

PROGRESS REPORT FOR PERIOD 10/1/06 – 12/31/06

(BUDGET PERIOD 8/1/06 – 4/30/07)

(U.S. DEPARTMENT OF ENERGY COOPERATIVE AGREEMENT)

AWARD # DE-FC26-06NT42648

**MICRO-MIXING LEAN PREMIX SYSTEM FOR ULTRA-LOW EMISSION
HYDROGEN COMBUSTION**

SUBMITTED BY:
LEAD ORGANIZATION

**PARKER HANNIFIN CORPORATION -GAS TURBINE FUEL SYSTEMS DIVISION
9200 TYLER BLVD.**

MENTOR, OHIO 44060 USA

PHONE: 440-954-8116

FAX: 440-954-8111

TAXPAYER I.D. NUMBER: 34-045-1060

DUNS NUMBER: 123575784

CAGE CODE: 2Y939

PRINCIPAL INVESTIGATOR:

DR. ADEL MANSOUR

**PARKER HANNIFIN CORPORATION - GAS TURBINE FUEL SYSTEMS DIV.
9200 TYLER BLVD.**

MENTOR, OHIO 44060 USA

PHONE: 440-954-8171

FAX: 440-954-8111

BUSINESS POINT OF CONTACT:

GARY GLOTZBECKER – CONTRACT ADMINISTRATOR

**PARKER HANNIFIN CORPORATION - GAS TURBINE FUEL SYSTEMS DIV.
9200 TYLER BLVD.**

MENTOR, OHIO 44060 USA

PHONE: 440-954-8116

FAX: 440-954-8111

DATE OF SUBMISSION: JANUARY 30, 2006



Aerospace
9200 Tyler Blvd
Mentor, OH 44060 USA
Phone (440) 954-8100
Fax: (440) 954-8111

**Micro-Mixing Lean-Premix System for Ultra-Low
Emission Hydrogen/Syngas Combustion
Cooperative Agreement DE-FC26-06NT42648
Phase I**

Progress Report: 10-01-2006 to 12-31-2006

**SUBMITTED TO:
Rondle E. Harp
Project Manager
Power Systems Project Division
U.S. Department of Energy
National Energy Technology Laboratory
P.O. Box 880 Mailstop E06
3610 Collins Ferry Road
Morgantown, WV 26507-0880**

PREPARED BY: *Erlendur Steinthorsson*
Erlendur Steinthorsson – Principal Engineer

1/31/07

APPROVED BY: *Adel Mansour*
Adel Mansour – Technology Team Leader

1/31/07

Micro-Mixing Lean-Premix System for Ultra-Low Emission Hydrogen/Syngas Combustion

Cooperative Agreement DE-FC26-06NT42648

Phase I

Progress Report: 10-01-2006 to 12-31-2006

Executive Summary

The objective of this DOE-supported research program is to develop and test a practical and scalable, high-performing multi-point injector module for hydrogen and syngas fuels that uses Parker Hannifin's Macrolamination technology. In the first reporting period of the project (see the last quarterly progress report) the focus of the development effort was on establishing a high-level conceptual design for the individual mixing cups, determining overall size of the mixing cup and conceiving of fuel-injection strategies. In this second reporting period, 10/01/2006 – 12/31/2006, effort on conceptual designs has continued. In addition, effort was started to determine probable fuel compositions in future applications of hydrogen/Syngas technology and on developing test and diagnostic plans for use in future tests.

Significant progress was made on determining likely fuel compositions for future power plants. Compositions for specific categories of fuels were identified, paving the way for a definitive specification of representative fuel compositions to be created for use in the remainder of the research program. Significant progress was made on the design tools that are needed for generating the multiple geometries to be evaluated in this research phase. A worksheet was added to the design spreadsheet introduced in the first progress report, with parameters driving feature creation in 3-D CAD models. In addition, the design tool now includes optional features for the addition of a liquid (water) atomizer at the base of a mixing cup. Two general mixing cup concepts were defined, each of which offers considerable geometric flexibility to vary parameters such as swirl strengths and mixing length. Three specific mixing cup designs were created and CFD analyses were conducted of fuel-air mixing achieved by those cup variants. The results of the analyses show that good mixing of fuel and air can be achieved within less than 10 mm of axial length. Initial reacting flow simulations were conducted for the purpose of evaluating performance of combustion models and for evaluating resource requirements for the CFD work that needs to be completed during Phase I. A review of testing and diagnostic needs for Phases II and III was started and is still underway, and suitable testing facilities at the University of California at Irvine Combustion Labs (UCICL) have been selected. The diagnostics methods to be used in Phase II of the program include extraction probe and Raman spectroscopy for fuel concentration, PIV for flow-field mapping, OH* radical imaging for flame studies, and extractive probes for emissions.

The project startup at University of California at Irvine (UCI) was held up due to an unforeseen delay in the signing of a Research Agreement between Parker Hannifin and UCI. An agreement was signed near the end of the reporting period, allowing the project to officially start at UCI on Dec. 20, 2006. Parker Hannifin applied for and received a three-

month no-cost extension to Phase I, extending the time for Phase I through April 30, 2007. This extension will not impact the overall project schedule as Phase II will be shortened by three months, from 21 months to 18 months, allowing final testing in Phase III to start on schedule.

Introduction

The objective of this DOE-Supported research program is to develop and test a practical and scalable, high-performing multi-point injector module for hydrogen and syngas fuels. The injector will use Parker Hannifin's demonstrated Macrolamination technology, incorporating a large number of small mixing cups for air and fuel, similar to what has been successfully demonstrated to yield ultra-low emissions for liquid-fuel injection. The specific objectives of this phase of the program are (i) to establish expected performance and operating conditions, (ii) to develop conceptual designs, (iii) to identify barrier issues, and (iv) to develop an R&D implementation plan for Phases II and III. Associated with these objectives are specific tasks, most of which proceed in parallel. The tasks are as follows:

Task 1.0 Definition of Operating Conditions – High Level Design Requirements

Task 2.0 High Level Conceptual Design of Parametric Macrolaminated Injector

Task 3.0 Drafting of Test and Diagnostics Plan

Task 4.0 Market Analysis

Task 5.0 R&D Implementation Plan

Task 6.0 Reporting

As in the first reporting period, the focus of effort in this second reporting period has been on Tasks 1.0 – 3.0. Of those tasks, the University of California at Irvine (UCI) is primarily responsible for Tasks 1.0 and 3.0 while Parker Hannifin is primarily responsible for Task 2.0 but with significant input from researchers at UCI, who will perform CFD analyses of proposed mixing cup configurations. In the following section, the progress made on each task is described. Thereafter, conclusions from the current work are summarized and the expected accomplishments in the third reporting period are outlined.

Technical Progress

Task 1.0—Definition of Operating Conditions—High Level Design Requirements

Significant progress was made relative to Task 1.0 objectives. In this task the general requirements of the fuel injector are to be defined, and fuel compositions and test conditions are to be identified to facilitate the development of a detailed test plan for atmospheric and high pressure tests. The known challenges associated hydrogen combustion are to be identified and possible solutions established. A summary of the results obtained to date are summarized below.

Fuel Compositions The composition of syngas can vary widely with the method of production, i.e. refinery gases or gasification. Similarly, large variation in composition also occurs depending on the feedstock, gasifier type, and choice of diluent. Literature searches confirm the gross variation among constituent concentrations. Therefore the idea of DOE-style matrix for fuel composition was abandoned. Instead, fuel compositions will be determined by likely future scenarios that involve high hydrogen fuels. One representative composition will be selected for each of the following scenarios in addition to the testing of pure hydrogen.

- Process and refinery gas
- Large scale IGCC power plant (>50MW)
- Small scale IGCC power plant (<50MW)

- Nitrogen dilution for NO_x abatement

Table 1 shows preliminary syngas compositions on a dry, volumetric basis that are representative of the above categories of fuels. Fine tuning of the exact concentrations of each constituent may be in order after further literature review is conducted.

Table 1 - Dry, clean syngas compositions

Mole Fractions	H2	CO	CH4	CO2	N2	LHV (Btu/ft3)	Wobbe Index
Pure H2	100	0	0	0	0	265	1006
Solar #10	54	11	25	10	0	398	603
Coal/Pet. Coke	37	46	1	14	2	247	289
Biomass	17	17	5	13	48	142	152
Nitrogen Dilution	23	31	1	10	35	165	183

Combustion Characteristics of Fuels UCI has compiled extensive information on the combustion characteristics of hydrogen and syngas, such as reaction rates, flame speeds, and auto-ignition times. Many kinetics reaction mechanisms have been evaluated at UCI. Furthermore, a substantial amount of data on laminar flame speeds and auto-ignition times have been compared to correlations. UCI currently has ongoing studies in the areas of flame speed determination and auto-ignition for syngas fuels.

Operating Conditions As with the fuel composition, the operating conditions will be determined based on platforms that are likely candidates for future applications of high hydrogen combustion. Trade studies are currently underway to determine the most probable engines and their respective operating conditions. The gas turbine manufacturers under consideration are Solar Turbines, General Electric, and Siemens.

Issues with Engine Balance of Plant The low Wobbe Index of syngas fuels leads to a number of challenges with syngas combustion (this is not the case for pure hydrogen). Modifications are likely required in the fuel delivery scheme. Also, hydrogen embrittlement has the potential to damage hardware associated with the fuel circuit; decreasing durability and raising O&M costs. Higher parasitic losses will be incurred from the need to compress a larger volume of fuel. Solar Turbines has commissioned a safety oriented study on the use of hydrogen in a gas turbine, whose findings will be included in the final Phase I report.

Technical Challenges and Barriers UCI and Solar Turbines have initiated discussions on identifying the technical challenges associated with lean premix operation on high hydrogen fuels. The list of possible hazards includes a number of materials-related issues, such as hydrogen embrittlement of fuel plumbing and components, and the enhanced heat transfer characteristics of syngas-based products. Moreover, the specific challenges in regards to combustion will also be addressed. These include flashback, the emergence of alternative pathways of NO_x formation, and the lack of availability of low temperature kinetics for hydrogen/syngas fuels.

Task 2.0—High Level Conceptual Design of Parametric Macrolaminated Injector

In the first reporting period, a range of options and geometric configurations for Macrolaminated mixing cup designs were defined, and approaches to approximately size a mixing cup and its features were explored. In this reporting period, the work continued and



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parametric CAD models for two mixing-cup concepts were created, enabling rapid creation of different detailed designs based on the underlying concepts. Also, CFD analyses (cold-flow) were carried out for several cup designs to evaluate the mixing performance of the concepts. Since the design space enabled by the Macrolamination technology and the mixing cup concept is large, systematic approach is needed to explore the possible mixing-cup concepts and detailed configurations. Below, the overall approach is described first, followed by a summary of accomplishments (results).

Approach The approach taken to explore the design space enabled by Parker's Macrolamination technology is as follows. First, the basic design options for the mixing cup are listed and classified according to geometry and function. The different design options for the various functions are then combined to create several different *mixing-cup concepts* which are distinctly different from other concepts in terms of the manner in which fuel and air are introduced into the mixing cup, or in the way air and fuel flow through the cup. From each distinct concept, numerous *instances* or variants can be created by varying the design parameters for that concept. The detailed implementation of each mixing-cup concept is then explored systematically, e.g., by altering the relative arrangement of fuel and air circuits and by adjusting geometric parameters to configure cups with different effective areas, different swirl numbers and different mixing and flame holding characteristics. The viability of the various design concepts are then explored using CFD. A schematic view of the approach is shown in Fig. 1. The basic design options are shown in Table II, which is reproduced from the first progress report with minor additions.

To facilitate systematic generation of design variants using the parametric CAD models, the mixing cup geometry is considered to consist of four regions according to the role of the fuel and air circuits which are contained within that region. The regions are shown in Fig. 2. Region 1 consists of the Macrolaminated layers near the bottom of the mixing cup where air is injected, with or without a swirl component. This region sets up the core air that flows along the cup's centerline. Region 2 consists of a subsequent series of layers where both fuel and air enter the cup. The arrangement of the air and fuel layers in this region with respect to other layers in the cup defines the overall mixing scheme of the cup. Region 3 consists of air layers downstream of Region 2 where swirling air may be added to further control the flow characteristics of the mixture as it exits the cup. In this region, the amount of air and the relative swirl strength in this region can be varied, for instance to help prevent. Region 4 is the exit region, which may utilize different geometric profiles (e.g., converging exit) to help control the flow. The four regions described above will provide a consistent basis for describing the concepts investigated in Phase I.

In any of the four regions described, multiple parameters define injection locations, swirl strength and orientation, and the interaction of multiple layers, resulting in an unbounded matrix of possible configurations. A design spreadsheet was created that drives the

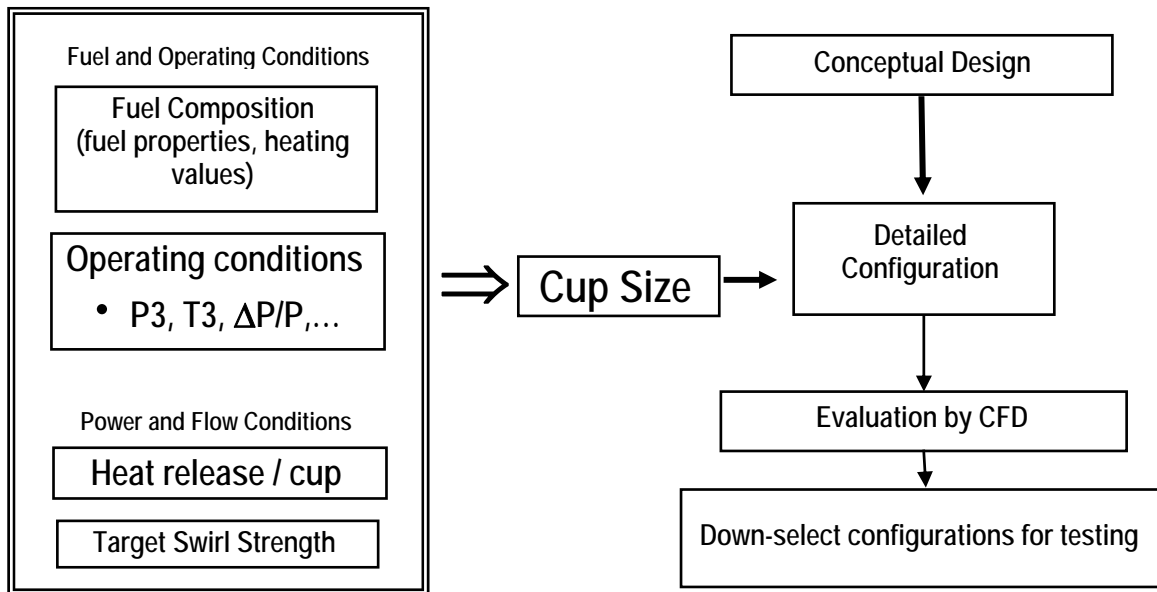


Figure 1. A diagram illustrating the design process for Phase I – engine operating conditions and overall swirl strength for each cup determine cup size; the design concept and required geometric parameters for the target mixing cup lead to a detailed design (an instance of the particular concept) which is then evaluated using CFD.

Table II Possible Mixing Cup Configurations

Fuel Injection	Air Flow Configuration	Mixing Cup Configuration	Exit Configuration	Flash-back prevention
Radial jets	Non-swirling—axial through-flow	Straight	Straight	Flow speed (high Δp)/high shear
Axial jets	Non-swirling—radial inflow	Converging	Converging	Air layer near wall at exit
Angled jets (swirling)	Radial swirler	Diverging	Diverging	
Axial swirling / non-swirling	Axial swirler		Burner cup at exit	
Radial-inflow swirling / non-swirling	Layered swirler (variable swirl based on axial location)			



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dimensions of relevant geometric features (see a sample sketch in Fig. 3). The spreadsheet was expanded in the current reporting period to drive creation of CAD models and was equipped to allow for liquid diluent atomization at the base of the cup, and axial injection of either air or fuel at various axial positions within the cup. As fuel compositions get further defined in this project phase, the impact of fuel composition on fuel circuit geometry will be investigated. Note that in addition to gas dilution circuits, the design tools developed for Phase I include optional features for the addition of a liquid (water) atomizer at the base of a mixing cup.

Results: Two different mixing cup concepts were defined and modeled in CAD by combining characteristics for different functions identified in Table II. The first concept is a mixing cup with radial-inflow swirling air and radial-inflow swirling fuel. This concept is considered a baseline concept. The second concept is a mixing cup with radially-inflow swirling air but axially-injected non-swirling fuel. The mixing cup concepts account for the all features needed in future incorporation of the mixing cups into a multi-point injection assembly. The features include a possible need for front-face cooling, selection of materials and space for manifolding. With adequate manifolding space, Macrolamination allows for the addition of networked passages for various fluid circuits within an array of mixing cups, connecting individual cups with circuits and external manifolds for fuel, cooling, and diluents. In this manner, by allocating space within the envelope of the single-point injector, concepts developed in Phase I, the scalability of the single-cup designs to future multi-cup embodiments of the concepts is ensured.

From the two mixing-cup concepts that were defined, three specific mixing cup configurations were created and analyzed using CFD. The first configuration comprised a Region 1 with two air layers, Region 2 with two fuel injection points and several air layers, and a Region 3 with a relatively strongly-swirling air layer. The second configuration was similar but used four injection points for hydrogen in Region 2 in stead of two injection points. The third configuration that was analyzed used axial injection of fuel. All three configurations used a straight exit region. The CFD analyses were done using Fluent and examined the mixing of air and fuel in the cups, utilizing a realizable k-e turbulence model with wall functions to account for the effects of turbulence on the flow. The grid systems were generated using Gambit. After conversion to polyhedral cells in Fluent, each grid contained 1.5 – 2 million cells. An example of a mixing profile near the exit of a cup is shown in Fig. 4, showing a profile with local equivalence ratio ranging from 0.16 to 0.42 for a cup with an overall equivalence ratio of 0.35. The results show a good level of mixing achieved in less than 10 mm of mixing length. Also, it is clear that further mixing can be achieved. Note, due to the proprietary nature of mixing cup designs, sketches are not shown in this report but can be provided to DOE in private meetings or non-publicly available documents. At the time of this writing, detailed information has been given to DOE during and following a meeting with DOE on January 19, 2007.

While awaiting the formal execution of the contract agreement documents between Parker Hannifin and UCI, efforts were taken at UCI to evaluate the computational requirements needed and to assess the time required to complete simulations. To accomplish this without a specific injector geometry, a ‘mock’ CFD model of the macrolamination injector was developed. The mock model has simpler geometry compared to the real injector but has similar macrolamination structure. Cold flow and reacting simulations were carried out which generated results including swirling flow structure, hydrogen/air mixing

performance, impacts of air injection angles, etc. Also, the two computational codes available to the UCICL, CFD-ACE and Fluent, were evaluated with the mock injector model.

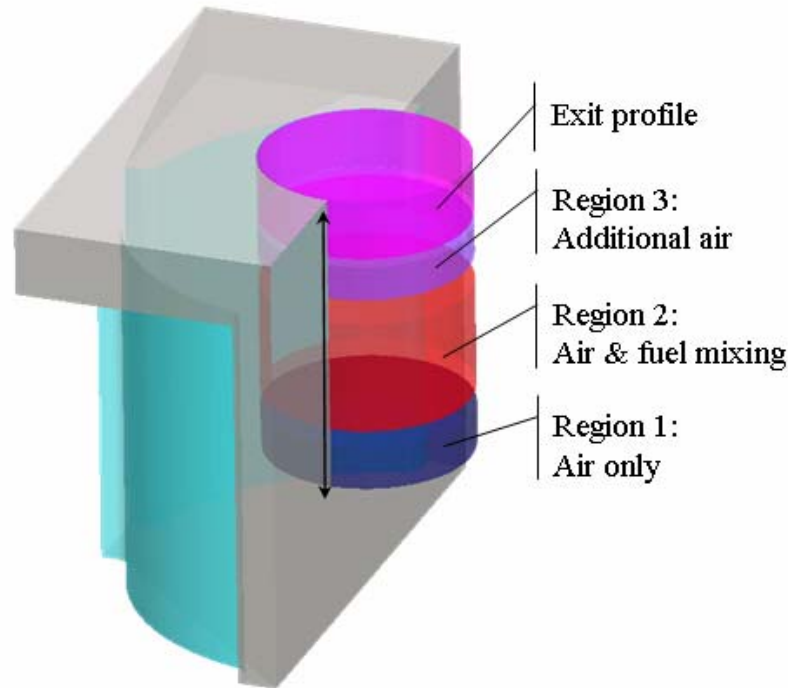


Figure 2. Schematic showing four regions in a mixing cup, defined according to the function of each region

Successful simulations were accomplished using both codes. Both codes appear to be appropriate and capable of accomplishing the simulations desired. However, Fluent was chosen for this project due to its wide application and convenient file exchange with Parker. A secure FTP was created for the purpose of allowing convenient file exchange of Fluent data, mesh files, etc., between UCI and Parker.

The result of the evaluation of the computational resources for CFD tasks at UCI indicates that the desktop PC used for meshing during the current reporting period cannot handle the large unstructured grids (over 1 million cells) due to memory limitation. As a result, a high performance workstation with 4GB memory and a 64bit OS will be obtained for meshing task. To accomplish the time intensive CFD tasks such as combustion modeling with multi step chemistry mechanism, a parallel version of Fluent, with a license for 8 CPUs, will be needed.

Late in the current reporting period, at the official project start at UCI, the first detailed Macrolaminated geometry was provided by Parker Hannifin. The mesh generated included several million cells. Preliminary cold flow results were obtained using 3 nodes (each with dual CPU Opteron processors) within the MPC cluster. These 3 nodes are owned by and dedicated to the UCICL. The results obtained suggest that additional nodes may be needed to accomplish 3D reacting flow simulations.

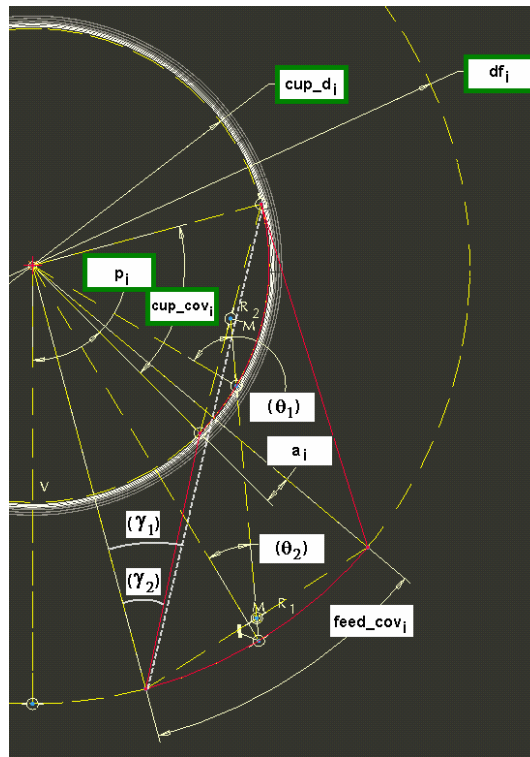


Figure 3. Schematic showing parameters that are used to define geometry of air and fuel circuits and to drive a parametric CAD model

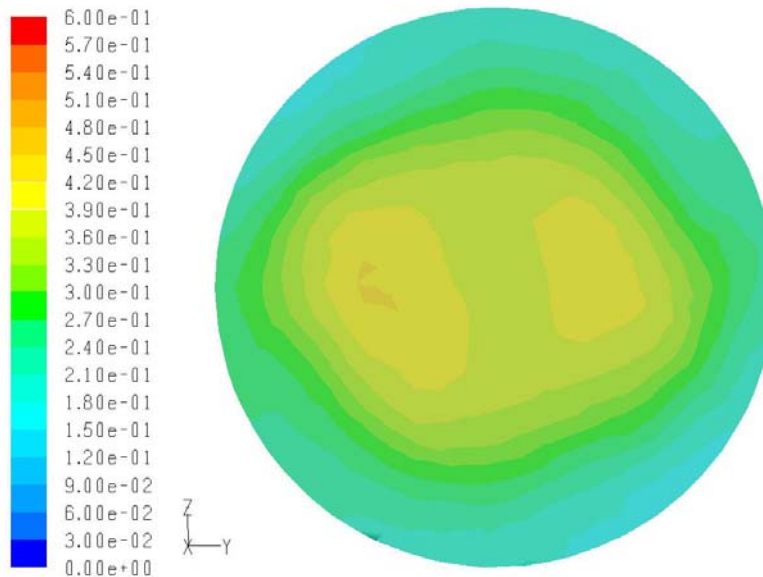


Figure 4. Sample results from CFD analysis of a mixing cup – contours of local equivalence ratio near the cup exit (overall equivalence ratio for this case was 0.35)



Task 3.0—Drafting of Test and Diagnostics Plan

Experimental studies are to be conducted in Phases II and III of the three year project. Phase II consists of the testing of single- and multi-cup concepts during Tasks 8.0 and 10.0 respectively. Under Task 8.0 (Phase II), a total of six single-cup prototypes are scheduled to be tested under atmospheric and high pressure conditions over a four month period. Based on the results of these experiments, two concepts will be selected for multi-cup studies. Atmospheric and high pressure tests will be conducted over another four month period. All phase II testing is to be performed at UCI. The final tests will be of a full scale (1MW) injector in phase III of the program. Atmospheric and high pressure tests of the injector will be conducted at UCI and Solar Turbines respectively. Task 3 is directed at developing a detailed Test Plan and Diagnostics Plan Report as a Deliverable for Phase I. Completion of this task requires specification of fuel compositions and operating conditions to be used in the tests, and identification of test facilities and diagnostics methods. Progress made during the current reporting period on Task 3 is summarized here.

Fuel Compositions and Operating Conditions Fuel compositions for the required tests will be defined under Task 1.0. Complete tests on the injector concepts will include operation on each of the five chosen fuel blends. Similarly, the operating conditions that will be defined in Task 1.0 will form the basis of the test conditions for Phases II and III.

Test Facilities UCI's facilities include a fuel blending station capable of simultaneous mixing of up to five gases. The gas blending station will be available for use throughout the duration of the project. UCI's atmospheric facilities are capable of 500 cfm of air at 120 psig and are all equipped with optical tables to facilitate the use of various laser diagnostic techniques. In addition, preheat temperatures of 1000 F are possible. The high pressure facilities at UCI can deliver 0.6 pps air at 20 atm and 0.2 pps nitrogen at 10 atm. The facility is equipped with a 550 kW electric preheater and has a large degree of optical access for making detailed measurements. Solar Turbines' high pressure single injector test rig is capable of 9 pps air at 20 atm and preheat temperatures up to 1000 F.

Experimental Methods Mixing profile studies of injector concepts will be pursued in two avenues. First, extractive probe measurements will be made. The small length scales of the mixing cups introduce the need for a very small probe, i.e. hypodermic needle, to achieve adequate spatial resolution. Two analyzers are available at UCI for sample measurements. Second, UCI will also explore the use of hydrogen Raman spectroscopy as a non-intrusive option for concentration measurements. Additional non-reacting tests will include characterization of the aerodynamics of the flow generated by the injector using particle image velocimetry (PIV). Global imaging of OH* radicals from hydrogen combustion serves as a flame indicator and will be used to study flame structure as well as for instantaneous monitoring of flashback. Other reacting tests include temperature profile and emissions measurements. Temperature measurements can be made by conventional thermocouple probes or by tunable diode laser absorption spectroscopy (TDLAS). The preclusion of thermocouples to sustain reaction temperatures gives merit to TDLAS despite it being a path averaged measurement. Emissions measurements will be made with the conventional extractive probe approach. Emissions sampling procedures at UCI are in accordance with the protocol of the CARB 100 test method.

Testing Approach Emphasis for the atmospheric tests will be to test as many configurations as possible in the time allotted using "screening" tests first. These screening



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tests will consist of cold flow mixing followed by reacting flow tests for emissions, lean blow off, and flashback determination. From these preliminary tests, promising injector prototypes will be selected for “complete” tests. Furthermore, the time intensiveness of high pressure tests may preclude the ability to tests all injector configurations at elevated pressure conditions during Task 8.0. Only injector concepts which are deemed most promising will be chosen for these studies.

Conclusion and Planned Accomplishments

At the end of the second quarterly reporting period, the methodology to be used for design exploration was well defined, as described in the previous section. Due to the multiple design options, the design space is still being explored and new mixing cup concepts being generated. Design tools have been created that can be used to drive generation of CAD models for new concepts, enabling the systematic exploration of the design space. CFD analysis on initial concepts show very promising results for fuel-air mixing and further enhancements are definitely possible. Some details of the CFD methodology are still being refined, especially the details of the chemistry models and turbulence-chemistry interaction models to be used for reacting-flow analyses. The project is proceeding on schedule.

In the next reporting period for this project, the expected accomplishments for Tasks 1.0 – 3.0 are as follows:

Task 1.0 The definition of operating conditions, necessary to develop a rigorous test plan, will be completed through further review of technical literature and trade studies. Also UCI and Solar Turbines will continue having discussions on issues related to engine balance of plant and technical challenges associated with hydrogen. Recommendations on these issues will be provided in the final Phase I report.

Task 2.0 Multiple mixing-cup configurations will be generated and efforts on evaluating the performance of the injector designs will begin in earnest. Based on the preliminary CFD results, additional computational resources are likely to be required at UCI. Also, selection of the chemistry approach to be used for the reacting flow computations will be established.

Task 3.0 The applicability of hydrogen Raman spectroscopy for mixing studies will be determined by simple experiments in the coming weeks. Comparisons will be made between this and the extractive probe method. Raman spectroscopy of hydrogen is expected to be a reliable tool that can be used instead of a physical probe. Drafting of the Test and Diagnostics Plan is underway and is expected to be completed.

Cost Plan Status

Baseline Reporting Period	Yr. 1 Start - 7/1/06 End - 6/30/07				Yr. 2 Start - 7/1/07 End - 6/30/08				Yr. 3 Start - 7/01/08 End - 6/30/09				
	* Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12	**Q13
Task Numbers	Task 1 - (9 months)				Task 2 - (18 Months)				Task 3 - (9 months)				
Baseline Cost Plan (from SF 424A)	\$70,132	\$105,198											
Federal Share	\$56,105	\$84,158											
Non-Federal Share	\$14,027	\$21,040											
Total Planned (Federal and Non-Federal)	\$70,132	\$105,198											
Cumul. Baseline Costs To Date	\$70,132	\$175,330											
Actual Incurred Costs	\$9,992	\$55,856											
Federal Share	\$7,994	\$44,685											
Non-Federal Share	\$1,998	\$11,171											
Total Incurred Costs-Quarterly (Federal and NonFederal)	\$9,992	\$55,856											
Cumul. Incurred Costs To Date	\$9,992	\$65,848											
Variance	-\$60,140	-\$49,342											
Federal Share	-\$48,111	-\$39,473											
Non-Federal Share	-\$12,029	-\$9,869											
Total Variance-Quarterly (Federal and Non-Federal)	-\$60,140	-\$49,342											
Cumulative Variance To Date	-\$60,140	-\$109,482											

* Q1 - reflects months of Aug. and Sept. 2006 only, since budget period - 8/1/06 - 4/30/07

** Q13 - will reflect the last month of the 3-yr. program (July 2009)

Note that adjustments have been made to above figures as appropriate to take into account that Phase 1 is now 9 months (previous report was only 6 months)

Milestone Plan / Status Report

Task / Subtask #	Critical Path Project Milestone Description	Project Duration - Start - 01AUG06 End - 31JUL09												Planned Start Date	Planned End Date	Actual Start Date	Actual End Date	Comments (notes, explanation of deviation from baseline path)	
		Project Year (PY) 1				PY 2				PY 3									
		Q1 - 8/2006	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12 - 7/2009						
1	Conceptual design	●	—	◆											10/6/2006	4/30/2007	10/6/2006		New baseline reflecting Phase I extension
2	R&D Implementation Plan			●◆											3/1/2006	4/30/2007			New baseline reflecting Phase I extension
3	Design & fabrication of single cups				●	—	◆								5/1/2007	9/24/2007			New baseline reflecting Phase I extension
4	Testing & analysis of single- cups					●	—	◆							9/25/2007	12/31/2007			New baseline reflecting Phase I extension
5	Design & fabrication of multi- cups						●	—	◆						1/1/2008	3/10/2008			New baseline reflecting Phase I extension
6	Testing & analysis of multi- cups							●	—	◆					3/11/2008	6/16/2008			New baseline reflecting Phase I extension
7	Multi-stage, full-scale design								●	—	◆				6/17/2008	10/31/2008			New baseline reflecting Phase I extension
8	System fabrication									●	—	◆			11/3/2008	4/10/2009			
9	System testing										●	—	◆		4/13/2009	7/31/2009			

Note that adjustments have been made to above figures as appropriate to take into account that Phase 1 is now 9 months (previous report was only 6 months)