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A versatile mass spectrometer gas analysis system is described which has been acquired under support from a DURIP grant. The system involves a quadrupole mass spectrometer, high vacuum turbomolecular pumping system, high speed data acquisition and control system and a quartz microprobe gas sampling apparatus. The system is supplemented by a gas chromatograph and related electronic diagnostic instrumentation. This apparatus will be used to study soot particle inception and growth under support from the Air Force Office of Scientific Research (AFOSR). Additional studies of metal oxide particle formation and combustion-generated emissions will also draw upon the capabilities of the acquired equipment.					
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Final Technical Report

on

DURIP

**Species and Temperature Measurements in Fuel Rich
Combustion Regions**

(AFOSR Contract AFOSR-89-0141)

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TABLE OF CONTENTS

	Abstract	i
1.	Introduction	1
2.	Mass Spectrometer Gas Analysis Apparatus	1
3.	Research Projects Impacted by the Instrumentation	2
4.	Equipment List	4

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Abstract

A versatile mass spectrometer gas analysis system is described which has been acquired under support from a DURIP grant. The system involves a quadrapole mass spectrometer, high vacuum turbomolecular pumping system, high speed data acquisition and control system and a quartz microprobe gas sampling apparatus. The system is supplemented by a gas chromatograph and related electronic diagnostic instrumentation. This apparatus will be used to study soot particle inception and growth under support from the Air Force Office of Scientific Research (AFOSR). Additional studies of metal oxide particle formation and combustion-generated emissions will also draw upon the capabilities of the acquired equipment.

1. Introduction

Over the past two decades, considerable progress has been made in the understanding of combustion phenomena. A good deal of this success can be traced to the application of sophisticated diagnostic techniques to these complex reacting flows. The complicated, coupled interaction between fluid mechanic and chemical kinetic effects typical of combustion phenomena requires high spatially resolved measurements of velocity, species concentration, and temperature. An array of novel diagnostic techniques have been developed recently to address these measurement needs. Despite these advances, there still remain significant problems for which measurements have only recently been undertaken or for which our present measurement capabilities are lacking.

An area which is particularly striking in this regard involves the study of fuel rich hydrocarbon combustion. Fuel rich regions of a combustion system present a host of problems from both a fundamental understanding and measurement point of view. Such regions are chemically complicated since the pyrolysis-like reaction sequence not only involves oxidative species such as CO, OH, O, H₂O, etc., but also contains a large number of hydrocarbon species. Eventually, these hydrocarbon species lead to the formation of large polynuclear aromatics as well as the onset of soot particle formation. Progress in understanding the controlling phenomena in fuel rich situations is limited by both the measurement techniques and the data base available. Presently, a major area for which study is needed involves the measurement of species concentration.

To address the need for an improved understanding of fuel rich combustion phenomena, a mass spectrometric gas analysis capability has been assembled under a grant from the DoD University Research Instrumentation Program (DURIP). The equipment acquired with this support provides capabilities for the study of fuel rich hydrocarbon systems and is being used in connection with an ongoing research program on soot formation funded by the Air Force Office of Scientific Research (AFOSR). Applications to the soot research area will focus on the particle inception region where little experimental data presently exists examining the complicated chemistry leading to soot particle formation. In addition, the equipment addresses the need for species concentration measurements important in the surface growth (e.g. C₂H₂) and particle oxidation (e.g. O₂) processes. This mass spectrometry capability augments techniques presently used to provide non-intrusive characterization of the soot particle and velocity fields in diffusion flames. In addition, the measurement capabilities provided by the equipment can be extended to a number of related combustion studies.

2. Mass Spectrometer Gas Analysis Apparatus

In keeping with the objectives outlined above, a quadrupole mass spectrometer system has been acquired to provide rapid on-line gas analysis capabilities. Because of the rapid advances occurring in the instrumentation field with respect to mass spectrometry, high vacuum turbomolecular pumping systems and computer based data acquisition, it was decided to assemble the mass spectrometer system from a number of vendors. This allowed for the assembly of a state-of-the-art instrument which had superior versatility and performance specifications as compared to single vendor systems.

The mass spectrometer system is composed of four major elements: 1) the quadrupole mass spectrometer, 2) the high vacuum turbomolecular pumping system which provides the high vacuum conditions for the mass spectrometer, 3) the data acquisition and control system and 4) the probe housing and positioning system. These major elements are supplemented by an appropriate sampling probe assembly and a variety of vacuum couplings needed to assemble the system, a gas chromatograph system and electronic modules for monitoring the system. A complete list of the various components, their suppliers and cost are included as section 4 of this report.

The major component of the system is, of course, the quadrupole mass spectrometer. For the present application a model EX500 quadrupole mass spectrometer manufactured by Extrel, Inc. has been selected. This unit has a mass range of 1-500 amu with a scan speed of 1000 amu/s. The mass resolution can be adjusted to suit a variety of measurement needs with a maximum resolution of 0.1 amu. Since the mass spectrometer requires a high vacuum environment for proper operation, a turbomolecular pumping system has been acquired separately from Balzer. This turbomolecular pump station has a rated pumping speed of 300 l/s which is required for the high sampling rate conditions

encountered in the present measurement applications. A turbomolecular pump has been selected because it does not require any pump oil for operation. This significantly reduces the hydrocarbon background in the mass spectrometer while also providing superior vacuum conditions. This main pumping system is supplemented by a smaller roughing pump which is placed on the probe inlet system. This pump has been purchased from Leybold and has a rated pumping speed of 3.4 cubic feet per minute. The vacuum conditions are monitored using both pirani and cold cathode gauges supplied from MKS Systems.

The mass spectra detected by the quadrupole mass spectrometer are in the form of analog electronic signals. Furthermore, enhanced performance and versatility can be obtained from this instrumentation if computer data acquisition and control are provided. For the present system, a Compaq 386 personal computer along with a Data Translation data acquisition system have been selected. The data system provides both an analog to digital conversion capability for data acquisition as well as a digital to analog output for control of the mass spectrometer. Suitable backup storage of the data is provided using a separate dual drive system from Bernoulli which has two 44MB disk drives. In addition to controlling the mass spectrometer, the computer system is also used to provide positioning control capability for the sample probe assembly. Two stepper motors which drive a pair of translating stages are used to position the flame system under study with respect to the probe inlet. These motors and stages are supplied from Exonic Inc. and are fully controllable via the Compaq computer.

The final major element of the mass spectrometer system is the sample probe and vacuum housing for the instrument. This assembly has been supplied from MDC Vacuum Components from their standard line of 8" vacuum fittings. This approach results in a modular system which allows for future expansion and modification. Appropriate vacuum couplings to match this system to the present vacuum pumping system are supplied by Leybold.

In addition to the previously described instrumentation, there are several support pieces of equipment. These include a printer for the system, an oscilloscope to monitor the analog signal from the mass spectrometer and a gas chromatograph unit. This latter system can be directly interfaced to the mass spectrometer to provide combined GC/MS capability or can be operated as an independent analysis unit. This unit was included to provide a more robust analysis capability for the intended research program.

The above described instrumentation represent a versatile, real time gas analysis system for combustion studies. Additional details regarding the system are contained in section 4. The mass spectrometer system is presently being applied to the study of soot formation in diffusion flames with an emphasis on the soot particle inception process. Current research impacted by the acquisition of this instrumentation as well future efforts to be influenced by its capabilities will be discussed in the next section.

3. Research Projects Impacted by the Instrumentation

The instrumentation obtained under the funding provided by the present DURIP grant directly impacts an ongoing AFOSR research grant on soot formation. These studies will use the mass spectrometer to investigate soot particle inception and surface growth in combustion environments. This work which was recently funded under AFOSR support (AFOSR-87-0145, "Soot Particle Inception and Growth Processes in Combustion") will provide direct measurements of soot precursor species in diffusion flames. Additional measurements of species involved in the early soot surface growth process will also be addressed. Of particular interest will be measurements of polycyclic aromatic hydrocarbons which are believed to be key building blocks on the route to soot particle inception. A focus of the present program is to provide measurements in regions containing significant amounts of soot particles. Previous studies have been unsuccessful in probing such regions due to plugging of the probes introduced into the flame. Present research is addressing novel approaches to avoiding such interferences. The data obtained in these studies is expected to provide new insights into the soot formation process.

Additional studies which will be impacted by the above described instrumentation include work

supported by DuPont on metal oxide particle formation. This program has been initiated as a related effort to the AFOSR soot particle studies. This research draws on the substantial diagnostic capabilities developed under AFOSR support in this laboratory and is an example of an industry-university-government interaction on related areas of interest. As with the soot studies, the mass spectrometer system will be used to probe for the chemical precursor species to the metal oxide particles.

The mass spectrometer system will also be utilized to investigate the effects of soot particles on the production of other combustion-generated species. Of particular interest is the production and emission CO from flames. Soot particles can significantly influence the temperature as well as compete for oxidizing species such as OH. Consequently, the presence of soot particles may have an impact on the emission products from combustion devices. This work will eventually be expanded to the consideration of other combustion-generated species such as NO_x and SO_x in a similar manner. All of these species are of concern from an emissions standpoint and are of interest to a wide variety of combustion driven systems.

Clearly, the instrumentation acquired under the DURIP Grant is having a substantial impact on the research directions in our laboratory. Problems of direct interest to DoD agencies are being investigated with the equipment acquired and future applications for the instrumentation hold significant potential for additional studies.

4. Equipment List

	Model No.	Description (Supplier)	Cost
1.	EX500	Mass Spectrometer System (Extrel Corporation)	\$36,900
2.	Model 5890A	Gas Chromatograph (Hewlett-Packard)	17,094
3.	DT 2823	Analog to Digital Converter System (Data Translation)	3,569
4.		Cold Cathode/Pirani Gauge Vacuum Monitoring System (MKS Systems)	1,490
5.	TSU332/8100	Turbo Station Vacuum System (Balzers)	12,713
6.	TVA-4224-23	Instrument Cabinet (Premier Metal Products)	589
7.	D4B-HC	Roughing Vacuum Pump (Leybold, Inc.)	1,188
8.		Stepper Motor System (Exonic Systems, Inc.)	7,295
9.	SR540	Mechanical Chopper (Stanford Research)	795
10.	386-25	Compaq Computer (Computer Discount Warehouse)	8,374
11.		Bernoulli Disk (PC Connection)	2,383
12.		Vacuum Chamber (MDC Vacuum)	2,027
13.	ML320	Okidata Printer (PC Brand)	345
14.	CPQ-GEN1MB	1MB Memory Module (Computer Discount Warehouse)	395
15.		Vacuum Connectors (Leybold)	326
16.	2245A	Oscilloscope (Tektronix)	1,895

Total			\$94,995

4. Equipment List (cont'd)

Funds

AFOSR DURIP	52,320
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University Matching	34,880
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Dept. Add'l Funds	7,795
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TOTAL	94,995
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