SANDIA REPORT

SAND2000-8202

Unlimited Release

Printed January 2000

RECEIVED

JAN 31 2000

OSTI

Department of Defense/Department of Energy Joint Demilitarization Technology Demonstration Program

Executive Summary of Phase II Demonstrations: The Low-Pressure Rocket Motor Burns in X-Tunnel

Prepared for
US Army Defense Ammunition Center

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation,
a Lockheed Martin Company, for the United States Department of
Energy under Contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States
Department of Energy by Sandia Corporation.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Prices available from (703) 605-6000
Web site: <http://www.ntis.gov/ordering.htm>

Available to the public from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd
Springfield, VA 22161

NTIS price codes
Printed copy: A04
Microfiche copy: A01

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

SAND2000-8202
Unlimited Release
Printed January 2000

**Department of Defense/Department of Energy
Joint Demilitarization Technology
Demonstration Program**

**Executive Summary of Phase II Demonstrations:
The Low-Pressure Rocket Motor Burns in X-Tunnel**

Prepared for
US Army Defense Ammunition Center

B. W. Bellow, A. E. Moeller, D. Steele, S. M. Williams
Bechtel Nevada

R. L. Heinle, C.O. Pruneda, C.A. Velsko, B. E. Watkins
Lawrence Livermore National Laboratory

C. J. Hewitt, H. Fry, J. A. Sanchez, J. R. Stephens
Los Alamos National Laboratory

J. R. Carson, W. C. Gray, W. C. Thomas, T. J. Tope
Radian International

S. W. Allendorf, L. R. Carrillo, H. H. Hirano, H. A. Johnsen, J. Lipkin,
D. K. Ottesen, R. L. Peabody, C. R. Shaddix, J. C. Swearengen
Sandia National Laboratories

R. F. Boehm, A. Smiecinski, K. J. Stetzenbach
University of Nevada, Las Vegas

* Currently at Washington State University

Dedication and Acknowledgement

This report is dedicated to the individuals and teams whose tireless efforts made it possible to complete the contained rocket motor burn tests at X-tunnel successfully. The financial and moral support of the program sponsor, Mr. James Q. Wheeler, Director of the US Army Defense Ammunition Center, is gratefully acknowledged.

Table of Contents

ABSTRACT	3
INTRODUCTION AND BACKGROUND.....	3
Data/Sampling Strategy	4
TEST CONFIGURATIONS AND ARMING AND FIRING PROCEDURES	5
RESULTS SUMMARY	7
Time-Averaged Measurements—Radian International, LLC (Appendix A).....	7
Time-Resolved Bulk Gas Analyses—LLNL/Bechtel Nevada (Appendix B)	8
Real-Time and Time-Averaged Aerosol Analyses—LANL (Appendix C).....	8
Real-Time Gas Species Analyses Using FTIR—LANL (Appendix D)	9
Post-Test Metal Residue Analyses—UNLV (Appendix E).....	9
In Situ Laser-Based Measurements of Gas Species Concentrations—SNL (Appendix F)	10
Real-Time Measurements of Test Chamber Pressure and Temperature— LLNL and Bechtel Nevada (Appendix G).....	11
SUMMARY AND CONCLUSIONS.....	11
REFERENCES.....	13
APPENDIX A	15
APPENDIX B	29
APPENDIX C	35
APPENDIX D	47
APPENDIX E	51
APPENDIX F.....	53
APPENDIX G.....	57

List of Figures

Figure 1. Plan view of rocket motor arrangement for SUNSPOT and DAZZLER tests	6
Figure 2. Plan view of rocket motor arrangement for THUNDERBIRD test.....	6
Figure B1. Early-time variation of O ₂ and CO ₂ gas concentrations in test chamber during SUNSPOT test.....	33
Figure B2. Variation of Nox gas concentrations in test chamber during SUNSPOT test	33
Figure B3. Complete history of CO ₂ concentration in SUNSPOT.....	34
Figure C1. Summary of LAASS streaker elemental composition data from SUNSPOT	42
Figure C2. Summary of LAASS streaker elemental composition data from THUNDERBIRD	43
Figure C3. Summary of LAASS streaker elemental composition data from DAZZLER.....	44
Figure C4. Summary of LAASS impactor data from SUNSPOT	45
Figure C5. Summary of LAASS impactor data from THUNDERBIRD.....	45
Figure C6. Summary of LAASS impactor data from DAZZLER	46
Figure D1. Absorbance spectra from first FTIR scan in THUNDERBIRD.....	47
Figure D2. Comparison between measured and simulated absorption features for water, CO and CO ₂	48
Figure D3. Representative spectra from DAZZLER (light background) compared with Simulated absorption features from the QASOFT database (dark background)	49
Figure F1. CO ₂ measured in invert during DAZZLER.....	55
Figure F2. CO ₂ measured in rid during DAZZLER.....	55
Figure F3. Water concentration measured in rib location during DAZZLER	56
Figure G1. Comparison of chamber pressure histories in rocket motor burn tests.....	58
Figure G2. Temperature histories from thermocouples array in SUNSPOT.....	58
Figure G3. Temperature histories from thermocouple array in THUNDERBIRD.....	59
Figure G4. Temperature histories from thermocouple array in DAZZLER	59

List of Tables

Table 1. Contained rocket motor burn tests in x-tunnel	4
Table 2. Sampling and measurements for Phase II test series.....	5
Table A1. Particulate Matter, HCN, and metal concentrations—NIKE rocket motor	16
Table A2. Particulate Matter, HCN, HCl, Cl ₂ , and Metal Concentrations—Improved HAWK rocket motor	17
Table A3. Selected VOC Concentrations—NIKE rocket motors	18
Table A4. Selected VOC Concentrations—Improved HAWK rocket motor	20
Table A5. SVOC Concentrations—NIKE rocket motor	21
Table A6. SVOC Concentrations—Improved HAWK rocket motor.....	22
Table A7. PCDD and PCDF Concentrations—Improved HAWK rocket motor	23
Table A8. Energetics in residue samples	24
Table A9. SVOCs in residue samples.....	25
Table A10. Total metals in residue samples	26
Table A11. TCLP metals analysis of residue samples	27
Table B1. Inventory of materials consumed in rocket motor burns	29
Table B2. Expected rocket burn combustion products and tracer gas amounts.....	30

List of Tables (continued)

Table B3. Data summary—comparison of computed and measured bulk gas species concentrations in the test chamber at the end of each burn	30
Table B4. Carbon balance	32
Table C1. Total (<10 μm) Elemental Concentrations—($\mu\text{g}/\text{m}^3$) for SUNSPOT	36
Table C2. Fine (< 2.5 μm) Elemental Concentrations—($\mu\text{g}/\text{m}^3$) for SUNSPOT	37
Table C3. Total (<10 μm) Elemental Concentrations—($\mu\text{g}/\text{m}^3$) for THUNDERBIRD	38
Table C4. Fine (< 2.5 μm) Elemental Concentrations—($\mu\text{g}/\text{m}^3$) for THUNDERBIRD	39
Table C5. Total (< 10 μm) Elemental Concentrations—($\mu\text{g}/\text{m}^3$) for DAZZLER	40
Table C6. Total (< 2.5 μm) Elemental Concentrations—($\mu\text{g}/\text{m}^3$) for DAZZLER	41
Table E1. Summary of metal concentrations (in ppb) found in coupon rinse solution obtained after each contained rocket motor burn test.	51
Table F1. TDL measurement summary for rocket motor burn experiments.....	54

This page intentionally left blank

Department of Defense/Department of Energy

Joint Demilitarization Technology

Demonstration Program

ABSTRACT

Three low-pressure rocket motor burn tests were executed in the May-June 1997 time frame at the X-tunnel complex located on the Department of Energy's Nevada Test Site. NIKE rocket motors containing double base propellant were used in two tests (two and four motors, respectively), and the third test used two Improved Hawk rocket motors containing composite propellant. Test procedures and the results of various measurements made during and after each test are described in detail in reference (1). That information is abstracted in this Executive Summary document, which is a companion to the Executive Summary of the Phase I Demonstrations in X-tunnel (2).

INTRODUCTION AND BACKGROUND

The Joint Demilitarization Technology (JDT) Program is a collaborative effort between the Departments of Defense and Energy (DoD and DOE) that is demonstrating and validating technologies for resource recovery, recycling, and alternative destruction/treatment technologies. The JDT Program is managed jointly by the Demil Technology Office in the Technology Directorate of the US Army Defense Ammunition Center, McAlester, OK, and the US DOE Nevada Operations Office, Las Vegas, NV.

In FY97, the JDT Program completed the first two Phases of a continuing study of full-scale, contained, and instrumented Open Burning/Open Detonation (OB/OD) events that are being executed in the X-tunnel complex in Area 25 at DOE's Nevada Test Site (NTS):

- Phase I—four detonation tests (employing 155mm HE M107 projectiles), and
- Phase II—three low-pressure rocket motor burn tests (employing NIKE and Improved Hawk rocket motors).

Test methods and results from Phase II are briefly described in this Executive Summary; a separate report provides detailed documentation of the test procedures and the results obtained from these three tests (1). An Executive Summary of the Phase I test results is also available (2).

The test facility established in the X-tunnel complex at NTS is a mined cavity (the test chamber) and a fabricated containment plug designed to withstand blast and pressure effects. The containment plug prevents the release of gases produced by munition detonations and rocket motor propellant burns. The volume of the test chamber is roughly 4644 m³ (164,000 ft³), and its dimensions are roughly 30.5 m long, 15.2 m wide, and 10.7 m high. Containment calculations performed by Burkhard at Lawrence Livermore National Laboratory (3) indicate that the test chamber and containment plug can safely contain a detonation of 1364 kg (3000 pounds) of double base propellant (roughly equivalent to 1023 kg of TNT).

The rocket motor burn tests used two different DoD tactical rocket motors: the NIKE M88 and the Improved Hawk. These motors contain propellants that are representative of the two most common formulations found in the demilitarization inventory, i.e., double base and composite. Each NIKE M88 rocket motor contains 341 kg (750 pounds) of double base type propellant, and each Improved Hawk motor contains 294 kg (647 pounds) of composite type propellant.

Three tests were performed: "SUNSPOT" and "THUNDERBIRD" using 2 and 4 NIKE motors, respectively; and "DAZZLER" using 2 Improved Hawk motors. In each test, linear shaped charges and explosive cutting tape were used to split the steel rocket motor cases longitudinally and partially around the circumference. These explosives also served to initiate the low-pressure (i.e., non-propulsive) propellant burns. Test parameters are summarized in Table 1.

Table 1. Contained rocket motor burn tests in x-tunnel

Test Name	Test Type ¹	Date Executed	Number of Assets	N.E.W. ² (pounds)	Inert Weight (pounds)
SUNSPOT	B1	14 May 97	2	1500 ³	888
THUNDERBIRD	B1	28 May 97	4	3000 ³	1776
DAZZLER	B2	11 June 97	2	1294 ⁴	490

1 - B1 = Burn of NIKE rocket motors; B2 = Burn of Improved Hawk rocket motors

2 - Net Explosive Weight (excluding initiating explosive charges)

3 - NC/NG (double base) Propellant

4 - Composite Propellant

Data/Sampling Strategy

The sampling procedures used in the Phase II tests are similar to those that were developed for Phase I (2). The data obtained from the Phase II tests focused on the following areas:

- laboratory analyses [using U.S. Environmental Protection Agency (EPA) standard methods] to identify EPA regulated chemicals in samples taken from the combustion cloud and residues recovered from the chamber after a test;
- rapid, time-resolved measurements of selected gas species and aerosol/particulate size distributions using both extraction and in situ methods;
- determination of the presence of toxic gases and explosive mixtures in the tunnel complex (as required by health and safety rules at NTS),
- in situ measurements of combustion cloud gas temperature (time histories and spatial variations); and
- in situ measurements of test chamber pressure histories.

Although some leakage from the test chamber was observed in SUNSPOT and THUNDERBIRD, the gases and aerosols produced in each test were substantially contained and sampled over several hours after test initiation. During this time, the gases cooled, most particulate matter settled out, and the temperature and pressure in the test chamber returned to near atmospheric values. Various measurements and sampling tools

were used in each test to obtain time-resolved and time-averaged measurements. The combustion gases were subsequently released to the atmosphere, and fresh air was pumped into the chamber prior to reentry by site personnel. The presence of hazardous materials (e.g., lead and asbestos) in the chamber as solid residues from the spent rocket motors necessitated the use of protective clothing and personal air respirators during reentry operations. These operations typically began 24 hours after a test. There was no effort to clean the test chamber between tests. That is, the solid residue generated from each test accumulated in the chamber and therefore was available to contribute to the non-volatile species identified in the measurements made in subsequent tests.

The types of measurements and analyses used to characterize the particulate and gaseous effluents in the Phase II tests are summarized in Table 2.

Table 2. Sampling and measurements for Phase II test series

Brief Description	Data Summary in Appendix	Responsible Organization*
EPA Standard Methods: VOCs, SVOCs, particulates, metals, HCN, HCl, Dioxins, residual energetic material	A	Radian International, LLC
Real Time Gas Analyses	B	LLNL/ Bechtel Nevada
Real Time and Time-Resolved Aerosol and Particulate Sampling/Analysis	C	LANL
FTIR Gas Species Analysis	D	LANL
Metal Residue Analyses	E	Radian/UNLV
Laser Measurement	F	SNL
Chamber pressure/gas temperature	G	LLNL/Bechtel Nevada

*LANL - Los Alamos National Laboratory

LLNL - Lawrence Livermore National Laboratory

SNL - Sandia National Laboratories

UNLV - University of Nevada, Las Vegas

TEST CONFIGURATIONS AND ARMING AND FIRING PROCEDURES

Plan views of the arrangements of the rocket motors in the test chamber for the SUNSPOT, THUNDERBIRD, and DAZZLER tests are shown in Figures 1 and 2. Note that the layout shown in Figure 1 is appropriate for both SUNSPOT and DAZZLER since two motors were used in each of these tests. The center of both rocket motor layouts shown in Figures 1 and 2 was located roughly 19 m from the containment plug. In all tests, the rocket motors, lying horizontally, were tied down to a concrete pad on the test chamber invert (floor). This procedure prevented them from moving during both the burn initiation event and the subsequent low-pressure burning of the propellant. The burn initiation process made use of the standard "crack and burn" DoD OB demilitarization process. In this method, copper linear shaped charges and explosive cutting tape are used to split the rocket motor cases along their length and partially around their circumference,

respectively. As can be seen in Figures 1 and 2, in each test the motors were physically offset to preclude any possibility of a sympathetic detonation if the propellant in one motor were to detonate because of the explosive initiation process.

Figure 1. Plan view of rocket motor arrangement for SUNSPOT and DAZZLER tests.

Figure 2. Plan view of rocket motor arrangement for THUNDERBIRD test.

In addition to using copper linear shaped charges and explosive cutting tape to initiate the propellant burns, separate copper linear shaped charge explosives were used to open standard sized compressed gas bottles of Krypton and, in DAZZLER only, Neon. These gases were released at test initiation time, and they were used as tracers for the real time gas measurements in each test. One bottle of Krypton was used in each of the SUNSPOT and THUNDERBIRD tests. For DAZZLER we released 2 compressed gas bottles; one bottle each of Krypton and Neon.

RESULTS SUMMARY

Abstracted data sets provided by each organization identified in Table 2 are given in Appendices A-G of this document. The key observations and principal conclusions drawn from these data sets are summarized below.

Time-Averaged Measurements—Radian International, LLC (Appendix A)

Radian collected time-averaged gas and particulate samples from the combustion clouds produced in each test by extracting high volumes of gas from the test chamber. They used several probes that passed through the containment barrier to extract these samples. In addition, they collected residue samples in the chamber after each test. Radian's probes were isolated from their sampling equipment by remotely operated valves. These valves are closed prior to a test initiation, and they are only opened after it is determined that the temperature and pressure in the test chamber are within safe limits for their sampling equipment. Nominal safe temperature and pressure limits were set at 100°C and 50 psig, respectively. The valves were opened at roughly 22, 10 and 5 minutes after test initiation in SUNSPOT, THUNDERBIRD, and DAZZLER, respectively. The delay in opening the sampling valves in the SUNSPOT test was excessive and likely compromised the time averaged data Radian and LANL obtained in this test. This delay was the result of seeing inconsistent temperature data from the thermocouple array in the test chamber (see Appendix G). The problem was resolved in THUNDERBIRD and DAZZLER by revising the thermocouple array location and by using a dedicated thermocouple located near the sampling ports in the test chamber.

The data obtained by Radian from post-test laboratory analyses of their samples reveal:

- substantial particulate loading in the combustion clouds of each test;
- high concentrations of lead and antimony in the NIKE rocket motor burns and of aluminum in DAZZLER;
- evidence of significant cross contamination of metals between tests;
- high concentrations of chlorine and HCl in DAZZLER;
- high concentrations of certain VOC's in all tests;
- high concentrations of certain SVOC's in all tests;
- the presence of dioxins and furans (in low concentrations) in DAZZLER;
- low concentrations of energetic materials in residue samples from each test; and
- the presence of high lead and chromium concentrations in the TCLP analysis of the DAZZLER residue samples.

Time-Resolved Bulk Gas Analyses—LLNL/Bechtel Nevada (Appendix B)

Two stainless steel sampling lines connected to a pumping station on the tunnel apron and two small ports in the test chamber were used to extract a continuous stream of gas from the combustion cloud in each test. Each sampling line was 12.7 mm in diameter and roughly 300 m long, and the transit time of a gas sample from the test chamber to the on-site instrumentation was roughly two minutes. One sampling line was coupled to a port located on the invert (floor) of the test chamber. The second sampling line used a port located on the chamber back (top) (roughly 10.7 m above the invert). A particulate filter was located at the chamber-end of each sampling line. The sampling lines were fabricated from stainless steel and were unheated. The gas stream extracted from the test chamber was used for real-time analyses of bulk gases, nitrogen oxides, and tracer gases released during each test. The on-site instrumentation used for these analyses included a gas chromatograph, mass spectrometer, and continuous emission monitors for CO₂, CO, O₂, O₂, and NO_x species.

The data obtained from these measurements were analyzed by LLNL (4). These analyses reveal:

- combustion products were well oxidized;
- the carbon available from rocket motor materials is converted primarily to CO₂;
- there appears to be evidence of excess CO₂ in DAZZLER;
- significant time and spatial variations in NO_x concentrations;
- there appears to be evidence of CO₂ saturation in test chamber after THUNDERBIRD; and
- species concentration data obtained at late times (i.e., times greater than about 80 minutes after test initiation) in SUNSPOT and THUNDERBIRD are potentially compromised by leaks of fresh air into the test chamber (5).

Real-Time and Time-Averaged Aerosol Analyses—LANL (Appendix C)

The Los Alamos Aerosol Sampling System (LAASS) was specially developed to measure aerosol concentrations as well as to collect aerosol samples during the rocket motor burn test series. Sampling port valves were opened remotely in each test at the same time Radian's valves were first opened, and the LAASS collected representative aerosol samples from the combustion cloud. These samples were obtained by drawing aerosol-laden gas through the containment barrier into two parallel sampling systems. One system (impactor) was used to collect aerosol samples from 0.1 to 10 μm in aerodynamic diameter¹ and measure their mass concentrations ($\mu\text{g}/\text{m}^3$) in real time. The second system (streaker) collected three aerosol size fractions, $> 10 \mu\text{m}$, 2.5 - 10 μm , and $< 2.5 \mu\text{m}$. The latter two size fractions were collected on rotating substrates thereby providing a time history of the aerosols in the test chamber. The streaker samples were subsequently analyzed using Proton-Induced X-ray Emission (PIXE) Spectroscopy to

¹ Aerodynamic diameter is the size of a unit density particle that has the same aerodynamic properties of the collected particle. This description is used because the transport properties of a particle are a function of its aerodynamic behavior.

determine the aerosol elemental composition for elements with atomic numbers greater than 11.

The data obtained from the LAASS system were analyzed by LANL. These analyses reveal:

- both the concentrations and the size distributions of the aerosols in the rocket motor burn combustion clouds are substantially different from those measured in the detonation tests;
- high aerosol concentrations required taking “grab” samples as opposed to continuous monitoring;
- time variation of aerosol size distributions is complex; perhaps because of competition between particle coagulation and settling mechanisms; and
- metal elemental concentration data that were obtained from the LAASS streaker instrument are consistent with the metals identified in independent analyses carried out by Radian and UNLV.

Real-Time Gas Species Analyses Using FTIR—LANL (Appendix D)

A Fourier Transform Infrared Spectroscopy (FTIR) diagnostic was deployed for analyzing the gas species that evolved during the THUNDERBIRD and DAZZLER tests. Unlike the other measurement techniques used in the rocket motor burn tests, the FTIR was not employed in the detonation test series. The FTIR system used in these tests was designed and deployed by LANL on a short time scale during the third quarter of FY97. This system was installed principally to detect and quantify the evolution of HCl gas generated from burning the composite propellant in the DAZZLER test. Gas samples for the FTIR instrument were extracted from the combustion chamber starting at 10 and 5 minutes after the THUNDERBIRD and DAZZLER tests were initiated, respectively. The insulated and heated sampling line between the combustion chamber and the FTIR gas cell was roughly 30 m long.

The data obtained from the FTIR diagnostic instrument were analyzed by LANL. These analyses reveal:

- only one spectrum was obtained in THUNDERBIRD due to particulate clogging of the sample line;
- data from THUNDERBIRD indicate presence of CO and CO₂ in concentrations similar to those measured by LLNL; and
- data from the 13 spectra analyzed from DAZZLER indicate HCl concentrations were below the detection limit of the instrument.

Post-Test Metal Residue Analyses—UNLV (Appendix E)

The Harry Reid Center for Environmental Studies at the University of Nevada, Las Vegas (UNLV) was contracted to analyze water/alcohol (50/50) rinse samples collected by Radian International. These samples were taken from two aluminum coupons (plates) that were exposed to the combustion clouds in the test chamber. The total surface area of the coupons was 0.75 m². The coupons were cleaned before each test and fixed vertically in the chamber at a height of roughly 3 m above the invert. The coupons were recovered

after each test and washed down with the water/alcohol mixture that UNLV analyzed. Samples were dried, digested, and analyzed using EPA method 200.8 (ICP-MS). The analyses were performed using an Inductively Coupled Plasma Mass Spectrometer (ICP-MS). Note that Radian also analyzed residue samples collected from the test chamber after each test. The results of Radian's analyses are summarized in Appendix A.

The data obtained by UNLV reveal:

- there is a reasonable correlation between the total amount of non-volatile metal species in released in each test and the metal concentrations observed in the rinse solution analyses
- all relevant metals are detected; and
- the test and analysis method employed here tends to reduce the effects of multi-test cross contamination from non-volatile metals.

In Situ Laser-Based Measurements of Gas Species Concentrations—SNL (Appendix F)

A modified commercial gas monitor based on tunable diode laser (TDL) spectroscopy was used to make in situ, real time measurements of several gas species as they evolved in the SUNSPOT and DAZZLER tests. Two TDL sampling sites were located in the test chamber: one in the invert and one on the left rib of the chamber at roughly 5 m above the invert. The development, installation and application of the TDL gas monitoring system were the responsibilities of SNL. The TDL monitor operates in the near infrared; and it detects molecular species using optical absorption by vibration transitions in overtone and combination modes at wavelengths near 1.30 μm and 1.55 μm . The monitor developed for this application can provide time-resolved concentrations of two different gas species in the test chamber (i.e., using two separate TDL modules). These data are obtained essentially simultaneously and in real time at a sampling rate on the order of 1 Hz.

The data obtained from the TDL monitors were analyzed by SNL (6). These analyses reveal:

- combustion cloud particulate characteristics are substantially different from those observed in detonation test series;
- potentially significant and persistent molecular stratification of gas species in the test chamber;
- quantitative and unique measurement of increased H_2O concentration in the test chamber; and
- good agreement with the on-line, real-time measurement of average CO_2 concentration obtained by LLNL in DAZZLER.

Real-Time Measurements of Test Chamber Pressure and Temperature— LLNL and Bechtel Nevada (Appendix G)

LLNL and Bechtel Nevada were responsible for obtaining time-resolved measurements of a variety of physical parameters during each rocket motor burn test. In addition to early-time shock, ground motion and strain gage measurements on the containment plug, the data for each test included:

- video coverage of the initiation and combustion processes;
- gas temperature measurements from vertically oriented, linear arrays of K-type thermocouples; and
- gas pressure history in the test chamber.

The video records are available upon request. The temperature and pressure data were recorded prior to test initiation (baseline data) and for roughly two hours after each propellant burn was complete. Long-term data were sampled at 1-Hz using the NTS Special Measurements Integrated Data System (SMIDS). Both the rapid rise and relatively slow decay in pressure and the transient gas temperatures associated with the propellant burning and the gas cool down after the burn were recorded in this way. Depending on the test, there were seven or eight thermocouples in a thermocouple array. These thermocouples were equally spaced in the array in an effort to measure gas temperature as a function of height in the test chamber. The array was positioned between the invert and the back of the test chamber for SUNSPOT and between the invert and the mid-height of the chamber in THUNDERBIRD and DAZZLER.

The temperature and pressure histories generated by the combustion process in the test chamber are presented in Appendix G. These data are of particular interest because they are relevant to understanding the highly dynamic chemistry and fluid flow processes that characterize each test.

The pressure and temperature data were analyzed by SNL. These analyses reveal:

- good correlation with pre-test estimates (1, 3) of propellant burn rates as well as the peak pressure amplitudes and decay rates;
- peak pressure values observed are consistent with pre-test estimates based on the assumption of complete conversion of CO to CO₂;
- thermal stratification in the test chamber is extreme at early times but decreases and persists as the gases cool; and
- gas cooling rates are consistent with pre-test estimates of dynamic heat transfer processes in the test chamber (1).

SUMMARY AND CONCLUSIONS

The three contained rocket motor burn tests in X-tunnel that are described in this report represent a significant step forward in efforts to quantify the environmental effects of using typical DoD OB procedures to dispose of excess rocket motors. This conclusion follows from the fact that these tests employed full sized motors for the first time in conjunction with contained and sampled effluents.

These tests, and the results obtained from them, can generally be judged as successful. However, several operational difficulties should be recognized when reviewing the results presented in Appendices A-G. These difficulties include:

- the quality of the time-averaged data from Radian and LANL measurements for the SUNSPOT test may be compromised due to the delayed opening of the valves that isolated their equipment from the test chamber, making it difficult to compare gas and particulate data sampling results between the two NIKE rocket motor tests (SUNSPOT and THUNDERBIRD);
- some measurements of non-volatile compounds obtained for THUNDERBIRD and DAZZLER are ambiguous due to cross contamination from the residues of previous tests in the chamber—the UNLV test methods and residue measurements are least affected by this problem; and
- there is evidence that the leak paths that developed between the test chamber and the tunnel drift during SUNSPOT and THUNDERBIRD allowed an in flow of fresh air into the test chamber that substantially reduced measured bulk gas concentrations at late times (greater than about 80 minutes after test initiation).

Nevertheless, the data provided by these tests are an invaluable source of information on the OB process. In addition, it is likely that further analyses of these data can be used to improve the execution and understanding of future munition testing campaigns in X-tunnel.

The extensive suite of data obtained from these tests includes gas species concentrations that were likely influenced by complex chemical kinetic processes occurring in the combustion clouds. In addition, the thermodynamic data from the tests define the local environmental conditions produced by the intense propellant combustion in the test chamber. It is likely that understanding the interaction between the chemical kinetic and thermodynamic processes occurring in these tests is a prerequisite to completely characterizing the contained burn events in X-Tunnel. Integrating such a characterization with the time-averaged and time-resolved gas species and particulate concentration data could then be expected to produce an improved understanding of the environmental consequences of OB demilitarization operations at DoD sites.

REFERENCES

1. "Contained Rocket Motor Burn Demonstrations in X-Tunnel: Final Report for the DoD/DOE Joint Demilitarization Technology Program", edited by Joel Lipkin, Sandia Report, in press
2. "Executive Summary of Phase I Demonstrations: Detonation of Conventional Weapons: 155-mm High-Explosive M107 Projectiles", Lawrence Livermore Laboratory Report # UCRL-ID-131252, July 1998
3. "Safety Factors and Design Criteria for U25x Complex (BANSHEE)", N. Burkhard, LLNL Memorandum to Distribution dated July 19, 1996
4. "Gas Sampling and Analysis Results for Low-Pressure Burn Demilitarization of Rocket Motors", C. Velsko, Lawrence Livermore Laboratory Report # UCRL-ID-136582, December 1998
5. "Chamber Leakage Effects on Measured Gas Concentrations During Contained Demilitarization Test at NTS X-Tunnel", C. R. Shaddix and J. Lipkin, Sandia Report, SAND2000-8209
6. "Tunable Diode Laser Spectroscopy: Report on JDT Contained Rocket Motor Burn Tests", S. W. Allendorf, et al., Sandia Report SAND98-8247, September 1998.

This page intentionally left blank

APPENDIX A

Time-Averaged Measurements—Radian International, LLC

Data obtained by Radian International LLC from post-test, laboratory analyses of samples extracted from the test chamber are summarized in Tables A1-A7. Particulate, HCN, and metal species concentrations in the combustion clouds for SUNSPOT and THUNDERBIRD (NIKE rocket motor tests) are summarized in Table A1. Table A2 summarizes measured concentrations of these same analytes, plus HCl and Cl₂, for DAZZLER (Improved HAWK rocket motor test).

Total nonmethane hydrocarbons and selected VOC concentrations for the NIKE and Improved HAWK rocket motor tests are presented in Tables A3 and A4, respectively. The VOCs presented in these tables were detected at concentrations >15 ppbv in the NIKE tests and > 5 ppbv in the Improved HAWK test. These cutpoints for inclusion in Tables A3 and A4 were chosen because they represent levels nominally five times greater than the sample detection limit.

Tables A5 and A6 present results for SVOCs for the NIKE and Improved HAWK rocket motor tests, respectively. Table A7 presents the PCDD and PCDF results for the Improved HAWK rocket motor test. Also included in Table A7 is the calculated 2,3,7,8-TCDD toxicity equivalence of the sample. These toxic equivalencies were calculated using procedures contained in Appendix IX of 40 CFR 266.

Table A1. Particulate Matter, HCN, and metal concentrations —NIKE rocket motor

Compound	Concentrations, mg/m ³		
	SUNSPOT	THUNDERBIRD	Average
Particulates			
TSP	9.08E+02	1.36E+03	1.13E+03
PM ₁₀	7.22E+01	4.84E+02	2.78E+02
HCN	2.63E+01	N/A	2.63E+01
Metals			
	Average Concentrations >1.0E+02		
Lead	2.58E+02	2.86E+02	2.72E+02
Antimony	1.42E+02	9.88E+01	1.21E+02
	Average Concentrations >1.0E+01 but <1.0E+02		
Phosphorus	4.36E+01	5.13E+01	4.75E+01
Calcium	1.52E+01	3.07E+01	2.30E+01
Potassium	4.75E+00	3.52E+01	2.00E+01
Iron	1.03E+01	2.71E+01	1.87E+01
Sodium	4.97E+00	1.66E+01	1.08E+01
	Average Concentrations >1.0E+00 but <1.0E+01		
Cadmium	6.88E+00	7.84E+00	7.36E+00
Aluminum	4.74E+00	6.61E+00	5.68E+00
Zinc	3.57E+00	6.72E+00	5.14E+00
Copper	3.65E+00	4.72E+00	4.19E+00
Magnesium	2.27E+00	4.42E+00	3.34E+00
Titanium	1.02E+00	1.92E+00	1.47E+00
	Average Concentrations >1.0E-01 but <1.0E+00		
Chromium	2.03E-01	3.22E-01	2.62E-01
Manganese	1.14E-01	2.73E-01	1.94E-01
Barium	1.30E-01	2.20E-01	1.75E-01
Nickel	1.12E-01	1.45E-01	1.28E-01
Strontium	8.86E-02	1.64E-01	1.26E-01
	Average Concentrations >1.0E-02 but <1.0E-01		
Arsenic	7.83E-02	9.52E-02	8.67E-02
Selenium	3.38E-02	5.48E-02	4.43E-02
Molybdenum	3.90E-02	3.09E-02	3.50E-02
Cobalt	1.63E-02	2.56E-02	2.09E-02
Vanadium	1.51E-02	1.35E-02	1.43E-02
Mercury	5.84E-03	2.05E-02	1.32E-02
Beryllium	4.54E-03	1.61E-02	1.03E-02

N/A = not available

Table A2. Particulate Matter, HCN, HCl, Cl₂, and Metal Concentrations —Improved HAWK rocket motor

Compound	Concentrations, mg/m ³
	DAZZLER
Particulates	
TSP	1.18E+03
PM ₁₀	1.04E+03
HCN	ND
HCl	1.43E+04
Chlorine	1.13E+02
Metals	
Average Concentrations >1.0E+01	
Aluminum	3.17E+02
Lead	1.92E+01
Iron	1.04E+01
Average Concentrations >1.0E+00 but <1.0E+01	
Copper	7.42E+00
Antimony	4.28E+00
Sodium	2.71E+00
Potassium	1.45E+00
Phosphorus	1.26E+00
Chromium	1.06E+00
Average Concentrations >1.0E-01 but <1.0E+00	
Calcium	8.60E-01
Zinc	6.22E-01
Titanium	3.78E-01
Nickel	2.78E-01
Cadmium	2.02E-01
Magnesium	1.65E-01
Manganese	1.29E-01
Average Concentrations >1.0E-02 but <1.0E-01	
Vanadium	4.53E-02
Molybdenum	3.95E-02
Thallium	2.81E-02
Cobalt	2.19E-02
Barium	1.77E-02
Average Concentrations <1.0E-02	
Mercury	5.93E-03
Strontium	3.11E-03
Silver	2.42E-03
Selenium	2.32E-03
Beryllium	8.13E-04

ND = not detected

Table A3. Selected VOC Concentrations —NIKE rocket motors

Compound	Concentrations, ppbv		
	SUNSPOT	THUNDERBIRD	Average
Average Concentrations >1.0E+04			
Total Nonmethane Hydrocarbons	2.91E+04	9.18E+04	6.04E+04
Acetone	5.96E+03	4.63E+04	2.61E+04
Ethanol	3.82E+03	2.94E+04	1.66E+04
Benzene	1.07E+04	1.66E+04	1.36E+04
Acetaldehyde	7.14E+03	1.98E+04	1.35E+04
Average Concentrations >1.0E+03 but <1.0E+04			
Chloromethane	1.08E+04	6.64E+03	8.69E+03
Acetonitrile	4.69E+03	9.29E+03	6.99E+03
Propylene	1.82E+03	6.13E+03	3.97E+03
Chloroethane	1.25E+03	5.45E+03	3.35E+03
Benzaldehyde	1.08E+03	2.37E+03	1.72E+03
1-Butene/Isobutene	5.56E+02	2.60E+03	1.58E+03
Average Concentrations >1.0E+02 but <1.0E+03			
Naphthalene	1.14E+03	7.70E+02	9.55E+02
Acrylonitrile	1.42E+03	4.61E+02	9.40E+02
2-Butanone	3.01E+02	1.44E+03	8.68E+02
1-Butanol	5.15E+02	1.22E+03	8.67E+02
Methylene chloride	1.88E+01	1.58E+03	7.97E+02
Toluene	5.21E+02	1.02E+03	7.72E+02
Chlorobenzene	3.89E+02	4.14E+02	4.02E+02
Vinyl acetate	1.56E+02	5.77E+02	3.66E+02
trans-2-Butene	1.06E+02	5.04E+02	3.05E+02
Propane	1.16E+02	4.58E+02	2.87E+02
Vinyl chloride	2.85E+02	1.76E+02	2.30E+02
Diethyl ether	1.97E+02	2.42E+02	2.20E+02
cis-2-Butene	7.21E+01	3.39E+02	2.05E+02
Butyraldehyde	1.31E+02	2.26E+02	1.78E+02
Ethylbenzene	5.63E+01	2.11E+02	1.33E+02
n-Butane	4.98E+01	1.85E+02	1.17E+02
m/p-Xylene	6.08E+01	1.49E+02	1.05E+02

Table A3. (Continued)

Compound	Concentrations, ppbv		
	SUNSPOT	THUNDERBIRD	Average
Average Concentrations >1.0E+01 but <1.0E+02			
Styrene	ND	9.96E+01	9.96E+01
Butyl acrylate	5.88E+01	9.66E+01	7.77E+01
1,4-Dioxane	8.50E+01	6.24E+01	7.37E+01
o-Xylene	3.70E+01	8.90E+01	6.30E+01
1-Hexene	2.89E+01	9.69E+01	6.29E+01
1-Pentene	2.54E+01	9.96E+01	6.25E+01
Isoheptane	2.27E+01	9.56E+01	5.91E+01
Chloroform	6.60E+00	8.02E+01	4.34E+01
1,2,4-Trimethylbenzene	3.69E+01	4.89E+01	4.29E+01
Chlorodifluoromethane	7.93E+01	4.65E+00	4.20E+01
2-Propanol	3.66E+01	3.38E+01	3.52E+01
Isobutane	1.55E+01	4.93E+01	3.24E+01
o-Dichlorobenzene	2.25E+01	3.92E+01	3.08E+01
trans-2-Pentene	9.92E+00	5.11E+01	3.05E+01
Hexanal	2.70E+01	2.68E+01	2.69E+01
1-Propanol	2.09E+01	3.02E+01	2.55E+01
1-Heptene	1.02E+01	3.93E+01	2.47E+01
n-Pentane	1.04E+01	3.40E+01	2.22E+01
Average Concentrations >1.0E+01 but <1.0E+02 (cont.)			
2-Methyl-1-pentene	2.17E+01	ND	2.17E+01
Cyclopentene	1.10E+01	3.00E+01	2.05E+01
1-Decene	ND	1.93E+01	1.93E+01
1,2-Dichloroethane	1.91E+01	ND	1.91E+01
Methylcyclopentene	ND	1.79E+01	1.79E+01
1,2,4-Trichlorobenzene	1.70E+01	ND	1.70E+01
3-Methyl-1-butene	6.44E+00	2.52E+01	1.58E+01
m-Ethyltoluene	9.67E+00	2.09E+01	1.53E+01
cis-2-Pentene	4.87E+00	2.35E+01	1.42E+01
n-Hexane	7.49E+00	1.57E+01	1.16E+01
1-Octene	5.12E+00	1.74E+01	1.12E+01
n-Heptane	4.71E+00	1.78E+01	1.12E+01
n-Propylbenzene	5.80E+00	1.63E+01	1.10E+01
1-Nonene	5.43E+00	1.61E+01	1.07E+01
Average Concentrations >1.0E+00 but <1.0E+01			
trans-2-Hexene	3.64E+00	1.61E+01	9.87E+00

ND = not detected

Table A4. Selected VOC Concentrations—Improved HAWK rocket motor

Compound	Concentrations, ppbv
	DAZZLER
Average Concentrations >1.0E+03	
Methylene chloride	1.46E+03
Total Nonmethane Hydrocarbons	2.57E+03
Concentrations >1.0E+02 but <1.0E+03	
Benzene	5.62E+02
Ethanol	2.69E+02
Acetaldehyde	1.87E+02
Chloromethane	1.86E+02
2-Propanol	1.44E+02
Acetonitrile	1.41E+02
Acetone	1.33E+02
1-Butanol	1.16E+02
Concentrations >1.0E+01 but <1.0E+02	
Carbon tetrachloride	9.46E+01
Propylene	8.56E+01
Chloroform	7.85E+01
Isobutane	6.62E+01
Benzaldehyde	6.50E+01
Tetrachloroethene	6.47E+01
Propane	6.13E+01
Toluene	5.63E+01
Vinyl chloride	3.13E+01
o-Dichlorobenzene	2.76E+01
Chlorobenzene	2.74E+01
Acrylonitrile	2.64E+01
Isopentane	2.38E+01
Naphthalene	2.14E+01
Butyraldehyde	2.13E+01
n-Butane	2.01E+01
Chloroethane	2.00E+01
m/p-Xylene	1.92E+01
1-Butene/Isobutene	1.62E+01
Trichloroethene	1.12E+01
Concentrations >1.0E+00 but <1.0E+01	
1,2-Dichloropropane	9.70E+00
1-Propanol	9.56E+00
1,2-Dichloroethane	7.92E+00
2-Butanone	7.62E+00
n-Pentane	7.43E+00
Chlorodifluoromethane	7.42E+00
Ethylbenzene	6.96E+00
Benzyl chloride	6.70E+00

Table A5. SVOC Concentrations —NIKE rocket motor

Compound	Concentrations, mg/m ³		
	SUNSPOT	THUNDERBIRD	Average
Average Concentrations >1.0E+01			
Diethylphthalate	9.46E+01	4.63E+01	7.05E+01
2-Nitrophenol	1.85E+01	2.04E+01	1.95E+01
Average Concentrations >1.0E+00 but <1.0E+01			
Phenol	1.21E+00	1.20E+01	6.58E+00
Benzoic acid	5.66E+00	6.44E+00	6.05E+00
4-Nitrophenol	3.59E+00	6.94E+00	5.27E+00
Naphthalene	7.06E+00	1.85E+00	4.45E+00
2,4-Dinitrophenol	ND	3.45E+00	3.45E+00
Dimethylphthalate	2.26E+00	3.85E+00	3.06E+00
Acetophenone	1.27E+00	3.55E+00	2.41E+00
Dibenzofuran	2.48E+00	1.43E+00	1.96E+00
Average Concentrations >1.0E-01 but <1.0E+00			
Nitrobenzene	3.37E-01	6.67E-01	5.02E-01
Phenanthrene	4.79E-01	1.11E-01	2.95E-01
bis(2-Ethylhexyl)phthalate	3.88E-01	8.45E-02	2.36E-01
2-Methylnaphthalene	3.18E-01	1.41E-01	2.29E-01
Chrysene	2.16E-01	ND	2.16E-01
1,2-Dichlorobenzene	2.37E-01	1.28E-01	1.82E-01
1,2,4-Trichlorobenzene	1.65E-01	ND	1.65E-01
4-Methylphenol/3-Methylphenol	7.47E-02	1.59E-01	1.17E-01
Benzyl alcohol	1.10E-01	ND	1.10E-01
1,4-Dichlorobenzene	1.02E-01	ND	1.02E-01
1,3-Dichlorobenzene	1.01E-01	ND	1.01E-01
Average Concentrations >1.0E-02 but <1.0E-01			
Fluoranthene	8.70E-02	ND	8.70E-02
2,4,6-Trichlorophenol	ND	7.49E-02	7.49E-02
2-Chlorophenol	3.10E-02	1.17E-01	7.42E-02
Benzo(b)fluoranthene	7.30E-02	ND	7.30E-02
Benzo(k)fluoranthene	7.30E-02	ND	7.30E-02
Fluorene	7.23E-02	2.66E-02	4.95E-02
1,2,4,5-Tetrachlorobenzene	2.30E-02	ND	2.30E-02
Di-n-butylphthalate	1.87E-02	1.99E-02	1.93E-02
Acenaphthylene	1.68E-02	ND	1.68E-02
Anthracene	1.39E-02	ND	1.39E-02
Average Concentrations >1.0E-03 but <1.0E-02			
Pyrene	6.18E-03	ND	6.18E-03

ND = not detected

Table A6. SVOC Concentrations —Improved HAWK rocket motor

Compound	Concentrations, mg/m ³
DAZZLER	
Concentrations>1.0E+00	
Benzoic acid	1.43E+00
Diethylphthalate	1.05E+00
Concentrations >1.0E-01 but <1.0E+00	
2-Nitrophenol	9.44E-01
2,4,6-Trichlorophenol	6.56E-01
1,2-Dichlorobenzene	3.30E-01
Naphthalene	2.81E-01
Hexachlorobenzene	2.40E-01
Pentachlorobenzene	1.94E-01
4-Nitrophenol	1.60E-01
Concentrations >1.0E-02 but <1.0E-01	
1,2,4,5-Tetrachlorobenzene	9.68E-02
Phenol	8.46E-02
Dibenzofuran	7.58E-02
1,2,4-Trichlorobenzene	6.10E-02
Dimethylphthalate	6.00E-02
4-Chloro-3-methylphenol	4.46E-02
2-Chloronaphthalene	4.36E-02
2,4-Dichlorophenol	4.13E-02
1,3-Dichlorobenzene	3.53E-02
Hexachlorobutadiene	3.47E-02
2-Chlorophenol	3.37E-02
4,6-Dinitro-2-methylphenol	3.35E-02
1,4-Dichlorobenzene	1.94E-02
Phenanthrene	1.03E-02

Table A7. PCDD and PCDF Concentrations—Improved HAWK rocket motor

Compound	Concentrations, mg/m ³
	DAZZLER
Polychlorinated dibenzo-p-dioxin	
2,3,7,8-TCDD	7.60E-05
1,2,3,7,8-PeCDD	1.20E-04
1,2,3,4,7,8-HxCDD	8.46E-05
1,2,3,6,7,8-HxCDD	1.42E-04
1,2,3,7,8,9-HxCDD	1.47E-04
1,2,3,4,6,7,8-HpCDD	4.95E-04
1,2,3,4,6,7,8,9-OCDD	1.11E-03
Total TCDD	1.86E-03
Total PeCDD	1.35E-03
Total HxCDD	1.49E-03
Total HpCDD	8.82E-04
Polychlorinated dibenzofurans	
2,3,7,8-TCDF	1.62E-03
1,2,3,7,8-PeCDF	1.05E-03
2,3,4,7,8-PeCDF	7.52E-04
1,2,3,4,7,8-HxCDF	3.32E-03
1,2,3,6,7,8-HxCDF	9.04E-04
2,3,4,6,7,8-HxCDF	7.09E-04
1,2,3,7,8,9-HxCDF	1.92E-04
1,2,3,4,6,7,8-HpCDF	4.81E-05
1,2,3,4,7,8,9-HpCDF	2.55E-03
1,2,3,4,6,7,8,9-OCDF	9.62E-05
Total TCDF	1.38E-02
Total PeCDF	8.56E-03
Total HxCDF	1.01E-02
Total HpCDF	1.30E-02
2,3,7,8-TCDD Toxicity Equivalence^a	1.31E-03

^aCalculated using procedures in Appendix IX of 40 CFR 266.

Samples of solid residue collected from the concrete pad on the invert of the test chamber after each test were analyzed for energetics, SVOC's and metals. These data are summarized in Tables A8-A11. Table A8 summarizes the results of the residue energetics analyses. SVOCs found in the residue samples are summarized in Table A9.

The concentrations of metals found in the residue samples are summarized in Table A10. The results of subjecting the residue to the Toxicity Characteristic Leaching Procedure (TCLP) are summarized in Table A11. For the residue from the SUNSPOT and THUNDERBIRD test burns, all the TCLP metals were detected at a level lower than their respective regulatory levels. For the DAZZLER residue, cadmium and lead from the TCLP exceeded the regulatory level for defining the material as "toxic." Since the total metals concentrations of cadmium and lead were similar in all residue samples, the TCLP results for the DAZZLER residue were somewhat unexpected. A possible explanation for the greater leachability of cadmium and lead from the DAZZLER residue is the high HCl content of the combustion gases from the DAZZLER test. Some of the HCl undoubtedly was absorbed on the residue. The acidity associated with the HCl could have caused the metals in the residue to be more readily leached by the TCLP.

Table A8. Energetics in residue samples

Analyte	Concentration, ppb		
	SUNSPOT	THUNDERBIRD	DAZZLER
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	ND	ND	411
Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	14950	7350	ND
1,3,5-Trinitrobenzene	ND	ND	1040
2-amino-4,6-dinitrotoluene	ND	ND	20
Net Explosive Weight (NEW), lb	1501.6	3002.8	1211

ND = not detected

Table A9. SVOCs in residue samples

SVOC	Concentration in Residue Samples, µg/kg		
	SUNSPOT	THUNDERBIRD	DAZZLER
2,4-Dinitrophenol	2020	1130	903
2-Methylnaphthalene	98	80	168
2-Nitrophenol	2550	5150	1540
4,6-Dinitro-2-methylphenol	205	ND	ND
4-Nitrophenol	2080	8540	1360
Anthracene	37	ND	ND
Benzo(b)fluoranthene	959	ND	ND
Benzoic Acid	852	999	3410
bis(2-Ethylhexyl)phthalate	4450	283	1040
Butylbenzylphthalate	1410	ND	ND
Chrysene	2270	ND	ND
Dibenzofuran	998	359	302
Diethylphthalate	87500	15500	44200
Dimethylphthalate	1710	657	3620
Di-n-butylphthalate	513	82	ND
Fluoranthene	368	15	ND
Fluorene	51	ND	ND
Hexachlorobutadiene	65	ND	ND
Naphthalene	288	480	90
Nitrobenzene	ND	58	ND
Phenanthrene	728	50	106
Phenol	11100	3930	ND

ND = not detected

Table A10. Total metals in residue samples

Metal	Concentration in Residue Samples, mg/kg		
	SUNSPOT	THUNDERBIRD	DAZZLER
Aluminum	NR	NR	19500
Antimony	2370	514	993
Arsenic	9.5	14.2	4.37
Barium	291	169	110
Beryllium	ND	0.464	ND
Cadmium	121	53.7	87.3
Cobalt	5.23	7.04	2.95
Chromium	42	24.7	68.9
Lead	14800	5880	8770
Manganese	283	176	163
Mercury	0.429	0.114	0.435
Nickel	23.5	11.0	12.2
Phosphorus	2360	1050	983
Selenium	1.89	1.15	1.44
Silver	ND	0.207	0.254
Thallium	1.39	2.18	1.04
Zinc	208	140	344

ND = not detected

NR = not reported

Table A11. TCLP metals analysis of residue samples

Metal	Concentration in Residue Leachate, mg/L			Regulatory Level, mg/L
	SUNSPOT	THUNDERBIRD	DAZZLER	
Arsenic	0.049	0.0185	0.007	5
Barium	0.237	0.215	0.313	100
Cadmium	0.0325	0.001	1.94	1
Chromium	0.0035	ND	0.0985	5
Lead	2.80	0.155	29.0	5
Mercury	0.0063	ND	0.00065	0.2
Selenium	0.0075	ND	ND	1
Silver	ND	ND	ND	5

ND = not detected

This page intentionally left blank

APPENDIX B

Time-Resolved Bulk Gas Analyses—LLNL/Bechtel Nevada

An inventory of the propellant and explosive materials consumed in each rocket motor burn test is shown in Table B1. This inventory indicates the carbon content of these materials. All of the carbon-bearing materials in each test must be identified in order to calculate the final distribution of carbon (i.e., the carbon balance) in all of the gaseous combustion products that were measured by LLNL and BN.

Assuming that the low pressure burns in the test chamber represent complete combustion, we can use the inventory information in Table B1 to estimate how much of each product gas will be produced in a given test. The calculated moles of the product gases are shown in Table B2 along with the quantities of inert tracer gas released in each test. Note that the results given in Table B2 generally depend on the assumptions that are made about the composition of the reaction products in a test. For example, the bottom two rows in Table B2 show how two different assumptions on the formation of HCl and Cl₂ affect the calculated moles of H₂O and O₂ in DAZZLER.

The combustion product gas concentrations expected for each test are obtained by using the estimated gas quantities in Table B2 and the initial gas composition in the test chamber. These concentrations are shown in the column labeled “*Expect*” in Table B3. Table B3 also includes a summary of all of the bulk gas species concentration data measured in the rocket motor burn test series.

Table B1. Inventory of materials consumed in rocket motor burns*.

Item Description	Test ID		
	SUNSPOT	THUNDERBIRD	DAZZLER
Total weight of carbon-containing materials	1606 lb, (2 NIKE) (29.34 wt% carbon)	3212 lb, (4 NIKE) (29.34 wt% carbon)	1334 lb (2 Imp. HAWK) (14.11 wt% carbon)
carbon-containing materials in each motor	OIO propellant, cellulose acetate liner	OIO propellant, cellulose acetate liner	composite propellant, liner, insert
RDX in Copper Linear Shaped Charge (CLSC) (for rocket mtr)	250gr/ft x 16=0.571lb	250gr/ft x 32=1.143lb	250gr/ft x 16=0.571lb
RDX in CLSC (for gas btl)	600gr/ft x 5=0.429lb	600gr/ft x 5=0.429lb	600gr/ft x 10=0.857lb
RDX in Cutting Tape	300g/ft x 10=0.429lb	300gr/ft x 20=0.857lb	300gr/ft x 13=0.571lb
RDX in RP1 Detonator	0.626g x 6=0.0084lb	0.626g x 10=0.014lb	0.626g x 8=0.0112lb
Total RDX Weight (C ₃ H ₆ O ₆ N ₆)	1.437 lb	2.443 lb	2.010 lb

*From R. L. Peabody, Sandia National Laboratories, Albuquerque, NM, and SPIA Data Sheets and T. Moore, Chemical Propulsion Information Agency, John Hopkins University, MD.

Table B2. Expected rocket burn combustion products and tracer gas amounts.*

Test ID	Test Weight, lbs	H ₂ O, moles	N ₂ , moles	CO ₂ , moles	O ₂ ,** moles	Neon, moles	Krypton, moles
SUNSPOT	1606	12095	3018	17796	-11277		412
THUNDERBIRD	3212	24186	6033	35590	-22553		379.8
DAZZLER (HCl)	1334	12107	2530	7115	-6830	446	380.8
DAZZLER (Cl ₂)	1334	13755	2530	7115	-7654	446	380.8

* Assume all metals are completely oxidized (i.e., PbO, Al₂O₃, Fe₃O₄), all nitrogen goes to N₂, all CO goes to CO₂, all hydrogen goes to H₂O or H₂O and HCl [in DAZZLER (HCl)], and all chlorine (in the two DAZZLER assumptions) reacted to either Cl₂ (1648 moles) or HCl (3295 moles).

** Negative values indicate consumption of atmospheric O₂ after all the oxygen in the carbon-bearing items (propellant+explosives+motor parts) is consumed.

Table B3. Data summary—comparison of computed and measured bulk gas species concentrations in the test chamber at the end of each burn *

Gas Species	SUNSPOT, % Vol,			THUNDERBIRD, % Vol			DAZZLER, % Vol		
	<i>Expect</i>	<i>Meas'd</i>	± %V	<i>Expect</i>	<i>Meas'd</i>	± %V	<i>Expect</i>	<i>Meas'd</i>	± %V
Nitrogen	75.42	75.63	0.10	73.20	75.13	0.5	76.45	77.10	0.1
Oxygen	13.45	13.14	0.10	6.75	4.48	0.5	16.22	16.20	0.1
Carbon Dioxide	10.01	9.95	0.10	19.00	19.01	0.5	4.10	4.17	0.1
Argon	0.88	0.87	0.02	0.84	0.85	0.02	0.90	0.90	0.02
Krypton	0.23	0.22	0.01	0.20	0.20	0.01	0.218	0.204	0.002
Neon							0.238	0.206	0.0006
Hydrogen Chloride							1.88	--	
		ppmv	±ppmv		ppmv	±ppmv		ppmv	±ppmv
Carbon Monoxide		682	42		1692	100		234	42
Hydrogen		64	6		299	20		497	6
Nitrogen oxides:									
NOx		1169	50		1324	50		1425	50
NO		1017	50		1164	50		1292	50
NO ₂ , by difference		152	50		159	50		133	
Methane		50	10		70	20		<10	10
Net Test Weight, lb ^{oo}		1606			3212			1334	

* *Expect* assumes only CO₂, N₂, H₂O, metal oxides and HCl (in DAZZLER) are formed and added to an initial atmosphere at 20°C, 60% relative humidity, and a pressure of 0.88 atmosphere with a volume of 4644 m³; note that initial CO₂ concentration was 200ppmv for SUNSPOT and THUNDERBIRD and 325ppmv for DAZZLER

* *Meas'd* values are obtained by extrapolating time-resolved gas concentration measurements back to test initiation time plus 60s (i.e., T=60s). These values are normalized to 100% on a water-free basis. Data from the sampling port on the tunnel back were used for obtaining the SUNSPOT and DAZZLER measurements. For THUNDERBIRD, the data shown represent an average from two measurements taken at the back and invert ports at 5 and 9 minutes, respectively. For this reason, it is assumed that the SUNSPOT and DAZZLER measurements represent maximum values, whereas the THUNDERBIRD measurements are an average.

* ± %V indicates the precision of the measured values except for values of NO₂, by difference and DAZZLER Kr and Ne. The uncertainty on NO₂ is the square root of the squared errors for NOx and NO. The uncertainty on the DAZZLER Kr and Ne values is the uncertainty on the intercept of a linear regression data fit.

^{oo} Initial weight of carbon bearing materials in the test

The gas species concentrations in Table B3 were measured in each test by extracting samples from the test chamber. These samples, composed of combustion product gases mixed with ambient air and tracer gas, were extracted from the test chamber using two sampling ports. One port was at the invert, and the second one was located on the back of the chamber. Stainless steel sampling lines from each port were routed out of the test chamber and over a distance of roughly 300 m to a pumping station located on the apron of the X-tunnel complex. The combustion gases were analyzed in real time by standard analytical instruments located near the pumping station. The transit time of the gases between the test chamber and the analysis station was roughly 120 s.

Since the gases in the test chamber tend to become stratified (i.e., hotter gases collecting near the tunnel back), we instituted a general procedure focused on analyzing the gas stream from the port on the chamber back. In general, this gas stream was analyzed for roughly 30 minutes before switching to the invert port for roughly 10 minutes before returning to the port at the chamber back. The one exception to this procedure occurred in the THUNDERBIRD test where we found the sampling port on the back of the chamber was non-operable roughly 7 minutes after the test was initiated. This failure was probably caused by high debris loading in the combustion cloud that clogged the sample port inlet filter. After the back sampling port became clogged, the invert port was used exclusively for gas sampling in THUNDERBIRD.

The histories of the O_2 and CO_2 concentrations during the first 20 minutes after initiation of the SUNSPOT test as given in Figure B1 are examples of the data obtained from these measurements. Similarly, the time histories of the NO_x species for 250 minutes in SUNSPOT are shown in Figure B2. It is evident from Figure B1 that, once the propellant burn is completed, the concentrations of the relatively stable O_2 and CO_2 gas species are essentially constant. It can also be seen that the measured concentrations of these species depend somewhat on sampling location. The full data record for the CO_2 concentration history in SUNSPOT is given in Figure B3. This record shows a gradual decrease in CO_2 concentration over the 3-4 hour sampling period for the test. In contrast, we see in Figure B2 over a comparable time scale that the concentration histories of the highly reactive NO_x species in the combustion cloud are characterized by:

- strong peaks followed by rapid decreases, and
- long-term molecular stratification in the chamber.

The occurrence of the concentration peaks in Figure B2 correlates well with the end of the propellant burn. The stratification is evident from the persistent factor of 2 difference in the NO_x gas concentrations measured at the invert and back sampling locations. However, in the interest of reporting conservative data in Table B3, we list only the highest values of the measured nitrogen oxide concentrations at the end of each test burn (i.e., derived from samples taken at the chamber back).

A summary of the carbon burn efficiency (overall carbon balance) computed from the test results is given in Table B4. These results suggest that the conversion of the carbon materials inventory in each test to carbon-containing gas species is complete. In the NIKE rocket motor burn tests, the CO₂ values are slightly greater than 100%, but within the 1-sigma uncertainty of the result. In contrast, the data from DAZZLER suggest the presence of excess CO₂ in the test chamber. A possible explanation for this anomaly is that some of the CO₂ absorbed in the chamber walls from previous tests may have been released in DAZZLER due to the elevated temperatures and the high concentration of acid gases in that test. Note also that less than 1% of the carbon was converted to CO and CH₄ in every test. This observation suggests that the combustion process in the test chamber proceeded very nearly to completion, which is consistent with the assumptions used above in calculating the expected gas species concentrations shown in Table B3.

Table B4. Carbon balance

	SUNSPOT		THUNDERBIRD		DAZZLER	
	% Total C	±%TC	% Total C	±%TC	% Total C	±%TC
CO ₂	103.89	3.85	101.89	5.75	108.85	2.80
CO	0.71	0.05	0.91	0.07	0.62	0.11
CH ₄	0.05	0.01	0.04	0.01		
Gas sum	105	4	103	6	109	3

% Total C = 100 x (moles carbon in gas product) / (initial total moles carbon in the test materials)

Figure B1. Early-time variation of O_2 and CO_2 gas concentrations in test chamber during SUNSPOT test. Samples extracted from chamber back and invert as indicated.

Figure B2. Variation of NO_x gas concentrations in test chamber during SUNSPOT test (samples taken from invert and back).

Figure B3. Complete history of CO₂ concentration in SUNSPOT.

APPENDIX C

Real-Time and Time-Averaged Aerosol Analyses—LANL

The LAASS impactor and streaker aerosol measurement elements provided data on the evolution, size distribution and composition of the particulate in the combustion cloud after each rocket motor burn test. Time-resolved elemental analyses (i.e., PIXE results) from the streaker are summarized in Tables C1-C6. Data from SUNSPOT are given in Tables C1 and C2 for the total ($<10\text{ }\mu\text{m}$) and fine ($<2.5\text{ }\mu\text{m}$) aerosol fractions, respectively. The same aerosol size distinction is used for streaker data obtained from the THUNDERBIRD (Tables C3 and C4) and DAZZLER (Tables C5 and C6) tests. These data also give us an indication of the evolution of the total aerosol concentrations in the test chamber. The sums of the elemental concentrations at each sampling time for the two aerosol size categories provide this information. These results for the SUNSPOT, THUNDERBIRD and DAZZLER tests are presented in Figures C1-C3, respectively. The rapid changes in the elemental concentration data shown in Figure C3 are physically unrealistic and may be the result of a measurement error. Additional analyses are required to resolve this issue.

The time histories of the aerosol size distributions obtained from the LAASS impactor measurements are reported in Figures C4-C6 for the SUNSPOT, THUNDERBIRD and DAZZLER tests, respectively. Figure C4 shows the aerosol size distribution obtained from the impactor 27 minutes after initiation of the motor burn in SUNSPOT. One of the impactor channels ($1.2 - 2.5\text{ }\mu\text{m}$) was inoperative during this test. In addition, because of an error in operating the flow controllers for the impactor, the impactor was not operated in an isokinetic condition for this sample. The aerosol concentration data therefore represent a lower limit to the actual aerosol concentration. Figure C5 shows the impactor data obtained for the first two sampling times in the THUNDERBIRD test. Note that dynamic processes in the test chamber (e.g., particle coagulation and thermally driven turbulence) likely affect the aerosol concentrations reported here. Thus, even though the quantities of propellant consumed in the SUNSPOT and THUNDERBIRD tests differ by a factor of two, the aerosol concentration in a given bin size will not show a similar scale dependence. A more meaningful test-to-test comparison is the aerosol mass integrated over all sizes. Finally, Figure C6 shows impactor data for the first three sampling times in the DAZZLER test. Unlike the comparable data from SUNSPOT and THUNDERBIRD, the results in Figure C6 suggest a shift in aerosol size distribution from larger to smaller sizes over the three sampling times. This shift may reflect propellant differences in the tests (smaller aerosols showing less coagulation than in previous tests), or it may be associated with the differing sample delay times in each test. The decrease in aerosol concentration observed for latter samples is also consistent with the streaker results for DAZZLER.

Table C1. Total (<10 µm) Elemental Concentrations—(µg/m³) for SUNSPOT

Sample Time (minutes):		26	39	62	79	101
Atomic Number	Element	Concentration				
		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
11	Na	0	0	0	0	0
12	Mg	0	0	0	0	0
13	Al	0	0	0	0	0
14	Si	3179.69	2176.42	2011.35	1583.43	1553.79
15	P	10372.5	7601.45	7956.44	5660.62	5794.44
16	S	0	0	0	1174.75	750.849
17	Cl	5759.18	5176.61	4804.79	2941.69	2905.63
18	Ar	0	0	0	0	0
19	K	992.051	779.297	812.712	535.771	532.807
20	Ca	3056.29	2218.89	1727.67	1292.55	1314.19
21	Sc	0	0	0	0	0
22	Ti	221.569	79.332	49.9231	87.9063	47.9999
23	V	0	0	0	0	0
24	Cr	42.2303	18.7993	40.884	17.413	15.4818
25	Mn	0	3.91852	0	0	0
26	Fe	2378.36	1742.1	1835.05	1324.6	1358.26
27	Co	0	0	0	0	0
28	Ni	0	0	0	0	0
29	Cu	1185.41	875.857	916.886	668.552	685.941
30	Zn	1198.15	884.191	926.341	680.893	685.941
31	Ga	0	41.8296	18.6711	0	15.3856
32	Ge	0	0	0	0	0
33	As	289.121	191.198	153.696	190.878	158.023
34	Se	8.26175	37.2299	11.5873	21.3716	9.3756
35	Br	170.444	134.408	176.053	117.155	123.566
48	Cd	2600.33	1915.99	2079.46	1792.58	1708.44
49	In	0	0	0	0	0
50	Sn	0	0	0	0	0
51	Sb	37622.6	27822.3	30170.2	21259.4	21900.4
82	Pb	118774	89541	96961.3	69804.1	71719.3

Table C2. Fine (< 2.5 µm) Elemental Concentrations—(µg/m³) for SUNSPOT

Sample Time (minutes):		26	39	62	79	101
Atomic Number	Element	Concentration				
		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
11	Na	0	0	0	0	0
12	Mg	0	0	0	0	0
13	Al	0	0	0	0	0
14	Si	2102.7	1410.35	1173.95	947.977	893.487
15	P	9023.01	6402.65	5320.85	4030.71	3966.6
16	S	0	0	0	1174.75	750.849
17	Cl	5304.83	4623.69	3421.69	2342.3	2228.51
18	Ar	0	0	0	0	0
19	K	769.28	611.417	512.052	361.401	344.573
20	Ca	2226.91	1667.57	1065.77	864.639	860.632
21	Sc	0	0	0	0	0
22	Ti	133.582	0	0	22.1168	0
23	V	0	0	0	0	0
24	Cr	42.2303	15.7061	32.8547	9.05507	10.6577
25	Mn	0	3.91852	0	0	0
26	Fe	1895.95	1338.23	1153.92	851.817	846.208
27	Co	0	0	0	0	0
28	Ni	0	0	0	0	0
29	Cu	967.209	687.544	579.364	432.72	431.919
30	Zn	954.388	669.113	570.549	426.309	404.673
31	Ga	0	41.8296	18.6711	0	15.3856
32	Ge	0	0	0	0	0
33	As	262.036	130.617	83.3387	73.8829	70.5975
34	Se	0	25.8029	0	8.81467	9.3756
35	Br	138.23	108.741	110.023	78.8512	84.0599
48	Cd	2314.25	1617.09	1370.28	1268.51	1123.47
49	In	0	0	0	0	0
50	Sn	0	0	0	0	0
51	Sb	32534.1	23198.6	19889.1	14680.4	14696.5
82	Pb	102651	74363.7	63385.5	46958.1	45996.5

Table C3. Total (<10 µm) Elemental Concentrations—(µg/m³) for THUNDERBIRD

Sample Time (minutes):		19	32	43	54	63
Atomic Number	Element	Concentration				
		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
14	Si	5755.18	5418.62	3365.6	3197.32	2452.08
15	P	9644.85	7712.03	5577.28	5067.63	4178.15
16	S	12563.3	12659.5	8173.6	8216.87	5288.8
17	Cl	5806.62	4086.8	3711.78	3192.51	3024.23
18	Ar	0	0	0	0	0
19	K	8308.22	6740.82	4740.69	4327.2	3557.92
20	Ca	5158.98	3726.2	2966.54	2658.82	1971.28
21	Sc	0	0	0	0	0
22	Ti	376.947	337.522	228.861	197.128	204.34
23	V	12.9335	0	0	0	13.7509
24	Cr	113.661	75.1971	40.3872	67.312	55.6766
25	Mn	53.3688	0	0	0	0
26	Fe	4870.5	3428.1	2639.59	2283.8	2149.18
27	Co	0	0	0	0	0
28	Ni	0	0	0	0	0
29	Cu	1485.19	1089.49	799.09	716.873	670.716
30	Zn	1941.95	1417.88	1064.97	945.253	840.438
35	Br	240.833	183.329	135.441	127.316	116.45
48	Cd	3405.03	2915.09	1716.94	1822.23	1591.45
49	In	0	0	0	0	0
50	Sn	0	0	0	0	0
51	Sb	29362.5	21549.5	15741.4	13875.9	13048.9
82	Pb	123325	91159.7	68129.4	60436.6	56061.3

Table C4. Fine (< 2.5 µm) Elemental Concentrations—(µg/m³) for THUNDERBIRD

Sample Time (minutes):		19	32	43	54	63
Atomic Number	Element	Concentration				
		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5
14	Si	4904.16	4707.03	2812.68	2456.89	1682.8
15	P	8558.24	6635.04	4399.32	3682.93	2841.53
16	S	11202.6	11106.5	7356.24	6538.88	3706.97
17	Cl	5481.12	3596.38	2875.18	2379.96	2211.68
18	Ar	0	0	0	0	0
19	K	7500.48	5961.92	3923.33	3312.71	2519.39
20	Ca	4519.52	3178.09	2456.89	2072.25	1394.32
21	Sc	0	0	0	0	0
22	Ti	272.614	260.594	169.242	129.816	115.873
23	V	0	0	0	0	0
24	Cr	100.968	62.504	40.3872	47.503	37.262
25	Mn	53.3688	0	0	0	0
26	Fe	4057.95	2788.64	1947.24	1572.22	1394.32
27	Co	0	0	0	0	0
28	Ni	0	0	0	0	0
29	Cu	1327.01	932.752	620.232	524.072	466.857
30	Zn	1682.8	1177.96	793.32	663.504	548.112
35	Br	205.302	154.818	94.7176	88.948	73.0816
48	Cd	3048.27	2548.24	1346.24	1317.39	1081.8
49	In	0	0	0	0	0
50	Sn	0	0	0	0	0
51	Sb	26155.5	18558.9	12020	10000.6	8894.8
82	Pb	107218	75966.4	50964.8	42118.1	36781.2

Table C5. Total (< 10 µm) Elemental Concentrations—(µg/m³) for DAZZLER

Sample Time Atomic Number	(minutes): Element	10	22	32	43	52	62	72	82
		Concentration							
		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6	Sample 7	Sample 8
11	Na	0	0	0	0	0	0	0	0
12	Mg	1877.52	2769.41	110.344	1177.96	805.34	1233.25	935.156	1012.08
13	Al	106690	113589	11419	67864.9	39666	35555.2	46829.9	47286.7
14	Si	0	158.424	0	0	0	245.208	0	0
15	P	0	0	0	0	0	0	0	0
16	S	644.272	926.982	0	399.064	153.616	163.472	310.116	147.365
17	Cl	668.072	1022.9	123.085	564.219	428.393	321.174	426.71	460.126
18	Ar	0	0	0	0	0	0	0	0
19	K	358.196	351.946	13.0537	205.542	104.814	99.2852	78.13	123.806
20	Ca	410.363	356.994	57.72	226.938	114.671	124.046	80.2936	116.594
21	Sc	0	0	0	0	0	0	0	0
22	Ti	66.4706	69.7641	11.669	53.3688	20.5542	26.6844	12.02	20.3378
23	V	0	0	0	0	0	0	0	0
24	Cr	210.614	199.556	35.8196	135.562	65.4369	60.8933	36.685	64.908
25	Mn	29.0884	0	0	19.9292	6.611	0	0	17.6934
26	Fe	1662.85	1230.37	169.722	674.562	360.36	330.31	189.676	364.206
27	Co	0	0	0	0	0	0	0	0
28	Ni	0	0	1.47125	1.51692	0	0	0	0
29	Cu	1791.7	1658.28	176.454	965.687	492.339	442.817	260.594	495.945
30	Zn	126.955	120.368	18.4868	71.0622	38.4159	34.1368	19.6407	37.9111
31	Ga	12.6931	11.1786	0	1.45923	0	0	0	4.30316
32	Ge	0	0	0	0	0	0	0	0
33	As	0	0	0	23.415	0	0	0	0
34	Se	0	0	0	0	0	0	0	0
35	Br	0	0	0	0.723604	3.87044	2.42804	0	1.61789
51	Sb	113.95	323.338	0	267.325	144	82.938	69.4756	157.222
82	Pb	1426.53	1361.14	171.165	764.712	416.132	372.62	226.938	432.239

Table C6. Fine (< 2.5 µm) Elemental Concentrations—(µg/m³) for DAZZLER

Sample Time (minutes):		10	22	32	43	52	62	72	82
Atomic Number	Element	Concentration							
		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6	Sample 7	Sample 8
11	Na	0	0	0	0	0	0	0	0
12	Mg	1334.22	1807.81	110.344	668.312	425.508	372.62	480.8	507.244
13	Al	85582.4	93275.2	6611	49522.4	21563.9	22020.6	30050	25482.4
14	Si	0	0	0	0	0	0	0	0
15	P	0	0	0	0	0	0	0	0
16	S	644.272	726.008	0	399.064	153.616	163.472	310.116	147.365
17	Cl	500.032	798.128	48.08	377.428	191.839	174.771	228.861	188.474
18	Ar	0	0	0	0	0	0	0	0
19	K	312.52	300.5	0	175.011	65.6292	68.514	42.3104	76.928
20	Ca	365.408	312.52	34.3772	185.108	74.7644	87.746	38.7044	65.8696
21	Sc	0	0	0	0	0	0	0	0
22	Ti	57.9364	63.706	9.47176	47.3588	14.7125	20.6744	6.58696	13.4864
23	V	0	0	0	0	0	0	0	0
24	Cr	189.195	179.819	26.9248	115.152	46.6376	42.7912	18.2704	40.3872
25	Mn	29.0884	0	0	19.9292	6.611	0	0	17.6934
26	Fe	1526.54	1110.65	131.499	569.748	257.228	233.428	93.5156	227.418
27	Co	0	0	0	0	0	0	0	0
28	Ni	0	0	0	0	0	0	0	0
29	Cu	1629.91	1502.5	137.028	831.784	355.792	319.732	131.98	317.328
30	Zn	115.392	109.622	14.5923	60.1	28.3672	24.5208	9.95256	24.7612
31	Ga	12.6931	11.1786	0	0	0	0	0	2.74056
32	Ge	0	0	0	0	0	0	0	0
33	As	0	0	0	23.415	0	0	0	0
34	Se	0	0	0	0	0	0	0	0
35	Br	0	0	0	0	3.87044	2.42804	0	1.61789
51	Sb	79.5724	281.268	0	233.669	93.9964	40.3872	25.7228	102.17
82	Pb	1281.33	1221.23	135.345	641.868	288.48	259.632	108.42	266.844

Figure C1. Summary of LAASS streaker elemental composition data from SUNSPOT

Figure C2. Summary of LAASS streaker elemental composition data from THUNDERBIRD

Figure C3. Summary of LAASS streaker elemental composition data from DAZZLER

Figure C4. Summary of LAASS impactor data from SUNSPOT

Figure C5. Summary of LAASS impactor data from THUNDERBIRD

Figure C6. Summary of LAASS impactor data from DAZZLER

APPENDIX D

Real-Time Gas Species Analyses Using FTIR—LANL

The FTIR diagnostic was implemented primarily to obtain time-resolved measurements of HCl gas concentrations in DAZZLER. Nevertheless, it was available to analyze gas samples extracted from the THUNDERBIRD test. The FTIR was therefore used in this test to establish operational procedures for it in X-tunnel, rather than for collecting critical data. Only a single FTIR spectrum was obtained in THUNDERBIRD because the substantial particulate loading in this test clogged an in-line, small-particulate filter located in the sampling line. This interruption occurred soon after the first sample was extracted from the test chamber. In addition, it appears that a water-based aerosol entered the sample cell despite the precaution of using a heated sample line.

To quantify the results for CO₂, CO and H₂O concentrations observed in this first scan, the background scan obtained prior to executing the THUNDERBIRD test was used as a reference to obtain the absorbance spectrum shown in Figure D1. This spectrum is a function of the concentrations of the gas species detected. We can obtain good estimates of these concentrations either by calculating the spectrum from known databases parameters or by adjusting tabulated spectra from available quantitative databases. The later was done here, using the QASOFT¹ database to quantify the concentrations of CO, CO₂ and H₂O in the sample at 0.2 %, 10 %, and 10 %, respectively. The spectra used for these analyses are shown in Figure D2.

Figure D1. Absorbance spectra from first FTIR scan in THUNDERBIRD (sample taken at test initiation time + 19 minutes)

¹ P. L. Hanst and S. T. Hanst, "Infrared Spectra for the Quantitative Analysis of Gases", Infrared Analysis, Inc., Anaheim, CA

Figure D2. Comparison between measured and simulated absorption features for water, CO and CO₂. Simulated spectra are derived from the QASOFT database. Estimated concentrations are indicated for each simulation.

Thirteen FTIR spectra were obtained using extracted samples from the DAZZLER test. This improved performance of the FTIR diagnostic (compared to the results in THUNDERBIRD) is related to changes in the sampling procedures implemented between the tests. In addition, a different combustion cloud aerosol size distribution in DAZZLER helped reduce particulate loading in the sampling line to the FTIR. However, no HCl peaks were observed in the thirteen spectra. Subsequent analysis of the FTIR diagnostic and comparison to QASOFT spectra suggest that an HCl concentration greater than 0.2 % should have been detectable by the instrument. The measurement of HCl concentration in DAZZLER obtained by Radian International from post-test analyses of

extracted samples was roughly 1.1%. Analyses of the the FTIR spectra from DAZZLER shown in Figure D3 indicate upper limits of 0.5%, 0.1%, 0.1% and 0.05% for the concentrations of NO, NO₂, N₂O, and HCN, respectively.

Figure D3. Representative spectra from DAZZLER (light background) compared with simulated absorption features from the QASOFT database (dark foreground).

This page intentionally left blank

APPENDIX E

Post-test Metal Residue Analyses—UNLV

The results of the UNLV analyses of the coupon rinse samples obtained after each rocket motor burn test are summarized in Table E1. These analyses identified the concentrations of non-volatile metal residues that remained on large aluminum plate coupons after they were exposed to the combustion clouds in the test chamber. The mounting of the plates before a test, and the recovery of the rinse solution (a 50/50 mixture of distilled water and alcohol) after a test, were the responsibility of Radian International. Since the plates were fixed vertically in the chamber at a height of roughly 3m above the invert, we speculate that the residue sample obtained from them was fairly representative of the non-volatile combustion cloud components in each test. Note that no effort was made to recover volatile or semi-volatile compounds from these samples.

Table E1. Summary of metal concentrations (in ppb) found in coupon rinse solution obtained after each contained rocket motor burn test.

Element	SUNSPOT M /SD	THUNDERBIRD M /SD	DAZZLER M /SD
Be 9	ND	ND	ND
Al 27	721 15	5411 56	1475000 13030
Cr 52	2.80 0.11	21.2 0.2	642 3
Cr 53	12.7 2.3	39.3 1.4	668 2
Mn 55	87.0 1.5	85.5 1.5	2683 58
Ni 60	10.4 0.2	8.73 0.45	179 1
Ni 62	10.8 0.4	10.1 1	179 5
Cu 63	78.8 1.4	640 11	1969 34
Cu 65	78.1 2.2	627 10	1954 53
Zn 66	311 7	409 14	272 3

Table E1. (Contd.)

Element	SUNSPOT M /SD	THUNDERBIRD M /SD	DAZZLER M /SD
Zn 68	301 14	409 8	270 8
As 75	6.65 0.81	25.2 0.7	16 0.3
Se 77	38.5 7.4	93.2 3	85.5 1
Se 82	0.273 0.889	2.46 0.78	0.51 0.55
Cd 111	56.9 2.1	317 11	60.2 1.7
Cd 114	56.2 0.6	315 6	60.5 1.5
Ba 135	19.1 0.4	67.6 2.5	32.8 0.8
Ba 137	19.6 0.2	69.4 2	33 0.5
Pb 207	2424 33	24200 434	2472 22
Pb 208	2459 44	24140 415	2467 33
Sb 121	364 5	6574 110	807 5
Sb 123	360 3	6564 57	796 14

M - Mean

SD -Standard Deviation

APPENDIX F

In Situ Laser-Based Measurements of Gas Species Concentrations—SNL

The tunable diode laser gas species monitor (TDL) was used in two of the three contained rocket motor burn tests in X-tunnel: SUNSPOT and DAZZLER. The TDL monitors were not used in THUNDERBIRD because it was anticipated that the transient high air temperature and substantial number of particles generated in that test would be detrimental to this instrumentation.

In these tests, the sensitivity of the TDL instrumentation at both its invert and rib locations was limited by laser transmittance. During SUNSPOT, laser transmittances at the rib location slowly decreased after initially recovering from a prompt attenuation at test initiation time, $T = 0$. Nevertheless, the optical paths for both lasers in the rib were completely blocked by $T = 2000$ s. Laser transmittance in the invert sample volume during SUNSPOT was essentially zero by $T = 40$ s. During DAZZLER, the overall laser transmittances increased somewhat after the initial drop-off at $T = 0$; allowing some gas species concentration measurements to be made during this test. The time history of the laser transmittance in DAZZLER was qualitatively similar to that observed in the detonation test series.

The results of the TDL measurements in the rocket motor burn tests are summarized in Table F1. Molecular species measurements during SUNSPOT are sparse: CO_2 and H_2O signals were detected and analyzed, but the laser transmittance was very low so the signals were weak. Conversely, during DAZZLER, CO_2 concentration histories were obtained in both locations, and the H_2O concentration history was measured at the rib location. While the CO_2 signal in the invert was characterized by a low signal: noise ratio, the measurements indicate that molecular stratification was present in DAZZLER, in qualitative agreement with results obtained in the detonation tests.

The CO_2 concentration histories measured at the invert and rib locations in DAZZLER are presented in Figures F1 and F2, respectively. Both curves have been smoothed using a binomial smoothing algorithm. This was particularly necessary for the invert measurements because of low laser transmittance. The final CO_2 concentrations are nominally 4% in the invert, and 6% in the rib. Equilibrium calculations for DAZZLER yield a fully-mixed final CO_2 concentration of 3.6%, compared to the on-line LLNL/BN measured value (early time) of 4.2%. Even with the large uncertainty seen in Figs. F1 and F2, these data suggest that the CO_2 concentration at the rib location is substantially higher than in the invert, even long after the combustion process is complete.

Table F1. TDL measurement summary for rocket motor burn experiments

	SUNSPOT	THUNDERBIRD	DAZZLER
<i>Execution date</i>	5/14/97	5/28/97	6/11/97
<i>Load</i>	2 Nike Rocket Motors	4 Nike Rocket Motors	2 Hawk Rocket Motors
<i>Species monitored</i>	HCN;CO; CO ₂ ; H ₂ O	Did not participate.	CO; CO ₂ ; H ₂ O
<i>Species detected</i>	CO ₂ ; H ₂ O	---	CO ₂ and H ₂ O
<i>CO concentration</i>	---	---	---
<i>CO₂ concentration, rib location</i>	9% peak	---	6%
<i>CO₂ concentration, invert location</i>	---	---	4%
<i>Fully mixed CO₂ concentration¹</i>	10.01%	19.00%	not available
<i>H₂O concentration added, rib location</i>	---	---	2.4%
<i>H₂O concentration added, invert location</i>	---	---	--
<i>Fully mixed H₂O concentration, 75% initial relative humidity</i>	7.23%	---	not available
<i>Final Transmittance (rib)</i>	0%	--	13%

Water concentration measurements were also obtained at the rib location in DAZZLER. Low transmittance prevented comparable measurements at the invert location. The results are shown in Figure F3. The pre-event water concentration in the chamber ambient air was estimated at 2.1%. The data in Figure F3 indicate that the total water concentration in the sealed chamber long after propellant combustion was completed was roughly 4.5%, corresponding to a water concentration increase of 2.4% from the combustion products. No other measurement of water concentration history was obtained in DAZZLER.

Figure F1. CO₂ measured in invert during DAZZLER.

Figure F2. CO₂ measured in rib during DAZZLER.

Figure F3. Water concentration measured in rib location during DAZZLER.

APPENDIX G

Time-Resolved Measurements of Test Chamber Pressure and Gas Temperatures—LLNL and Bechtel Nevada

The pressure transients produced by the hot combustion gases mixing with and heating the ambient air in the test chamber are shown in Figure G1. The first 500 s of the data from each test are overlaid in this figure. The times to reach maximum pressure differ somewhat from test-to-test, but they correlate well with the burn times of the propellant that are observed in the video records of the tests. The characteristics of the pressure decay in each test also correlate with the cooling rates of the gases observed from the thermocouple records from each test. We note, however, that a containment seal failure in the THUNDERBIRD test resulted in a significant pressure leak at roughly the same time that the peak pressure was reached in this test. It is likely that this leak reduced the magnitude of the maximum pressure recorded in this test.

Representative temperature histories obtained from the thermocouple arrays are shown in Figures G2-G4 for the SUNSPOT, THUNDERBIRD, and DAZZLER tests, respectively. The thermocouple array used in SUNSPOT was positioned over the two motors and attached at the invert near the left rib and to the back, near the center, of the chamber. We see in Figure G2 that the thermocouples near the back of the chamber recorded extremely high temperature transients when the propellant was burning, whereas the thermocouples near the invert recorded much more gradual temperature increases. These data are consistent with the presence of significant thermal stratification in the test chamber as the gases are heated by the burning propellant. It is also evident in Figure G2 that the remnants of this stratification persist as the gases cool. Similar observations apply to the recorded temperature histories for THUNDERBIRD and DAZZLER that are shown in Figures G3 and G4, respectively. However, the thermocouple array was in a different location in the test chamber for these tests compared to its location in SUNSPOT. In THUNDERBIRD and DAZZLER, the array was oriented away from direct contact with the propellant flame and was anchored between the chamber invert and the mid-height of the chamber rib near the containment plug. The temperature variations seen in Figures G3 and G4, while still significant, are therefore not as severe as observed in Figure G2 for SUNSPOT.

Figure G1. Comparison of chamber pressure histories in rocket motor burn tests.

Figure G2. Temperature histories from thermocouple array in SUNSPOT.

Figure G3. Temperature histories from thermocouple array in THUNDERBIRD.

Figure G4. Temperature histories from thermocouple array in DAZZLER.

Distribution:

- 2 The Johns Hopkins University
Chemical Propulsion Information Agency
10630 Little Patuxent Parkway, Suite 202
Columbia, MD 2104-3200
Jim Cocchiaro
Tom Moore
- 1 US Environmental Protection Agency
Mail Drop 46 – ERC Annex
79 T. W. Alexander Dr
Research Triangle Park, NC 27711
William Mitchell
- 4 University of California
Los Alamos National Laboratory
P.O. Box 1663
Los Alamos, New Mexico 87545
John Stephens, CST-1
John Sanchez, DX-2
Herb Fry, CST-6
Cliff Hewitt, CST-6
- 4 University of California
Lawrence Livermore National Laboratory
P.O. Box 808
Livermore, CA 94550
Bruce Watkins, L 282
Carol Velsko, L 231
César Prunada, L 282
Ray Heinle, L 221
- 2 Bechtel Nevada
2621 Losee Road
North Las Vegas, NV 89030-4134
Sam Williams
Al Moeller
- 1 Thiokol Propulsion Group
M/S: 130
P.O. Box 707
Brigham City, UT 84302-0689
William Munson

Distribution: (continued)

- 1 US Department of Energy/Nevada Operations Office
P.O. Box 98518
Las Vegas, NV 89193-8518
Deborah Howard
- 2 University of Nevada Las Vegas
Energy Research Center
P.O. Box 454027
Las Vegas, NV 89124-4027
Bob Boehm
Klaus Stezenbach
- 3 US Army Defense Ammunition Center
1 C Tree Road
McAlester, OK 74501-9002
Jim Wheeler
Solim Kwak
Ed Ansell
- 3 Radian International LLC
1093 Commerce Park Drive, Suite 100
Oak Ridge, TN 37830
John Carson
Tim Tope
Walt Gray
- 1 MS9001 M. E. John, 8000
Attn: R. C. Wayne, 2200
J. Vitko, 8100
W. J. Mclean, 8300
D. R. Henson, 8400
P. N. Smith, 8500
T. M. Dyer, 8700
K. E. Washington, 8900
D. L. Crawford, 9900
- 1 MS9052 Don Hardesty, 8361
- 1 MS9052 Chris Shaddix, 8361
- 1 MS9052 Sarah Allendorf, 8361
- 1 MS9403 Jim Wang, 8723
- 1 MS9403 Dave Ottesen, 8723
- 1 MS9403 Howard Johnsen, 8723
- 1 MS9409 Larry Carrillo, 8421
- 1 MS9105 Jane Ann Lamph, 8119
- 10 MS9105 Joel Lipkin, 8119

Distribution: (continued)

1	MS1156	Rob Tachau, 15322
1	MS1157	Ray Peabody, 153221
1	MS1391	Harold Roberts, 153221
1	MS1167	Larry Posey, 15343
3	MS 9018	Central Technical Files, 8940-2
1	MS 0899	Technical Library, 4916
1	MS 9021	Technical Communications Department, 8528/ Technical Library, MS 0899, 4916
1	MS 9021	Technical Communications Department, 8528 For DOE/OSTI