Combustion Characterization and Modeling of Fuel Blends for Power Generation Gas Turbines
Contract # 04-01-SR114

FACT SHEET

I. PROJECT PARTICIPANTS

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II. PROJECT DESCRIPTION

A. Objectives

A multidisciplinary team consisting of the University of Central Florida, Flow Parametrics, and The Aerospace Corporation has been assembled to provide the blend of experimental measurements, chemical kinetics modeling, and computational fluid dynamics modeling required to produce an experimental and analytical database on fuel variability effects in gas turbines. The primary objectives for the 3-year program are as follows.

1. Create efficient test matrices to explore a wide range of fuel mixtures, stoichiometry, and test conditions in an aggressively short period of time.
2. Measure ignition delay times for a range of syngas and natural gas blends at temperatures between 800 and 1800 K and pressures up to 30 atm.
3. Develop ignition delay time correlations from the ignition data that can be utilized immediately by combustion engineers.
4. Perform flame speed measurements for a range of syngas blends at realistic temperatures and pressures.

5. Formulate flame speed correlations from the data that can be used immediately.
6. Validate computational fluid dynamics models including finite-rate chemistry of a typical premixed gas turbine combustor and a diffusion flame combustor.
7. Test mixtures from fuel matrices in the CFD gas turbine combustors using the kinetics mechanisms identified in this program.
8. Identify appropriate full chemical kinetics mechanisms to model the ignition and flame speed data, compare with the new data, and make required improvements.
9. Assemble a reduced chemical kinetics mechanism for use in the CFD calculations.
10. Acquire detailed kinetics information such as species concentration time histories for the validation and improvement of the chemical kinetics model(s).
11. Characterize experimentally and analytically the formation of NOx for the same range of mixtures and conditions identified for the ignition and flame speed measurements.
12. Compare the ignition behavior of liquid-fuel sprays experimentally.

B. **Background/Relevancy**

Much challenge remains for the gas turbine industry to meet the DOE Vision 21 goals, especially with the requirement of burning a variety of fuels such as coal, natural gas, biomass, petroleum, coke, and municipal waste. Similar complications related to fuel composition variations are even more severe when gas turbines manufactured for use in the United States are installed in other countries, where even the natural gas blends, not to mention more exotic fuel makeups, can be distinctly different from those in the U.S. Such wide variations in fuel composition often produce wide variations in the chemical behavior of the fuels, not only in terms of their overall energy content but also in important parameters such as reactivity and flame speed. 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 characteristic ignition delay time, has a direct impact on the performance and stability of a given combustor design. However, very little if any fundamental flame speed and ignition data are available for uncommon fuel mixtures, much less at realistic engine pressures and concentrations.

C. **Period of Performance**

Start: May 1, 2004
End: April 30, 2007

D. Project Summary

This project is divided into seven major tasks, based on the team strengths and program objectives: 1) test matrix and literature review; 2) autoignition measurements; 3) flame speed measurements; 4) chemical kinetics modeling; 5) CFD modeling; 6) NOx measurements; and, 7) mechanism validation experiments.

III. PROJECT COSTS

A. *$405,590 (total, UTSR)*

IV. MAJOR ACCOMPLISHMENTS SINCE BEGINNING OF PROJECT

1. Many ignition delay time experiments were performed for mixtures of methane with hydrogen, ethane, propane, butane, and pentane at pressures up to about 30 atm and undiluted fuel/air mixtures at lean equivalence ratios ($\phi = 0.5$).
2. Several shock-tube experiments of syngas mixtures have been performed, covering a range of CO/H_2 blends from 90/10 to 10/90% by volume and pressures up to 15 atm.
3. A chemical kinetics mechanism for electronically excited OH radicals was developed.
4. A gas dynamic technique for extending the test time in the PI's shock-tube facility was demonstrated.
5. A 21-test design-of-experiments test matrix was derived for the autoignition experiments, and each "test" represents a fuel blend mixture of methane with various combinations of H_2, C_2H_6, C_3H_8, C_4H_{10}, and C_5H_{12}.
6. The 21-test matrix was run at a pressure and temperature reflective of gas turbine premixers (800 K, 20 atm) to determine whether there is autoignition within 10 ms.
7. The detail design and analysis for a new, high-pressure flame speed experiment were performed, and fabrication is complete.
8. A model CFD burner was assembled by Flow Parametrics for application to fuel-flexibility simulations.
9. The chemical time scale for methane ignition, using the experimental ignition data obtained under this program, was correlated into one expression for use in CFD simulations.
10. Performed high-pressure experiments for a particular syngas blend ($H_2/CO/CO_2$/other) at temperatures less than 1000 K, showing extreme disagreement with current kinetics models. Results compare favorable with new flow reactor data from UCI (McDonell et al.).

V. MAJOR ACTIVITIES PLANNED DURING THE NEXT 6 MONTHS

1. Use CFD model and revised methane chemistry model to probe interactions between chemistry and fluid mechanics in premixer regions.
2. Perform first laminar flame speed experiments on target syngas mixtures.
3. Suggest improvements required to CO/H_2 kinetics models.
4. Continue ignition measurements of syngas mixtures at engine pressures.
5. Wrap up natural gas-based ignition measurements.

VI. MAJOR ACCOMPLISHMENTS PLANNED IN OUTMONTHS (6-18 MONTHS)

1. Complete flame speed measurements.
2. Complete CFD simulations of fluid/chemistry interaction.
3. Complete ignition delay time measurements.
4. Write final report.

VII. ISSUES - none

VIII. ATTACHMENTS – None.