench" configuration can more than double the film cooling effectiveness, η, over a wide range of coolant blowing ratios, M, even when the surface is significantly roughened by deposited contaminants.

Approach

A key part of this project is the use of a new technique for film injection that incorporates shallow transverse trenches that redistributes the coolant and provides a more uniform coolant coverage over the surface. Recent experiments in our laboratories have shown that this film cooling configuration maintains good performance even with significant depositions on the surface. However, for these previous studies the effects of deposition have been determined using somewhat simplistic models of obstructions located upstream and downstream of the coolant holes. An important part of this study is the development of techniques for simulating the active deposition of particles on turbine components. Once these techniques for active deposition of particulates are developed, new film cooling configurations will be designed

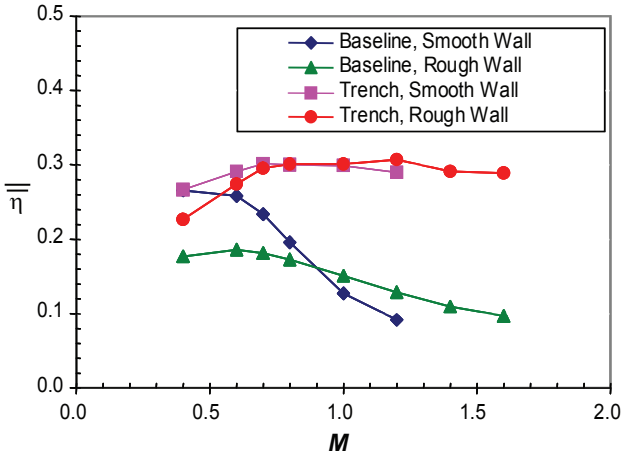

FIGURE 1. Experimental Results Showing the Increase in Film Effectiveness for the New Trench Configuration for Smooth and Rough Surfaces Compared to Standard Film Cooling Holes (Baseline)

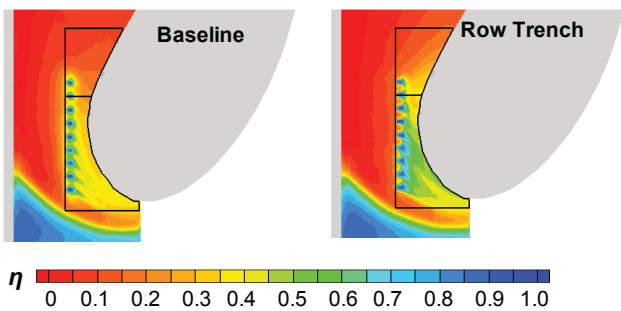

FIGURE 2. Contours Showing Improved Film Coolant Coverage Due to a Trench on the Endwall Approaching a Turbine Vane

that will minimize depositions on vane and endwall surfaces. Furthermore, new endwall contours will also be designed that minimize deposition rates to the surface. These new endwall contours will also be designed to reduce secondary flows and therefore reduce aerodynamic losses. The end result of the proposed research will be robust film cooling and endwall designs that perform well even with large contaminant levels in the mainstream.

Results

The project is due to begin August 1, 2007.

Conclusions and Future Directions

The initial task when this project starts in August, 2007 is to develop a methodology for injecting and collecting particles in the main gas path that simulates the deposition on surfaces. Both Penn State University and the University of Texas will work together to develop a method to generate simulated contaminant particles, injection method, and airfoil surface tackiness that will simulate depositions in a hot environment. A second method for simulating particle deposition will developed in which various materials that can be liquefied with a modest increase in temperature (e.g. wax) will be used as contaminant particles. These particles will be impacted on conduction component parts that will be cooled internally and via film cooling so that the molten particles will solidify and fuse to the surface. These deposition simulations will be compared with actual engine hardware through discussions with our industry partners to ensure that we are qualitatively simulating accurate deposition locations and amounts.

V.A.5 Syngas Particulate Deposition and Erosion at the Leading Edge of a Turbine Blade with Film Cooling

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Objectives

- The primary objectives of this research are to provide design data and tools to engineers by studying fluid-thermal particle dynamics in the leading edge region of a turbine blade in the presence of film-cooling jets and to quantify the potential deposition and erosion under different flow, thermal, and particle dynamics.
- Investigate the effect of particle size on deposition and find the critical particle diameter below which there is no deposition. Investigate whether deposition in cooling holes and subsequent blockage is a possibility and, if so, under what conditions this happens and what can be done to avoid this phenomenon.
- Investigate the effect of coolant injection ratio on particle trajectory. Smaller particles tend to follow the flow streamlines while larger particles deviate from the flow considerably and have a much larger propensity to collide with the blade surface.
- Investigate the effect of coolant temperature. Coolant jets can aid the condensation of corrosive vapors on the blade surface, while on the other hand they can solidify molten ash such that it does not stick to the surface. However, this can lead to increased erosion. Formulate design guidelines on the effect of gas, coolant, and surface temperature on deposition, erosion, and corrosion.
- Investigate the effect of deposition and ensuing surface roughness on heat transfer coefficient and adiabatic effectiveness. Investigate whether deposition is self-limiting or can result in a runaway cycle.
- Investigate whether commercial computational fluid dynamics tools predict deposition and erosion patterns with accuracy using a steady calculation procedure. The use of a steady flow assumption is the only viable alternative in a design environment, while the actual flow is highly unsteady in which time-dependent turbulent eddies have a large effect on particle transport.

Accomplishments

The project will start in August 2007.

Introduction

The vision of DOE's fossil energy turbine program is to provide power generation technology essential to the success of advanced fossil energy power systems in the 2008 to 2015 time frame. One of the key capabilities needed to achieve this goal is coal gasification. One of the issues in achieving this goal relates to the durability of turbine components subjected to a harsh high temperature, high pressure, and high velocity environment in the gas path immediately downstream of the combustor.

Coal gasification and combustion can introduce contaminants in the vapor as well as solid or molten state depending on the gas clean up procedures used, coal composition and operating conditions. These byproducts, when combined with high temperatures and high gas stream velocities, can cause deposition, erosion, and corrosion (DEC) of turbine components. Some of the common compounds which lead to DEC are trace amounts of sulphates, chlorides, and hydroxides of alkali metals such as calcium, sodium, potassium, and magnesium. Other metallic compounds of antimony, beryllium, chromium, mercury, selenium and vanadium are also threats for DEC. The extent of damage done by DEC in the gas path is directly dependent on the impaction of solid or molten particulates on surfaces, which lead to erosion and deposition. One surface which is particularly vulnerable is the leading edge of vanes and blades in the presence of film cooling.

Approach

This project will be performed at near engine conditions combining unique computational and experimental equipment and facilities for conditions relevant to the design of systems. A blade with a cylindrical leading edge and a camberless after body in a linear cascade will be tested. The work will use the method of time-accurate large-eddy simulations (LES) as a theoretical tool for simulating particle dynamics

and a high temperature experimental facility matched to relevant engine conditions. LES, by accurately representing the unsteady nature of the flow and temperature fields and the relevant turbulent length scales, will leave little uncertainty in modeling the trajectory of particles which will be very sensitive to these factors. By using carefully derived similarity parameters, the high temperature experimental facility will provide an inexpensive and effective testing environment, with much relevancy to industry.

To maintain a high degree of relevancy to industrial design, experimental and computational conditions represent real engine conditions. By using a high temperature test facility (up to 800 K) which can generate velocities up to 200 m/s in a 2”x5” cross-section, engine-like conditions are created in the test section. The use of this facility allows the matching of key similarity parameters relevant to the flow and thermal fields and particle dynamics such that experimental and computational observations can be extrapolated to the engine in a straightforward manner.

The computations will be performed using a state-of-the-art LES code developed by the principal investigator and applied extensively to complex turbulent flows in heat exchangers and in blade internal cooling geometries and leading edge film cooling, amongst other turbulent flows. It is highly parallel and uses hundreds of processors for quick turnaround time. It solves the Navier-Stokes and energy equations in a multi-block structured/unstructured generalized coordinate system. Its turbulence modeling capabilities include solving the Reynolds-Averaged Navier-Stokes equations using k-ω-based models, LES using the Smagorinsky and dynamic Smagorinsky models, and a hybrid detached-eddy simulation capability.

V. UNIVERSITY TURBINE SYSTEMS RESEARCH

B. Combustion

V.B.1 Turbulent Flame Speed Measurements and Modeling of Syngas Fuels

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Objectives

- Improve understanding of turbulent flame speeds of synthesis gas (syngas) fuels.
- Measure turbulent flame speeds of syngas fuels at conditions relevant to gas turbine combustors.
- Develop predictive flame speed models that can be used by gas turbine manufacturers to develop syngas combustors.

Accomplishments

This is a new project, just beginning.

Introduction

Turbulent flame speed, S_T, is a key combustion parameter that impacts the performance of low emission combustion systems. The turbulent flame speed is measure of how fast (e.g., at what velocity) the fuel and air can be consumed in modern, low emissions combustors, which operate with premixed fuel and air. Unanticipated changes in S_T during operation from the expected (design) conditions can therefore alter gas turbine pollutant emissions and combustor operability. While most current ground power gas turbines operate on natural gas fuel, there is great interest in allowing systems to operate on more available and secure sources, such as fuel gas synthesized from coal. These coal-derived syngas fuels contain varying amounts of H_2, CO and diluents, along with some hydrocarbons. The ability to operate on gases with high H_2 content may also permit reductions in CO_2 emissions.

Therefore, system designers and operators need information on S_T for the wide range of syngas fuel compositions. However, little is known about S_T for syngas fuels, in particular at the temperatures and pressures of interest to both simple cycle and recuperated gas turbines. The measurements that have been obtained were made primarily at atmospheric conditions and are of extremely limited usefulness for gas turbine (GT) operations.

Approach

The required effort consists of two basic tasks. First is the measurement task. An existing high pressure facility (Figure 1) is being modified to accommodate the burners needed to make quantitative turbulent flame speed measurements. Measurements of turbulent flame speeds are being acquired over a broad range of temperatures, pressure, and fuel compositions. The range of operating conditions is being determined in close coordination with gas turbine manufacturers. The second part of this project involves development of physics-based correlations of the turbulent flame speed data and models for predicting the flame speed characteristics of other fuels. The key end work product will be a model and a validating data set that can be used by industry for calculating the turbulent flame speed of syngas mixtures at temperatures and pressures of practical interest.

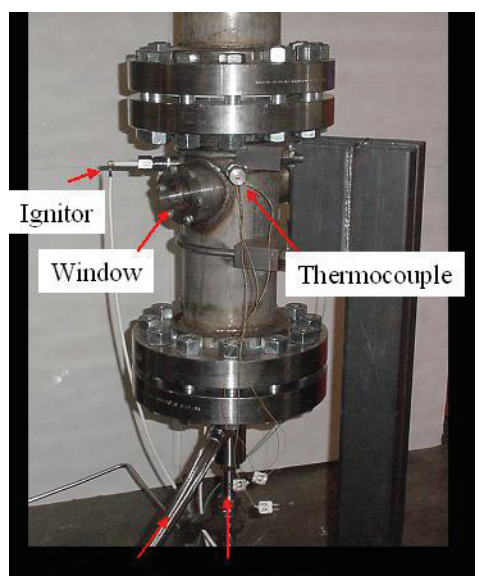

FIGURE 1. Photograph of High Pressure, Preheated Combustion Facility

Conclusions and Future Directions

Modification of the facility is underway. The first tasks to be accomplished in the upcoming year are determination of the range of measurement conditions in concert with our industrial collaborators, and S_T measurements over the composition and temperature matrix at low pressure.

V.B.2 Fundamental Studies in Syngas Premixed Combustion Dynamics

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Objectives

- Study lean syngas and hydrogen combustion over a range of gas compositions.
- Quantify syngas combustion lean flammability limits.
- Examine combustion dynamics in configurations that resemble gas turbine combustors.
- Propose ways of extending the syngas lean flammability limits while avoiding dynamics.

Accomplishments

- Conducted syngas tests in a model combustor to explore the effects of equivalence ratio and fuel composition on combustor stability.
- Completed the design, fabrication and installation of a new axisymmetric swirl stabilized combustor, with flexible modular construction, optically accessible test section.
- Conducted initial tests in the swirl combustor by changing the equivalence ratio, Reynolds number and syngas composition.
- Experimented with microjet stabilization in the swirl-stabilized combustor.

Introduction

Syngas, produced by the partial oxidation of coal in pure oxygen and steam inside high-pressure gasifiers, has been proposed as the fuel of choice for modern high efficiency low emission combined cycle power plants. In these integrated gasifier combined cycle (IGCC) plants, gas turbine engines are used as topping cycles that take advantage of high temperature combustion products of syngas to improve the overall energy conversion efficiency. Incorporating technologies to filter out turbine-corroding gases from the gasifier products and deliver clean syngas to the gas turbine combustor enables the use of syngas in gas turbines. The sequestration of carbon dioxide, e.g., following the production of steam for the bottoming cycle, makes this plant environmentally ideal.

Combustion of syngas differs fundamentally from that of other complex hydrocarbons for a number of reasons, including the high hydrogen content, the short ignition delay, and the high flame speed. The objective of this study is to investigate experimentally the fundamental properties of syngas combustion over a wide range of conditions. Data and models necessary for the design of stable, efficient and clean combustors for gas turbine engines running on syngas are being collected and assembled, and insight into the mechanisms governing the stability limits and the ensuing dynamics is being acquired, with the goal of proposing solutions that lead to efficient, clean and stable burning at high temperatures and high efficiency. Innovative solutions for stabilizing combustion at lean and ultra-lean conditions will be demonstrated in the laboratory, as well as abstracted in design guidelines.

Approach

We are constructing stability maps for premixed syngas combustion, whose coordinates are the fuel composition, that is, the ratio of hydrogen to carbon monoxide, the equivalence ratio, the Reynolds number, and the inlet temperature for a step-stabilized combustor and a swirl stabilized combustor. The focuses of our experiments are the lean and ultra lean limits, the associated dynamics observed as the equivalence ratio is reduced and the flow velocity is increased, and how the gas composition and other factors affect the blowout limits of the combustor. Mechanisms and precursors of dynamics, and the relationship between the dynamics and the blowout limits will be investigated using extensive, spatially resolved non-intrusive measurements and modeling analysis. Besides the static stability limits measured in the experiments, dynamics associated with unstable operation are being categorized under different operating conditions. The experimental measurements will be used to suggest means of modifying the stabilization zone passively so as to improve the stability limits without impacting other performance metrics such as emissions and efficiency. Modeling of flame propagation in syngas mixtures will be used to support the analysis of the experimental data.

Results

We conducted tests in the step-stabilized combustor over a range of Reynolds numbers, defined by the inlet flow velocity and inlet channel height, ranging from 5,000 to 8,500. The syngas composition was varied from 80% CO and 10% H_2 to 20% CO and 80% H_2, in 10% increments. At each syngas composition and Reynolds number, we collected data over the range of equivalence ratios at which a flame could be established in the system. The lower limit in each case is the lean flammability limit, below which flame blowout is observed. The upper stability limit is reached when the flame flashes back upstream of the test section.

Figure 1 shows the overall sound pressure level (OASPL) for syngas mixtures with compositions varying from 20% CO and 80% H_2 to 80% CO and 20% H_2 over a range of equivalence ratios at a Reynolds number of 8,500. Three distinct regimes can be identified: stable regime, quasi-stable regime and unstable regime. As the amount of hydrogen in the fuel is increased, the lean flammability limit is extended and transitions between operating regimes shifting to lower equivalence ratios. Decreasing the Reynolds number causes the unstable region to become narrower and the stable region to become wider. The transition to flashback at high equivalence ratio is more abrupt at high Reynolds numbers.

As expected from the strong distinction in the pressure levels among the identified modes, there are also substantial differences in the flame structure. A series of still images taken from a single cycle of the combustor's unsteady mode is compared with a similar sequence from the stable mode in Figure 2. The unstable mode is dominated by the periodic shedding of large-scale vortices. In the stable mode, the thin flame extending from the step tends to wrap around much smaller vortices that are shed at a higher rate. The temporal variation in the heat release rate is much smaller than that observed during the unstable operation.

We have also conducted a similar range of tests in our recently-constructed swirl-stabilized combustor. Despite the substantial differences in combustor geometry, we observe a family of operating modes similar to those seen in the backward-facing step. The OASPL for syngas mixtures with composition varying from 30% CO to 70% CO as a function of equivalence ratio is shown in Figure 3. As in the step combustor, there is a stable region at low equivalence ratios, a quasi-

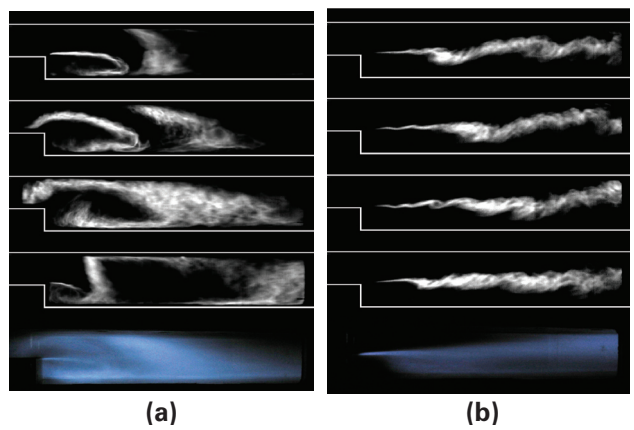

FIGURE 2. Image sequences of (a) an unstable flame in the backward-facing step combustor at equivalence ratio 0.38 and (b) a stable flame in the backward-facing step combustor at equivalence ratio 0.42. Both flames have 80% CO fuel composition. The inter-frame timing is approximately 9.2 ms. The exposure time is 0.47 ms. The final frame in each sequence is a 100 ms exposure showing the average flame structure.

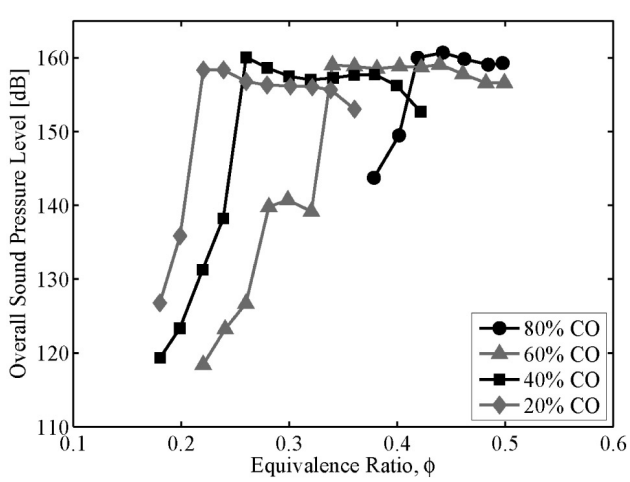

FIGURE 1. Dependence of Overall Sound Pressure Level on Equivalence Ratio and Syngas Composition in the Backward-Facing Step Combustor at a Reynolds Number of 8,500

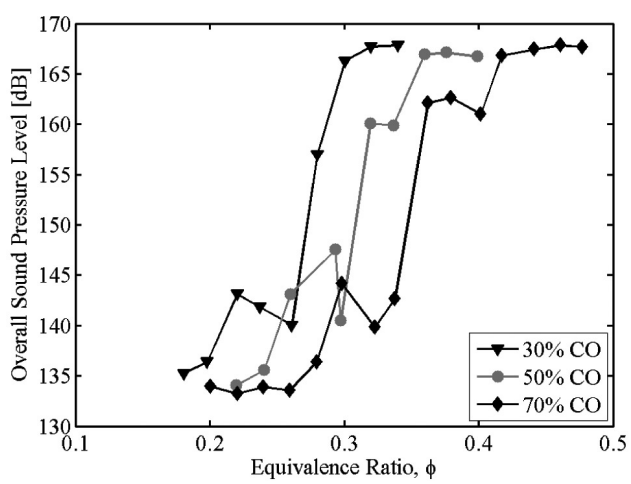

FIGURE 3. Dependence of Overall Sound Pressure Level on Equivalence Ratio and Syngas Composition in the Swirl-stabilized Combustor at a Reynolds Number of 25,000

stable region at intermediate equivalence ratios, and an unstable region at high equivalence ratios. Unlike in the step combustor, the OASPL in the quasi-stable region is only slightly lower than in the unstable region. Image sequences extracted from high-speed videos of typical unstable and stable flames in the swirl combustor are shown in Figures 4a and 4b, respectively. In the stable case, the flame is shaped like a funnel, with the majority of the burning occurring in the vortex break-down region downstream of the swirler. The base of the flame extends upstream of the expansion plane, where it is anchored on the swirler centerbody. The flame burns steadily, and the intensity in the burning zone varies only slightly with time. In the unstable case, the fuel burns in pulses, with a frequency corresponding to the observed pressure oscillations. The rapidly-burning flame is convoluted around a vortex which is periodically shed at the expansion plane. The enhanced mixing of the vortical interaction produces the rapid burning and produces a flame which is much more compact than the stable case.

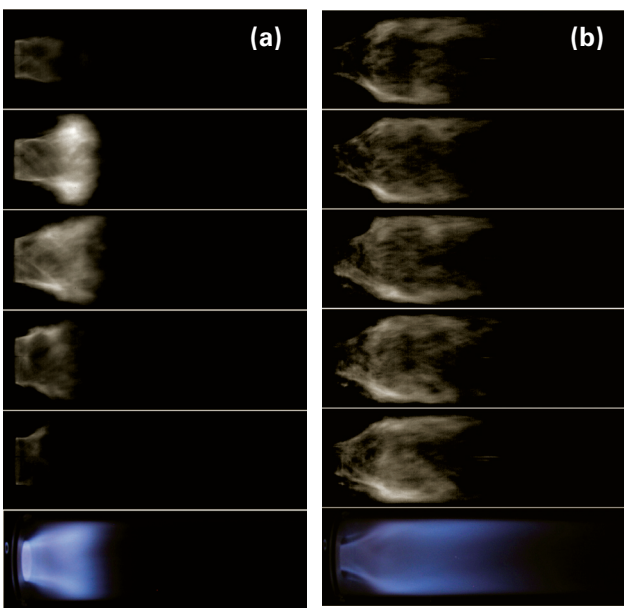

FIGURE 4. Image sequences of (a) an unstable flame in the swirl-stabilized combustor at equivalence ratio 0.44 and (b) a stable flame in swirl-stabilized combustor at equivalence ratio 0.32. Both flames have 60% CO fuel composition. The inter-frame timing is approximately 2 ms. The exposure time is 1 ms. The final frame in each sequence is a 500 ms exposure showing the average flame structure.

Conclusions and Future Directions

Results show that while the stability characteristics of synfuel, as defined by the dependence of the OASPL on the equivalence ratio, is rather similar for all fuel compositions tested so far; the entire curve shifts to lower fuel concentrations and to lower pressures as the hydrogen percentage in the fuel increases. Thus, higher hydrogen concentration in the fuel enables leaner operation, at lower pressure amplitudes. It should be stated however that the stability window, in terms of the range of equivalence ratio within which pressure oscillations are acceptably low, is rather narrow and does not change appreciably with increasing the hydrogen concentration. The trends observed in the swirl combustor correspond closely with those previously noted in the step-stabilized combustor, indicating that these phenomena are robust and that similar trends may be expected in a range of combustor designs. Future experiments will expand the parameter space to include a range of inlet temperatures.

In addition to the experimental data that have been collected, we are also positioned to examine the mechanisms responsible for the transition between stable and unstable operation as the fuel composition and mixture quality change. It is already apparent that flame-vortex-acoustics interactions depend on the local burning characteristics; burning speed and other combustion related parameters change. We will use our modeling experience and computational tools to gain insight into these mechanisms and to propose measures for extending the stability window of syngas combustion. We will also experiment with the use of microjets to stabilize combustion in the two configurations.

FY 2007 Publications/Presentations

1. H. M. Altay, R. L. Speth, D. Snarheim, D. E. Hudgins, A. F. Ghoniem and A. M. Annaswamy. "Impact of Microjet Actuation on Stability of a Backward-facing Step combustor." 45th AIAA Aerospace Sciences Meeting and Exhibit. Reno, Nevada, January, 2007.

2. R. L. Speth, H. M. Altay and A. F. Ghoniem. "Dynamics and Stability Limits of Syngas Combustion in a Backward-facing Step Combustor." Proceedings of ASME Turbo Expo 2007. Montreal, Canada, May, 2007.

V.B.3 Autoignition Studies of Syngas and Hydrogen (SGH) Fuels

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Objectives

- Parametrically determine the autoignition delay time for CO/H_2 mixtures as function of CO concentration, equivalence ratio, pressure and temperature.
- Determine effect of water concentration on autoignition using mixtures of $CO/H_2/H_2O$.
- Conduct studies at operating pressures up to 3.0 MPa (30 atm) and 950 K (1,250°F) and typical air mass flow rates of 0.5 kg/s (1 lbm/s).

Accomplishments

- Completed literature review of reported measurements of autoignition times for H_2/CO mixtures for application to syngas fuels planned for use in FutureGen, the DOE Integrated Sequestration and Hydrogen Research Initiative.
- Compared literature results with current chemical kinetic models that indicated a significant discrepancy between chemical kinetic model predictions and measurements from previous work of other researchers.
- Redesigned the originally proposed test rig based on this literature review to achieve a higher temperature capability in order overlap with current shock tube results.
- Completed fabrication of the test rig and substantially completed assembly that will be followed by initial characterization and autoignition measurements of syngas.
- Completed measurements of the laminar flame speed for syngas.

Introduction

The renewed interest in coal-based integrated gasification combined cycle (IGCC) plants is due to the desire for greater fuel supply flexibility using the large known resources of coal in the United States. The use of coal will reduce U.S. dependence on foreign supplies of oil and natural gas currently used to generate electric power. Current Department of Energy plans through the FutureGen initiative strive for efficient, environmentally clean IGCC technologies that can provide both electrical generation and hydrogen production capabilities. Combustion of syngas produced from coal gasification, as well as a broader range of syngas and hydrogen (SGH) fuels, is a key technology research area as syngas is, in a sense, a new fuel. Furthermore, although syngas is largely composed of CO and H_2, the amount of each of these components in the fuel can vary widely depending on the source of the coal and gasification technology used. Consequently, there is a critical need for fundamental properties such as autoignition (when will it ignite?) and flame speed (how fast will it burn?). The determination of the autoignition time for premixed syngas-air mixtures is critical to the operation of gas turbine power systems using lean premixed technology since the syngas is mixed with high temperature air before introduction to the combustion chamber. If this mixture autoignites before entering the combustion chamber due to long residence times in the gas turbine inlet section, significant and costly damage can occur to the gas turbine. The study of autoignition is thus a key issue and is the main focus of the present research project. In particular, the determination of the autoignition time for syngas-air mixtures must be done under conditions relevant to gas turbine engines used for power generation, that is, studies must be done at high-pressure (up to 30 atm) and high-temperatures (up to 950 K). Such measurements are challenging in terms of the facilities needed to conduct the measurements and the diagnostics required to accurately measure the autoignition time, which can vary from one-thousandth of a second to a few seconds. Thus, a major accomplish of the research to date has been the design, fabrication and assembly of a high-pressure autoignition test facility that will be described in the following section.

Approach

Syngas autoignition experiments are being conducted at Penn State using a flow reactor based on the design used by Spadaccini and TeVelde [1]. A schematic of the flow reactor is shown in Figure 1. Air flow at a maximum flowrate of 2.5 kg/s (5.5 lbm/s)

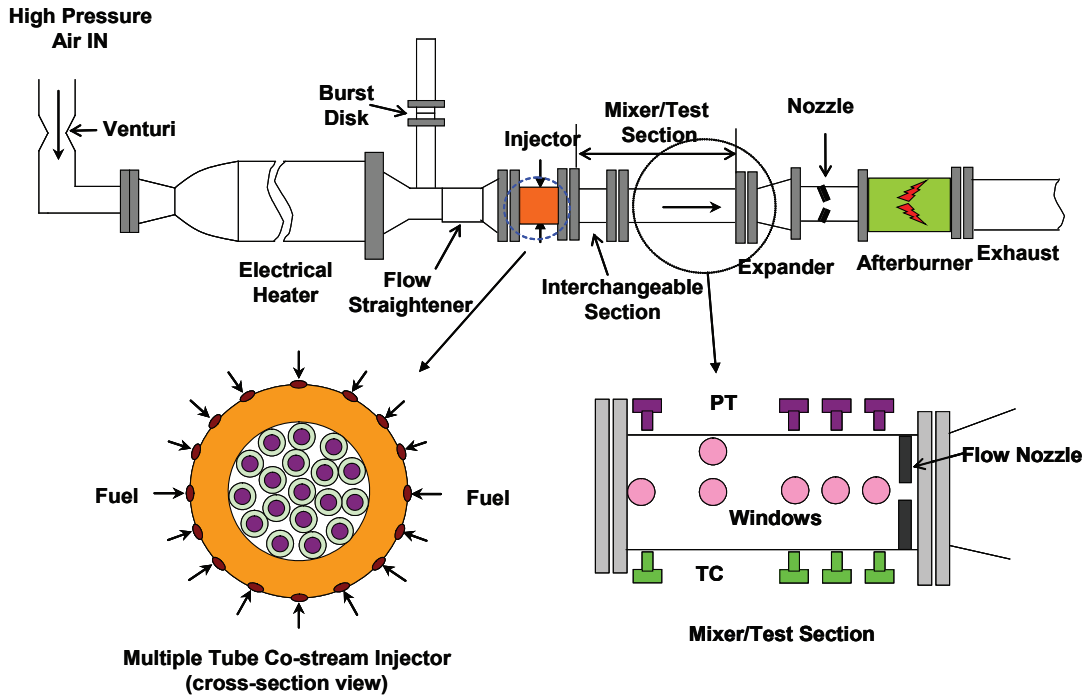

FIGURE 1. Simplified Schematic of Flow Reactor

is supplied from two blowdown tanks to an electric resistance-type air heater that can heat 0.5 kg/s (1.1 lbm/s) of air to a maximum temperature of 800 K (980°F). The heated air can be further heated using a heat exchanger and then flows through a flow straightener section and subsequently mixes with the fuel in the mixer section. The fuel-air mixture then flows through a constant-diameter variable-length instrumented test section followed by a flow nozzle and diffuser section before being burned in an afterburner. A distributed strut type fuel injector with aerodynamic surfaces and a design that features multiple converging-diverging nozzles with fuel injection in the converging section of the nozzles is utilized to mix the fuel and air streams within a short distance from the injection point. The variable-length test section with a circular cross section (diameter of 43 mm) provides the capability to determine autoignition times for various syngas and sygas/hydrogen mixtures. The range of ignition delay times that can be measured depends on the length from the injection point to the flow nozzle, *L*, and the average flow velocity, *U*, of the fuel/air mixture. The test conditions can be varied from pressures between 10 to 30 atm (147 to 440 psi) and mixture temperatures between 700 to 950 K (800°F to 1,250°F), which adequately replicate practical gas turbine operating conditions.

Results

The most significant result for the past year has been the completion of the fabrication and assembly of the flow reactor that is being used to study the autoignition of syngas and syngas-hydrogen mixtures. Figure 2 shows a picture of the flow reactor that illustrates the variable-length capability as well as pointing out the major components of the device. A particularly important design feature of this flow reactor is the injector that is shown in Figure 3. This injector is a distributed strut type fuel injector with aerodynamic surfaces and a design that features multiple converging-diverging nozzles with fuel injection in the converging section of the nozzles. This design provides rapid mixing of the syngas and air streams within a short distance from the injection point, which is critical for achieving an accurate measurement of autoignition time. Also the aerodynamic surfaces eliminate or minimize the potential for flow recirculation occurring at the injector face that would complicate the measurements. Recent tests have focused on characterizing the temperature uniformity in the flow reactor. Measurements of the axial profile within the flow reactor indicate that the temperature varies by less than 1.7°C (3°F) along the 2.13-m (7-ft) test section. Such a small variation in the temperature in the reactor defines the precision to which the autoignition temperature can be determined, which is more than adequate for the present studies.

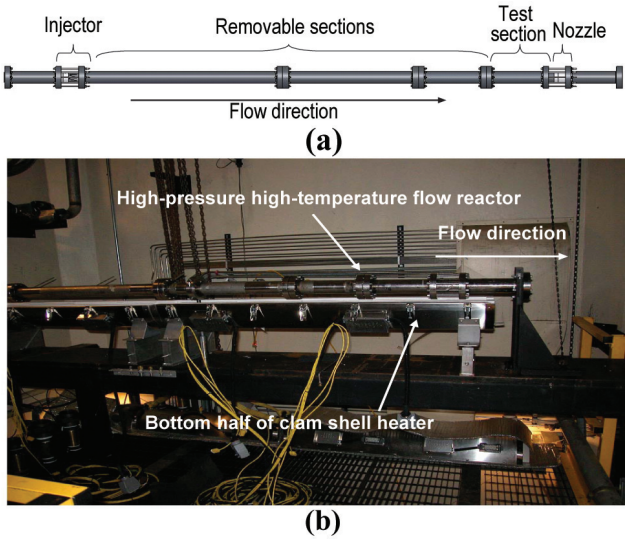

FIGURE 2. Picture of the Assembled Flow Reactor for Autoignition Studies of Syngas

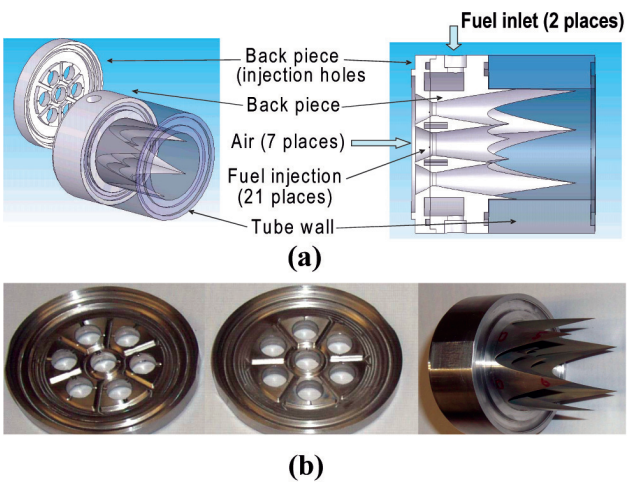

FIGURE 3. Schematic diagram and pictures of the distributed strut type fuel injector. The figure shows the multiple converging-diverging nozzles with fuel injection in the converging section of the nozzles that is utilized to mix the fuel and air streams within a short distance from the injection point.

During the first year of our research project, comparisons were made between current chemical kinetic models for syngas combustion and measured autoignition times obtained by other researchers [2]. These comparisons showed that current models predicted longer autoignition times that differ by as much as three orders of magnitude from measurements made at temperatures close to 1,000 K (1,340°F). These comparisons were particularly important since gas turbines operate at inlet air temperatures below these temperatures where little data currently exists [2]. Since there appears to be some concern regarding the accuracy of chemical kinetic models for syngas combustion, a set

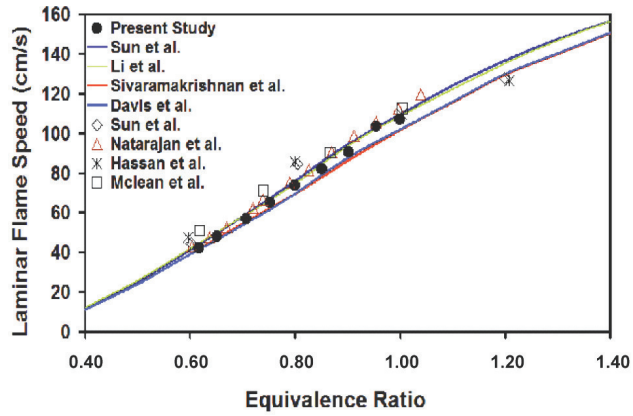

FIGURE 4. Laminar flame speeds of 50/50% H_2/CO/air mixture. Symbols represent experimental data and lines represent computations.

of experiments was conducted to determine the laminar flame speed for syngas-air mixtures and compare it to current kinetic model predictions. Since laminar flame speed measurements involve higher temperatures than autoignition studies, the objective of these studies was to narrow the temperature range of uncertainty for current models of syngas-air combustion.

These laminar flame speed experiments were conducted using straight steel tubes of various diameters through which mixtures of varying molar percentages of H_2 and CO were combusted. The resulting flames have a conical shape and the angle of the flame cone can then be used to determine the laminar flame speed. Natarajan et al. [3] have recently reported results for syngas using a similar technique. Figure 4 shows the results obtained in our recent experiments for a 50%H_2/50%CO mixture along with data obtained by other workers as well as comparisons with four chemical kinetic models that show good agreement with the data. The details regarding the specific references and data presented in Figure 4 can be found in reference 4. These results confirm that differences between experiments and predictions of autoignition time recently observed results from either inaccuracy in the chemical kinetic rates for the temperature range of 600 K to 950 K (800°F to 1,250°F) or systematic errors in the experiments. Future studies conducted under the present research project will address these issues.

Conclusions and Future Directions

Work done over the last year has resulted in the completion of the flow reactor to be used to determine the autoignition time for syngas-air mixtures under relevant gas turbine conditions. Additionally, studies of the laminar flame speed for syngas-air mixtures have been completed and confirm that current chemical kinetic models for syngas-air mixtures accurately predict the laminar flame speed for these mixtures. Future work

will focus on obtaining autoignition time measurements for a variety of syngas-air mixtures at high-pressure and high-temperature conditions. These experiments are aimed at providing data needed for implementing the use of syngas as a fuel for gas turbine power systems and helping to resolve current discrepancies between chemical kinetic models and experiments with respect to the prediction of autoignition time.

FY 2007 Publications/Presentations

1. "Autoignition Studies of Syngas and Hydrogen (SGH) Fuels," Semi-Annual Report for February 1, 2006 to July 31, 2006, February, 2007.

2. "Autoignition Studies of Syngas and Hydrogen (SGH) Fuels," Semi-Annual Report for August 1, 2006 to January 31, 2007, March 2007.

3. "Autoignition Studies of Syngas and Hydrogen (SGH) Fuels", presented at the UTSR Peer Review Workshop IV, October 17–19, 2006, Clemson University, Clemson, SC.

4. "Autoignition Studies of Syngas and Hydrogen (SGH) Fuels", presented at the Workshop on Hydrogen Combustion in Gas Turbines, March 22, 2007, EPRI Washington, D.C. Office.

5. "Laminar Flame Speed of Syngas Mixtures (H_2-CO) With Straight and Nozzle Burners," AIAA-2007-5658 presented at the 43rd Joint Propulsion Conference and Exhibit, July 8-11, 2007, Cincinnati, OH.

6. "Autoignition and Flame Holding Studies for Gas Turbine Applications," presentation to Rich Dennis (NETL), June 5, 2007, The Pennsylvania State University, University Park, PA.

References

1. Spadaccini, L. J. and TeVelde, J. A., "Autoignition Characteristics of Aircraft-Type Fuels," Combustion and Flame, Vol. 46, 1982, pp. 283-300.

2. Petersen, E. L., Kalitan, D. M., Barrett, A. B., Reehal S. C., John D. Mertens J. D., Beerer D. J., Hack R. L, and McDonell V. G., "New syngas/air ignition data at lower temperature and elevated pressure and comparison to current kinetics models," Combustion and Flame, 149:244-247 (2007).

3. Natarajan, J., Nabdula, S., Lieuwen, T.,and Seitzman, J., "Laminar Flame Speeds of Synthetic Gas Fuel Mixtures", Proceedings of GT2005, ASME Turbo Expo 2005, GT2005-68917, June 2005.

4. Bouvet, N., Gokalp, I., Lee, S.-Y., and Santoro, R. J., "Laminar Flame Speed of Syngas Mixtures (H_2-CO) With Straight and Nozzle Burners," AIAA-2007-5658, 43rd Joint Propulsion Conference and Exhibit, July 8-11, 2007, Cincinnati, OH.

V.B.4 Combustion Characterization and Modeling of Fuel Blends for Power Generation Gas Turbines

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Subcontractors:
- Flow Parametrics, Hartford, CT
- The Aerospace Corporation, Los Angeles, CA

Objectives

- Complete and demonstrate facility for measuring laminar flame speeds at high pressures.
- Develop correlations for representing methane combustion chemistry for use in computational fluid dynamics (CFD).
- Perform ignition delay time measurements of synthesis gas mixtures at engine conditions.

Accomplishments

- Obtained new syngas data from our shock tube for a mixture that overlaps with flow reactor data from the United Technologies Research Center (UTRC) and University of California, Irvine (UCI) that show significantly faster ignition than what is predicted by the chemical kinetics models, which are reasonably well known. This result is significant in that the ignition in this regime may not be purely kinetic.
- Derived a reduced chemistry model for methane combustion for use in CFD models. The reduced model takes the form of correlations for chemical times; these correlations are comprehensive in that they take the place of the detailed methane kinetics mechanism, but without having to couple the full mechanism with the CFD.
- Completed and demonstrated a new facility for the measurement of laminar flame speeds at elevated initial pressures (up to 30 atm). Some sample experiments for methane-air mixtures were obtained.
- Began work on a reduced chemistry model for syngas fuels for use in CFD models.

Introduction

For several years now, natural gas has been widely used as a fuel for stationary power generation gas turbine engines [1]. Although composed primarily of methane, natural gas can contain from a few percent up to as much as 18% of other gases, depending on the international source [2]. These natural gas impurities are usually higher-order hydrocarbons such as ethane and propane. Composition variations in native and foreign natural gas can cause changes in the combustion chemistry, emissions formation, and stability, among other concerns [3-5]. However, in the near future, power generation gas turbines may be required to burn ever more exotic gaseous fuel blends in addition to indigenous natural gas. Typical fuel blends can include potentially high concentrations (>10%) of hydrogen and even larger concentrations of hydrocarbons than what are common in natural gas. In addition to changes in the heating value of the fuel blends, significant changes in the ignition chemistry occur when gases such as H_2 and C_2H_6 are added to methane. Even larger changes in the combustion chemistry may then occur if the methane-based fuel were to contain significant levels of hydrogen or hydrocarbons. In particular, recent interests in coal-derived synthesis gases containing mostly hydrogen and carbon monoxide have generated similar concern. Such chemical effects can have dramatic impacts on existing gas turbine combustors designed to operate on natural gas typical of those found, for example, in the United States. These concerns are complicated by the fact that few data exist on the fundamental effects of fuel composition variation at the fuel/air mixture ratios, temperatures, and pressures of interest to the designers of power generation gas turbines.

Of primary concern, ultimately, is how fuel variability impacts the operation of a stationary gas turbine. For example, the flame speed of the fuel-oxidizer mixture in the combustor relates to its flashback or blowoff tendencies. Likewise, the fuel reactivity, often expressed in terms of its autoignition delay time, has a direct impact on the performance and stability of a given combustor design. Assuming a gas turbine designer or field engineer is aware of the flashback and ignition limitations of a given combustor, a determination as to whether or not a certain fuel will behave adequately in that particular combustor can be made if that fuel's flame speed and ignition characteristics were known *a priori*. However, very little if any fundamental flame speed and ignition data are available for uncommon fuel

mixtures such as those mentioned above, much less at realistic engine pressures and concentrations.

Approach

We are conducting a research project to study ignition delay times, flame speeds, and related chemical kinetics over a wide range of fuel composition, mixture stoichiometry, temperature, and pressure, with emphasis on real fuel-air mixtures at engine conditions of elevated pressure. This project is providing data related to fuel flexibility issues, allowing gas turbine designers and field engineers to predict the effects of fuel flexibility on the likelihood of autoignition in premixed regions, flashback, combustor efficiency, emissions, and combustion instability. Provided in the next section is an outline of the research effort.

Efforts at the University of Central Florida (UCF) involve overall project management and the generation of fundamental measurements of ignition delay times and flame speeds. All experiments are conducted at UCF and The Aerospace Corporation, who provide the use of the high-pressure shock tube capability. The results of the chemical kinetics experiments are combined with the fluid mechanics of stationary power generation gas turbines through CFD, and Flow Parametrics is working on the CFD modeling.

Results

During this fiscal year, we presented new data for synthesis gas ignition at practical conditions that, when used in conjunction with an earlier set of data from UTRC, show considerable disagreement with what is predicted by state-of-the-art chemical kinetics models (Figure 1). This result is significant because coal-derived synthesis gas (i.e., syngas) is comprised primarily of H_2 and CO along with varying levels of CO_2 and other gases, and the CO/H_2 kinetics are often considered to be reasonably well known, even at elevated pressures and lower temperatures. The reason for this discrepancy is not known at this time.

Computational fluid dynamics modeling of the complex processes that occur within the burner of a gas turbine engine has become a critical step in the design process. However, due to computer limitations, it is very difficult to completely couple the fluid mechanics solver with the full combustion chemistry. Therefore, simplified chemistry models are required, and one topic of this research was to provide reduced chemistry models for CH_4/O_2 gas turbine flow fields to be integrated into CFD codes for the simulation of flow fields of natural gas-fueled burners. The reduction procedure for the CH_4/O_2 model utilized a response modeling technique wherein the full mechanism was solved over a range of temperatures, pressures,

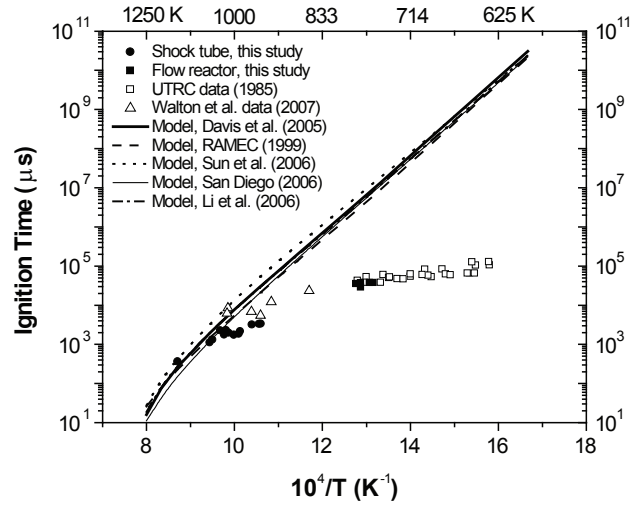

FIGURE 1. Comparison of syngas ignition delay times and chemical kinetics models, showing the greatly accelerated ignition in the experiments. This may indicate that the ignition of these mixtures may not be completely controlled by the chemical kinetics.

and mixture ratios to establish the response of a particular variable such as chemical reaction time. The conditions covered were between 1,000 and 2,500 K for temperature, 0.1 and 2 for equivalence ratio, and 0.1 and 50 for pressure. The kinetic times include the time to ignition, the time to equilibrium H_2O formation, the time to equilibrium CO formation, and the time to equilibrium NO formation. The kinetic time models are given in Arrhenius-type formulas as functions of equivalence ratio, temperature, and pressure; or fuel-to-air ratio, temperature and pressure. A single global kinetics model was obtained for the entire range of conditions, and separate models for the low-temperature and high-temperature regions as well as for fuel-lean and rich cases were also derived. Predictions using the reduced model were verified using results from the full mechanism and empirical correlations from experiments. The models are intended for (but not limited to) use in CFD codes for flow field simulations of gas turbine combustors in which initial conditions and degree of mixedness of the fuel and air are key factors in achieving stable and robust combustion processes and acceptable emissions levels. The new model was applied to CFD simulations of a typical gas turbine burner with premixer with good results.

A constant-pressure cylindrical flame speed vessel (30-cm internal diameter, 36.2-cm length) has been built for the study of constant-pressure, freely propagating, spherical flames. A Z-type schlieren setup, using either a vertical or a circular knife edge, in combination with a high-speed camera is used to capture the progression of the flame. Flame speed data were analyzed using special image tracking software. A linear regression of flame speed versus stretch was obtained, giving the Markstein

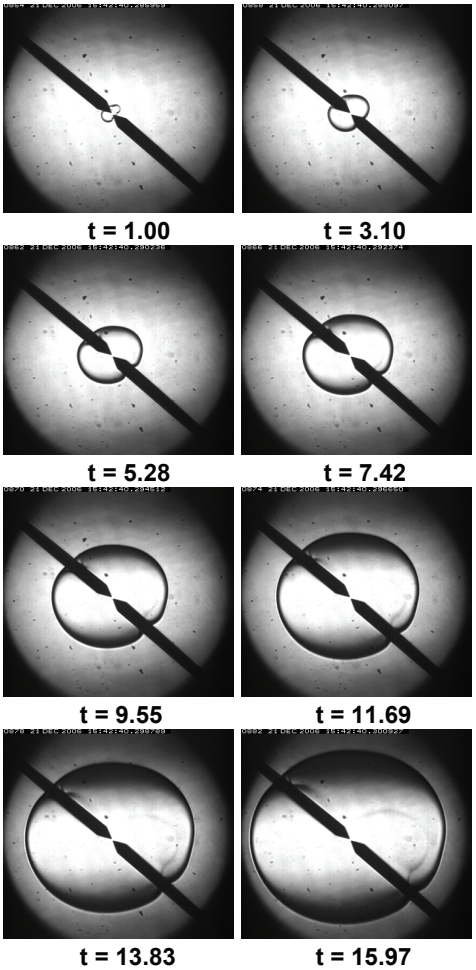

FIGURE 2. Typical Laminar Flame Speed Results for CH_4/Air, 1 atm, $\phi = 0.8$, Time in ms

length and the unstretched flame speed. A high-speed, piezo-resistive pressure transducer is used to obtain pressure data during the experiment and guarantees constant-pressure conditions. The vessel was designed for initial pressures up to 30 atm, where full use of the 12.7-cm aperture can be utilized within 3.5% of the pressure rise. Several methane-air mixtures have been tested around 1 atm and show good agreement with published data. Figure 2 shows some typical results from the schlieren diagnostic for a stoichiometric methane-air mixture.

Conclusions and Future Directions

We are in the last year of the 3-year grant from the UTSR program. Fuel-flexibility experiments on hydrocarbon mixtures, namely for ignition delay times, flame speeds, and chemical kinetics, should continue. Demonstration of the reduced chemistry in the form of correlations in CFD models for wider conditions and applications should be performed. Also important will be resolution of the discrepancy in hydrogen and syngas-based mixtures with regard to the much earlier ignition seen at practical conditions than what is predicted by kinetics models.

FY 2007 Publications/Presentations

1. E. L. Petersen, D. M. Kalitan, A. Barrett, S. C. Reehal, J. D. Mertens, D. J. Beerer, R. Hack, and V. McDonell, "New Syngas/Air Ignition Data at Elevated Pressure and Comparison to Current Kinetics Models," *Combustion and Flame*, Vol. 149, 2007, pp. 244–247.

2. E. L. Petersen, D. M. Kalitan, S. L. Simmons, G. Bourque, H. J. Curran, and J. M. Simmie, "Methane/Propane Oxidation at High Pressures: Experimental and Detailed Chemical Kinetic Modeling," *Proceedings of the Combustion Institute*, Vol. 31, 2007, pp. 447–454.

3. J. de Vries and E. L. Petersen, "Autoignition of Methane-Based Fuel Blends under Gas Turbine Conditions," *Proceedings of the Combustion Institute*, Vol. 31, 2007, pp. 3163-3171.

4. E. L. Petersen, J. M. Hall, S. D. Smith, J. de Vries, A.R. Amadio, and M. W. Crofton, "Ignition of Lean Methane-Based Fuel Blends at Gas Turbine Pressures," *Journal of Engineering for Gas Turbines and Power*, in press.

5. T. Lieuwen, V. McDonell, E. Petersen, and D. Santavicca, "Fuel Flexibility Influences on Premixed-Combustor Blowout, Flashback, Autoignition, and Instability," *Journal of Engineering for Gas Turbines and Power*, in press.

6. D. M. Kalitan, E. L. Petersen, and M. W. Crofton, "Ignition and Oxidation of Lean CO/H_2 Fuel Blends in Air," submitted to *Journal of Propulsion and Power*, in press.

7. J. de Vries, B. A. Corbin, and E. L. Petersen, "A Facility for High-Pressure Laminar Flame Speed Measurements," Paper A20, 5th U.S. Combustion Meeting, March 25–27, 2007, San Diego, CA.

8. A. B. Barrett, S. C. Reehal, and E. L. Petersen, "Measurement of Ignition Delay Time for a Syngas/Air Mixture Containing Water Vapor," Paper C25, 5th U.S. Combustion Meeting, March 25-27, 2007, San Diego, CA.

9. M. Lamnaouer, E. L. Petersen, R. C. Ryder, and A. Brankovic, "Reduced Combustion Time Model for Methane in Gas Turbine Flow Fields," AIAA Paper 2007-0385, 45th AIAA Aerospace Sciences Meeting and Exhibit, January 8-11, 2007, Reno, NV.

10. E. L. Petersen, "Hydrocarbon-Air Ignition Experiments at Elevated Pressures," 41st JANNAF Combustion Subcommittee Meeting, December 4–8, 2006, San Diego, CA.

References

1. Lefebvre, A. H., 1999, *Gas Turbine Combustion*, 2nd Ed, Taylor & Francis, Philadelphia, PA.

2. Spadaccini, L. J. and Colket, M. B. III, 1994, "Ignition Delay Characteristics of Methane Fuels," *Progress in Energy and Combustion Science*, **20**, pp. 431–460.

3. Naber, J. D., Siebers, D. L., Di Julio, S. S., and Westbrook, C. K., 1994, "Effects of Natural Gas Composition on Ignition Delay under Diesel Conditions," *Combustion and Flame*, **99**, pp. 192-200.

4. Flores, R. M., Miyasato, M. M., McDonell, V. G., and Samuelsen, G. S., 2001, "Response of a Model Gas Turbine Combustor to Variation in Gaseous Fuel Composition," *Journal of Engineering for Gas Turbines and Power*, **123**, pp. 824–831.

5. Flores, R. M., McDonell, V. G., and Samuelsen, G. S., 2003, "Impact of Ethane and Propane Variation in Natural Gas on Performance of a Model Gas Turbine Combustor," *Journal of Engineering for Gas Turbines and Power*, **125**, pp. 701–708.

V.B.5 High Pressure Kinetics of Syngas and Nearly Pure Hydrogen Fuels

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Objectives

- Develop the necessary chemical kinetics information to understand the combustion of syngas and nearly pure hydrogen fuels at conditions of interest in gas turbine combustion.
- Explore high-pressure kinetics by making detailed composition measurements of combustion intermediates and products in a high-pressure flow reactor using molecular beam/mass spectrometry (MB/MS) and matrix isolation spectroscopy (MIS).
- Compare experimental data with calculations using existing mechanisms.
- Use theoretical methods to improve the predictability of existing mechanisms.

Accomplishments

This project has not started yet.

Introduction

The objective of this project is to develop the necessary chemical kinetics information to understand the combustion of syngas and nearly pure hydrogen fuels at conditions of interest in gas turbine combustion. Syngas is the product of the gasification of coal and/or biomass. The composition of syngas can vary considerably, but typically contains mostly hydrogen, CO and CO_2 with smaller amounts of CH_4, O_2, N_2, other hydrocarbons and water vapor. With further processing, the hydrogen content can be increased to fairly high levels. Both syngas and nearly pure H_2 mixtures can be oxidized either with air, or with pure oxygen, or any combination thereof. The use of any particular fuel/oxidizer combination in gas turbines will require an ability to predict important combustion properties such as laminar flame speed, autoignition conditions, flammability limits and NOx formation rates.

Approach

Combustion properties depend on the chemical kinetics of the fuel/oxidzer combination. Existing reaction mechanisms do a satisfactory job of predicting these properties at pressures close to atmospheric and below, but are less well tested at higher pressures in the range of 15-20 bar, especially at lower temperatures. We will explore the high-pressure kinetics by making detailed composition measurements of combustion intermediates and products in a high-pressure flow reactor using MB/MS and MIS. The data would then be compared with calculations using existing mechanisms. The appearance of new species, or substantial differences in concentrations of previously modeled species, would drive a detailed examination of those parts of the mechanisms affected. Theoretical methods such as transition state theory would be used to estimate unknown reaction rates and existing mechanisms would be modified based on differences in observed composition and concentrations. The main advantage of this approach is that it offers a direct validation path for the reaction mechanism because of the ability to identify reactive intermediates.

Results

The project has not yet started. We anticipate that funding will be in place shortly.

Conclusions and Future Directions

Our approach will be as described above. We will be taking particular care to explore and isolate the possibility that surface catalytic reactions or unknown gas phase reactions play an important role on low temperature H_2 oxidation kinetics.

V. UNIVERSITY TURBINE SYSTEMS RESEARCH

C. Materials

V.C.1 Evaluating Coatings for Current and Future Service

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Objectives

- To provide quantitative nondestructive measurements of thermal protection offered by coatings on serviceable engine parts.
- To understand how individual elements of service-related changes affect the thermal protection provided by a coating.
- Monitoring the complex physical changes that precede coating failure.

Accomplishments

- Demonstrated feasibility of measurements to reveal the thermal contact resistance between coating and base metal material.
- Developed a process by which localized delamination of the coating can be visualized.

Introduction

The advancement of new coatings requires the evaluation of candidate materials under environmental tests designed to reflect service conditions, either current or future. While it is unrealistic to envision a single measurement that provides all conceivable information, it is arguable that the capability for the single most important measurement is still lacking. A quantitative nondestructive measurement of the thermal protection offered by a coating is not currently among the measurements one can employ on serviceable engine parts (or even on many experimental specimens). Our research concerns a first-principle measurement for quantifying thermal properties of the coating without specialized sample preparation. These measurements carry sufficient quantitative value to make meaningful assessments and comparisons of different coating materials, and may be richly descriptive of the multifaceted nature of service-related change over the lifetime of a coating.

Approach

The principle of our measurement is to determine coating properties from indirect interrogation of the temperature established in a coating by periodic heating. The experimental measurement is shown schematically in Figure 1. A CO_2 laser is used as the heating source. An analytic model has been developed to calculate the transient temperature in the coating as a function of unknown material properties and known geometric parameters and heating conditions. The temperature field is interrogated through thermal emission from the coating. The calculated phase of the thermal emission is compared with experimental measurements to evaluate candidate solutions to the coating properties. A set of measurements is performed by recording the phase of the thermal emission as a function of laser frequency. Measurement frequencies are selected such that the thermal penetration depths span from less than to greater than the coating thickness. We have shown that

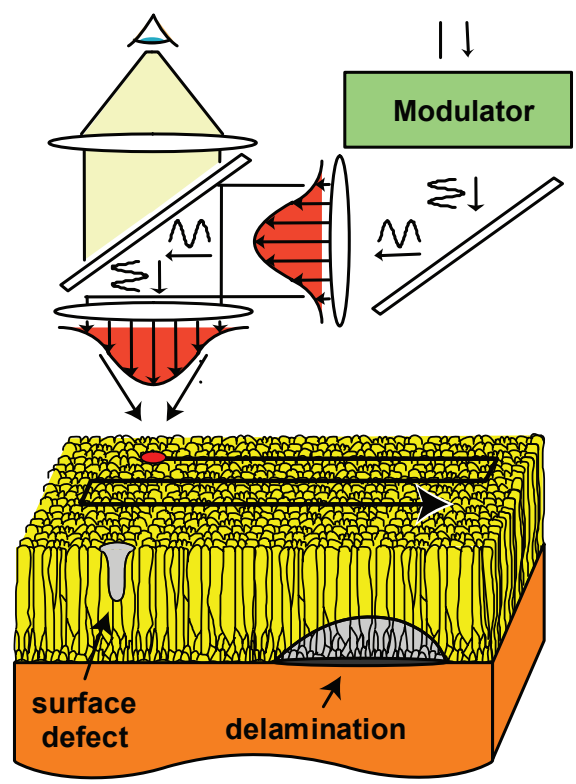

FIGURE 1. Schematic of Experimental Measurement

measurement will determine four unknown properties of the coating [1,2].

Results

In a preliminary investigation, our measurement technique has been exploited for surface mapping measurements to illustrate the capability to detect coating defects and resolve their relative locations. The initial investigation used specimens with local delaminations caused by thermal-acoustic shock resulting from pulsed laser heating. Figure 2 shows the defect mapping of the sample taken with two laser frequencies, 100 Hz and 500 Hz. At high frequencies, only defects near the surface are seen. At low frequencies, defects as deep as the interface can be resolved. When contrasting maps at both high and low frequencies, delaminations are present in the low frequency map, but absent in the high frequency map. In contrast, near surface defects are present in both frequency maps. In this manner, the relative depth of a defect in the thermal barrier coating (TBC) can be established.

Thermal property measurements were made at two locations on the thermal-acoustic shock damaged sample, one where the coating was in good thermal contact with the substrate, and the other where the coating was debonded. Using the analysis described in reference [3], measurements revealed that the debonded region of the coating has an interfacial resistance of about 3.5×10^{-6} m^2 K/W. This is approximately "equivalent" to the thermal resistance of a 0.14 µm air gap, and represents about 5% of the topcoat's thermal resistance. This air-gap thickness is consistent with cross-sectional microscopy observations of partially separated TBC interfaces. In contrast, the thermal contact resistance of the intact coating was determined to be at least one order of magnitude smaller than the debonded region. The thermal conductivity of the coating overlying the debonded region is measured to be 1.4 W/m/K and indistinguishable (within ~10%) from the conductivity of the coating measured away for the debonded region [3]. Close agreement is expected since the laser shock used to separate the coating should not alter any of its thermal properties. The uncertainty in fitted values of both the thermal properties and optical penetration depth for the laser is less than 10%, but the uncertainty in the thermal contact resistance is about 50%. This is a reasonable outcome considering the contact resistance of the debonded region represents only 5% of the entire resistance of the coating.

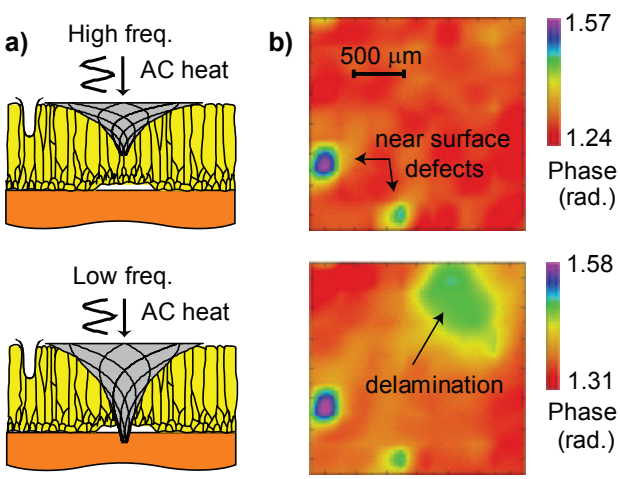

FIGURE 2. Defect Mapping of a Coating at Two Laser Frequencies

Conclusions and Future Directions

A proof-of-concept measurement has demonstrated the ability to resolve and differentiate interfacial delimitation from the intrinsic properties of the coating. More work is needed to understand how the thermal contact resistance evolves with service conditions. Monitoring such changes through thermal property measurements may supplement or offer an even better predictive measure for the remaining life to failure. Additional, studies will be conducted to address the needs for quantitative thermal properties measurements of coatings over a service lifetime, and, second, to develop and capitalize on the thermal property measurements to assess and track degradation of coatings under new service conditions. Future work will also look at the effects of foreign deposits with respect to thermal performance of the coatings.

References

1. T. D. Bennett and F. Yu, "A nondestructive technique for determining thermal properties of thermal barrier coatings" Journal of Applied Physics, 97(1) 2005 13520-1-12.

2. T. D. Bennett, F. Yu, "Linear radiation model for phase of thermal emission spectroscopy", Journal of Applied Physics, vol.98, no.9, 1 November 2005, pp. 93516-1-7.

3. F. Yu and T. D. Bennett, "Phase of thermal emission spectroscopy for properties measurements of delaminating thermal barrier coatings" Journal of Applied Physics, vol. 98, no.10, 15 November 2005, pp. 103501-1-8.

V.C.2 Degradation of Thermal Barrier Coatings with Syngas Combustion: Testing by Hyperbaric Advanced Development Environmental Simulator and Characterization by Advanced Electron Microscopy

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Objectives

- Identify degradation (e.g., hot corrosion) mechanisms (e.g., yttria-stabilized zirconia [YSZ] destabilization, deposit penetration and reaction, etc.).
- Generate critical materials data (e.g., solubility, eutectic compositions and degradation kinetics for realistic natural gas [NG] and syngas [SG] combustion turbine environment).
- Provide feasible approaches to improve resistance against thermal barrier coating (TBC) degradation in a fuel-flexible combustion environment.

Accomplishments

- Understanding of TBC degradation via successful characterization of TBC-coated turbine blades that were employed in industrial turbines with SG combustion.
  - Deposits consisting of cubic Fe_3O_4 with a large solubility and monoclinic Fe_2O_3 with minimal solubility.
  - Thermally grown oxide (TGO) scale consisting of α-Al_2O_3 and tetragonal spinel-$(Ni,Co)(Al,Cr)_2O_4$.
  - Internal oxidation in NiCoCrAlY bond coats consisted of α-Al_2O_3 and cubic NiO.
- Fabrication of air plasma spray (APS) YSZ TBC coatings (t' phase) at UCF.
- Fundamental study of TBCs and Ni-base superalloys degradation in SG, sulfur-poisoned SG, deposits of V_2O_5, P_2O_5, and other potential fuel contaminants.

Introduction

The main driver of technology development in modern turbines for energy generation is to increase turbine power plant fuel flexibility and efficiency as well as reliability, availability, and maintainability, with low emissions and life cycle costs. Critical tasks to achieve this objective include the development of turbine technologies that enable low-cost and environmentally acceptable use of its large reserves of coal and operation at high turbine inlet temperature for efficient energy production with reduced emissions. Inevitably, turbines need advanced hot section components and coatings that can tolerate higher operating temperatures while being significantly more resistant to the contaminations that erode, corrode, and make deposits. The development of advanced TBCs that can tolerate the more aggressive combustion byproducts, while still enabling high turbine inlet temperatures, increased power output, and high power plant efficiency is highly warranted [1].

The evaluation of TBCs in SG combustion environments proposed in this project will help develop IGCC power generation technologies; leading to less expensive and more reliable energy sources, and reduced U.S. dependence on foreign resources. Development of reliable and durable TBCs for integrated gasification combined cycle (IGCC) based on decreased fuel cost will increase the performance efficiency of turbines by 2.2%, equivalent to CO_2 emission reduction by 300 million tons per year per unit and operational savings of 6.3% (assuming 40/60 split in fuel/capital cost).

Approach

This project is designed to provide, for the first time, investigation on the mechanism of TBC degradation in SG combustion environment by using the Hyperbaric Advanced Development Environmental Simulator (HADES). The use of HADES provides realistic test conditions and real time monitoring/controlling of high temperature, high pressure, temperature gradient, erosion, and turbine operation from real SG combustion. These offer a significant advantage over furnace or burner-rig testing, which requires several assumptions (e.g., effects of total and partial pressures, deposit constituents, gas or oxide constituents, etc.). State-of-the-art characterization techniques such as

focused ion beam *in situ* lift-out (FIB-INLO) and transmission electron microscopy/scanning transmission electron microcopy (TEM/STEM) will be employed to identify deposit constituents and hot corrosion reactions to understand the mode and mechanisms of TBC degradation in realistic syngas combustion environments. Use of FIB-INLO and TEM/STEM will enable detailed identification of phase constituents of deposits, penetrants and reaction products, thus providing the exact mechanisms for degradation of TBCs in a syngas combustion environments. Critical materials information, such as deposit solubility and eutectic composition, and reaction/hot corrosion rates in the light of TBC constituents will be provided from the selected in-laboratory thermodynamic/kinetics experiment/modeling. The following lists the technical approaches taken to achieve the objectives of this project:

- Degradation testing of various TBCs in air and in a SG combustion environment.
- Identification and characterization of the degradation using advanced microstructurel characterization techniques.
- Development of fundamental understanding of the difference in degradation behavior of TBCs in NG and SG.
- Generate critical materials data (e.g., solubility, eutectic compositions and degradation kinetics for realistic turbine environments).
- Provide feasible approaches to improve resistance against TBC degradation in a SG combustion environments.
- Transfer to industrial partners the attained knowledge on TBC degradation in a SG combustion environment.
- Provide two pairs of student research teams, with interdisciplinary team-based research activities in collaboration with industrial partners.

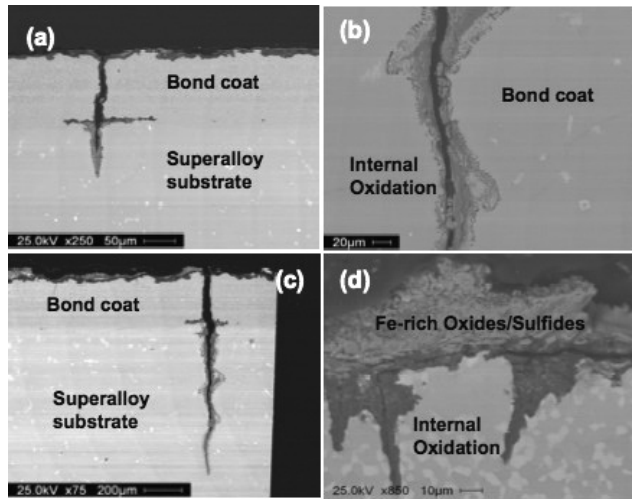

FIGURE 1. Internal Oxidation Damage after TBC Spallation: (a,b) Internal Oxidation through the Bond Coat; (c) Penetration into the Superalloy Substrate; (d) Fe-rich Deposits on the TGO Scale after TBC Spallation

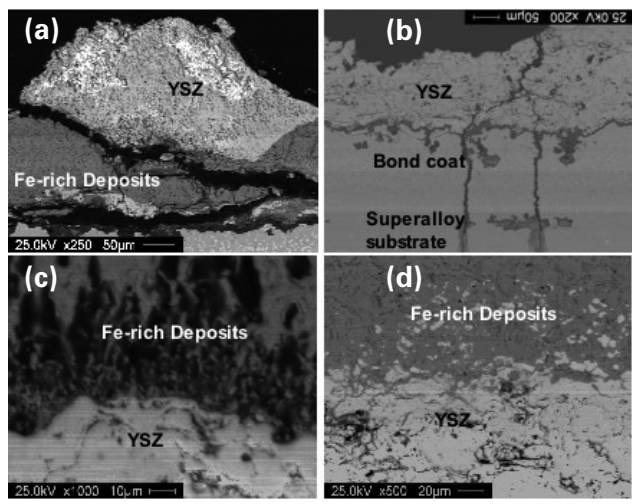

FIGURE 2. Degradation of the YSZ Topcoat in the Form of: (a) YSZ Spallation; (b) Deposit Penetration through YSZ; (c) Deposit; (d) YSZ Dissolution

Results

SG turbine components coated with NiCoCrAlY coatings and TBCs were successfully characterized and provided detailed information for the first time on identity of deposits and how they interact with coatings on turbine components. In regions where TBCs had spalled, a significant local-internal oxidation was observed as presented in Figure 1. This penetration attack through the length of the bond coat extended into the superalloy substrate as shown in Figures 1(a) and 1(c). The interface between internal oxidation and bond coat revealed a distinctive microstructure as seen in Figure 1(b). Additional deposits on top of the TGO scale were observed without any indication of TGO/deposit interaction as shown in Figure 1(d). In regions where TBC is still adherent, several distinctive degradation modes were observed as shown in Figure 2. Clearly, deposits arising from fuel contaminates (a) spalled, (b) penetrated, (c) deposited, and (d) dissolved the YSZ topcoat. Closer examination via TEM/STEM via FIB-INLO revealed that the deposits consisted of cubic Fe_3O_4 with a large solubility and monoclinic Fe_2O_3 with minimal solubility as presented in Figure 3.

In order to provide a basic understanding through laboratory testing, we have successfully produced free-standing APS YSZ coatings (t' phase) at UCF's Thermal Spray Facility (UCF-TSF). Using these controlled specimens, degradation of APS YSZ TBCs by potential

fuel contaminants such as V_2O_5, P_2O_5, and $NaSO_4$ were examined. This study provided valuable information on how the fuel contaminants react with the constituents of TBCs with an emphasis on the YSZ topcoat [2]. The following summarizes the findings that are new relative to the existing knowledge in the open literature:

- Formation of YVO_4 and ZrV_2O_7 above and below 750°C, respectively (see Figure 4).
- YSZ destabilization with the formation of YVO_4 via incongruent melting of ZrV_2O_7.
- Na_2SO_4 (sodium sulfate) had no effect on YSZ coatings at high temperature without the presence of gaseous SO_3.

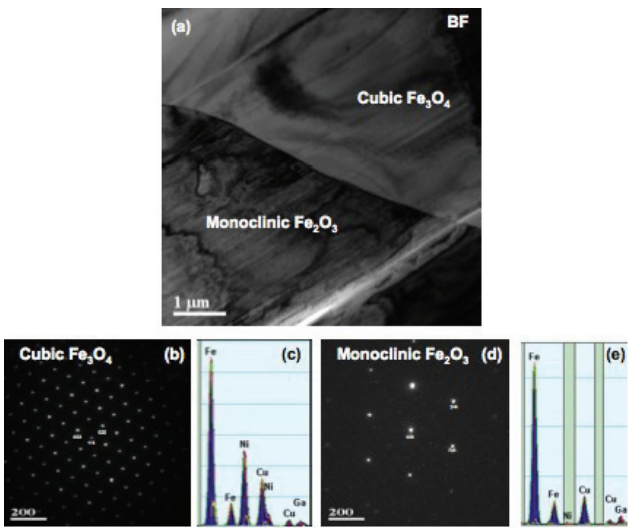

FIGURE 3. (a) Bright-Field TEM Micrograph of Two-phase Deposit Identified as (b) Cubic Fe_3O_4 with (c) a Large Solubility of Ni and (d) Monoclinic Fe_2O_3 with (d) Minimal Solubility

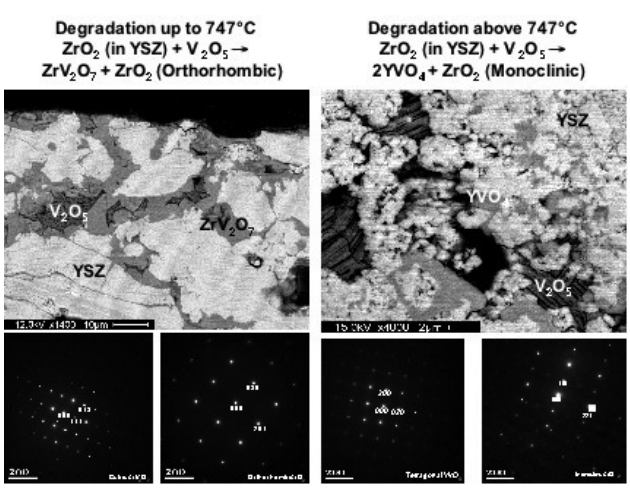

FIGURE 4. Temperature-Dependent Reaction of V_2O_5 with APS YSZ Topcoat

- A reaction between ZrO_2 (in YSZ) and P_2O_5 results in the formation of ZrP_2O_7 at all temperatures (200°C through 1,400°C). Thus the presence of P in fuel should not affect the stability of the YSZ topcoats.

Conclusions and Future Directions

This project has provided an understanding for the mechanism of TBC degradation in SG combustion environments by using in-laboratory experiments and realistic SG combustion environments. State-of-the-art characterization techniques such as FIB INLO and TEM/STEM will be employed to identify deposit constituents and hot corrosion reactions to understand the mode and mechanisms of TBC degradation in realistic SG combustion environments. Use of FIB-INLO and TEM/STEM will enable detailed identification of phase constituents of deposits, penetrants and reaction products, thus providing the exact mechanisms for degradation of TBCs in a syngas combustion environment. Critical materials information, such as deposits and reaction/hot corrosion rates in the light of TBC constituents will be provided from the selected in-laboratory thermodynamic/kinetics experiment/modeling in addition to HADES testing. Microstructural characterizations were carried out for TBC- and MCrAlY-coated blades that were employed in turbines with SG fuel. TBC-coated button specimens thermally treated in SG and sulfur-poisoned SG environment. In-laboratory examination of APS YSZ in the presence of V_2O_5, P_2O_5, and Na_2SO_4 has also provided valuable and new information regarding degradation of TBCs due to fuel contaminants. Siemens Power Generation has acquired HADES, and HADES is going through installation and testing.

FY 2007 Publications/Presentations

1. P. Mohan, B. Yuan, V.H. Desai, Y.H. Sohn, "Degradation of Yttria Stabilized Zirconia Topcoat in Thermal Barrier Coatings by V_2O_5 and P_2O_5." *Journal of the American Ceramic Society*, Accepted for Publication, 2007.

2. V. Krishnan, S. Bharani, J.S. Kapat, Y.H. Sohn, V.H. Desai, "A Simplistic Model to Study the Influence of Film Cooling on Low Temperature Hot Corrosion Rate in Coal Gas/Syngas Fired Gas Turbines," *International Journal of Heat and Mass Transfer*, Accepted for Publication, 2007.

3. P. Mohan, B. Yuan, V.H. Desai, Y.H. Sohn, "Degradation of Yttria Stabilized Zirconia Topcoat in Thermal Barrier Coatings by V_2O_5 and P_2O_5," Presented at the 2007 International Conference on Metallurgical Coatings and Thin Films - ICMCTF, April 23–27, 2007, San Diego, CA.

4. P. Mohan, B. Yuan, V.H. Desai, Y.H. Sohn, "Degradation Mechanisms of Yttria Stabilized Zirconia Topcoat in Thermal Barrier Coatings by V_2O_5," Presented at TMS 2007: 136th Annual Meeting and Exposition, February 25 – March 1, 2007, Orlando, FL.

References

1. Materials and Practices to Improve Resistance to Fuel Derived Environmental Damage in Land- and Sea-Based Turbines, ed. D. Olson, G. Edwards, P. Bollinger, A. Lasseigne, G. Atkins, EPRI, Palo Alto, CA, CSM, Golden, CO, ONR, Arlington, VA, DOE, Oak Ridge, TN, 2003.

2. P. Mohan, B. Yuan, V.H. Desai, Y.H. Sohn, J. Am. Ceram. Soc., in Press, 2007.

V.C.3 Investigation of Material Performance in High Moisture Environments Including Corrosive Contaminants Typical of Those Arising by Using Alternate Fuels in Gas Turbines

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Objectives

- Develop a fundamental understanding of the degradation processes in moisture environments and in such environments where the specimens have deposits which are typical of deposits that will be encountered from alternate fuels, namely, CaO and $CaSO_4$.
- Attempt to describe how moisture/contaminant levels and temperature affect the corrosion processes.
- Determine the alloy compositions and coatings that are most resistant to corrosion induced by deposits from alternate fuels.
- Compare and describe the failure mechanisms of state-of-the-art thermal barrier coatings (TBCs) operating with conventional fuels and with alternate fuels.

Accomplishments

- Specimens of three superalloys, namely, René N5, GTD 111 and IN 738, as well as specimens of these alloys with CoNiCrAlY, NiCrAlY and platinum aluminide coatings have been fabricated.
- The fabricated specimens have been subjected to tests at 750°C, 950°C and 1,150°C using deposits of Na_2SO_4, $CaSO_4$ and CaO. It was determined that the test conditions of CaO deposits at 950°C in dry and wet air (P_{H2O}=0.1 atm) represented conditions typical of those that may be encountered in gas turbines using alternate fuels.
- The fabricated alloys and coatings have been exposed to CaO deposits in dry and wet air at 950°C. All three of the uncoated alloys were severely degraded. The superalloy René N5 was more severely degraded than GTD 111 and IN 738. This attack appeared to be more severe in water vapor compared to that in dry air.
- Such tests have also been performed using the coated alloy specimens. It has been determined that CaO deposits caused degradation of all three coatings.
- It has been determined the larger the amount of the CaO deposit, the more severe the alloy degradation.

Introduction

Much of the previous materials development for power generating turbines has been performed with natural gas as the fuel of choice. More recently, the need for fuel flexibility has caused alternate fuels such as syngas to be considered for use in gas turbines. Preliminary testing with a variety of alternative fuels has shown increased deposition of ash as well as highly aggressive corrosion of turbine materials that was more severe in the presence of moisture [1]. This project is directed at investigating the corrosion induced by ash deposition and moisture from use of alternative fuels. The alloys and coatings to be studied are typical of those used in current power generating gas turbines, as well as those that may be used in advanced systems.

Approach

To achieve the objectives presented previously in this report, the alloys René N5, GTD 111 and IN 738 as well as these alloys coated with CoNiCrAlY, NiCrAlY and platinum aluminide have been exposed to conditions relevant to corrosion induced using alternate fuels. The initial test conditions involved a number of deposits including Na_2SO_4, $CaSO_4$ and CaO in dry and wet air at temperatures from 750°C to 1,150°C. Based upon these results, in order to compare these alloys and coatings in a manageable number of experiments, it was decided to perform subsequent experiments at 950°C using CaO deposits (0.5–1.0 mg/cm^2) in dry and wet air (P_{H2O}=0.1 atm), since these conditions were considered to be representative of those that may be encountered when using syngas.

Results

Specimens of René N5, GTD 111 and IN 738 have been exposed to cyclic oxidation conditions at 950°C with deposits of CaO in dry and wet air. It has been found that all three of these alloys were attacked more severely when CaO deposits were present and this attack became even more severe in wet compared to dry air. However, the increase in attack due to the presence of water vapor was small compared to the attack caused the CaO deposit. It was also found that the degradation induced via CaO deposits caused more severe degradation of René N5 compared to GTD 111 and IN 738. The attack induced by CaO caused similar amounts of degradation of GTD 111 and IN 738. The attack of the three alloys in dry air with no deposits can be seen in Figure 1, and these micrographs can be compared to those in Figure 2 where CaO was present as a deposit.

Tests using CaO deposits and cyclic oxidation conditions at 950°C in dry and wet air have also been performed for the three coatings on the three alloy substrates. All three coatings were significantly degraded by attack induced by the CaO deposits. No effect of the alloy substrate on coatings performances was

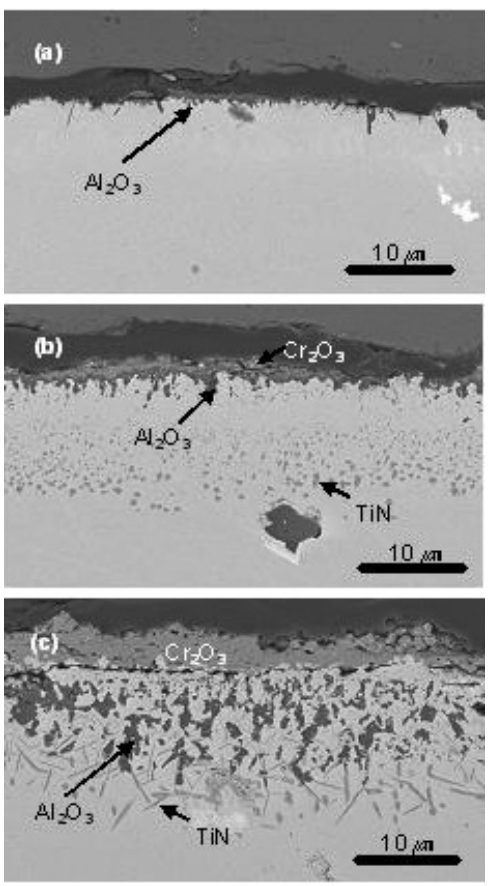

FIGURE 1. Scanning Electron Micrographs Comparing the Oxidation Products Formed on (a) René N5, (b) GTD 111 and (c) IN 738 after 140 Hours of Cyclic Oxidation at 950°C in Dry Air

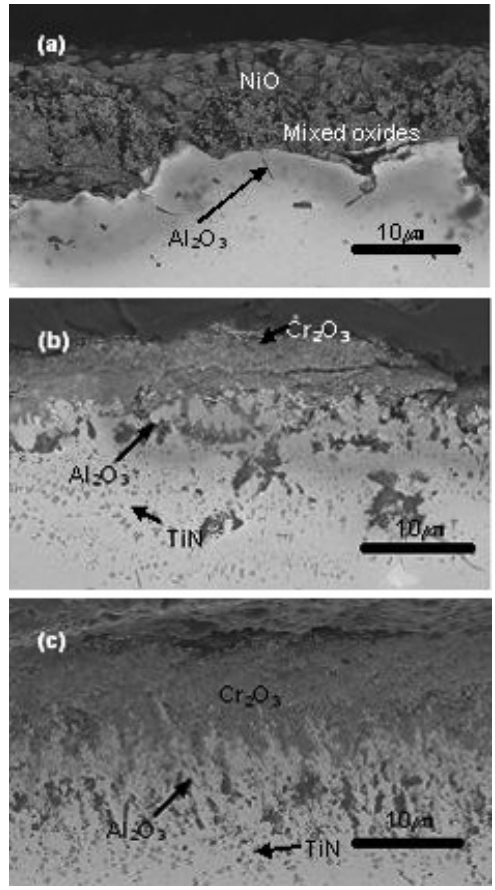

FIGURE 2. Scanning Electron Micrographs of Cross-Sections through (a) René N5, (b) GTD 111 and (c) IN 738 after 80 Hours of Cyclic Oxidation at 950°C in Dry Air with CaO Deposits on Their Surfaces

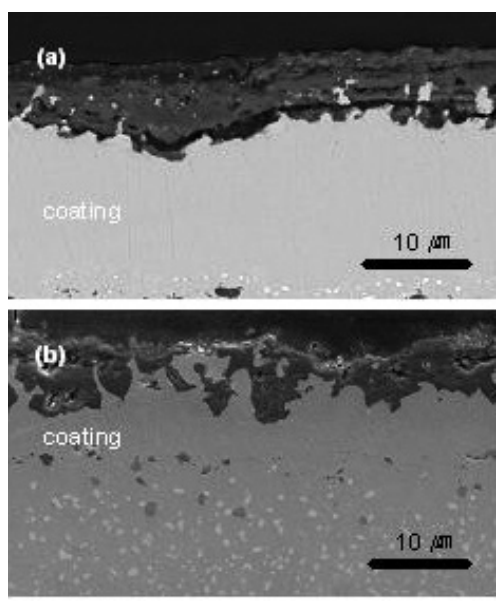

FIGURE 3. Micrographs Showing Cross-Sections of the Platinum Aluminide Coating on René N5 after 200 hours at 950°C, (a) in Dry Air and (b) in Dry Air with a CaO Deposit

apparent. The attack of the platinum aluminide coating on René N5 induced by the CaO deposit can be seen by comparing the two micrographs presented in Figure 3. Work is in progress to compare the degradation of all of the coatings and to formulate approaches to inhibit or prevent the degradation induced by the CaO deposits.

Conclusions and Future Directions

The results that have been obtained in this research show that the deposits, which may be encountered in using alternate fuels, will cause increased degradation of the alloys and coatings that are currently used in power generating gas turbines. This degradation appears to occur by the CaO deposits reacting with the oxide scales, that form on the alloys and coatings, whereby the resulting products do not afford protection to the underlying metallic substrates.

Future work will be directed at determining in more detail the processes by which the CaO causes increased degradation and procedures to inhibit or prevent such effects.

FY 2007 Publications/Presentations

1. M. J. Stiger, G. H. Meier, F. S. Pettit, Q. Ma, J. L. Beuth and M. J. Lance, "Accelerated Cyclic Oxidation Testing Protocols for Thermal Barrier Coatings and Alumina-Forming Alloys and Coatings," Corrosion, 57, 1 (2006).

References

1. R. R. Wenglarz, "Turbine Flow Path Issues for Syngas and Other Alternate Fuels," Impact of Alternative Fuels on Turbine Materials, Materials Workshop III, DOE, University of Connecticut, October 14-16, 2002.

VI. Acronyms and Abbreviations

°C	Degrees Celsius
°F	Degrees Fahrenheit
$/kW	Dollars per kilowatt
2D	Two-dimensional
3D	Three-dimensional
AAB	Academic Advisory Board
AC	Alternating current
AIAA	American Institute of Aeronautics and Astronautics
Al	Aluminum
Al_2O_3	Alumina
ANL	Argonne National Laboratory
APEP	Advanced Power and Energy Program (University of California Irvine)
APU	Auxiliary power unit
APS	Air plasma sprayed
Ar	Argon
ASME	American Society of Mechanical Engineers
ASU	Air separation unit
ATI	Allegheny Technologies, Inc.
atm	Atmosphere(s)
ATS	Advanced Turbine Systems
AVC	Advanced vortex combustor
BFW	Boiler feed water
BHP	Brake horsepower
Btu, BTU	British thermal unit
Btu/lb	British thermal unit(s) per pound
C	Carbon
C	Celsius
Ca	Calcium
CA	California
CaO	Calcium oxide
CASPT2	Complete active space second order perturbation theory
CBS	Complete basis set
CC	Combined cycle
CCADS	Combustion control and diagnostics sensor
CCSD	Coupled-cluster single and double excitation
CES	Clean Energy Systems
CFD	Computational fluid dynamics
CH_4	Methane
CHN	Carbon, hydrogen, nitrogen
Cl	Chlorine
cm	Centimeter(s)
cm^2	Square centimeter(s)
cm^2	Cubic centimeter(s)
cm/sec, cm/s	Centimeter(s) per second
CMC	Ceramic matrix composite
CO	Carbon monoxide
CO	Colorado
CO_2	Carbon dioxide
Cond.	Condition
COS	Carbonyl sulfide
Cr	Chromium
CRADA	Cooperative Research and Development Agreement
CSLM	Cofocal scanning laser microscopy
CT	Connecticut
CTE	Coefficient of thermal expansion
DACRS	Dual annular counter-rotating
dB	Decibel
DC	Direct current
DEC	Deposition erosion and corrosion
deg, DEG	Degree(s)
DETE	Discrete-error transport equation
DGTC	Dynamic gas turbine combustor
DLN	Dry low NOx
DOE	U.S. Department of Energy
DOE-FE	U.S. Department of Energy, Office of Fossil Energy
DWTS	Direct Write thermal spray
EBC	Environmental barrier coating
e.g.	*Exempli gratia*: for example
EMF	Electromotive force
EOR	Enhanced oil recovery
EPD	Electrophoretic deposition
EPRI	Electric Power Research Institute
et al.	*Et alibi*: and others
ESEM	Environmental scanning electron microscope
F	Fahrentheit
FEM	Finite element methods
FL, Fl.	Florida
FSNB-CK	Fitted statistical narrow band correlated-k
FIB-INLO	Focused ion beam *in situ* lift-out
FTT	Florida Turbine Technologies

FY	Fiscal year
g	Gram(s)
g/s	Gram(s) per second
GA	Georgia
GE	General Electric
GmbH	Gesellschaft mit beschränkter Haftung - a limited liability company
GPa	Gigapascal(s)
GRI	Gas Research Institute
GT	Gas turbine
GT	Georgia Institute of Technology
GTI	Gas Technology Institute
H	Hydrogen
H_2	Diatomic hydrogen
H_2O	Water
H_2S	Hydrogen sulphide
HADES	Hyperbaric Advanced Development Environmental Simulator
HAT	Humid air turbine
Hf	Hafnium
Hg	Mercury
HHV	Higher heating value
HP	High pressure
HPT	High pressure turbine
hr	Hour(s)
HRSG	Heat recovery steam generator
I	Current
IA	Iowa
ICE	Intelligent CCADS (combustion control and diagnostics sensor) electronics
ICEPAG	International Colloquium on Environmentally Preferred Advanced Power Generation
i.e.	id est: that is
IEEE	Institute of Electrical and Electronics Engineers, Inc.
IGCC	Integrated gasification combined cycle
IGTI	International Gas Turbine Institute
ID	Idaho
IL	Illinois
in	Inch(es)
IP	Intermediate pressure
IPT	Intermediate pressure turbine
IRB	Industrial Review Board
ISO	International Organization for Standardization
K	Potassium
K	Kelvin
kcal	Kilocalorie(s)
kcal/mol	Kilocalorie(s) per mole
kg	Kilogram(s)
kW	Kilowatt(s)
LA	Louisiana
lb	Pound(s)
lbm	Pound(s) mass
LBNL	Lawrence Berkeley National Laboratory
LCF	Low cycle fatigue
LES	Large eddy simulation
LP	Low pressure
LPT	Low pressure turbine
LSC	Low-swirl combustion
LSI	Low-swirl injectors
LT	Low temperature
m	Meter(s)
MA	Massachusetts
MB/MS	Molecular beam/mass spectrometry
MI	Michigan
μin	Micro-inch(es)
MIS	Matrix isolation spectroscopy
m/sec	Meter(s) per second
mg	Milligram(s)
mg/cm^2	Milligram(s) per square centimeter
mm	Millimeter(s)
MP	Medium pressure
MPa	Megapascal(s)
ms	Microsecond(s)
MS&T	Materials Science and Technology
MSRI	Materials and Systems Research, Inc.
MT	Montana
MW	Megawatt(s)
MWh	Megawatt hour(s)
MW_{th}	Megawatt(s) thermal
N	Nitrogen
N_2	Diatomic nitrogen
NASA	National Aeronautics and Space Administration
NEMS	National Energy Modeling System
NETL	National Energy Technology Laboratory
NG	Natural gas
NH_3	Hydrogen nitride (ammonia)
Na	Sodium
Nb	Niobium
ND	North Dakota
Ni	Nickel
NiO	Nickel oxide

NO	Nitrogen oxide
NOx	Oxides of nitrogen
NIST	National Institute for Standards and Technology
NJ	New Jersey
NRPM	Normalized revolutions per minute
NU	Northwestern University
NV	Nevada
NY	New York
O	Oxygen
O_2	Diatomic oxygen
OASPL	Overall sound pressure level
ODS	Oxide dispersion-strengthened
OEM	Original equipment manufacturer
OH	Ohio
OH-PLIF	Planar laser-induced fluorescence
OPPDIF	A FORTRAN program for computing opposed-flow diffusion flames
ORNL	Oak Ridge National Laboratory
OSU	Ohio State University
P	Phosphorus
P	Pressure
P&ID	Piping and instrumentation diagram
PA	Pennsylvania
Pb	Lead
PCI	Precision Combustion, Inc.
PGM	Platinum group metal
PIV	Particle image velocimetry
PLC	Programmable logic controller
POGT	Partial oxidation gas turbine
POR	Partial oxidation reactor
PLIF	Planar laser-induced fluorescence
ppm	Part(s) per million
ppmvd, ppmVd	Part(s) per million by volume dry
psi	Pound(s) per square inch
psia	Pound(s) per square inch absolute
Pt	Platinum
PVC	Polyvinyl chloride
PWB	Printed wiring board
RCL, RCL™	Rich catalytic lean-burn
RCM	Rapid compression machine
R&D	Research and development
RDS	Research and Development Solutions
RFP	Request for proposals
RGB	Red green blue
RIT	Rotor inlet temperature
RMS	Root mean square
s	second(s)
S	Sulfur
S	Swirl
SAIC	Science Applications International Corporation
SAMA	Scientific Apparatus Makers Association
SBIR	Small Business Innovation Research
SC	South Carolina
SCFH	Standard cubic feet per hour
SCIES	South Carolina Institute for Energy Studies
SCR	Selective catalytic reduction
SECA	Solid State Energy Conversion Alliance
SEM	Scanning electron microscopy
SG	Synthesis gas (syngas)
SGH	Synthesis gas and hydrogen
SimVal	Simulation and validation
SimVal/DGTC	Simulation and Validation/Dynamic Gas Turbine Combustor
S_L	Laminar flame speed
SO_2	Sulfur dioxide
SPG	Siemens Power Generation
SRI	Stanford Research Institute
SOFC	Solid oxide fuel cell
SPPS	Small particle plasma spray
S_T	Turbulent flame speed
SwRI	Southwest Research Institute
T	Temperature
T70	Solar Taurus 70 engine
T_{ad}	Adiabatic flame temperature
TADF	Turbine Accelerated Deposition Facility
TBC	Thermal barrier coating
TC	Thermocouple
TE	Trailing edge
TEM/STEM	Transmission electron microscopy/ scanning transmission electron microscopy
TET	Turbine entry temperature
TIT	Turbine inlet temperature
Ti	Titanium
TMF	Thermal-metal-fatigue
TO_2	Temperature of oxygen
TN	Tennessee
TTU	Tennessee Tech University
TVC	Trapped vortex combustor
TX	Texas

u’	Turbulence intensity
uA	Milliampere(s)
UC	University of Cincinnati
UC	University of California
UCF	University of Central Florida
UCI	University of California, Irvine
UConn	University of Connecticut
UMR	University of Missouri – Rolla
UND	University of North Dakota
U.S.	United States
UT	Utah
UTRC	United Technologies Research Center
UTSA	University of Texas at San Antonio
UTSR	University Turbine Systems Research
V	Vanadium
VA	Virginia
Vol	Volume
W	Watt(s)
W/m/K	Watt(s) per meter per Kelvin
WA	Washington
WV	West Virginia
Wt%	Weight percent
XtL	Coal, gas, or biomass to Liquids
Y	Yttrium
YSZ	Yttria-stabilized zirconia

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