LANL TA-14 1997

Department of Energy
Albuquerque Operations Office
Los Alamos Area Office
Los Alamos, New Mexico 87544

MAR 4 1997

Mr. Filiberto Dominguez
Air Pollution Control Bureau
New Mexico Environment Department
2048 Galisteo Street
Santa Fe, NM 87505

Dear Mr. Dominguez:

Enclosed for your approval is an application for open burning at Technical Area (TA) 14. Open burning is conducted at this area of the Los Alamos National Laboratory in order to diminish the safety risks associated with high explosives contaminated waste generated.

The application request is for a single burn scheduled for early March. Approval to conduct open burns at TA-14 is included in the five (5) year permit application being prepared for submittal to your office. As you are aware, open burning is allowed only when approved by the State of New Mexico as specified under Title 20, Chapter 2, Part 60 of the New Mexico Administrative Code. The enclosed application was prepared to satisfy the information requirements specified under this regulation.

If you have any questions concerning this permit application, please contact Steve Fong of my staff at (505) 665-5534.

Sincerely,

Mathew P. Johansen, P.E.
Acting Assistant Area Manager
Office of Environment and Projects

LAAMEP:9SF-094

Enclosure

cc w/enclosure:
S. Fong, LAAMEP, LAAO
E. Christie, LAAMEP, LAAO
L. Maez, ESH-17, LANL, MS-J978

3851

STATE OF NEW MEXICO
Environment
Department

PERMIT NO. AQB 97 1[illegible]
(AQB assigned)

NEW MEXICO ENVIRONMENT DEPARTMENT/AIR QUALITY BUREAU PERMIT APPLICATION AND REPORTING OF OPEN BURNING FOR PRESCRIBED/PRESCRIBED NATURAL FIRE AREAS

PERMITTEE: USDA___ USDI___ BLM___ MILITARY___ DOE X PRIVATE___ OTHER___

ADMINISTRATIVE UNIT: Technical Area 14 COUNTY: Los Alamos

CONTACT: Steve Fong/Leland Maez PHONE: 665-5534/665-1240

NAME OF BURN: Burn Cage LOCATION: Los Alamos National Laboratory
(Township, Range, Section)

PROPOSED ACREAGE See Attach. FUEL LOADING DETERMINATION METHOD See attachment

TYPE OF FUEL See attachment TONS/ACRE See attachment

Is burn likely to impact a smoke sensitive area? Yes___ No X
If yes, please attach a map of smoke sensitive areas (Include distance and direction).

Smoke sensitive areas include: Class I areas as well as other scenic and important views, urban and rural population centers, hospitals, nursing homes, schools, transportation facilities such as roads, highways, and airports, recreational areas, and other locations that may be sensitive to smoke impacts for health, safety, and/or aesthetic reasons.

Signed [illegible] Date 3/4/97
Name and Title
Joseph Vozella, Asst. Area Manager, Office of Environment & Projects

Submit to: New Mexico Environment Department, Air Quality Bureau
2048 Galisteo
Santa Fe, NM 87505

This application has been received by the New Mexico Environment Department and is
APPROVED X **DENIED** ___ **for the following reasons:**
AS PER 20 NMAC 2.60, SUBSECTION H3

This permit is approved for the following dates: 3/5/97 - 12/31/97
and is subject to the conditions set forth in 20 NMAC 2.60 and the following conditions:
RESTRICT IGNITION TO DAYS W/ GOOD DISPERSION TO BETTER DILUTE SMOKE

The Department reserves the right to cancel this permit at any time if the public interest so warrants it. The holder of this permit is therefore cautioned and charged that he/she, and he/she alone, assumes full responsibility to exercise the utmost care and judgement before igniting any prescribed fires. The Environment Department hereby disclaims any and all liability of itself or it's agents that might be incurred by petitioner's acts.

Signed [illegible] Date 3/5/97
Name and Title

NMED 8/96 White - Applicant; Canary - Applicant Main Office; Pink - Air Quality Bureau;

ATTACHMENT A

LOS ALAMOS NATIONAL LABORATORY APPLICATION FOR OPEN-BURNING PERMIT IN TECHNICAL AREA 14, BURN CAGE

DATES BURNING REQUESTED:

A single burn scheduled for either March 4th or 5th is requested in order to mitigate the safety hazards posed by high explosive (HE) contaminated burnable waste. This burn is required to keep the HE waste from accumulating to dangerous levels. Safety and storage requirements dictate that waste burning must occur every 90 days as needed.

EXACT LOCATION AND DIRECTION TO SITE:

The burn will be conducted within Los Alamos National Laboratory boundaries at Technical Area 14, in the burn cage located near mound 3, just south of the Control Building (Q-23), and south of the magazine storage building (Q-22) (Attachment B). The site known as Q-Site East can be accessed by properly cleared or escorted personnel via a paved road off R-Site Road. However, the road is not accessible to the public and is administratively controlled.

TYPE AND QUANTITY OF MATERIALS TO BE BURNED:

The burn contains a maximum of 50 pounds of HE contaminated combustible waste placed inside the bottom grill of the burn cage. Each burn requires approximately a 1/2 gallon of excelsior or non-metal and non-halogen containing volatile organic compound to be used as a starter fluid. The starter fluid is placed in the bottom section of the burn cage or sprinkled over the HE-contaminated waste to aid in ignition and combustion of the waste. The waste consists of small amounts of HE, rags, paper, sample containers, Kimwipes, toothpicks, and other processing and clean-up waste.

METHOD OF IGNITION AND HOW BURNING WILL BE MAINTAINED AND CONTROLLED:

The Standard Operating Procedure (SOP) that will be followed during the burn is attached (Attachment C). It covers the hazards involved and precautions to be taken during the burn setup, method of ignition, and the post burn observation period. The SOP also covers unburnable material inspection procedures, receiving and placement for the burn, and disposal of the flashed material. The ignition method is a remotely operated electric match.

WHY IS BURNING NECESSARY:

The burning is necessary to mitigate the hazards associated with HE contaminated material generated during testing and operations of new HE having unknown properties and characteristics. Open burning is very effective in eliminating HE contamination of burnable waste so the safety concerns associated with burial disposal can be minimized.

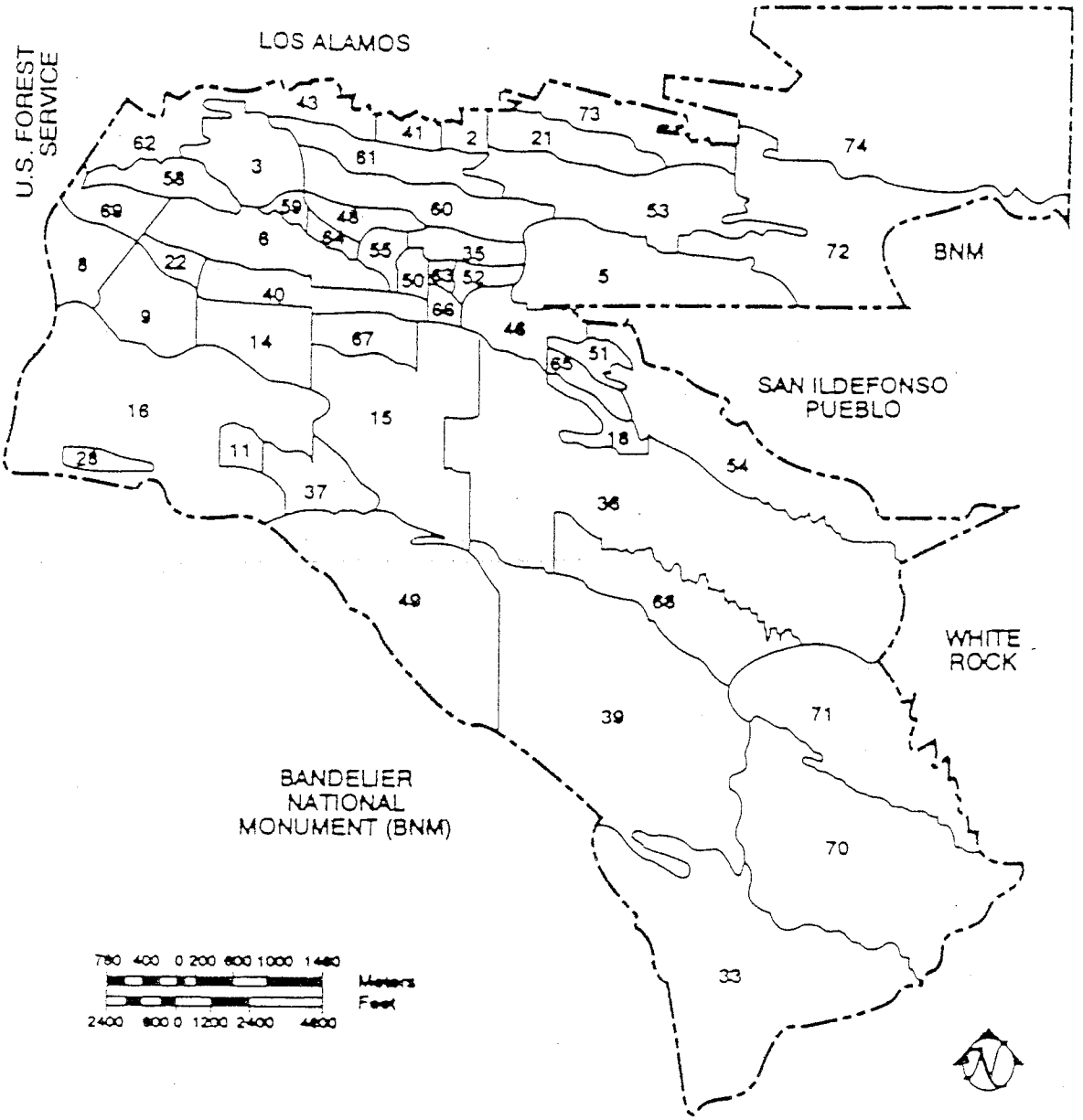
ALTERNATIVES TO BURNING AND REASONS WHY ALTERNATIVES ARE NOT FEASIBLE:

There are two alternatives to open burning. First, the direct burial of HE contaminated material is possible. However, this practice is contrary to the Laboratory's policy not to transport or move material resulting from any process associated with high explosives for safety reasons. For HE contaminated waste generated during testing and operations of new HE, this policy prevents accidents which might occur from the presence of HE residue remaining on the burnable materials. While this scenario is unlikely, there is a finite probability of its occurrence.

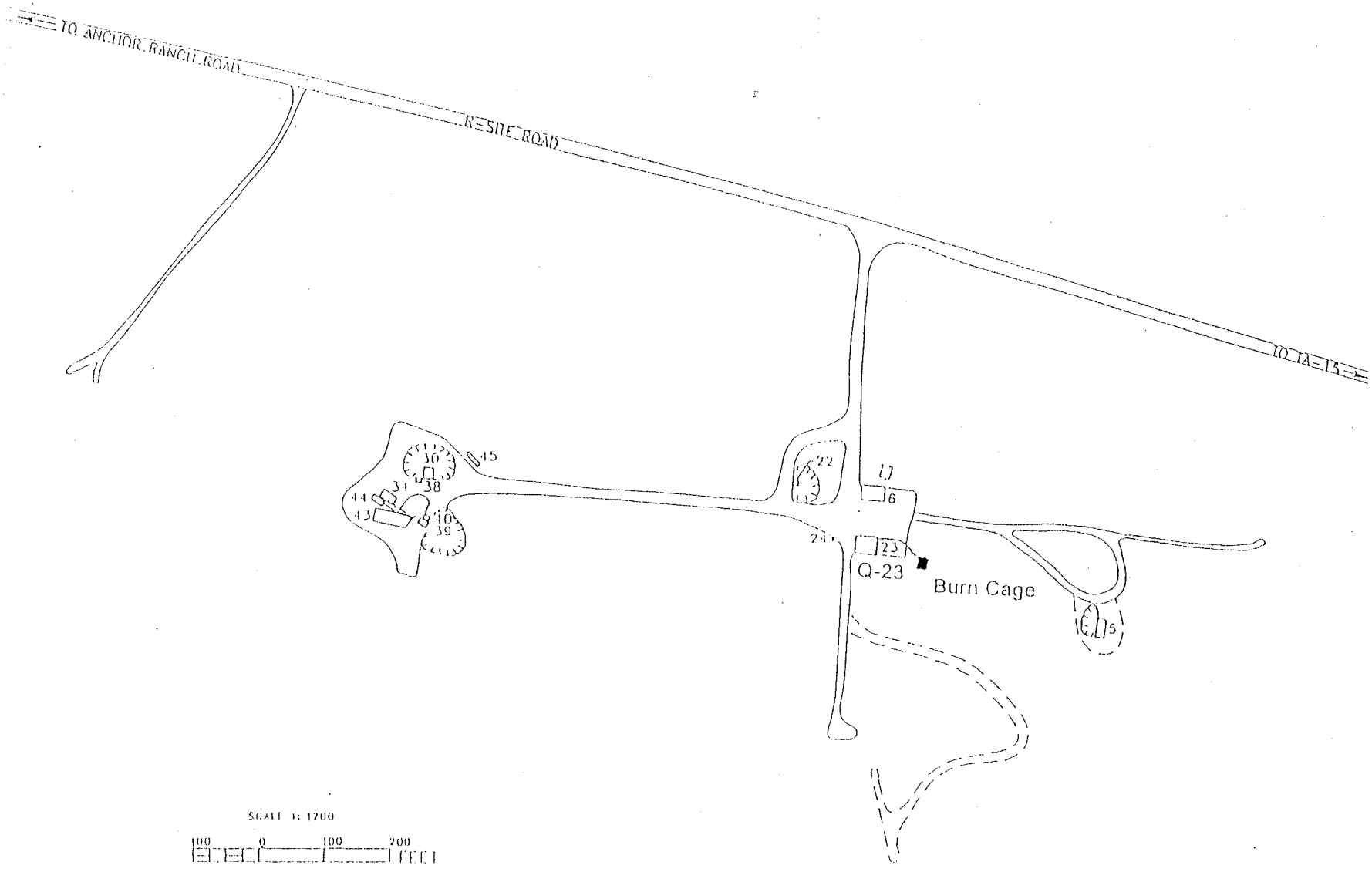
The second option would be to thermally treat the waste material in a thermal treatment oven or an incinerator. Due to the possibility of detonation at high temperatures occurring from contamination on the waste as well as some of the potentially explosive solvents, the treatment unit would have to be constructed of special materials.

Emission estimates and impacts are presented in attachment D.

ATTACHMENT B


LOS ALAMOS
U.S. FOREST SERVICE
BNM
SAN ILDEFONSO PUEBLO
WHITE ROCK
BANDELIER NATIONAL MONUMENT (BNM)
Meters
Feet

Technical Area 14



ATTACHMENT C

M-1

STANDARD OPERATING PROCEDURE

FOR

DESTRUCTION OF
HE-CONTAMINATED WASTE AND HE WASTE

6.1.5

Prepared by: _____ Date: 5/7/93
J. R. Stine, M-1

Approved by: _____ Date: 5/7/93
John C. Dallman, M-1 Group Leader

Approved by: _____ Date: _____
M-DO

Approved by: _____ Date: _____
HS-5

Final Approval: _____ Date: _____
C. B. Bieri, Group M-1 ES&H Officer

This SOP has been approved by M-1 and M-DO. While we await final review from HS and other groups as determined by HS, we are using this SOP as written. If more than 30 days have elapsed without action by reviewing Groups outside M Division, this SOP will be regarded by the M-1 Group Office as having the full force of complete and unqualified endorsement.

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1.0 INTRODUCTION

Group M-1 does tests and operations on new high-explosives that have unknown properties and characteristics. These operations generate waste that cannot be sent to WX-3 for disposal because of its uncharacterized nature or experimental history. These wastes are destroyed at Q-Site East by either burning or detonation.

2.0 PURPOSE

The purpose of this operation is to safely destroy HE waste and HE-contaminated waste originating in Group M-1. This SOP is closely tied to M-1:SOP 6.1.

3.0 SCOPE

This SOP applies to all M-1 personnel who perform the burning and detonation operations. These operations shall only be performed by Group M-1 personnel at Technical Area (TA) 14 (Q-site), Building 23 and the adjacent firing area.

4.0 DEFINITIONS

HE-Contaminated Waste:	Materials such as rags; paper; sample containers; Kimwipes; toothpicks; other process and clean-up waste.
HE Waste:	Damaged or suspect devices, explosives that have undergone severe testing, experimental explosives, explosives of temporary interest, newly synthesized compounds, new mixtures, and some salvage explosives.

5.0 RESPONSIBILITIES

5.1 Group Leader

- Ensures that the necessary policies, procedures, equipment, expertise (training), and manpower are available for this operation and delegates the responsibility for implementation of details to a Line Supervisor.

5.2 Line Supervisor

- Implements the details for safely performing these operations.
- Chooses, along with the Group Leader, the Firing Site Leader.

5.3 Firing Site Leader

- Has primary responsibility for safe operations.
- Supervises routine burning and detonation operations.
- Trains operators.

6.1.2 Detonation Operation

HE waste shall be destroyed by detonation on Mound 3.

6.1.3 Weight Limitations

Weight limitations are as follows.

Operation	Weight Limitation
Burning	50 lb of combustibles in each burn
Detonation	10 lb per shot

6.2 Personnel Limits

The personnel limits in M-1:SOP 6.1 shall be followed for this operation.

6.3 Transportation

The requirements for transporting HE-contaminated waste and small samples of HE waste for burning and detonation are listed below.

- Waste shall be transported to TA-14 (Q-Site) in accordance with M-1:SOP 1.9 for on-site transportation.
- No quantity greater than that which can be disposed of in a single day shall be transported to Q-Site.
- Operators will be told where HE waste is stored.

6.4 Storage

The following storage precautions shall be taken for materials to be burned and to be detonated:

- HE-contaminated wastes are stored in Magazine AE-208A at TA-9 while awaiting destruction at Q-Site. The waste will be labeled with its contents by the generator and labeled "Hazardous Waste" by the Waste Management Coordinator.
- At Q-Site, the explosive-contaminated waste will be kept in Room 104 of Building 23 while "in process."

7.2 Burning Operation

Follow the steps below for destroying HE-contaminated waste.

Step	Action
1	Short the end of the detonator cable.
2	Attach one or two ignitors in parallel to the firing cable and place them in the fuel space.
3	Sprinkle fuel on the HE-contaminated waste to enhance destruction of the waste and aid in ignition. Note: Use only volatile hydrocarbons, such as acetone, toluene, fuel oil, hexane, as a fuel. **CAUTION** DO NOT use any material that contains metals or halogens in its molecular composition. If in doubt, check with the experimenter in charge of Q-Site.
4	Cover the top of the burn cage with the wire mesh provided to minimize the escape of burning particles.
5	Fire the ignitors using the firing control unit in Room 101 of Building Q-23 (see M-1:SOP 6.1). Note: The siren will go through its normal sequence, but the Firing Supervisor may turn the siren off after determining that the burn is progressing satisfactorily.
6	• Wait for at least 10 minutes after visible flaming has stopped and • Then sound the "all-clear" signal. Note: If there is still a considerable amount of smoke, the Firing Site Leader must use his judgment about delaying the all-clear signal.
7	In the event of a misfire, do not approach the area until at least 10 minutes have elapsed without any evidence of flames or smoke in the burn cage.
8	DO NOT use the burn cage for another burn operation for 24 hours.
9	After 24 hours or more, remove the ashes and place in the satellite storage outside Building 23.
10	Cover the burn cage with a tarp.

7.4 Disposing of Waste

Waste generated from these operations shall be packaged and disposed of according to M-1:SOP 1.5. Waste minimization will be handled according to the M-Division Operations Manual.

7.5 Emergency Procedures

In the event of an emergency situation, the Building Emergency Plan (BEP)/ Site Emergency Plan (SEP) shall be followed. The BEP/SEP shall be available in Building Q-23 and the operators shall be familiar with its contents.

8.0 REQUIRED RECORDS

- M-1:SOP 6.1
- Completed and signed Shot Sheet (for detonation or burning)
- M-1 Q-Site Check List, Burning of HE-Contaminated Waste

9.0 REFERENCES

- DOE Explosives Safety Manual
- Los Alamos Environment, Safety, and Health Manual
- M-Division Operation Manual
- M-1:SOP 1.5, Disposal of Hazardous Materials
- M-1:SOP 1.9, Packaging and On-Site Transportation of Explosives
- M-1:SOP 6.1, Q-Site East (TA-14) Firing Operations

10.0 ATTACHMENTS

I. M-1 Q-Site Check List, Burning of HE-Contaminated Waste

II. Hazardous Waste Facility Permit

Attachment I

M-1 Q-Site Check List
Burning of HE-Contaminated Waste

Requester _____ Date Burned _____

Charge Code _____ Shot No. _____

This checklist is intended for use as a safety supplement to M-1:SOP 6.1.5 "Destruction of HE-Contaminated Waste and Waste HE." All Q-Site users must be familiar with Group M-1 SOPs 6.1 and 6.1.5. This checklist should be referred to by the Firing Supervisor subsequent to burning in the burn cage and prior to final arming. In the event of a misfire follow the checklist on the other side of this page.

OK	N/A	
☐	☐	1) Secure and clear area.
☐	☐	2) Ensure burn cage is clean.
☐	☐	3) Open all glass and plastic containers.
☐	☐	4) Place containers to be burned on grate.
☐	☐	5) Place fuel material in bottom of burn cage.
☐	☐	6) Short end of detonator cable.
☐	☐	7) Attach ignitors to detonator cable and place igniters in fuel material.
☐	☐	8) Sprinkle fuel on waste material.
☐	☐	9) Cover top of burn cage with wire mesh.
☐	☐	10) Connect detonator cable to CDU.
☐	☐	11) Start firing sequence.
☐	☐	12) Fire ignitors.
☐	☐	13) Observe burning.
☐	☐	14) Turn off siren (do NOT sound "all-clear").
☐	☐	15) Wait 10 min. after flame has stopped and sound "all-clear."
☐	☐	16) Another batch cannot be burned until 24 hours has elapsed.
☐	☐	17) Clean up ashes (after 24 hours) and place in satellite storage outside TA-23.
☐	☐	18) Cover burn cage with tarp.

Signature _____ Date _____
Firing Supervisor

FORM DATE 8/7/91 Approved By: _____ Date: _____

Attachment II

Hazardous Waste Facility Permit

PERMITTEE: U.S. Department of Energy
University of California Regents
ID NUMBER: NM0890010515

LOCATION: Los Alamos National Laboratory,
Los Alamos, NM 87545
PERMIT NUMBER:
NM 0890010515-1

Pursuant to the Solid Waste Disposal Act, as amended by the Resource Conservation and Recovery Act (RCRA), as amended (42 U.S.C. 6901, et seq.), and the New Mexico Hazardous Waste Act (§§ 74-4-1 et seq. NMSA 1978), a permit is issued to the U.S. Department of Energy's Los Alamos Area Office and the University of California Regents, doing business as Los Alamos National Laboratory, (hereafter called the Permittee) to operate a hazardous waste incinerator, container storage and tank treatment and storage facility at the location stated above.

The Permittee must comply with all the terms and conditions of this permit. This permit consists of the conditions contained herein including the attachments. Applicable provisions of regulations cited are those which are in effect on the effective date of this permit, New Mexico Hazardous Waste Management Regulations (HWMR-5, as amended 1989). This permit shall become effective in accordance with HWMR-5, Part IX, sections 902.F. and 902.G. and shall run for a period of ten years.

This permit is based on the provisions of HWMR-5. This permit is also based on the assumption that all information contained in the permit application is accurate and that the facility will be operated as specified in the application. The permit application consists of information submitted on March 27, 1986; revised on November 13, 1987 and November 25, 1987; and supplemented on November 8, 1988 and through numerous technical discussions.

Any inaccuracies found in the information may be grounds for the termination or modification of this permit and potential enforcement action.

Signed this 8th day of November, 1989

by _____

Richard Mitzelfelt, Director, H.M.E.I.D.

New Mexico
Health and Environment Department
Environmental Improvement Division

ATTACHMENT D

TECHNICAL APPROACH TO ESTIMATING EMISSIONS AND THE AIR QUALITY IMPACTS FROM THE OPEN BURNING OF HIGH EXPLOSIVES CONTAMINATED WASTE CONDUCTED AT TECHNICAL AREA 14

Air emissions resulting from the combustion of high explosives (HE) contaminated waste consist primarily of carbon monoxide (CO), oxides of nitrogen (NOx), particulate matter (PM), volatile organic compounds (VOC's), sulfur dioxide (SO_2), and heavy metals such as lead (Pb). Detailed emission estimates for wood, paper, and plastics were performed for this analysis using AP-42 emission factors developed by the Environmental Protection Agency (EPA) found in the July 1995, Version 4.0 of EPA's Air Chief; available on CD ROM. In addition, emission estimates for the combustion of solvents were performed using emission factors and equations presented in the document titled "Prediction of Fire Properties of Fuels," A. Tewarson, Factory Mutual Research Corporation, 1986 (Attachment E). Emission estimates for the combustion of HE were performed using emission factors compiled from data provided in the documents titled: "Emissions from the Open Burning or Detonation of High Explosives," R.V. Carter, U.S. Army Environmental Hygiene Agency, 1978; "Air Quality Impact Analysis, Open Burning of Explosives," Department of Energy, Pantex Plant, Amarillo, Texas, Radian Corp., 1990; "Lawrence Livermore National Laboratory (LLNL) Explosives Handbook Properties of Chemical Explosives and Explosive Simulants," B. M. Dobratz, 1981. Table 1 shows the typical profile of the constants of a burn as well as the emission factors from the sources described above.

TABLE 1. BURN CONSTITUENTS AND ASSOCIATED EMISSION FACTORS

Waste Type	Amount Burned	Emission Factors (lb/lb of material burned)							
		CO	NOx	VOC	PM	SO_2	HF	HCl	Pb
Wood/ Cardboard	10 lb	0.13	0.001	0.11	0.02	0.001	N/A	N/A	1E-07
Plastics/ Paper	30 lb	0.04	0.003	0.02	0.01	0.001	0.0001	0.004	N/A
HE	2 lb	0.05	0.13	0.005	0.27	N/A	0.050	0.028	N/A
Solvents	8 lb (≈ 1 gal)	0.01	N/A	0.02	0.04	0.05	N/A	N/A	1E-06
Emission Totals (lbs)	**50 lb**	**2.66**	**0.30**	**1.86**	**1.16**	**0.44**	**0.07**	**0.16**	**9E-06**

HE Contaminated Waste Solvent Mixtures

Approximately one gallon of HE contaminated dilute solvents generated during HE processing operations at LANL are included in the waste burn at TA-14. The average make-up of the dilute solvent solution is 30% methanol, 25% water, 20% acetonitrile, 20% tetrahydrofuran, 5% of any the solvents in Table 2. Combustion emissions were estimated using emission factors and equations from A. Tewarson, Prediction of Fire Properties of Fuels, Factory Mutual Research Corporation, 1985. Table 2 gives the chemical properties and assumptions required for the emission calculations. Emission estimates from solvent burning are shown above in Table 1.

TABLE 2. CHEMICAL PROPERTIES OF HE CONTAMINATED WASTE SOLVENTS

SOLVENT TYPE	MOLECULAR WEIGHT (g/mole)	DENSITY (g/ml)	NUMBER OF CARBONS	ASSUMPTIONS USED FOR CALCULATIONS
methanol	32	0.7914	1	experimental data available
acetonitrile	41	0.7868	2	C_2 linear alkanes
tetrahydrofuran	72	0.8888	4	C_3-C_6 linear ketones
methyl ethyl ketone	72	0.8054	4	C_3-C_6 linear ketones
butyl acetate	116	0.8825	6	C_5-C_{10} acetate
ethyl acetate	88	0.9003	4	C_4 acetate
toluene	92	0.8669	7	experimental data available
ethanol	46	0.7893	2	experimental data available
acetone	58	0.7899	3	experimental data available
cyclohexane	84	0.7785	6	C_5 -C_{10} cyclo alkane

High Explosives (HE) Waste

Waste HE, generated during HE processing, can consist of a number of different types of HE and associated binders. Table 3 gives a representative list of the HE waste composition found in process waste burned as well as amount of combustion products formed.

TABLE 3. EMISSIONS FROM THE OPEN BURNING OF HIGH EXPLOSIVES

High Explosives, Propellants, and Binders	Composition Fraction	Quantity Burned (lb/burn)	Combustion Products (lb)			
			CO	NOx	VOC	PM
TATB[1,2]	0.21	0.42	1.09E-02	2.92E-02	1.93E-04	8.17E-02
NTO[1,2]	0.18	0.36	1.01E-02	2.70E-02	1.80E-04	7.56E-02
Pyroxylin[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
Comp B[1,2]	0.04	0.08	2.00E-04	1.48E-03	N/A	N/A
LAX 112[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
RDX[1,2]	0.04	0.08	2.09E-04	1.50E-03	4.17E-03	N/A
DNT[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
Nitroguanidine[1,2]	0.04	0.08	2.22E-04	1.50E-03	N/A	2.34E-03
HMX[1,2]	0.04	0.08	2.22E-04	1.50E-03	N/A	2.34E-03
PETN[1,2]	0.04	0.08	2.00E-04	1.48E-03	N/A	N/A
TNT[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
HNS[1,2]	0.04	0.08	2.18E-04	1.15E-03	1.58E-04	6.48E-03
Barium nitrate[3,4]	0.01	0.02	N/A	7.00E-03	N/A	N/A
Cyanuric acid[3,4]	0.01	0.02	2.20E-03	1.76E-02	N/A	1.76E-02
Pentek[3,4]	0.01	0.02	2.20E-03	1.76E-02	N/A	1.76E-02
Exxon461[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
KFE[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
Polystyrene[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
Estane[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
Viton[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
BDNPA-F[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
DBP[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
DOP[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
CEF[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
TOTAL	**1**	**2**	**5.06E-02**	**1.31E-01**	**4.86E-03**	**2.71E-01**

1 Emission factors from Roy V. Carter (June 1978), Emissions from the Open Burning and Detonation of Explosives.

2 Emission factors from U.S. Environmental Protection Agency (June 1995), AP-42 Air Pollution Emission Factors.

3 Emission factors from Radian Corp. (July 1990), Air Quality Impact Analysis, Open Burning of Explosives, Department of Energy, Pantex Plant, Amarillo, Texas.

4 Emission factors based on chemical structures from B. M. Dobratz (March 1981), LLNL Explosives Handbook Properties of Chemical Explosives and Explosive Simulants.

Air Quality Impact Modeling

Air emissions from the open burning of HE contaminated waste at TA-14 are regulated under National and New Mexico Ambient Air Quality Standards. Air emissions from this operation include criteria pollutants such as carbon monoxide (CO), oxides of nitrogen (NOx), particulate matter (PM), sulfur dioxide (SO_2), volatile organic compounds (VOC's), and lead (Pb). In addition, some hazardous air pollutants such as hydrogen chloride (HCl) and hydrogen fluoride (HF) are emitted as a result of combustion of some binders used to form HE. Impacts from operations of this type* must meet ambient air standards for all criteria pollutants. Compliance with the ambient air quality standards was determined using the SCREEN 3 air emissions dispersion model.

The SCREEN 3 model was developed and approved by the Environmental Protection Agency (EPA) as a screening procedure for estimating air quality impacts of stationary sources. SCREEN 3 is a conservative model which uses worst case meteorological data to determine emission impacts. Input parameters supplied for this analysis included: a heat release rate of 15,748 cal/sec; a one hour burn duration; a 2.5 m/sec wind speed; and a one meter source height using a flare source type. Emission impacts are shown in Table 4 for the maximum impact (61 meters) and for the two nearest off-site locations, Pajarito Road 2,042 meters to the north/northeast and State Road 4 bordering Bandelier National Monument 2,286 meters to the south/southeast. The impacts are shown to be will below the ambient standards at all affected locations.

TABLE 4. AIR QUALITY IMPACTS FROM HE PROCESS WASTE BURNING

CHEMICAL	MODELING PARAMETERS	AMBIENT AIR QUALITY STANDARD			AIR CONCENTRATION AT: 61 M (Max.)	2042 M (Pajarito Rd.)	2286 M (SR 4)
CO	D Stability	8-hour average	0.5 mg/m³	(8.7 ppm)	0.53 ppm	3.8E-03 ppm	3.2E-03 ppm
		1-hour average	2.0 mg/m³	(13.1 ppm)	0.76 ppm	5.5E-03 ppm	4.6E-03 ppm
NOx		24-hour average	5.0 μg/m³	(0.1 ppm)	1.4E-02 ppm	1.0E-04 ppm	8.6E-05 ppm
		Annual arithmetic average	1.0 μg/m³	(0.05 ppm)	2.9E-03 ppm	2.1E-05 ppm	1.7E-05 ppm
PM	2.5 meters/sec. wind speed	24-hour average	150 μg/m³		136.6 μg/m³	1.0 μg/m³	0.8 μg/m³
		7-day average	110 μg/m³		19.5 μg/m³	0.1 μg/m³	0.1 μg/m³
		30-day average	90 μg/m³		4.6 μg/m³	3.3E-02 μg/m³	2.8E-02 μg/m³
		Annual geometric mean	60 μg/m³		27.3 μg/m³	0.2 μg/m³	0.2 μg/m³
SO_2	Heat Released 15,748 cal/sec.	24-hour average	5.0 μg/m³	(0.1 ppm)	0.03 ppm	2.1E-04 ppm	1.8E-04 ppm
		Annual arithmetic average	1.0 μg/m³	(0.02 ppm)	0.006 ppm	4.3E-05 ppm	3.6E-05 ppm
Lead		3-month average	0.03 μg/m³		8.9E-06 μg/m³	6.4E-08 μg/m³	5.4E-08 μg/m³
Photo Chemical Oxidant (VOC)		1-hour average		(0.06 ppm)	0.14 ppm	1.0E-03 ppm	8.0E-04 ppm

* HAP's emission standards are regulated under 20 NMAC 2.70 for the facility at 10 tons per year for any one HAP or 25 tons per year for any combination of HAP's. Subsequently, impacts for HCl and HF releases were not included in this modeling analysis.

ATTACHMENT E

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PREDICTION OF FIRE PROPERTIES OF FUELS

by

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Subject Categories

(3) Combustion and Practical Systems

(9) Fire

(18) Modeling and Scaling

For presentation at the Twenty-First International Symposium on Combustion, Technical University of Munich, West Germany, August 3-8, 1986

Factory Mutual Research

1151 Boston-Providence Turnpike
Norwood, Massachusetts 02062

RC86-TP-3

1. INTRODUCTION

Fire properties are defined as the parameters which characterize the combustion and pyrolysis behavior of fuels in fires[1]. In conjunction with fire models, fire properties are used to assess hazards presented by various types of fires and protection needs. A fundamental understanding of diffusion flames has always been found to be very useful in the prediction of fires. In this paper, an attempt has thus been made to use the understanding of the soot formation in diffusion flames to develop relationships for the prediction of fire properties.

The soot formation in diffusion flames has been of great interest because of the relationship with flame radiation and heat transfer, combustion efficiency, and emission of particulates and other chemical compounds some of which may be toxic and corrosive in nature.

In this study, we have used the concept of the smoke point height, L_s, which has been used by many investigators to describe the sooting tendency of fuels. L_s is defined as the height of an overventilated diffusion flame at which soot just begins to be released at the flame tip. The smaller the value of L_s, the greater the tendency to soot. Extensive data for L_s are available in the literature for liquid and gaseous fuels[2-8]. Many investigators find that L_s depends on the nature of chemical bonds and flame turbulence. It has been shown that L_s is related to flame temperature (flame convection)[6] and to flame radiation[9].

In order to use the literature data for L_s to develop predictions for fire properties, it was necessary to perform experiments in our flammability apparatus. In the experiments, simultaneous measurements were made for L_s and fire properties of fuels of known chemical structures and L_s values. In addition to gaseous and liquid fuels, solid fuels were used in the experiments.

The radiative component of the combustion efficiency, χ_R, is defined as

$$\chi_R = \chi_A - \chi_c \cdot \tag{7}$$

3. EXPERIMENTS

Experiments were performed in our apparatus, shown in Fig. 1[10]. For gaseous samples, a burner tube very similar to one in Ref. 9 was used. For liquid and solid samples, a 250 ml Pyrex Erlenmeyer flask with a 14/35 ground glass joint was used. The ground glass joint was attached to a 0.12-m long Pyrex glass tube with an internal diameter of 0.009 m to reduce the effects of temperature on L_s values. External heat flux was used for solid and low vapor pressure liquids; for high vapor pressure liquids, a heating mantle placed around the flask was used. The rate of generation of the fuel vapors and flame height were varied by varying either the external heat flux or the heating rate of the mantle.

L_s value was measured visually and for the measurement of fire properties, all the combustion products were captured along with air in the sampling duct of our apparatus. In the duct, measurements were made for the gas temperature, mass fractions of CO_2, CO, total gaseous hydrocarbons (CH), soot (S), and O_2, and $\dot{m}_T$. Measurements were also made for optical transmission through soot, but data have not been discussed in this paper. The generation rate of fuel vapors was measured by a load cell assembly.

In the experiments, data were recorded by a computer at a time interval of about one second. Data were averaged by the computer at the steady state, lasting for about 10 minutes. Each experiment was performed at least twice and the data were averaged. The accuracy of all the averaged experimental data is about ±2%.

All the experiments were performed under natural air flow conditions and thus represent overventilated fire conditions.

The relationship between f_{CO_2} and L_s is same as between χ_A and L_s as expected from Eq. (5) for overventilated fires.

Predictions of Fire Properties of Fuels

If it is assumed that the relationships given in Eqs. (8) to (13) are of general applicability, then it is possible to use the L_s values from the literature to predict χ_i and f_j values for many fuels. The literature values for L_s, however, cannot be used directly because of variations due to differences in the experimental conditions used by various investigators.[11] The following approach was thus taken in this study: 1) relationships between L_s values measured by us and reported in the literature, for selected fuels, were established separately for each investigator; 2) these relationships were then used to recalculate all other L values separately for each investigator; and 3) for fuels which were used by several investigators, the recalculated values of L_s were averaged. The recalculated values of L_s were then used in Eqs. (8) to (13) to predict the χ_i and f_j values. The predicted values of χ_i and f_j are listed in Table II. The detailed tabulation of the data is given in Ref. 12. Values of f_{others} in the table are calculated from the atom balance, i.e., $f_{others} = 1 - \Sigma f_j$.

5. DISCUSSION

Comparison Between the Predicted and Measured Values of Fire Properties

Table III lists the experimental and predicated data for some selected fire properties (f_{CO_2} or χ_A and f_S). A reasonable agreement can be noted between the predicted and measured values. Also our predictions for f_S and those of Pagni's[15], based on entirely different principles, are very similar, except for octane and polystyrene. The new measurements suggest that our older f_S value of 0.18 for polystyrene[17], referred in Ref. 15, appears to be somewhat higher.

and soot, in that order. Butadiene, which is at the top within the aliphatic fuels group, is expected to follow the above aromatic group of compounds.

Relationship Between the Generation Efficiencies of CO and CO_2

In combustion systems, the ratio of CO to CO_2 is used as an indicator of the burning efficiency of fuels. For fuels burning under overventilated conditions, the ratio will vary with the chemical structure of the fuels. For fuels with fixed chemical structure, the ratio will vary with ventilation.

For fuels with variable chemical structure, burning under overventilated conditions, the relationship between f_{CO} and f_{CO_2} can be predicted from Eqs. (10) and (11). The predicted relationship is shown by the solid line in Fig. 3. Experimental data obtained under variable ventilation conditions for wood cribs, heptane, and PMMA from Ref. (18) to (20) have also been included in Fig. 3. Data for enclosure fires of wood cribs with variable ventilation were averaged for similar f_{CO_2} values, and were restricted to the flaming fires only. Data in Fig. 3 indicate that as f_{CO_2} decreases, f_{CO} approaches an asymptotic limit, which is about 0.12 for wood, which is a char forming fuel, and about 0.08 for heptane and PMMA, which are non-char forming fuels.

The results in Fig. 3 indicate that, up to the asymptotic limit of f_{CO}, the relationship between f_{CO} and f_{CO_2} is expected to be the same for the combustion of fuels with: 1) fixed chemical structure and variable ventilation; and 2) variable chemical structure with overventilation. It may be possible to define the asymptotic limit for f_{CO} for underventilated fires of fuels based on their chemical structure.

Relationship Between the Generation Efficiencies of CO and Soot

Emissions of CO and soot from combustion systems are associated with reduced ventilation and/or involvement of fuels which burn inefficiently because of their chemical structures.

From Eqs. (3), (4), and (14),

$$\boxed{\dot{E}''_j = (f_j\ k_j / [\int_0^{T_v} c_p\ dT + H_v])\ (\dot{q}''_{fs} - \dot{q}''_{rr})\ ,} \tag{16}$$

where $\dot{E}''_j$ is the emission rate of a compound j per unit fuel surface area (kg/m^{2}s). In Eqs. (14), (15), and (16), $\int_0^{T_v} c_p\ dT + H_v$ is defined as heat of gasification of the fuel, L_g (kJ/kg). H_T values are known from the literature and k_j values can be calculated from the elemental composition of the fuel.

Heat of Gasification

L_g values can also be calculated from the literature values for c_p, T_v, and H_v[21], or can be measured. Within a generic group of fuels, L_g increases with the molecular weight of the fuel, primarily due to increase in T_v, and can be estimated for fuels of higher molecular weight. The measured value of L_g for PE is 1750 kJ/kg[17], and from the relationship between L_g and the molecular weight of alkenes, it can be estimated that the molecular weight of the oligomer produced by the vaporization of PE is about 0.601 kg/mole, which is reasonably close to a value of 0.692 kg/mole reported for the molecular weight of the PE oligomer in pyrolysis[22]. In a similar fashion, the molecular weight of PP oligomer is estimated to be 0.720 kg/mole.

From the values of L_g, H_T, k_j, and the data from Table II, emission rates can be calculated for the fuel vapors and the combustion products for defined values of $\dot{q}''_{fs} - \dot{q}''_{rr}$, for example, at the asymptotic limit of $\dot{q}''_{fs} - \dot{q}''_{rr}$, which is approximately constant for fuels with variable molecular weight within a generic group of fuels. Within the aliphatic fuels group, the asymptotic limit for $\dot{q}''_{fs} - \dot{q}''_{rr}$ is equal to 41 kW/m^2, with a variation of ± 15% (as derived from the data for polyoxymethylene, PMMA, heptane, polyethylene, and polypropylene[1,10,16,17]). The emission rates for heat, CO, and soot calculated in this fashion for alkanes and alkenes, as examples, are shown in Figs. 5 and 6, respectively. Experimental data for PE and PP are also included in Fig. 6. The emission rates decrease with increase in the molecular weight of the fuel, because of the increase of L_g due to increase of T_v.

NOMENCLATURE

C_p	specific heat (kJ/kg K)
$\dot{E}''$	emission rate per unit fuel surface area (kg/m^{2}s)
f_j	generation efficiency of compounds j or oxygen depletion efficiency (-)
$\dot{G}_f$	generation rate of fuel vapors (kg/s)
H_{CO}	heat of combustion of CO (kJ/kg)
H_T	net heat of complete combustion (kJ/kg)
H_v	heat of vaporization (kJ/kg)
k_j	maximum possible total (theoretical) yield of compound j or stoichiometric mass oxygen to fuel ratio (kg/kg)
L_g	heat of gasification of the fuel (kJ/kg)
L_s	smoke point height (m)
$\dot{m}_T$	total mass flow rate of combustion product-air mixture (kg/s)
$\dot{Q}_A$	actual heat release rate (kW)
$\dot{Q}_T$	total (theoretical) heat release rate (kW)
$\dot{q}''_{fs}$	flame heat to the surface of the fuel (kW/m^2)
$\dot{q}''_{rr}$	surface heat loss due to reradiation (kW/m^2)
ΔT	gas temperature above ambient (K)
T_v	vaporization temperature (K)
X_j	mass fraction of compound j (kg/kg)
Y_j	yield of compound j (kg/kg)
χ_A	combustion efficiency (-)
χ_C	convective component of combustion efficiency
χ_R	radiative component of combustion efficiency

Subscripts

f	fuel vapors
i	heat
j	chemical compound

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TABLE I

Experimental Data for Smoke Point Height and

Selected Fire Properties of Fuels

Fuel	L (m)	χ_A	χ_c	χ_R	f_{CO_2}	f_{CO}	f_{CH}	f_S
Methanol	N	0.97	0.83	0.14	0.97	0.001	0.001	N
Ethanol	0.225	0.97	0.74	0.23	0.97	0.001	0.001	0.021
Acetone	0.205	0.96	0.73	0.23	0.96	0.001	0.001	0.022
Pentane	0.155	0.94	0.65	0.29	0.94	0.002	0.001	N
Isopropanol	0.148	0.94	0.65	0.29	0.94	0.002	0.001	N
Hexane	0.125	0.93	0.63	0.30	0.93	0.004	0.002	N
Nylon	0.120	0.90	0.58	0.32	0.90	0.004	0.002	0.030
Ethylene	0.106	0.91	0.61	0.30	0.91	0.003	0.002	0.032
Heptane	0.110	0.93	0.61	0.32	0.93	0.004	0.003	0.032
PMMA	0.105	0.95	0.63	0.32	0.95	0.006	0.001	0.027
Cyclohexane	0.085	0.91	0.56	0.35	0.91	0.005	0.001	N
Isooctane	0.080	0.91	0.60	0.31	0.91	0.007	0.003	N
Polypropylene	0.050	0.89	0.52	0.37	0.89	0.015	0.003	0.050
Polyethylene	0.045	0.87	0.50	0.37	0.86	0.013	0.002	0.060
Propylene	0.029	0.81	0.41	0.40	0.81	0.011	0.006	0.064
Polystyrene	0.015	0.66	0.26	0.40	0.65	0.027	0.023	0.101
Toluene	0.005	0.68	0.28	0.40	0.68	0.030	0.023	0.190

N not measured

TABLE II

(continued)

Fuel	C atoms	X_A	X_C	X_R	f_{CO_2}	f_{CO} x100	f_{CH} x100	f_S x10	f_{others} x10
Butyrate	5 to 6	0.97	0.72	0.25	0.97	0.20	0.11	0.24	0.04
	7 to 8	0.93	0.63	0.30	0.93	0.31	0.15	0.30	0.35
Laurate, oxalate, malonate, lactate	4 to 14	0.97	0.71	0.26	0.97	0.22	0.11	0.24	0.03
C-H-N Structure									
Amines	4 to 12	0.90	0.57	0.33	0.90	0.43	0.21	0.36	0.58
C-H-S Structure									
Mercaptans and Sulfides	6 to 12	0.90	0.57	0.33	0.90	0.43	0.21	0.36	0.58
				Aromatic Fuels					
C-H Structure									
Arenes	6 to 21	0.71	0.30	0.41	0.70	3.80	1.58	1.32	1.14
Cyclic Arenes	10 to 12	0.76	0.36	0.40	0.75	1.96	0.85	0.89	1.32
PAH	9 to 12	0.68	0.27	0.41	0.68	5.20	2.13	1.59	0.88
polycyclic aromatic HC → 3or more rings									
C-H-O Structure									
Alcohols	7 to 8	0.71	0.30	0.41	0.71	3.49	1.46	1.25	1.16
Ketones	11	0.76	0.36	0.40	0.76	2.01	0.87	0.90	1.20
Aldehydes	7	0.75	0.35	0.40	0.75	2.26	0.97	0.97	1.21
Esters	9	0.76	0.36	0.40	0.76	1.96	0.85	0.89	1.22
C-H-N Structure									
Amines and Heterocylics	6 to 11	0.73	0.32	0.41	0.73	3.00	1.26	1.14	1.13
C-H-S Structure									
Mercaptans and Sulfides	6 to 8	0.67	0.26	0.41	0.67	6.18	2.50	1.76	0.67

N: not predicted

FIGURE CAPTIONS

Fig. 1 Flammability apparatus

Fig. 2 Combustion efficiency and its convective and radiative components as functions of smoke point height

Fig. 3 Relationship between the generation efficiencies of CO and CO_2. Solid line represents our predictions for fuels with variable chemical structures. Experimental data points connected by dashed lines are for variable ventilation conditions: O, enclosure fires of wood cribs, Ref. 18; ●, Heptane, Ref. 19; ■, wood cribs, Ref. 18; *, PMMA, Ref. 20.

Fig. 4 Relationship between the generation efficiencies of soot and CO. Solid line represents our predictions for fuels with variable chemical structures. Symbols connected by dashed lines represent experimental data for PMMA with variable ventilation conditions, Ref. 20.

Fig. 5 Estimated emission rates of heat, CO, and soot as functions of the molecular weight of alkanes for overventilated fires.

Fig. 6 Estimated emission rates of heat, CO, and soot as functions of molecular weight of alkenes for overventilated fires. Dark symbols represent experimental data for polyethylene and polypropylene.

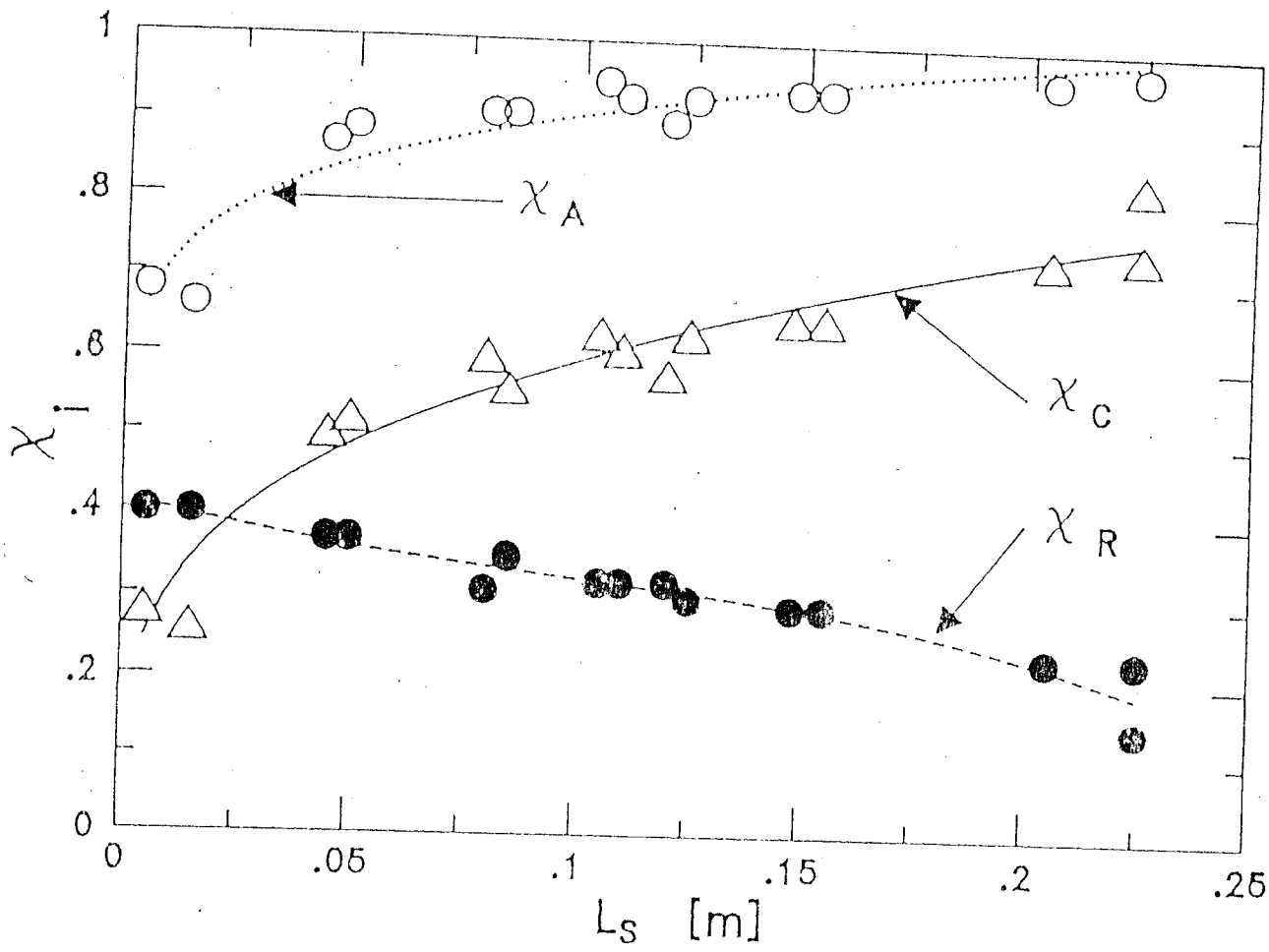


Fig. 2/ Rewarson

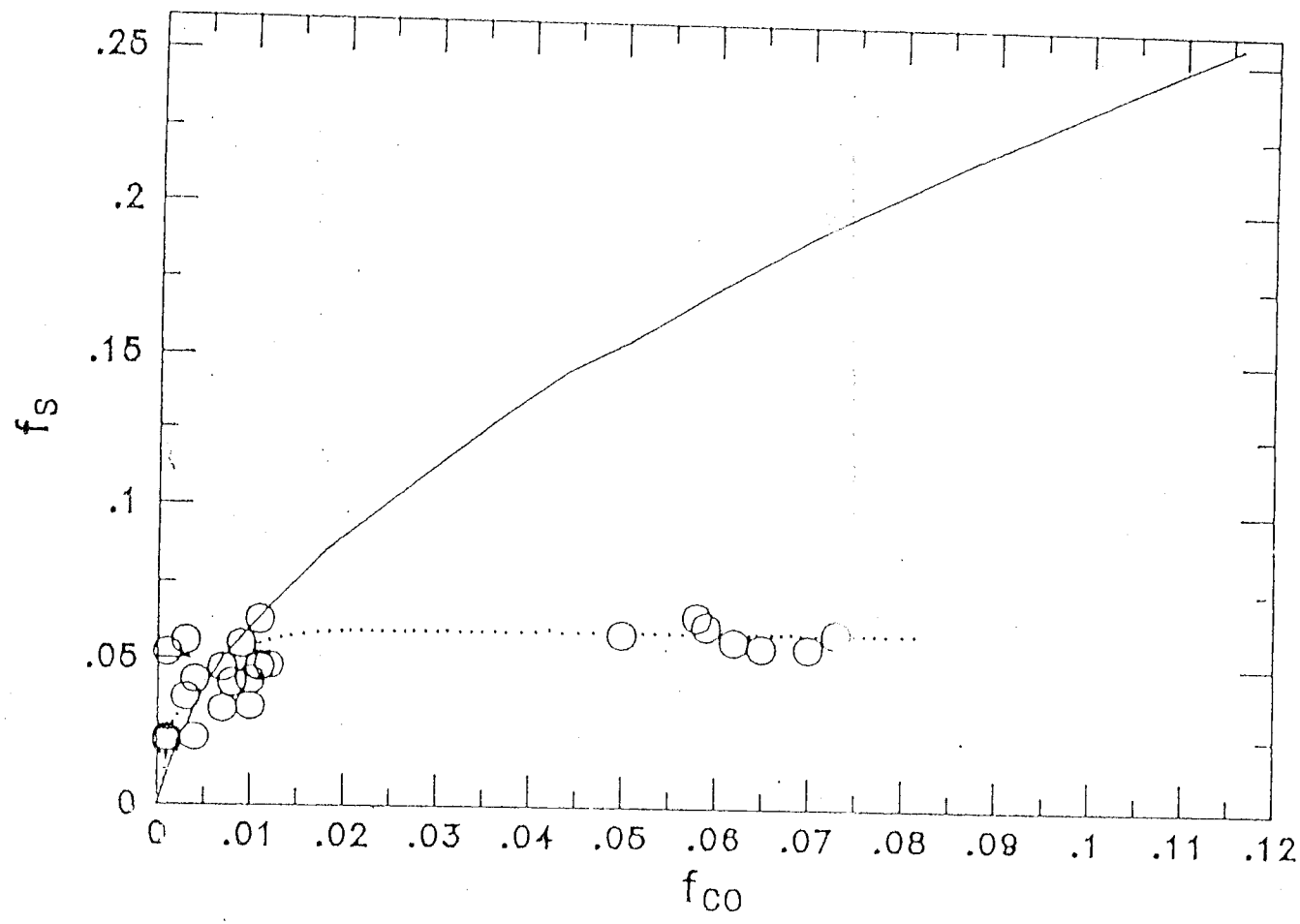


Fig. 4/ Tawarson

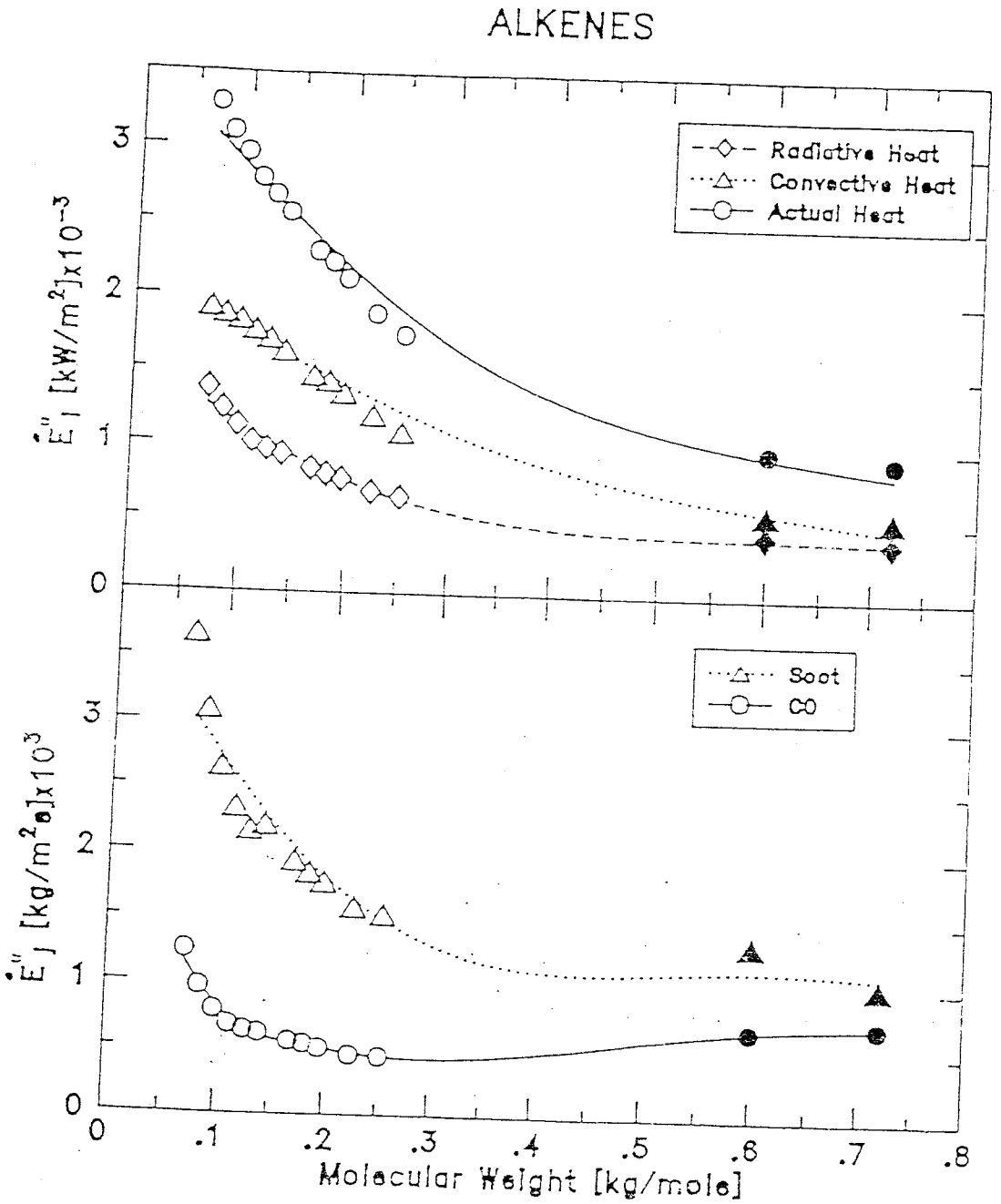


Fig. 6/ Tewarson

STATE OF NEW MEXICO
Environment
Department

PERMIT NO. _____
(AQB assigned)

NEW MEXICO ENVIRONMENT DEPARTMENT/AIR QUALITY BUREAU PERMIT APPLICATION AND REPORTING OF OPEN BURNING FOR PRESCRIBED/PRESCRIBED NATURAL FIRE AREAS

PERMITTEE: USDA___ USDI___ BLM___ MILITARY___ DOE X PRIVATE___ OTHER___

ADMINISTRATIVE UNIT: Technical Area 14 COUNTY: Los Alamos

CONTACT: Steve Fong/Leland Maez PHONE: 665-5534/665-1240

NAME OF BURN: Burn Cage LOCATION: Los Alamos National Laboratory
(Township, Range, Section)

PROPOSED ACREAGE See Attach. FUEL LOADING DETERMINATION METHOD See attachment

TYPE OF FUEL See attachment TONS/ACRE See attachment

Is burn likely to impact a smoke sensitive area? Yes___ No X
If yes, please attach a map of smoke sensitive areas (Include distance and direction).

Smoke sensitive areas include: Class I areas as well as other scenic and important views, urban and rural population centers, hospitals, nursing homes, schools, transportation facilities such as roads, highways, and airports, recreational areas, and other locations that may be sensitive to smoke impacts for health, safety, and/or aesthetic reasons.

Signed_____ Date_____
Name and Title
Joseph Vozella, Asst. Area Manager, Office of Environment & Projects

Submit to: New Mexico Environment Department, Air Quality Bureau
2048 Galisteo
Santa Fe, NM 87505

This application has been received by the New Mexico Environment Department and is
APPROVED ____ DENIED ____ for the following reasons:_____

This permit is approved for the following dates:_____
and is subject to the conditions set forth in 20 NMAC 2.60 and the following conditions:

The Department reserves the right to cancel this permit at any time if the public interest so warrants it. The holder of this permit is therefore cautioned and charged that he/she, and he/she alone, assumes full responsibility to exercise the utmost care and judgement before igniting any prescribed fires. The Environment Department hereby disclaims any and all liability of itself or it's agents that might be incurred by petitioner's acts.

Signed_____ Date_____
Name and Title

ATTACHMENT A

LOS ALAMOS NATIONAL LABORATORY APPLICATION FOR OPEN-BURNING PERMIT IN TECHNICAL AREA 14, BURN CAGE

DATES BURNING REQUESTED:

A single burn scheduled for either March 4th or 5th is requested in order to mitigate the safety hazards posed by high explosive (HE) contaminated burnable waste. This burn is required to keep the HE waste from accumulating to dangerous levels. Safety and storage requirements dictate that waste burning must occur every 90 days as needed.

EXACT LOCATION AND DIRECTION TO SITE:

The burn will be conducted within Los Alamos National Laboratory boundaries at Technical Area 14, in the burn cage located near mound 3, just south of the Control Building (Q-23), and south of the magazine storage building (Q-22) (Attachment B). The site known as Q-Site East can be accessed by properly cleared or escorted personnel via a paved road off R-Site Road. However, the road is not accessible to the public and is administratively controlled.

TYPE AND QUANTITY OF MATERIALS TO BE BURNED:

The burn contains a maximum of 50 pounds of HE contaminated combustible waste placed inside the bottom grill of the burn cage. Each burn requires approximately a 1/2 gallon of excelsior or non-metal and non-halogen containing volatile organic compound to be used as a starter fluid. The starter fluid is placed in the bottom section of the burn cage or sprinkled over the HE-contaminated waste to aid in ignition and combustion of the waste. The waste consists of small amounts of HE, rags, paper, sample containers, Kimwipes, toothpicks, and other processing and clean-up waste.

METHOD OF IGNITION AND HOW BURNING WILL BE MAINTAINED AND CONTROLLED:

The Standard Operating Procedure (SOP) that will be followed during the burn is attached (Attachment C). It covers the hazards involved and precautions to be taken during the burn setup, method of ignition, and the post burn observation period. The SOP also covers unburnable material inspection procedures, receiving and placement for the burn, and disposal of the flashed material. The ignition method is a remotely operated electric match.

WHY IS BURNING NECESSARY:

The burning is necessary to mitigate the hazards associated with HE contaminated material generated during testing and operations of new HE having unknown properties and characteristics. Open burning is very effective in eliminating HE contamination of burnable waste so the safety concerns associated with burial disposal can be minimized.

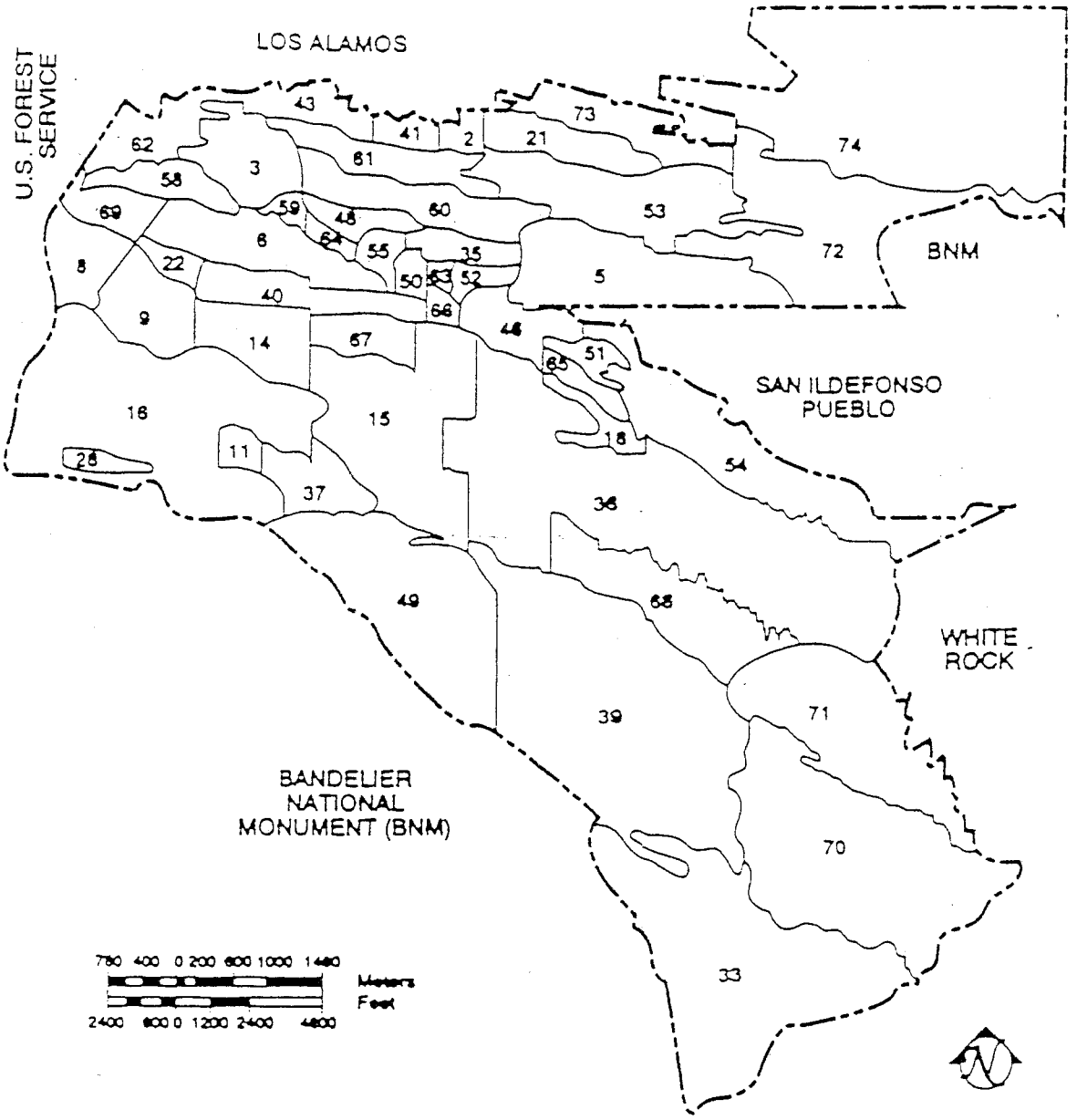
ALTERNATIVES TO BURNING AND REASONS WHY ALTERNATIVES ARE NOT FEASIBLE:

There are two alternatives to open burning. First, the direct burial of HE contaminated material is possible. However, this practice is contrary to the Laboratory's policy not to transport or move material resulting from any process associated with high explosives for safety reasons. For HE contaminated waste generated during testing and operations of new HE, this policy prevents accidents which might occur from the presence of HE residue remaining on the burnable materials. While this scenario is unlikely, there is a finite probability of its occurrence.

The second option would be to thermally treat the waste material in a thermal treatment oven or an incinerator. Due to the possibility of detonation at high temperatures occurring from contamination on the waste as well as some of the potentially explosive solvents, the treatment unit would have to be constructed of special materials.

Emission estimates and impacts are presented in attachment D.

ATTACHMENT B


LOS ALAMOS
U.S. FOREST SERVICE
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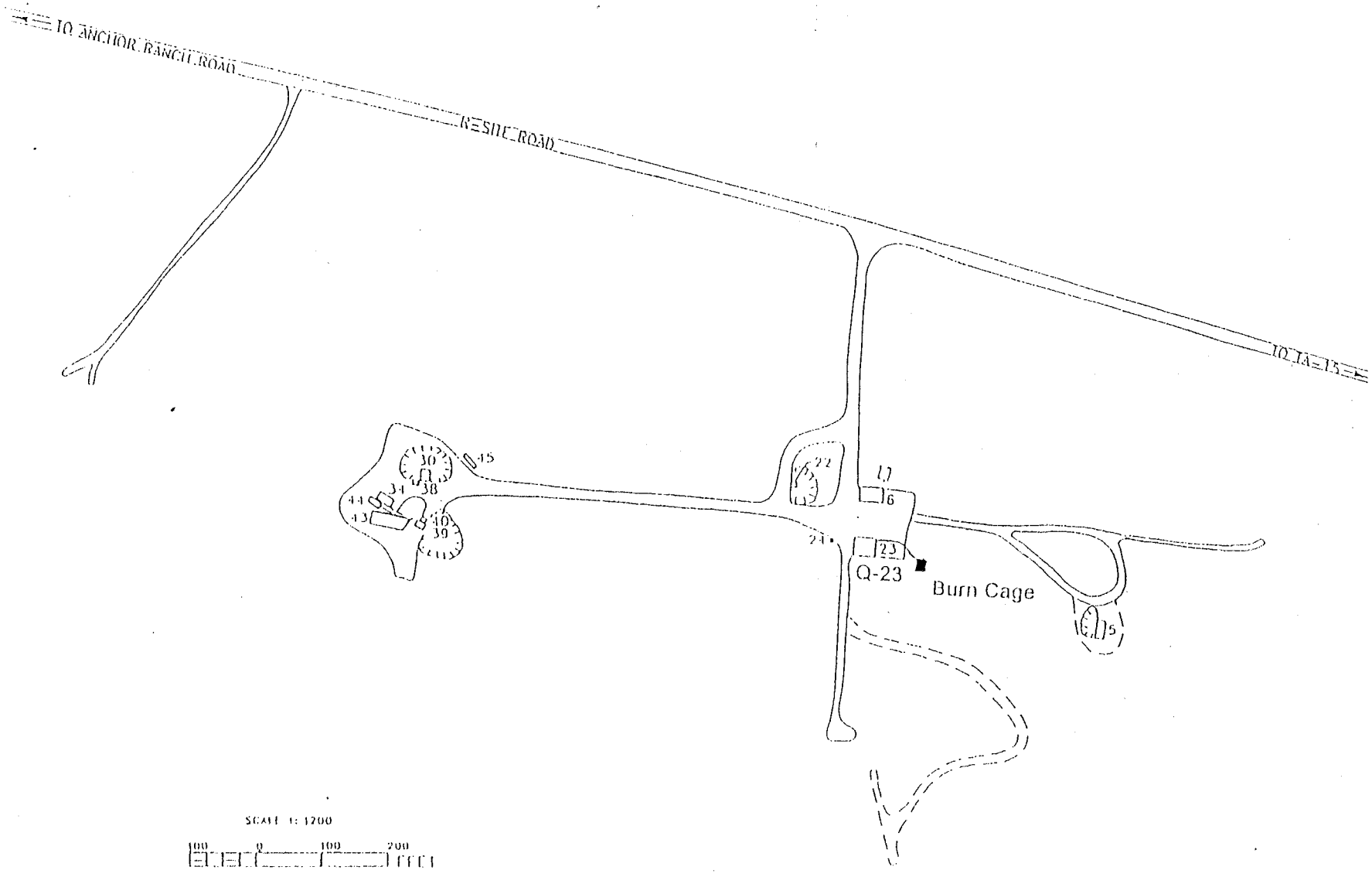
WHITE ROCK
BANDELIER NATIONAL MONUMENT (BNM)
Meters
Feet

Technical Area 14



ATTACHMENT C

M-1

STANDARD OPERATING PROCEDURE

FOR

DESTRUCTION OF
HE-CONTAMINATED WASTE AND HE WASTE

6.1.5

Prepared by: _____ Date: 5/7/93
J. R. Stine, M-1

Approved by: _____ Date: 5/7/93
John C. Dallman, M-1 Group Leader

Approved by: _____ Date: _____
M-DO

Approved by: _____ Date: _____
HS-5

Final Approval: _____ Date: _____
C. B. Bieri, Group M-1 ES&H Officer

This SOP has been approved by M-1 and M-DO. While we await final review from HS and other groups as determined by HS, we are using this SOP as written. If more than 30 days have elapsed without action by reviewing Groups outside M Division, this SOP will be regarded by the M-1 Group Office as having the full force of complete and unqualified endorsement.

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1.0 INTRODUCTION

Group M-1 does tests and operations on new high-explosives that have unknown properties and characteristics. These operations generate waste that cannot be sent to WX-3 for disposal because of its uncharacterized nature or experimental history. These wastes are destroyed at Q-Site East by either burning or detonation.

2.0 PURPOSE

The purpose of this operation is to safely destroy HE waste and HE-contaminated waste originating in Group M-1. This SOP is closely tied to M-1:SOP 6.1.

3.0 SCOPE

This SOP applies to all M-1 personnel who perform the burning and detonation operations. These operations shall only be performed by Group M-1 personnel at Technical Area (TA) 14 (Q-site), Building 23 and the adjacent firing area.

4.0 DEFINITIONS

HE-Contaminated Waste:	Materials such as rags; paper; sample containers; Kimwipes; toothpicks; other process and clean-up waste.
HE Waste:	Damaged or suspect devices, explosives that have undergone severe testing, experimental explosives, explosives of temporary interest, newly synthesized compounds, new mixtures, and some salvage explosives.

5.0 RESPONSIBILITIES

5.1 Group Leader

- Ensures that the necessary policies, procedures, equipment, expertise (training), and manpower are available for this operation and delegates the responsibility for implementation of details to a Line Supervisor.

5.2 Line Supervisor

- Implements the details for safely performing these operations.
- Chooses, along with the Group Leader, the Firing Site Leader.

5.3 Firing Site Leader

- Has primary responsibility for safe operations.
- Supervises routine burning and detonation operations.
- Trains operators.

6.1.2 Detonation Operation

HE waste shall be destroyed by detonation on Mound 3.

6.1.3 Weight Limitations

Weight limitations are as follows.

Operation	Weight Limitation
Burning	50 lb of combustibles in each burn
Detonation	10 lb per shot

6.2 Personnel Limits

The personnel limits in M-1:SOP 6.1 shall be followed for this operation.

6.3 Transportation

The requirements for transporting HE-contaminated waste and small samples of HE waste for burning and detonation are listed below.

- Waste shall be transported to TA-14 (Q-Site) in accordance with M-1:SOP 1.9 for on-site transportation.
- No quantity greater than that which can be disposed of in a single day shall be transported to Q-Site.
- Operators will be told where HE waste is stored.

6.4 Storage

The following storage precautions shall be taken for materials to be burned and to be detonated:

- HE-contaminated wastes are stored in Magazine AE-208A at TA-9 while awaiting destruction at Q-Site. The waste will be labeled with its contents by the generator and labeled "Hazardous Waste" by the Waste Management Coordinator.
- At Q-Site, the explosive-contaminated waste will be kept in Room 104 of Building 23 while "in process."

7.2 Burning Operation

Follow the steps below for destroying HE-contaminated waste.

Step	Action
1	Short the end of the detonator cable.
2	Attach one or two ignitors in parallel to the firing cable and place them in the fuel space.
3	Sprinkle fuel on the HE-contaminated waste to enhance destruction of the waste and aid in ignition. Note: Use only volatile hydrocarbons, such as acetone, toluene, fuel oil, hexane, as a fuel. **CAUTION** DO NOT use any material that contains metals or halogens in its molecular composition. If in doubt, check with the experimenter in charge of Q-Site.
4	Cover the top of the burn cage with the wire mesh provided to minimize the escape of burning particles.
5	Fire the ignitors using the firing control unit in Room 101 of Building Q-23 (see M-1:SOP 6.1). Note: The siren will go through its normal sequence, but the Firing Supervisor may turn the siren off after determining that the burn is progressing satisfactorily.
6	• Wait for at least 10 minutes after visible flaming has stopped and • Then sound the "all-clear" signal. Note: If there is still a considerable amount of smoke, the Firing Site Leader must use his judgment about delaying the all-clear signal.
7	In the event of a misfire, do not approach the area until at least 10 minutes have elapsed without any evidence of flames or smoke in the burn cage.
8	DO NOT use the burn cage for another burn operation for 24 hours.
9	After 24 hours or more, remove the ashes and place in the satellite storage outside Building 23.
10	Cover the burn cage with a tarp.

7.4 Disposing of Waste

Waste generated from these operations shall be packaged and disposed of according to M-1:SOP 1.5. Waste minimization will be handled according to the M-Division Operations Manual.

7.5 Emergency Procedures

In the event of an emergency situation, the Building Emergency Plan (BEP)/ Site Emergency Plan (SEP) shall be followed. The BEP/SEP shall be available in Building Q-23 and the operators shall be familiar with its contents.

8.0 REQUIRED RECORDS

- M-1:SOP 6.1
- Completed and signed Shot Sheet (for detonation or burning)
- M-1 Q-Site Check List, Burning of HE-Contaminated Waste

9.0 REFERENCES

- DOE Explosives Safety Manual
- Los Alamos Environment, Safety, and Health Manual
- M-Division Operation Manual
- M-1:SOP 1.5, Disposal of Hazardous Materials
- M-1:SOP 1.9, Packaging and On-Site Transportation of Explosives
- M-1:SOP 6.1, Q-Site East (TA-14) Firing Operations

10.0 ATTACHMENTS

I. M-1 Q-Site Check List, Burning of HE-Contaminated Waste

II. Hazardous Waste Facility Permit

Attachment I

M-1 Q-Site Check List
Burning of HE-Contaminated Waste

Requester _____ Date Burned _____

Charge Code _____ Shot No. _____

This checklist is intended for use as a safety supplement to M-1:SOP 6.1.5 "Destruction of HE-Contaminated Waste and Waste HE." All Q-Site users must be familiar with Group M-1 SOPs 6.1 and 6.1.5. This checklist should be referred to by the Firing Supervisor subsequent to burning in the burn cage and prior to final arming. In the event of a misfire follow the checklist on the other side of this page.

OK	N/A	
☐	☐	1) Secure and clear area.
☐	☐	2) Ensure burn cage is clean.
☐	☐	3) Open all glass and plastic containers.
☐	☐	4) Place containers to be burned on grate.
☐	☐	5) Place fuel material in bottom of burn cage.
☐	☐	6) Short end of detonator cable..
☐	☐	7) Attach ignitors to detonator cable and place igniters in fuel material.
☐	☐	8) Sprinkle fuel on waste material.
☐	☐	9) Cover top of burn cage with wire mesh.
☐	☐	10) Connect detonator cable to CDU.
☐	☐	11) Start firing sequence.
☐	☐	12) Fire ignitors.
☐	☐	13) Observe burning.
☐	☐	14) Turn off siren (do NOT sound "all-clear").
☐	☐	15) Wait 10 min. after flame has stopped and sound "all-clear."
☐	☐	16) Another batch cannot be burned until 24 hours has elapsed.
☐	☐	17) Clean up ashes (after 24 hours) and place in satellite storage outside TA-23.
☐	☐	18) Cover burn cage with tarp.

Signature _____ Date _____
Firing Supervisor

FORM DATE 8/7/91 Approved By: _____ Date: _____

Attachment II

Hazardous Waste Facility Permit

PERMITTEE: U.S. Department of Energy
University of California Regents
ID NUMBER: NM0890010515

LOCATION: Los Alamos National Laboratory,
Los Alamos, NM 87545
PERMIT NUMBER:
NM 0890010515-1

Pursuant to the Solid Waste Disposal Act, as amended by the Resource Conservation and Recovery Act (RCRA), as amended (42 U.S.C. 6901, et seq.), and the New Mexico Hazardous Waste Act (§§ 74-4-1 et seq. NMSA 1978), a permit is issued to the U.S. Department of Energy's Los Alamos Area Office and the University of California Regents, doing business as Los Alamos National Laboratory, (hereafter called the Permittee) to operate a hazardous waste incinerator, container storage and tank treatment and storage facility at the location stated above.

The Permittee must comply with all the terms and conditions of this permit. This permit consists of the conditions contained herein including the attachments. Applicable provisions of regulations cited are those which are in effect on the effective date of this permit. New Mexico Hazardous Waste Management Regulations (HWMR-5, as amended 1989). This permit shall become effective in accordance with HWMR-5, Part IX, sections 902.F. and 902.G. and shall run for a period of ten years.

This permit is based on the provisions of HWMR-5. This permit is also based on the assumption that all information contained in the permit application is accurate and that the facility will be operated as specified in the application. The permit application consists of information submitted on March 27, 1986; revised on November 13, 1986 and November 25, 1987; and supplemented on November 8, 1988 and through numerous technical discussions.

Any inaccuracies found in the information may be grounds for the termination or modification of this permit and potential enforcement action.

Signed this 8th day of November 1989

by _____

Richard Mitzelfelt, Director, H.M.E.I.D.

New Mexico
Health and Environment Department
Environmental Improvement Division

ATTACHMENT D

TECHNICAL APPROACH TO ESTIMATING EMISSIONS AND THE AIR QUALITY IMPACTS FROM THE OPEN BURNING OF HIGH EXPLOSIVES CONTAMINATED WASTE CONDUCTED AT TECHNICAL AREA 14

Air emissions resulting from the combustion of high explosives (HE) contaminated waste consist primarily of carbon monoxide (CO), oxides of nitrogen (NOx), particulate matter (PM), volatile organic compounds (VOC's), sulfur dioxide (SO_2), and heavy metals such as lead (Pb). Detailed emission estimates for wood, paper, and plastics were performed for this analysis using AP-42 emission factors developed by the Environmental Protection Agency (EPA) found in the July 1995, Version 4.0 of EPA's Air Chief; available on CD ROM. In addition, emission estimates for the combustion of solvents were performed using emission factors and equations presented in the document titled "Prediction of Fire Properties of Fuels," A. Tewarson, Factory Mutual Research Corporation, 1986 (Attachment E). Emission estimates for the combustion of HE were performed using emission factors compiled from data provided in the documents titled: "Emissions from the Open Burning or Detonation of High Explosives," R.V. Carter, U.S. Army Environmental Hygiene Agency, 1978; "Air Quality Impact Analysis, Open Burning of Explosives," Department of Energy, Pantex Plant, Amarillo, Texas, Radian Corp., 1990; "Lawrence Livermore National Laboratory (LLNL) Explosives Handbook Properties of Chemical Explosives and Explosive Simulants," B. M. Dobratz, 1981. Table 1 shows the typical profile of the constants of a burn as well as the emission factors from the sources described above.

TABLE 1. BURN CONSTITUENTS AND ASSOCIATED EMISSION FACTORS

Waste Type	Amount Burned	Emission Factors (lb/lb of material burned)							
		CO	NOx	VOC	PM	SO_2	HF	HCl	Pb
Wood/ Cardboard	10 lb	0.13	0.001	0.11	0.02	0.001	N/A	N/A	1E-07
Plastics/ Paper	30 lb	0.04	0.003	0.02	0.01	0.001	0.0001	0.004	N/A
HE	2 lb	0.05	0.13	0.005	0.27	N/A	0.050	0.028	N/A
Solvents	8 lb (≈ 1 gal)	0.01	N/A	0.02	0.04	0.05	N/A	N/A	1E-06
Emission Totals (lbs)	**50 lb**	**2.66**	**0.30**	**1.86**	**1.16**	**0.44**	**0.07**	**0.16**	**9E-06**

HE Contaminated Waste Solvent Mixtures

Approximately one gallon of HE contaminated dilute solvents generated during HE processing operations at LANL are included in the waste burn at TA-14. The average make-up of the dilute solvent solution is 30% methanol, 25% water, 20% acetonitrile, 20% tetrahydrofuran, 5% of any the solvents in Table 2. Combustion emissions were estimated using emission factors and equations from A. Tewarson, Prediction of Fire Properties of Fuels, Factory Mutual Research Corporation, 1985. Table 2 gives the chemical properties and assumptions required for the emission calculations. Emission estimates from solvent burning are shown above in Table 1.

TABLE 2. CHEMICAL PROPERTIES OF HE CONTAMINATED WASTE SOLVENTS

SOLVENT TYPE	MOLECULAR WEIGHT (g/mole)	DENSITY (g/ml)	NUMBER OF CARBONS	ASSUMPTIONS USED FOR CALCULATIONS
methanol	32	0.7914	1	experimental data available
acetonitrile	41	0.7868	2	C_2 linear alkanes
tetrahydrofuran	72	0.8888	4	C_3-C_6 linear ketones
methyl ethyl ketone	72	0.8054	4	C_3-C_6 linear ketones
butyl acetate	116	0.8825	6	C_5-C_{10} acetate
ethyl acetate	88	0.9003	4	C_4 acetate
toluene	92	0.8669	7	experimental data available
ethanol	46	0.7893	2	experimental data available
acetone	58	0.7899	3	experimental data available
cyclohexane	84	0.7785	6	C_5 -C_{10} cyclo alkane

High Explosives (HE) Waste

Waste HE, generated during HE processing, can consist of a number of different types of HE and associated binders. Table 3 gives a representative list of the HE waste composition found in process waste burned as well as amount of combustion products formed.

TABLE 3. EMISSIONS FROM THE OPEN BURNING OF HIGH EXPLOSIVES

High Explosives, Propellants, and Binders	Composition Fraction	Quantity Burned (lb/burn)	Combustion Products (lb)			
			CO	NOx	VOC	PM
TATB[1,2]	0.21	0.42	1.09E-02	2.92E-02	1.93E-04	8.17E-02
NTO[1,2]	0.18	0.36	1.01E-02	2.70E-02	1.80E-04	7.56E-02
Pyroxylin[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
Comp B[1,2]	0.04	0.08	2.00E-04	1.48E-03	N/A	N/A
LAX 112[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
RDX[1,2]	0.04	0.08	2.09E-04	1.50E-03	4.17E-03	N/A
DNT[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
Nitroguanidine[1,2]	0.04	0.08	2.22E-04	1.50E-03	N/A	2.34E-03
HMX[1,2]	0.04	0.08	2.22E-04	1.50E-03	N/A	2.34E-03
PETN[1,2]	0.04	0.08	2.00E-04	1.48E-03	N/A	N/A
TNT[1,2]	0.04	0.08	2.24E-03	6.00E-03	4.00E-05	1.68E-02
HNS[1,2]	0.04	0.08	2.18E-04	1.15E-03	1.58E-04	6.48E-03
Barium nitrate[3,4]	0.01	0.02	N/A	7.00E-03	N/A	N/A
Cyanuric acid[3,4]	0.01	0.02	2.20E-03	1.76E-02	N/A	1.76E-02
Pentek[3,4]	0.01	0.02	2.20E-03	1.76E-02	N/A	1.76E-02
Exxon461[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
KFE[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
Polystyrene[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
Estane[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
Viton[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
BDNPA-F[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
DBP[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
DOP[3,4]	0.02	0.04	2.20E-03	N/A	N/A	N/A
CEF[3,4]	0.02	0.04	1.00E-03	N/A	N/A	N/A
TOTAL	**1**	**2**	**5.06E-02**	**1.31E-01**	**4.86E-03**	**2.71E-01**

1 Emission factors from Roy V. Carter (June 1978), Emissions from the Open Burning and Detonation of Explosives.

2 Emission factors from U.S. Environmental Protection Agency (June 1995), AP-42 Air Pollution Emission Factors.

3 Emission factors from Radian Corp. (July 1990), Air Quality Impact Analysis, Open Burning of Explosives, Department of Energy, Pantex Plant, Amarillo, Texas.

4 Emission factors based on chemical structures from B. M. Dobratz (March 1981), LLNL Explosives Handbook Properties of Chemical Explosives and Explosive Simulants.

Air Quality Impact Modeling

Air emissions from the open burning of HE contaminated waste at TA-14 are regulated under National and New Mexico Ambient Air Quality Standards. Air emissions from this operation include criteria pollutants such as carbon monoxide (CO), oxides of nitrogen (NOx), particulate matter (PM), sulfur dioxide (SO_2), volatile organic compounds (VOC's), and lead (Pb). In addition, some hazardous air pollutants such as hydrogen chloride (HCl) and hydrogen fluoride (HF) are emitted as a result of combustion of some binders used to form HE. Impacts from operations of this type* must meet ambient air standards for all criteria pollutants. Compliance with the ambient air quality standards was determined using the SCREEN 3 air emissions dispersion model.

The SCREEN 3 model was developed and approved by the Environmental Protection Agency (EPA) as a screening procedure for estimating air quality impacts of stationary sources. SCREEN 3 is a conservative model which uses worst case meteorological data to determine emission impacts. Input parameters supplied for this analysis included: a heat release rate of 15,748 cal/sec; a one hour burn duration; a 2.5 m/sec wind speed; and a one meter source height using a flare source type. Emission impacts are shown in Table 4 for the maximum impact (61 meters) and for the two nearest off-site locations, Pajarito Road 2,042 meters to the north/northeast and State Road 4 bordering Bandelier National Monument 2,286 meters to the south/southeast. The impacts are shown to be will below the ambient standards at all affected locations.

TABLE 4. AIR QUALITY IMPACTS FROM HE PROCESS WASTE BURNING

CHEMICAL	MODELING PARAMETERS	AMBIENT AIR QUALITY STANDARD			AIR CONCENTRATION AT: 61 M (Max.)	2042 M (Pajarito Rd.)	2286 M (SR 4)
CO	D Stability	8-hour average	0.5 mg/m³	(8.7 ppm)	0.53 ppm	3.8E-03 ppm	3.2E-03 ppm
		1-hour average	2.0 mg/m³	(13.1 ppm)	0.76 ppm	5.5E-03 ppm	4.6E-03 ppm
NOx		24-hour average	5.0 μg/m³	(0.1 ppm)	1.4E-02 ppm	1.0E-04 ppm	8.6E-05 ppm
		Annual arithmetic average	1.0 μg/m³	(0.05 ppm)	2.9E-03 ppm	2.1E-05 ppm	1.7E-05 ppm
PM	2.5 meters/sec. wind speed	24-hour average	150 μg/m³		136.6 μg/m³	1.0 μg/m³	0.8 μg/m³
		7-day average	110 μg/m³		19.5 μg/m³	0.1 μg/m³	0.1 μg/m³
		30-day average	90 μg/m³		4.6 μg/m³	3.3E-02 μg/m³	2.8E-02 μg/m³
		Annual geometric mean	60 μg/m³		27.3 μg/m³	0.2 μg/m³	0.2 μg/m³
SO_2	Heat Released 15,748 cal/sec.	24-hour average	5.0 μg/m³	(0.1 ppm)	0.03 ppm	2.1E-04 ppm	1.8E-04 ppm
		Annual arithmetic average	1.0 μg/m³	(0.02 ppm)	0.006 ppm	4.3E-05 ppm	3.6E-05 ppm
Lead		3-month average	0.03 μg/m³		8.9E-06 μg/m³	6.4E-08 μg/m³	5.4E-08 μg/m³
Photo Chemical Oxidant (VOC)		1-hour average		(0.06 ppm)	0.14 ppm	1.0E-03 ppm	8.0E-04 ppm

* HAP's emission standards are regulated under 20 NMAC 2.70 for the facility at 10 tons per year for any one HAP or 25 tons per year for any combination of HAP's. Subsequently, impacts for HCl and HF releases were not included in this modeling analysis.

ATTACHMENT E

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PREDICTION OF FIRE PROPERTIES OF FUELS

by

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Subject Categories

(3) Combustion and Practical Systems

(9) Fire

(18) Modeling and Scaling

For presentation at the Twenty-First International Symposium on Combustion, Technical University of Munich, West Germany, August 3-8, 1986

Factory Mutual Research

1151 Boston-Providence Turnpike
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2086-TR-2

1. INTRODUCTION

Fire properties are defined as the parameters which characterize the combustion and pyrolysis behavior of fuels in fires[1]. In conjunction with fire models, fire properties are used to assess hazards presented by various types of fires and protection needs. A fundamental understanding of diffusion flames has always been found to be very useful in the prediction of fires. In this paper, an attempt has thus been made to use the understanding of the soot formation in diffusion flames to develop relationships for the prediction of fire properties.

The soot formation in diffusion flames has been of great interest because of the relationship with flame radiation and heat transfer, combustion efficiency, and emission of particulates and other chemical compounds some of which may be toxic and corrosive in nature.

In this study, we have used the concept of the smoke point height, L_s, which has been used by many investigators to describe the sooting tendency of fuels. L_s is defined as the height of an overventilated diffusion flame at which soot just begins to be released at the flame tip. The smaller the value of L_s, the greater the tendency to soot. Extensive data for L_s are available in the literature for liquid and gaseous fuels[2-8]. Many investigators find that L_s depends on the nature of chemical bonds and flame turbulence. It has been shown that L_s is related to flame temperature (flame convection)[6] and to flame radiation[9].

In order to use the literature data for L_s to develop predictions for fire properties, it was necessary to perform experiments in our flammability apparatus. In the experiments, simultaneous measurements were made for L_s and fire properties of fuels of known chemical structures and L_s values. In addition to gaseous and liquid fuels, solid fuels were used in the experiments.

The radiative component of the combustion efficiency, χ_R, is defined as

$$\chi_R = \chi_A - \chi_C \ . \tag{7}$$

3. EXPERIMENTS

Experiments were performed in our apparatus, shown in Fig. 1[10]. For gaseous samples, a burner tube very similar to one in Ref. 9 was used. For liquid and solid samples, a 250 ml Pyrex Erlenmeyer flask with a 14/35 ground glass joint was used. The ground glass joint was attached to a 0.12-m long Pyrex glass tube with an internal diameter of 0.009 m to reduce the effects of temperature on L_s values. External heat flux was used for solid and low vapor pressure liquids; for high vapor pressure liquids, a heating mantle placed around the flask was used. The rate of generation of the fuel vapors and flame height were varied by varying either the external heat flux or the heating rate of the mantle.

L_s value was measured visually and for the measurement of fire properties, all the combustion products were captured along with air in the sampling duct of our apparatus. In the duct, measurements were made for the gas temperature, mass fractions of CO_2, CO, total gaseous hydrocarbons (CH), soot (S), and O_2, and $\dot{m}_T$. Measurements were also made for optical transmission through soot, but data have not been discussed in this paper. The generation rate of fuel vapors was measured by a load cell assembly.

In the experiments, data were recorded by a computer at a time interval of about one second. Data were averaged by the computer at the steady state, lasting for about 10 minutes. Each experiment was performed at least twice and the data were averaged. The accuracy of all the averaged experimental data is about ±2%.

All the experiments were performed under natural air flow conditions and thus represent overventilated fire conditions.

The relationship between f_{CO_2} and L_s is same as between χ_A and L_s as expected from Eq. (5) for overventilated fires.

Predictions of Fire Properties of Fuels

If it is assumed that the relationships given in Eqs. (8) to (13) are of general applicability, then it is possible to use the L_s values from the literature to predict χ_i and f_j values for many fuels. The literature values for L_s, however, cannot be used directly because of variations due to differences in the experimental conditions used by various investigators.[11] The following approach was thus taken in this study: 1) relationships between L_s values measured by us and reported in the literature, for selected fuels, were established separately for each investigator; 2) these relationships were then used to recalculate all other L values separately for each investigator; and 3) for fuels which were used by several investigators, the recalculated values of L_s were averaged. The recalculated values of L_s were then used in Eqs. (8) to (13) to predict the χ_i and f_j values. The predicted values of χ_i and f_j are listed in Table II. The detailed tabulation of the data is given in Ref. 12. Values of f_{others} in the table are calculated from the atom balance, i.e., $f_{others} = 1 - \Sigma f_j$.

5. DISCUSSION

Comparison Between the Predicted and Measured Values of Fire Properties

Table III lists the experimental and predicated data for some selected fire properties (f_{CO_2} or χ_A and f_S). A reasonable agreement can be noted between the predicted and measured values. Also our predictions for f_S and those of Pagni's[15], based on entirely different principles, are very similar, except for octane and polystyrene. The new measurements suggest that our older f_S value of 0.18 for polystyrene[17], referred in Ref. 15, appears to be somewhat higher.

and soot, in that order. Butadiene, which is at the top within the aliphatic fuels group, is expected to follow the above aromatic group of compounds.

Relationship Between the Generation Efficiencies of CO and CO_2

In combustion systems, the ratio of CO to CO_2 is used as an indicator of the burning efficiency of fuels. For fuels burning under overventilated conditions, the ratio will vary with the chemical structure of the fuels. For fuels with fixed chemical structure, the ratio will vary with ventilation.

For fuels with variable chemical structure, burning under overventilated conditions, the relationship between f_{CO} and f_{CO_2} can be predicted from Eqs. (10) and (11). The predicted relationship is shown by the solid line in Fig. 3. Experimental data obtained under variable ventilation conditions for wood cribs, heptane, and PMMA from Ref. (18) to (20) have also been included in Fig. 3. Data for enclosure fires of wood cribs with variable ventilation were averaged for similar f_{CO_2} values, and were restricted to the flaming fires only. Data in Fig. 3 indicate that as f_{CO_2} decreases, f_{CO} approaches an asymptotic limit, which is about 0.12 for wood, which is a char forming fuel, and about 0.08 for heptane and PMMA, which are non-char forming fuels.

The results in Fig. 3 indicate that, up to the asymptotic limit of f_{CO}, the relationship between f_{CO} and f_{CO_2} is expected to be the same for the combustion of fuels with: 1) fixed chemical structure and variable ventilation; and 2) variable chemical structure with overventilation. It may be possible to define the asymptotic limit for f_{CO} for underventilated fires of fuels based on their chemical structure.

Relationship Between the Generation Efficiencies of CO and Soot

Emissions of CO and soot from combustion systems are associated with reduced ventilation and/or involvement of fuels which burn inefficiently because of their chemical structures.

From Eqs. (3), (4), and (14),

$$\boxed{\dot{E}''_j = (f_j\ k_j / [\int_0^{T_v} c_p\ dT + H_v])\ (\dot{q}''_{fs} - \dot{q}''_{rr})\ ,} \qquad (16)$$

where $\dot{E}''_j$ is the emission rate of a compound j per unit fuel surface area (kg/m^{2}s). In Eqs. (14), (15), and (16), $\int_0^{T_v} c_p\ dT + H_v$ is defined as heat of gasification of the fuel, L_g (kJ/kg). H_T values are known from the literature and k_j values can be calculated from the elemental composition of the fuel.

L_g values can also be calculated from the literature values for c_p, T_v, and H_v[21], or can be measured. Within a generic group of fuels, L_g increases with the molecular weight of the fuel, primarily due to increase in T_v, and can be estimated for fuels of higher molecular weight. The measured value of L_g for PE is 1750 kJ/kg[17], and from the relationship between L_g and the molecular weight of alkenes, it can be estimated that the molecular weight of the oligomer produced by the vaporization of PE is about 0.601 kg/mole, which is reasonably close to a value of 0.692 kg/mole reported for the molecular weight of the PE oligomer in pyrolysis[22]. In a similar fashion, the molecular weight of PP oligomer is estimated to be 0.720 kg/mole.

From the values of L_g, H_T, k_j, and the data from Table II, emission rates can be calculated for the fuel vapors and the combustion products for defined values of $\dot{q}''_{fs} - \dot{q}''_{rr}$, for example, at the asymptotic limit of $\dot{q}''_{fs} - \dot{q}''_{rr}$, which is approximately constant for fuels with variable molecular weight within a generic group of fuels. Within the aliphatic fuels group, the asymptotic limit for $\dot{q}''_{fs} - \dot{q}''_{rr}$ is equal to 41 kW/m^2, with a variation of ± 15% (as derived from the data for polyoxymethylene, PMMA, heptane, polyethylene, and polypropylene[1,10,16,17]). The emission rates for heat, CO, and soot calculated in this fashion for alkanes and alkenes, as examples, are shown in Figs. 5 and 6, respectively. Experimental data for PE and PP are also included in Fig. 6. The emission rates decrease with increase in the molecular weight of the fuel, because of the increase of L_g due to increase of T_v.

NOMENCLATURE

C_p	specific heat (kJ/kg K)
$\dot{E}''$	emission rate per unit fuel surface area (kg/m^2s)
f_j	generation efficiency of compounds j or oxygen depletion efficiency (-)
$\dot{G}_f$	generation rate of fuel vapors (kg/s)
H_{CO}	heat of combustion of CO (kJ/kg)
H_T	net heat of complete combustion (kJ/kg)
H_v	heat of vaporization (kJ/kg)
k_j	maximum possible total (theoretical) yield of compound j or stoichiometric mass oxygen to fuel ratio (kg/kg)
L_g	heat of gasification of the fuel (kJ/kg)
L_s	smoke point height (m)
$\dot{m}_T$	total mass flow rate of combustion product-air mixture (kg/s)
$\dot{Q}_A$	actual heat release rate (kW)
$\dot{Q}_T$	total (theoretical) heat release rate (kW)
$\dot{q}''_{fs}$	flame heat to the surface of the fuel (kW/m^2)
$\dot{q}''_{rr}$	surface heat loss due to reradiation (kW/m^2)
ΔT	gas temperature above ambient (K)
T_v	vaporization temperature (K)
X_j	mass fraction of compound j (kg/kg)
Y_j	yield of compound j (kg/kg)
χ_A	combustion efficiency (-)
χ_C	convective component of combustion efficiency
χ_R	radiative component of combustion efficiency

Subscripts

f	fuel vapors
i	heat
j	chemical compound

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TABLE I

Experimental Data for Smoke Point Height and

Selected Fire Properties of Fuels

Fuel	L (m)	χ_A	χ_c	χ_R	f_{CO_2}	f_{CO}	f_{CH}	f_S
Methanol	N	0.97	0.83	0.14	0.97	0.001	0.001	N
Ethanol	0.225	0.97	0.74	0.23	0.97	0.001	0.001	0.021
Acetone	0.205	0.96	0.73	0.23	0.96	0.001	0.001	0.022
Pentane	0.155	0.94	0.65	0.29	0.94	0.002	0.001	N
Isopropanol	0.148	0.94	0.65	0.29	0.94	0.002	0.001	N
Hexane	0.125	0.93	0.63	0.30	0.93	0.004	0.002	N
Nylon	0.120	0.90	0.58	0.32	0.90	0.004	0.002	0.030
Ethylene	0.106	0.91	0.61	0.30	0.91	0.003	0.002	0.032
Heptane	0.110	0.93	0.61	0.32	0.93	0.004	0.003	0.032
PMMA	0.105	0.95	0.63	0.32	0.95	0.006	0.001	0.027
Cyclohexane	0.085	0.91	0.56	0.35	0.91	0.005	0.001	N
Isooctane	0.080	0.91	0.60	0.31	0.91	0.007	0.003	N
Polypropylene	0.050	0.89	0.52	0.37	0.89	0.015	0.003	0.050
Polyethylene	0.045	0.87	0.50	0.37	0.86	0.013	0.002	0.060
Propylene	0.029	0.81	0.41	0.40	0.81	0.011	0.006	0.064
Polystyrene	0.015	0.66	0.26	0.40	0.65	0.027	0.023	0.101
Toluene	0.005	0.68	0.28	0.40	0.68	0.030	0.023	0.190

N not measured

TABLE II

(continued)

Fuel	C atoms	X_A	X_C	X_R	f_{CO_2}	f_{CO} x100	f_{CH} x100	f_S x10	f_{others} x10
Butyrate	5 to 6	0.97	0.72	0.25	0.97	0.20	0.11	0.24	0.04
	7 to 8	0.93	0.63	0.30	0.93	0.31	0.15	0.30	0.35
Laurate, oxalate, malonate, lactate	4 to 14	0.97	0.71	0.26	0.97	0.22	0.11	0.24	0.03
C-H-N Structure									
Amines	4 to 12	0.90	0.57	0.33	0.90	0.43	0.21	0.36	0.58
C-H-S Structure									
Mercaptans and Sulfides	6 to 12	0.90	0.57	0.33	0.90	0.43	0.21	0.36	0.58
				Aromatic Fuels					
C-H Structure									
Arenes	6 to 21	0.71	0.30	0.41	0.70	3.80	1.58	1.32	1.14
Cyclic Arenes	10 to 12	0.76	0.36	0.40	0.75	1.96	0.85	0.89	1.32
PAH	9 to 12	0.68	0.27	0.41	0.68	5.20	2.13	1.59	0.88
[illegible] aromatic [illegible] → 3 or more rings									
C-H-O Structure									
Alcohols	7 to 8	0.71	0.30	0.41	0.71	3.49	1.46	1.25	1.16
Ketones	11	0.76	0.36	0.40	0.76	2.01	0.87	0.90	1.20
Aldehydes	7	0.75	0.35	0.40	0.75	2.26	0.97	0.97	1.21
Esters	9	0.76	0.36	0.40	0.76	1.96	0.85	0.89	1.22
C-H-N Structure									
Amines and Heterocylics	6 to 11	0.73	0.32	0.41	0.73	3.00	1.26	1.14	1.13
C-H-S Structure									
Mercaptans and Sulfides	6 to 8	0.67	0.26	0.41	0.67	6.18	2.50	1.76	0.67

N: not predicted

FIGURE CAPTIONS

Fig. 1 Flammability apparatus

Fig. 2 Combustion efficiency and its convective and radiative components as functions of smoke point height

Fig. 3 Relationship between the generation efficiencies of CO and CO_2. Solid line represents our predictions for fuels with variable chemical structures. Experimental data points connected by dashed lines are for variable ventilation conditions: O, enclosure fires of wood cribs, Ref. 18; ●, Heptane, Ref. 19; ■, wood cribs, Ref. 18; *, PMMA, Ref. 20.

Fig. 4 Relationship between the generation efficiencies of soot and CO. Solid line represents our predictions for fuels with variable chemical structures. Symbols connected by dashed lines represent experimental data for PMMA with variable ventilation conditions, Ref. 20.

Fig. 5 Estimated emission rates of heat, CO, and soot as functions of the molecular weight of alkanes for overventilated fires.

Fig. 6 Estimated emission rates of heat, CO, and soot as functions of molecular weight of alkenes for overventilated fires. Dark symbols represent experimental data for polyethylene and polypropylene.

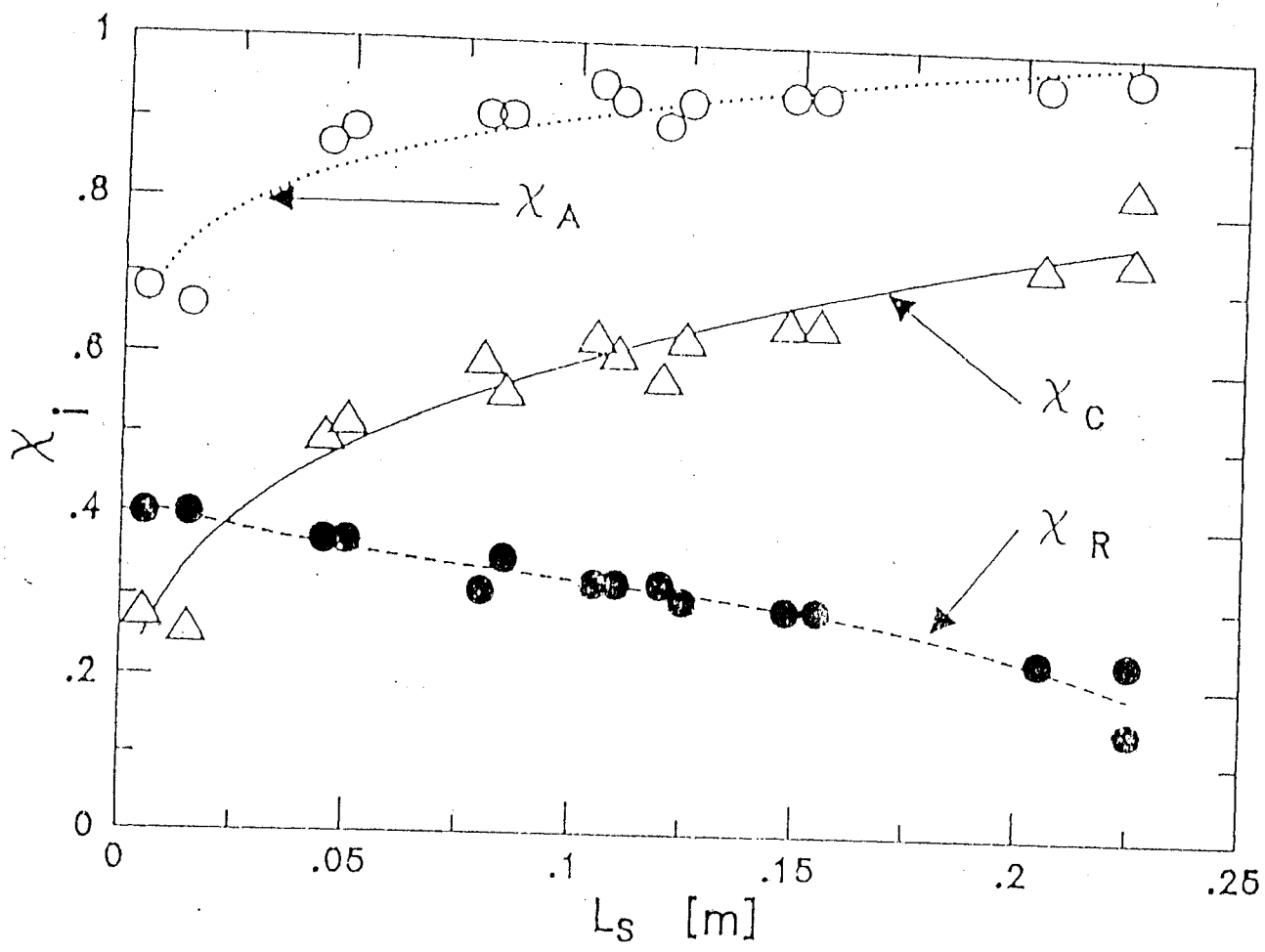

Fig. 2/ Pawarson

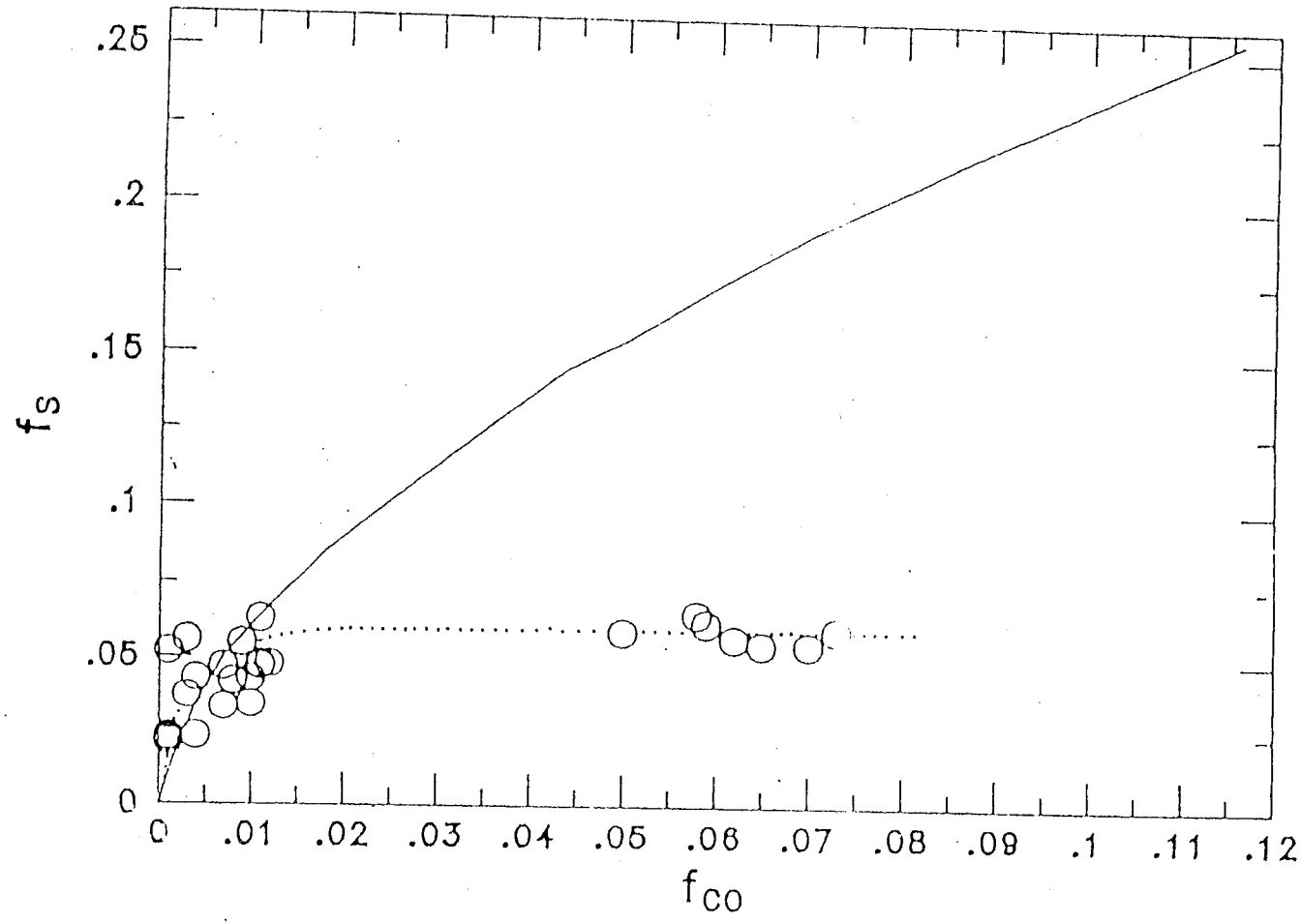

Fig. 4/ Tewarson

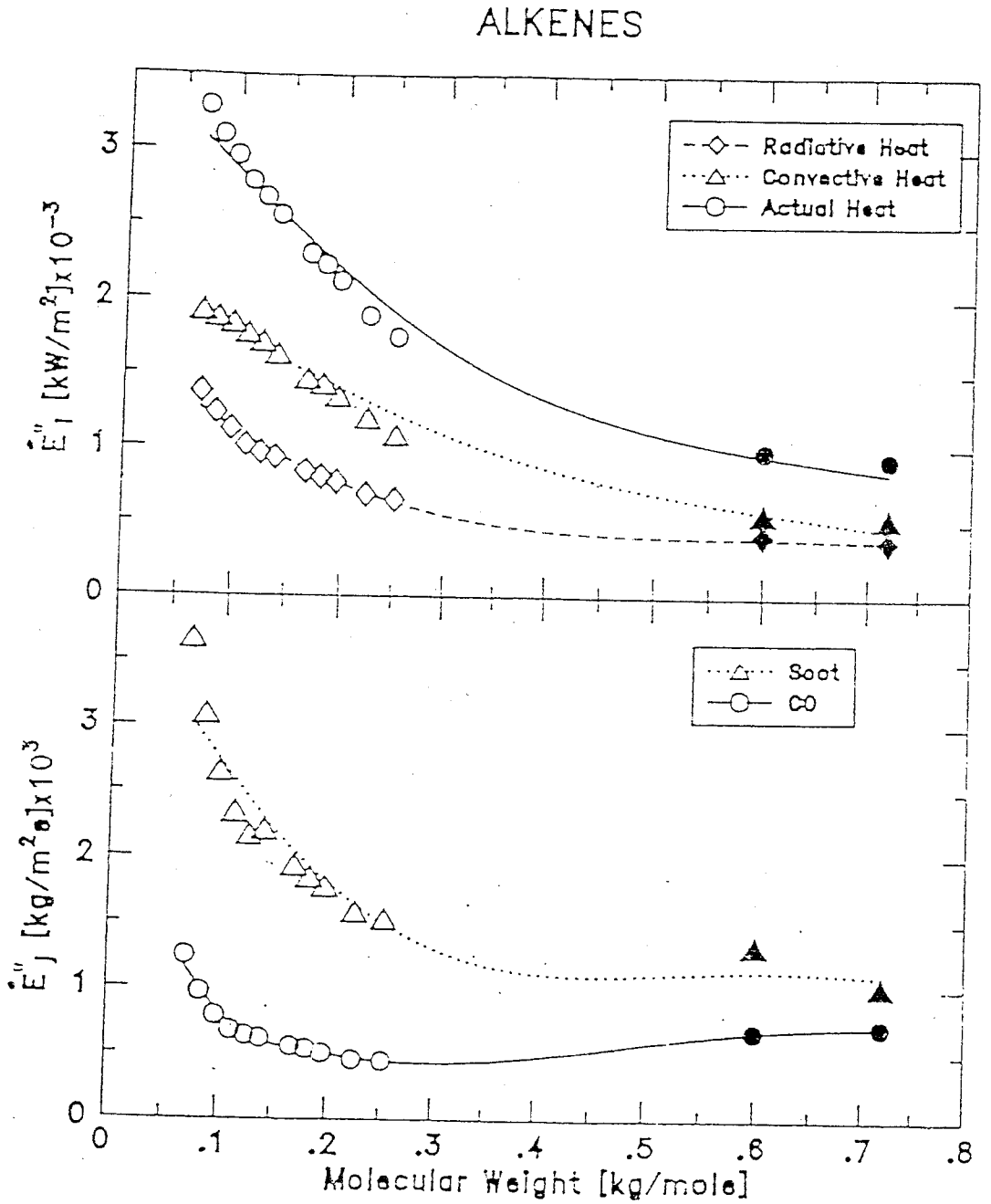

Fig. 6/ Tewarson

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Memorandum

DATE: NOV. 6, 2001

TO: New Mexico Environment Department
Air Quality Bureau
Phone Number: (505) 827-1494
Fax Number: (505) 827-1523

Attention: John Volkerding, Enforcement

Subject: OPEN BURN NOTIFICATION

FROM: HAROLD A. MARTINEZ

Technical Area: 14 **Operation:** BURN AT Q-SITE (30 gal BARREL)

Proposed Burn Date: WEEK OF NOV 5th 2001

Comments:

For further information, please call Harold Martinez at (505) 665-8863.

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Memorandum

DATE: DEC. 10, 2001

TO: New Mexico Environment Department
Air Quality Bureau
Phone Number: (505) 827-1494
Fax Number: (505) 827-1523

Attention: John Volkerding, Enforcement

Subject: OPEN BURN NOTIFICATION

FROM: Harold A. MARTINEZ

Technical Area: 14 Operation: BURN AT Q-SITE (30 gal. BARREL

Proposed Burn Date: WEEK OF DECEMBER 10TH 2001

Comments:

For further information, please call Harold Martinez at (505) 665-8863.

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Memorandum

DATE: FEB. 1, 2002

TO: ***New Mexico Environment Department***
Air Quality Bureau
Phone Number: (505) 827-1494
Fax Number: (505) 827-1523

Attention: John Volkerding, Enforcement

Subject: OPEN BURN NOTIFICATION

FROM: HAROLD A MARTINEZ

Technical Area: 14 ***Operation:*** BURN AT Q-SITE 30 gal. BARREL

Proposed Burn Date: WEEK OF FEB. 4, 2002

Comments:

For further information, please call Harold Martinez at (505) 665-8863.