FUNDAMENTAL CHARACTERIZATION OF ALTERNATE FUEL EFFECTS IN CONTINUOUS COMBUSTION SYSTEMS. TECHNICAL PROGRESS REPORT NO. 2, 15 NOVEMBER 1977--14 FEBRUARY 1978

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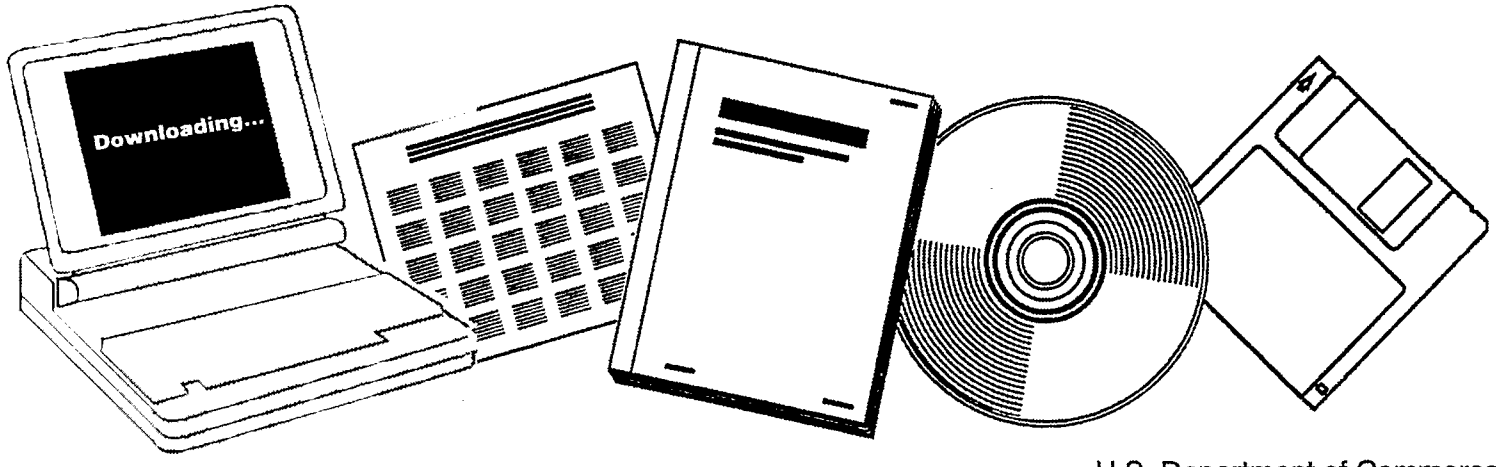
12 JUN 1978



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FUNDAMENTAL CHARACTERIZATION OF ALTERNATE FUEL EFFECTS IN CONTINUOUS COMBUSTION SYSTEMS

Technical Progress Report No. 2
for the Period
15 November 1977 - 14 February 1978

William S. Blazowski

June 12, 1978

Work Performed Under Contract EC-77-C-03-1543

Exxon Research and Engineering Company
Government Research Laboratories
P.O. Box 8
Linden, New Jersey 07036

government research

REA

FOREWORD

This is the second Technical Progress Report for DOE Contract EC-77-C-03-1543, "Fundamental Characterization of Alternate Fuel Effects in Continuous Combustion Systems." It includes brief descriptions of initial experimental and analytical information generated during months four through six of the program. Experimental information was generated by Exxon Research and Engineering Company (ER&E) and analytical work was performed by Science Applications Inc. (SAI). Dr. Raymond Edelman is responsible for activities at SAI. ER&E is the prime contractor for this program and is responsible for overall program direction and performance.

The data and findings of our work during this quarter must be regarded as preliminary. Much further analysis and confirming data will be provided during the balance of the first program year. Consequently, the description of progress contained herein is of a general nature. The first year Interim Report will provide a full, detailed accounting of the technical data, analysis, interpretation, and conclusions.

William S. Blazowski
Principal Investigator

INTRODUCTION

Alternate fuels derived from coal, oil, shale, and tar sands are expected to play an increasingly important role in meeting the future national energy demand. The properties of these fuels can result in significantly different combustion performance compared with conventional specification fuels. For example, decreased hydrogen content can result in increased flame luminosity and exhaust smoke emission, higher fuel bound nitrogen can result in increased NO_x emissions, and fuel impurities can result in deposition within the combustion device. Although additional refining and fuel treatment can mitigate these problems to some extent, the approach of adapting the combustion system to utilize fuels having "unconventional" properties while operating in an environmentally acceptable manner seems to be most cost effective and energy efficient. This program will provide vital fundamental information necessary for the efficient pursuit of this approach.

The subject program is a multi-year effort to provide an improved fundamental understanding of the relationships between fuel properties and combustion characteristics and to develop analytical modeling/correlation capabilities for the prediction of fuel effects. The work will be limited to investigation of alternate liquid and gaseous fuels used in continuous combustion systems, with gas turbine systems receiving special attention. The program philosophy is to relate fundamental combustion phenomena to fuel characteristics using analytical models developed with and eventually verified by data obtained in carefully designed experiments. Consequently, the program will proceed along two parallel paths, modeling and experimental. ER&E will be responsible for overall program direction and experimentation, while Science Applications, Inc. (SAI) will be responsible for analytical modeling under subcontract to ER&E.

Effort during the first phase of this program (to be undertaken in the first year) will provide a well-developed plan for subsequent years of the program. Key combustion properties and ranges of fuel variation of interest to our subsequent efforts will be surveyed. Experimental work will include the utilization of unique ER&E experimental equipment for evaluation of fuel combustion characteristics. The analytical modeling effort will include new applications of quasi-global modeling techniques as well as predictions of and comparisons with the experimental results generated. Efforts during the second two years of this program will concentrate on solving the problems identified using the approaches defined in Phase 1. These efforts will be characterized by the broad application of experimental combustion facilities available at ER&E. The SAI modeling work will not only attempt to better describe chemical and physical phenomena, but will also provide valuable guidance concerning the design of experiments. This cooperative, iterative procedure will optimize the improvements to fundamental understanding and the generation of an analytical model during this program.

Tasks 1 and 2 of the first year of this effort were completed in January with the Task 1/2 presentation to DOE representatives on the 12th and the submittal of the first Technical Progress Report. The report provides background information which describes the current understanding of alternate fuel effects in gas turbines. A survey of analytical model capability for prediction of fuel effects in continuous combustion systems was provided and sections on computational methods for recirculating reacting flows, turbulent flow modeling, and the phenomena of unmixedness, droplet and spray combustion, and fuel decomposition and combustion were included. Key technical areas requiring additional study and analysis have been identified and prioritized. The presentation summarized this information and described current planning of the second and third program years. An expanded program involving more concentrated effort and larger scale experimentation is envisioned.

Experimental Developments

A reliable procedure for jet-stirred reactor ignition has been developed which does not involve hydrogen injection. Ethylene-air mixtures, with inlet temperatures as low as 25°C, have been utilized. Air and fuel flow rates are reduced gradually until a condition is reached where the combustion of the mixture external to the reactor flashes into the internal reaction zone and ignites the jet mixed combustion process. This occurs with fuel-air injection velocities far below sonic. Flow rates are then increased to an idle condition--an equivalence ratio of about 0.35 and air flow of 200 l/min--for reactor warm-up. Experience during the past quarter has also provided guidance for ethylene-air mixture conditions which should be avoided to prevent reactor overtemperature and refractory melting. At the high preheat reactor temperatures (>250°C) equivalence ratios of 0.6-2.0 should be avoided. A narrowing of this zone will be possible with fuels other than ethylene and with N_2 dilution of the inlet air, or with decreased inlet mixture temperature.

A carbon balance between the inlet mixture and combustion product measurements has been used to verify proper functioning of the exhaust system. The carbon mass fraction calculated from the measured inlet fuel and air flows and the exhaust carbon mass fraction calculated from measured values of CO, CO_2, and hydrocarbons have been compared. Agreement between the two calculations for fuel-lean conditions is within $\pm$10% for most data obtained.

Lean blow out limits for ethylene-air combustion as a function of total mass flow and inlet temperature have been acquired. The trends observed are in agreement with expectations. Gaseous exhaust product concentrations for lean operation have also been determined. Hydrocarbons are only present near the lean blow out limit. Carbon monoxide increases as the fuel-air ratio is lowered to approach the lean blow out point and increases at the high fuel-air ratio. Consequently, a minimum value is observed. These results will be of value in developing quasi-global models of hydrocarbon combustion in well-mixed combustion zones. These data have been acquired for both 1.5-inch and 2-inch diameter stirred combustors and the results will be analyzed for indication of surface effects which may impact the global chemistry being studied.

Soot data has been obtained for rich ethylene-air operation. Results to date represent observations of soot deposits on filters, but not gravimetric analysis. Data was obtained by testing at increasing equivalence ratio increments of 0.1 and results represent an equivalence ratio value midway between test points at which soot was first observed. Incipient sooting equivalence ratio for ethylene-air combustion has been obtained to determine the dependencies on inlet mixture flow rate as well as inlet temperature. Gaseous species concentrations at the incipient soot limit were also determined. The predominant carbon species is CO (present at about 20 mole percent) with hydrocarbon concentrations also being significant (up to 8% as methane).

Liquid fuels to be tested in future program months were acquired. The complete fuel list is:

ethylene	ortho-xylene
n-octene	meta-xylene
cyclo-octane	para-xylene
hexane	cumene
cyclo-hexane	tetralin
n-octane	decalin
iso-octane	1-methyl napthalene
toluene	dicyclopentadiene

Study of toluene-air combustion was initiated during this quarter. Data were acquired for both lean and rich operation. The results indicate sooting at much lower equivalence ratios and the production of much larger quantities of soot.

Analytical Developments

Analytical work during the past quarter has concerned comparison of the existing quasi-global model for hydrocarbon combustion with available data and extension of the quasi-global modeling concept. Comparisons with existing data have shown that the present quasi-global model predicts well the ignition delay time for propane, but underestimates ignition delay times of ethane and butane. The rate of the oxidation reaction in the quasi-global model was determined from a series of comparisons between experimental results and calculations pertaining to ten different fuels. However, while propane was included in the group of the fuels studied, both ethane and butane were absent. Another reason for these complications is that the data with which comparisons are being made are available for only a limited distance of a plug flow reactor (combustion time). It is impossible to conclude whether the predictions would agree with the data for longer times as the equilibrium temperature is approached.

Computer coding has been changed to account for the extension of the quasi-global model. The objective of the model under development is to include both bound nitrogen and soot formation, as well as pyrolysis and oxidation of the fuel. However, in a first step we are concentrating on a model of the gas phase reactions pertaining to pyrolysis and oxidation of the fuel. This model includes three quasi-global steps, instead of one. For example, for propane, the one step oxidation to CO and H_2 is now replaced by

$$C_3H_8 \xrightarrow{k_1} \frac{3}{2} C_2H_4 + H_2$$

$$C_2H_4 + O_2 \xrightarrow{k_2} 2\ CO + 2\ H_2$$

$$C_3H_8 + \frac{3}{2} O_2 \xrightarrow{k_3} 3\ CO + 4\ H_2$$

This new mechanism is suggested by the fact that data from Princeton University show that CO appearance in significant quantities lags behind propane disappearance. For this reason, it is suggested here that, as described in our previous report, the fuel first pyrolyses to an intermediate species (which is here chosen to be ethylene) and only then is oxidized.

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