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PRELIMINARY INVESTIGATION INTO THE EXPLOSION POTENTIAL OF VOLATILE ORGANIC COMPOUNDS IN WIPP CH-TRU WASTE

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Environmental Evaluation Group
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CONTENTS

Title	Page
Foreword	iii
Staff	iv
Summary	v
1. STATEMENT OF THE PROBLEM	1
2. WASTE FORMS CONTAINING VOLATILE ORGANIC COMPOUNDS	2
2.1 Table 1 - Flammable Organic Compounds Selected from a List of Compounds Identified by Drez and James-Lipponer in the Preliminary Inventory of Nonradioactive Waste Constituents to be emplaced in the WIPP (Brush, 1990)	5
3. REVIEW OF REPORTS AND MEMOS	6
3.1 Review of EPA Memo (Smith, 1989)	6
3.2 Summary of Report Prepared by Dzombak, Nair, & Small (1990) Addressing the issue of Explosibility	10
3.3 Natural Resources Defense Council et al (1990)	11
3.4 Summary of Documents	12
3.5 Use of Acetone at Rocky Flats Plant	12
3.6 Analysis of Sludge Samples	13
3.6.1 Table 2 - Analyses Photocopied from DOE's No Migration Variance Petition, Attachment J of Appendix B	15
3.6.2 Table 3 - Photocopied from DOE's No Migration Variance Petition, Attachment H of Appendix B	18
3.6 WIPP WAC and TRAMPAC	19
3.7 Bin-Scale and Alcove-Scale Test-Plan (Molecke 1990a; Molecke, 1990b)	19
4. EXPLOSIBILITY OF ACETONE	21
4.1 Explosibility of Acetone	21
4.2 Potential References on Acetone Explosibility	22

5. SUMMARY OF CONCLUSIONS AND RECOMMENDATIONS..... 23

5.1 Conclusions..... 23
5.2 Recommendations..... 25

6. REFERENCES..... 26

7. APPENDICES
Appendix A From Brush, 1989, "Organic Compounds Identified in the Preliminary Inventory of Nonradioactive Waste Constituents to be Emplaced in the WIPP"..... 28
Appendix B From Molecke, 1990a, "WIPP Test Gases to be Quantified"..... 29
Appendix C From Molecke, 1990b, "WIPP Test Gases to Be Quantified"..... 30
Appendix D From FSEIS, 1990, "Hazardous chemical constituents reported in CH-TRU mixed waste for which no estimates on concentrations are available"..... 31
Appendix E From FSEIS, 1990, "Estimated concentrations of hazardous constituents in TRU mixed waste from the Rocky Flats Plant"..... 32

FOREWORD

The purpose of the Environmental Evaluation Group (EEG) is to conduct an independent technical evaluation of the Waste Isolation Pilot Plant (WIPP) Project to ensure protection of the public health and safety and the environment. The WIPP Project, located in southeastern New Mexico, is being constructed as a repository for permanent disposal of transuranic (TRU) radioactive wastes generated by the national defense programs. The EEG was established in 1978 with funds provided by the U. S. Department of Energy (DOE) to the State of New Mexico. Public Law 100-456, the National Defense Authorization Act, Fiscal Year 1989, Section 1433, assigned EEG to the New Mexico Institute of Mining and Technology and provided for continued funding from DOE through a contract (DE-AC04-89AL58309).

EEG performs independent technical analyses of the suitability of the proposed site; the design of the repository, its planned operation, and its long-term integrity; suitability and safety of the transportation systems; suitability of the Waste Acceptance Criteria and the generator sites' compliance with them; and related subjects. These analyses include assessments of reports issued by the DOE and its contractors, other federal agencies and organizations, as they relate to the potential health, safety and environmental impacts from WIPP. Another important function of EEG is independent environmental monitoring of background radioactivity in air, water, and soil, both on-site and in surrounding communities.

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SUMMARY

The U.S. EPA conducted hearings for the DOE's No-Migration Variance Petition. At the May 29th, 1990 hearing in Santa Fe, a memo was cited as raising serious concerns about possibility of an explosion at WIPP caused by volatile organic compounds in the waste. Acetone and alcohols were identified as the potentially dangerous components.

Long recognized concerns for an explosion resulting from hydrogen and/or methane gas generation are not addressed here. Those discussions can be found elsewhere. This report focuses on determining if volatile, flammable organic compounds such as acetone will be in the waste in sufficient quantities to represent a credible risk of explosion. This investigation draws the following conclusions.

The halogenated organic compounds are non-flammable and do not represent a credible threat of explosion.

Compliance with the WIPP WAC and TRAMPAC will minimize the risk of explosion from volatile, flammable organic compounds during transportation. TRAMPAC limits the amount of potentially flammable organic compounds to a concentration of less than 500 ppm, which is well below the lower limits of flammability for organic compounds that could be in the WIPP inventory.

The precautions outlined by Molecke (1990a & 1990b) are designed to mitigate the risk of explosion during the bin-scale and alcove-scale tests.

A responsible determination of the risk of explosion during the operational or long term disposal phase requires an estimate of the amount of flammable organic compounds to be stored or generated in the repository. The bin-scale and alcove-scale experiments are designed to provide that kind of information.

1. STATEMENT OF THE PROBLEM

An August 23, 1989 memo from Ben Smith of the Land Disposal Restriction Branch of the Office of Solid Waste and Emergency Response of the U.S. EPA to Matt Hale and Matt Straus, directors of the WIPP Work Group of the EPA, was cited by Jim Werner of the Natural Resources Defense Council at hearings held by the EPA in Santa Fe, on May 29, 1990. The memo raised serious questions about the safety of the WIPP project due to the "significant ... possibility" of an underground explosion at WIPP. In summary, the memo suggested that the DOE has been concealing the fact that volatile and potentially explosive components such as acetone and alcohols were present in the drums containing contact-handled transuranic (CH-TRU) waste to be sent to WIPP. Raising the issue of explosibility has prompted a number of responses, some of which include inaccurate information about the potential explosibility of material that is intended for shipment to the repository.

This report examines the potential for an explosion from the non-radioactive components in the waste that can be sent to WIPP and the known flammable or explosive nature of any of those components or other combustible components that would be generated. The potential danger of explosion due to hydrogen gas or methane gas generation will not be discussed in this report. Discussions of that yet to be resolved issue can be found elsewhere (Lappin & Slezak, 1990; Molecke, 1990b & 1989; Neill & Channell, 1983). Included in this report are reviews of the EPA memo filed by Smith (1989), the follow-up analysis prepared by Dzombak, Nair, and Small (1990), a survey of the use of acetone at Rocky Flats Plant (Duff, 1990), and the comments prepared by the Natural Resources Defense Council, et al (1990). An analysis of those reviews coupled with information from various DOE documents, memos, letters, and information in the published literature leads to the conclusions and recommendations.

2. WASTE FORMS CONTAINING VOLATILE ORGANIC COMPOUNDS

There are eight CH-TRU mixed waste forms. From the descriptions given in the DOE No-Migration Variance Petition (U.S. DOE 1990a, v. 1, p. 3-2), three of these forms possibly contain volatile organic compounds. Those three include 1) the cemented and uncemented aqueous waste, 2) the cemented and uncemented organic waste, and 3) the solidified process and laboratory solids.

> The cemented and uncemented aqueous waste form consists of wastewater treatment sludge.... Immobilization involves solidification with portland cement. Prior to 1984, this waste was not cemented and exists today as a damp solid. WIPP WAC certification requires that only residual quantities of free liquids (i.e., less than one percent by weight) may exist in TRU waste. Alcohols and halogenated organic compounds in the sludge are derived from the cleaning of equipment and glassware and the degreasing of metal.
>
> The cemented and uncemented organic waste form contains oil and halogenated organic solvents solidified using Envirostone cement and an emulsifier. Prior to 1984, this waste form was solidified with calcium silicates and currently exists as a damp solid without free liquids, as required by the WIPP WAC. Organic waste consists of lathe coolants and degreasing solvents used in plutonium fabrication.
>
> The solidified process and laboratory solids waste form consists of anion and cation resins and incinerator ash which are neutralized and immobilized with portland cement, as well as organic acids immobilized with magnesia cement. Solvents in this waste are from plutonium recovery operations and research and development laboratories.

A more detailed description of the TRU waste forms generated at each site can be found in the TRUPACT II Contents Document (TRUCON, U.S. DOE, 1989). Molecke (1990a) notes that only TRU waste described in the TRUCON are shippable at present. After

some cross-categorization, Molecke (1990a) classifies the waste types in terms of 1) high organic, newly generated, 2) high organic, old waste, 3) low organic, newly generated and old, and 4) process sludges. Volatile organic compounds are present in each of these four catagories and Molecke's (1990a) estimate of the percentage of each waste type from RFP and INEL cannot be used to calculate the fraction of waste that will potentially contain organic volatile components. Nor can the TRUCON codes themselves be used to estimate the distribution of volatile components.

For this investigation, the volatile organic compounds can be classified into two groups: halogenated and non-halogenated. The halogenated compounds are nonflammable (Windholz et al., 1983) and include tetrachloroethylene, trichloroethylene, methylene chloride, 1,1,1-trichloroethane (methylchloroform), carbon tetrachloride, and 1,1,2-trichloro-1,2,2-trifloroethane (Freon 113). These non-flammable organic constituents do not represent an explosion hazard.

Conversely, some of the non-halogenated organic compounds are flammable. These include the alcohols and glycols, saturated and unsaturated aliphatic hydrocarbons, aromatic hydrocarbons and the ketones. Table 1 lists some of organic compounds identified in the preliminary inventory of nonradioactive waste constituents to be emplaced in the WIPP (Brush, 1989). The organic compounds included in the list include those which are described as flammable by either the Merck Index (Windholz et al, 1983) or by Sax (1984) and for which limits of flammability and autoignition temperatures could be found in either Lange's Handbook of Chemistry (Dean, 1985) or National Bureau of Mines Bulletin 503 (1952). The lower limits of flammability indicate the concentration of vapor in air below which a burning reaction cannot be sustained. The upper limit of flammability indicates the maximum concentration of the vapor in air above which a flame

is not propagated. The autoignition temperature of a substance is the minimum temperature required to initiate or cause self-sustained combustion independent of the heat source (Committee on Hazardous Substances, 1981). The handbooks do not specify the lower limit of explosibility; the concentration of vapor below which an explosion cannot occur (U.S. DOE, 1990b). However, the Committee on Hazardous Substances (p. 58, 1981) identifies the explosive range and flammable range as one and the same. The TRAMPAC limit of 500 ppm flammable organic vapor is well below each of the lower limits of flammability for components given in Table 1. However, it should be noted that the range presented in Table 1 is determined for ambient conditions of temperature and pressure. Increasing temperature or pressure can widen the range of flammability.

2.1 Table 1 - Flammable Organic Compounds Selected from a List of Compounds Identified by Drez and James-Lipponer in the Preliminary Inventory of Nonradioactive Waste Constituents to be emplaced in the WIPP (BRUSH, 1990)

GAS OR VAPOR	*LIMITS OF FLAMMABILITY IN AIR (PERCENT)		*AUTO IGNITION TEMPERATURE (°C)
	LOWER	HIGHER	
Acids, Organic			
Acetic Acid	5.4	16.0	465
Alcohols			
Butanol	1.4	11.2	365
Ethanol	3.3	19	365
Isopropanol	2.1	13.5	440
Methanol	6.7	36.0	385
Aldehydes			
Formaldehyde	7.0	73	429
Hydrocarbons, Aliphatic Saturated			
Decane	0.8	5.4	210
Hexane	1.1	7.5	225
Kerosene	0.7	5	-
Nonane	0.8	2.9	205
Pentane	2.2	22	260
Octane	1.0	6.5	220
Hydrocarbons, Aliphatic Unsaturated			
Butadiene	2.0	11.5	-
Styrene	1.1	6.1	490
Hydrocarbons, Aromatic			
Ethyl Benzene	1.0	6.7	432
Toluene	1.2	7.1	480
Xylene, m- and p-	1.1	7.0	530
Xylene, 0-	1.0	6.0	465
Ketones			
Acetone	2.6	12.8	465
Methyl Ethyl Ketone	1.8	10	-
Methyl Isobutyl Ketone	1.4	7.5	-

* VALUES FROM LANGE'S HANDBOOK OF CHEMISTRY (Dean, 1985) AND/OR NATIONAL BUREAU OF MINES, BULLETIN 503 (1952).

3. REVIEW OF REPORTS AND MEMOS

3.1 Review of EPA Memo (Smith, 1989)

The DOE submitted to the U.S. Environmental Protection Agency the No-Migration Variance Petition (U.S. DOE, 1990a). Smith's (1989) investigation was intended to determine whether or not the DOE has satisfactorily demonstrated that there would be no migration of hazardous constituents beyond the boundary of the unit. Smith evaluated various DOE reports and reviewed the regional files on waste generation and management practices at the Rocky Flats Plant. His investigation led him to conclude that "emissions from the WIPP could occur in excess of health based numbers." (Smith, 1989, p. 1) Apparently the conclusions support his long held position on the need to pretreat any waste scheduled for disposal at WIPP. "As I have stated on numerous occasions in the past, the only realistic way I see for DOE to make a successful demonstration is to consider some pretreatment of the wastes, especially the combustible and sludge waste forms." (Smith, 1989, p. 6)

Smith (1989) argues that, based on low level waste data, some hazardous constituents have been routinely underreported. Specifically, he maintains that "INEL and RFP deny the presence of acetone in the waste" (Smith, 1989, p. 3) in spite of evidence that acetone and alcohols are used as commercially available solvents for cleanup and that DOE "has based its organic constituent characterization on some rather focused headspace analyses of drums stored at INEL." (Smith, 1989, p. 2) Smith also asserts that files maintained at the Rocky Flats Plant suggest widespread use of acetone and various alcohols as clean-up solvents. Smith claimed that the solvents would promote the significant possibility of reaching the explosive limits in a waste storage room.

Contrary to Smith's allegations, the potential presence of a number of volatile organic compounds is widely recognized in several DOE reports including the Final Supplement Environmental Impact Statement (U.S. DOE, 1990c), the No-Migration Variance Petition (U.S. DOE, 1990a), the WIPP Bin-Scale CH-TRU Waste Test Plan (Molecke, 1990a), the WIPP In-Situ Alcove CH-TRU Waste Test Plan (Molecke, 1990b), and the Test Plan for Laboratory and Modeling Studies of Repository and Radionuclide Chemistry for the WIPP (Brush, 1989). Tables from those documents are reproduced in the appendices of this report and clearly show that DOE plans to include analyses for acetone during the experimental phase of the project.

Table 5-1 of the DOE No-Migration Variance Petition (U.S. DOE, 1990a) and Table 5.31 of the DOE FSEIS (U.S. DOE, 1990c) are identical and estimate the concentration of a number of hazardous constituents including methyl and butyl alcohol. Table 5.32 (see Appendix) of the FSEIS identifies acetone as a hazardous constituent in CH-TRU mixed waste for which no estimates on concentration are available. Table 7.2 (see Appendix) of the laboratory test plan (Brush, 1989) was compiled by Drez and James-Lipponer in their preliminary inventory of the non-radioactive waste constituents to be emplaced in the WIPP. Various alcohols and ketones, including acetone, are identified as being used in the Rocky Flats Plant. A footnote to the table states that these organic compounds may be present in trace amounts only. Table 11.1 of the Bin Scale Test Plan and Table 12.2 (see Appendix) of the In Situ Alcove Test Plan identify several volatile organic compounds to be quantified including methyl alcohol, butyl alcohol, and acetone.

Smith's expressed concerns about the potential explosibility of acetone are not totally unfounded. Acetone is a volatile, highly flammable liquid (Windholz et al, 1983) and should be

kept away from heat, sparks, and flames (Kirk-Othmer Encyclopedia of Chemical Technology, 1978). The explosion hazard is classified as moderate even when acetone vapor is exposed to an open flame (Sax, 1984).

Smith argues that "isopropyl alcohol is converted to acetone under the probable waste storage conditions." Smith's report does not identify the probable conversion mechanism nor does the report provide a reference.

The commercial production of acetone by dehydrogenation of isopropyl alcohol is endothermic requiring substantial amounts of energy and a catalyst.

$$CH_3CHOHCH_3 + 66.5\ kJ/mol\ (at\ 327^oC) \rightarrow CH_3COCH_3 + H_2$$

In theory, a 98% conversion is possible at 325°C [617°F]. In practice, the conversion is generally run at 400-600°C [752-1112°F], although some reactions having been successfully run at a temperature as low as 315°C [594°F] (Kirk-Othmer, 1978). Thus, while dehydrogenation of isopropyl alcohol is the preferred commercial alcohol to acetone conversion, it requires high temperatures which are not expected in the repository. Temperatures in the repository are not expected to rise more than a few degrees above the ambient temperature of about 27°C.

The catalytic oxidation of isopropyl alcohol, on the other hand, is highly exothermic. The process produces energy and will proceed if oxygen is present. High yield, commercial production requires a catalyst and reactors maintained at 400-600°C [752-1112°F]. Again, the temperature requirements are much higher than is anticipated in the repository. Given above energy requirements for commercial conversion, it is difficult to accept

Smith's argument that isopropyl alcohol in the drums would be converted to acetone by this mechanism under the anticipated repository temperatures.

Again, the exact conversion was not specified in Smith's memo. Therefore, one can only speculate that Smith may have been referring to a bio-oxidation process. For example, acetic acid bacteria such as acetobacter or gluconobacter normally oxidize ethanol into acetic acid. These bacteria can also oxidize isopropanol into acetone (Gottschalk, 1986). Hence, it is possible to generate acetone biologically, but it would require isopropyl alcohol, oxygen, and the acetic acid bacteria.

There are anaerobic bacteria that can generate acetone from either the cellulosic material present or alcohols. These would include Clostridium cytophagia (cellulose fermenter), Clostridium acetobutylicum and Clostridium butyricum (grain and alcohol fermenters). Clostridium acetobutylicum was used in Germany to produce acetone from grain during World War II (Spencer, 1990).

Whether or not a potentially explosive amount of acetone can be generated would depend on the amount of isopropyl alcohol present, the efficiency of the conversion under the repository conditions, and the presence of other organisms that could use acetone to generate yet another organic compound. It is worth noting that a potentially explosive situation requires oxygen and, in the long run, both corrosion and microbial activity are expected to remove the available oxygen from the rooms.

3.2 Summary of Report Prepared by Dzombak, Nain, & Small (1990) Addressing the issue of Explosibility

Dzombak et al. (1990) issued a report to address the issue of explosibility during the test phase of WIPP. The report focused on the generation of gases in individual drums of TRU waste by the mechanisms of thermal degradation, biodegradation, corrosion, radiolysis, and evaporation. Dzomback et al (1990, p.36) conclude that, during the test phase, "so long as some minimum level of ventilation is maintained in the barrels and in the room, flammability limits should be safely avoided...." The issues of long term gas generation and pressure build-up once the room is sealed were not addressed.

The issue of potential explosibility is discussed in Section 6.0 titled "Estimates of Storage Room Concentrations." The volatile organic compounds included in these calculations are different than the components used in the calculations cited by Smith (1989). There was no reason given for selecting different components. Dzombak et al (1990) discuss the volatilization rates for methylene chloride, 1,1,1 trichloroethane, and trichloroethylene. They conclude that even under conditions of non-ventilation, the partial pressure for these constituents will lie "still well below the 1 percent by volume lower bound typically found for flammability. Thus, flammability conditions resulting from organic emissions to the room appear to be a remote possibility." (Dzombak et al, 1990, p. 36.)

The conclusion is correct, but for an entirely different reason. The organic materials cited above are simply not flammable according to a variety of sources including, the Merck Index (Windholz et al, 1983).

3.3 Natural Resources Defense Council et al (1990)

The Natural Resources Defense Council (NRDC) et al (1990) strongly opposes approval of the DOE No-Migration Variance Petition (U.S. DOE, 1990). Unfortunately, the NRDC et al. report further confused the issue of flammability when it also incorrectly identified two organic compounds as flammable: methyl chloroform (1,1,1-trichloroethane) and carbon tetrachloride. Not only are these chemicals classified as nonflammable, the Merck Index (Windholz et al, 1983) notes that carbon tetrachloride (which is now well documented as highly toxic) has been used to extinguish fires.

It is not clear why the Natural Resources Defense Council et al (1990) chose to cite the low flash point of the various alcohols as an additional cause for concern. By definition, the flash point is "the lowest temperature at which a liquid gives off vapor in sufficient concentration to form an ignitable mixture with air near the surface of the liquid ..." (Committee on Hazardous Substances in the Laboratory, 1981, p. 58). Normal butyl alcohol, for instance, will not ignite at a temperature below 34°C [95°F]. Hence, the flash point explosion hazard for that alcohol is classified as "moderate when exposed to flame." (Sax, 1984, p. 563)

As shown in Table 1, the autoignition temperature for normal butanol, at ambient conditions, is 365°C [689°F] and requires a minimum vapor concentration in air of 1.4%. The autoignition temperatures for methanol, ethanol, and isopropanol are also quite high, ranging from 365-440°C [689-824°F]. A repository temperature of 27°C would not promote spontaneous combustion of these components even if they and oxygen were present in sufficient quantity.

3.4 Summary of Documents

Thus far, this report has reviewed documents that discuss the potential for an explosion due to the presence of volatile organic compounds. Halogenated organic compounds have been identified as nonflammable. A few other organic compounds, such as acetone and the alcohols, have been identified as flammable. Estimating the risk of an explosion due to the presence of acetone requires knowledge of the quantity of acetone that will be sent to WIPP given 1) process information, 2) available waste analysis, and 3) the TRUPACT-II Authorized Methods for Payload Control (TRAMPAC) and the WIPP Waste Acceptance Criteria (WIPP WAC). Process information given in the next section suggests that the amount of acetone in the waste may be negligible.

3.5 Use of Acetone at Rocky Flats Plant

A March 20th, 1990 memo from Mark Duff of the DOE to Matt Hale of the EPA included an attachment describing the use of flammable solvents such as acetone at Rocky Flats Plant (RFP). The attachment described in detail how acetone is used and in which buildings. In summary,

> ....the dominant use of acetone at the Rocky Flats Plant is for the cleaning of glassware and metals that contain minimal or no radioactive contamination and disposal of the materials in non-line generated waste (almost always low-level). RFP safety regulations preclude the use of flammable solvents (e.g. acetone) inside any glovebox system where the majority of the transuranic waste is generated, except under special circumstances. Therefore, it is highly unlikely that flammable solvents, including acetone, would be present in any transuranic solid waste. None of the headspace analyses (Appendix B of the No-Migration Petition) have detected the presence of acetone in any drums of TRU waste.

Some acetone residuals could occur in waste waters that pass through Buildings 374 or 774, prior to processing as a sludge. Analysis of liquids samples from tanks in Buildings 374, 707, and 779 do show detectable quantities of acetone (Appendix B, Attachment H of the No-Migration Petition). However, the liquids in these tanks would merge with liquid wastes from other buildings prior to further processing by vacuum filtration into a solidified inorganic sludge. The effluent, liquid from filtration, becomes low level waste that is processed into saltcrete by an evaporation method. It is highly unlikely that any residual acetone would persist in the final transuranic sludge wasteform after vacuum filtration and cementation. Analyses of several TRU waste sludge samples (Appendix B, Attachment H of the No-Migration Variance Petition) did not detect any acetone in the waste (Duff, 1990, p. 4).

3.6 Analysis of Sludge Samples

A leaching procedure was used to analyze solidified inorganic sludges from several drums of low-level (non-TRU) waste. The analyses detected very small quantities of acetone, on the order of 22-73 μg/l or approximately 22-73 parts per billion. (Section 1 of Attachment J of Appendix B of DOE's No-Migration Variance Petition and reproduced here as Table 2.) However, similar quantities were detected in blank samples which are prepared to be devoid of acetone. Thus, the acetone detected in the sludge samples may have been due to a source of contamination inherent to the sample preparation or analyses. It can not be known for certain if the detectable amount of acetone reflects the actual presence of acetone in the sludge.

The analytical results from leaching procedures on two organic and five inorganic sludges (Attachments H of Appendix B of DOE's No-Migration Variance Petition and reproduced here as Table 3)

showed no flammable organic compounds in six of the drums and, in one inorganic drum, very low amounts (a few parts per billion) of toluene, ethylbenzene, styrene, and xylenes. Gas samples from the same drums showed no trace of any of 36 organic compounds, including acetone.

In spite of the argument that "it is highly unlikely that acetone would persist in the final TRU sludge form after vacuum filtration," (Duff, 1990, p. 4) it is still uncertain as to how much acetone or other flammable organic compounds, if any, would remain. A direct analysis of the volatile organic compounds in the various waste forms would resolve that issue.

TABLE 2 - ANALYSES PHOTOCOPIED FROM DOE'S
NO MIGRATION VARIANCE PETITION, ATTACHMENT J OF APPENDIX B

TOXICITY CHARACTERISTICS LEACHING PROCEDURES (TCLP) TEST RESULTS - INORGANIC SLUDGES, ROCKY FLATS PLANT

VOLATILE ORGANIC AROMATIC COMPOUNDS@

VOA COMPOUND	DETECTION LIMITS (µ g/kg)	VFS-08-88-01 (µ g/l)	VFS-08-88-02 (µ g/l)	VFS-08-88-03 (µ g/l)
Acetone	10	36	24	22
n-Butyl alcohol	*	ND	ND	ND
Carbon disulfide	5	ND	ND	ND
Carbon Tetrachloride	5	ND	ND	ND
Chlorobenzene	5	ND	ND	ND
Cyclohexanone	*	ND	ND	ND
1,2-Dichlorobenzene	*	ND	ND	ND
Ethyl Acetate	*	ND	ND	ND
Ethylbenzene	5	ND	ND	ND
Ethyl ether	*	ND	ND	ND
Isobutanol	*	ND	ND	ND
Methyl Isobutyl ketone	10	ND	ND	ND
Methylene chloride	5	30	26	26
Methyl ethyl ketone	10	ND	ND	ND
Tetrachloroethylene	5	ND	ND	ND
Toluene	5	ND	ND	ND
1,1,1-trichloroethane	5	ND	ND	ND
1,1,2-trichloro-1,2,2-trifluoroethane	*	ND	ND	ND
Trichloroethylene	5	ND	ND	ND
Trichlorofluoromethane	10	ND	ND	ND
Xylene	5	ND	ND	ND

SURROGATE COMPOUNDS	PERCENT RECOVERY	PERCENT RECOVERY	PERCENT RECOVERY
1,2-Dichloroethane-D4	90	92	92
Toluene-D8	100	99	99
p-BFB	102	101	102

ND= None Detected.
* = Library Search had no detection limit.
@ Copied from Envirodyne Engineers Report of Analysis 12161 Lackland Road, St. Louis, MO 63146. Report Date: September 30, 1988.

WIP:0497-T/1

TABLE 2 (continued)

TOXICITY CHARACTERISTICS LEACHING PROCEDURES (TCLP) TEST RESULTS - INORGANIC SLUDGES, ROCKY FLATS PLANT

VOLATILE ORGANIC AROMATIC COMPOUNDS@

VOA COMPOUND	DETECTION LIMITS (µ g/kg)	METHOD BLANK (µ g/l)	METHOD BLANK (µ g/l)	METHOD BLANK (µ g/l)
Acetone	10	3	20	14
n-Butyl alcohol	*	ND	ND	ND
Carbon disulfide	5	ND	ND	ND
Carbon Tetrachloride	5	ND	ND	ND
Chlorobenzene	5	ND	ND	ND
Cyclohexanone	*	ND	ND	ND
1,2-Dichlorobenzene	*	ND	ND	ND
Ethyl Acetate	*	ND	ND	ND
Ethylbenzene	5	ND	ND	ND
Ethyl ether	*	ND	ND	ND
Isobutanol	*	ND	ND	ND
Methyl Isobutyl ketone	10	ND	ND	ND
Methylene chloride	5	23	11	9
Methyl ethyl ketone	10	ND	ND	ND
Tetrachloroethylene	5	ND	ND	ND
Toluene	5	ND	ND	ND
1,1,1-trichloroethane	5	ND	ND	ND
1,1,2-trichloro-1,2,2-trifluoroethane	*	ND	ND	ND
Trichloroethylene	5	ND	ND	ND
Trichlorofluoromethane	10	ND	ND	ND
Xylene	5	ND	ND	ND

SURROGATE COMPOUNDS	PERCENT RECOVERY	PERCENT RECOVERY	PERCENT RECOVERY
1,2-Dichloroethane-D4	95	92	93
Toluene-D8	99	99	101
p-BFB	86	100	99

ND= None Detected.
* = *Library Search had no detection limit.*
@ Copied from Envirodyne Engineers Report of Analysis 12161 Lackland Road, St. Louis, MO 63146.
Report Date: September 30, 1988.

WIP:0497-T/3

TABLE 2 (continued)

TOXICITY CHARACTERISTICS LEACHING PROCEDURE (TCLP) TEST RESULTS - INORGANIC SLUDGES, ROCKY FLATS PLANT

VOLATILE ORGANIC AROMATIC COMPOUNDS@

VOA COMPOUND	DETECTION LIMITS (µ g/kg)	EXTR. BLANK (µ g/l)	EXTR. BLANK (µ g/l)	METHOD BLANK (µ g/l)
Acetone	10	5	37	4
n-Butyl alcohol	*	ND	ND	ND
Carbon disulfide	5	ND	ND	ND
Carbon Tetrachloride	5	ND	ND	ND
Chlorobenzene	5	ND	ND	ND
Cyclohexanone	*	ND	ND	ND
1,2-Dichlorobenzene	*	ND	ND	ND
Ethyl Acetate	*	ND	ND	ND
Ethylbenzene	5	ND	ND	ND
Ethyl ether	*	ND	ND	ND
Isobutanol	*	ND	ND	ND
Methyl isobutyl ketone	10	ND	ND	ND
Methylene chloride	5	29	27	21
Methyl ethyl ketone	10	ND	ND	ND
Tetrachloroethylene	5	ND	ND	ND
Toluene	5	ND	ND	ND
1,1,1-trichloroethane	5	ND	ND	ND
1,1,2-trichloro-1,2,2-trifluoroethane	*	ND	ND	ND
Trichloroethylene	5	ND	ND	ND
Trichlorofluoromethane	10	ND	ND	ND
Xylene	5	ND	ND	ND

SURROGATE COMPOUNDS	PERCENT RECOVERY	PERCENT RECOVERY	PERCENT RECOVERY
1,2-Dichloroethane-D4	105	93	108
Toluene-D8	103	99	103
p-BFB	102	101	102

ND= None Detected.
* = Library Search had no detection limit.
@ Copied from Envirodyne Engineers Report of Analysis 12161 Lackland Road, St. Louis, MO 63146. Report Date: September 30, 1988.

TABLE 3 - PHOTOCOPIED FROM DOE'S
NO MIGRATION VARIANCE PETITION, ATTACHMENT H OF APPENDIX B

TABLE H-1[a]

VOLATILE ORGANIC ANALYSIS OF SLUDGE SAMPLES[a]

IDC Volatile Compounds (ppm)	001 7411- 2808	001 7412- 02917	001 7412- 03492	001 7412- 03850	001 7411- 2578	003 7431- 6930	003 250- 0484
1,1-Dichloroethene	.1U	.1U	.1U	.1U	.1U	.1U	80[b]
1,2-Dichloroethene(Total)	7.8	.1U	.1U	.1U	.1U	.1U	.1U
Chloroform	1.8	.1U	.1U	.1U	.1U	.1U	.1U
1,1,1-Trichloroethane	8.8	.1U	.1U	.1U	.1U	.1U	.1U
Tetrachloroethene	1.7	.1U	.1U	.1U	.1U	1.2	40[b]
1,1,2,2-Tetrachloroethane	4.7	.1U	.1U	.1U	.1U	.1U	.1U
Toluene	0.9	.1U	.1U	.1U	.1U	.1U	.1U
Ethylbenzene	5.3	.1U	.1U	.1U	.1U	.1U	.1U
Styrene	9.6	.1U	.1U	.1U	.1U	.1U	.1U
Total Xylenes	19.0	.1U	.1U	.1U	.1U	.1U	.1U
Carbon Tetrachloride	.1U	.1U	.1U	.1U	.1U	2.2	700[b]
Freon TF	.2U	.2U	.2U	.2U	.2U	4.0	.2U

U Analyzed, not detected

[a] Other volatile organic compounds analyzed for but were not detected include: 1) propanol, 2) butanol, 3) chloroethane, 4) methylene chloride, 5) acetone, 6) carbon disulfide, 7: 1,1-dichloroethane, 8) 1,2-dichloroethane, 9) 2-Butanone, 10) vinyl acetate, 11) bromodichloromethane, 12) 1,2-dichloropropane, 13) cis-1,3-dichloropropene, 14) trichloroethene, 15) dibromochloromethane, 16) 1,1,2-trichloroethane, 17) benzene, 18) trans-1,3-dichloropropene, 19) bromoform, 20) 4-methyl-2-pentanone, 21) 2-hexanone, 22) chlorobenzene, 23) chloromethane, and 24) bromomethane. All detection limits are .2 or .1 ppm for above compounds. Modifed from the TRUPACT-II Safety Analysis Report.

[b] Concentrations in ppb

[a] Modified from the TRUPACT-II Safety Analysis Report

3.6 WIPP WAC and TRAMPAC

For waste to be accepted at WIPP, compliance must be demonstrated with the WIPP Waste Acceptance Criteria (WIPP WAC) (U.S. DOE, 1989) and the TRUPACT Authorized Methods for Payload Control (TRAMPAC) (Nuclear Packaging, 1989). TRAMPAC specifically requires that potentially flammable organic compounds shall be limited to 500 ppm, which is well below the lower limits of flammability for the materials to be sent to WIPP. WIPP WAC (4.2.1 and 4.2.2) specifies that TRU waste shall not be in a free liquid form and only minor liquid residues remaining in well-drained bottles, cans, and other containers are acceptable. Furthermore, the TRAMPAC (Vol 1, 1.3.7-13) and WIPP WAC (4.4.1 and 4.4.2) explicitly prohibit transporting explosive materials or compressed gases.

3.7 Bin-Scale and Alcove-Scale Test-Plan (Molecke, 1990a; Molecke, 1990b)

The bin-scale tests (Molecke, 1990a) are designed to measure gas generation and depletion rates and gas compositions that occur with actual TRU waste, as a function of waste type, time, and interaction with brine and engineered barrier materials. The waste types include:

- High organic, newly generated
- High-organic, old waste
- Low-organic waste (old and new)
- Process sludges (old and new)

One objective of the test phase is to determine the amount of volatile organic gases (VOC's) that will be released in the bins. Quantitative analyses of the VOC's will be accomplished using a gas chromatograph equipped with a methyl silicone

capillary column and a flame ionization detector. Method development is in progress (Greenlee, 1990) and will include analyses for what are anticipated to be minor amounts of the volatile organic compounds (Molecke, p. 31, 1990a). The list of components to be analyzed (see Table 11.1 of Molecke, 1990a in the Appendix) includes the alcohols, acetone, the xylenes, and the alkanes (Molecke, 1990a and Greenlee, 1990).

The explosibility potential of hydrogen and/or methane gas within the bins has been recognized and addressed (Molecke, p. 167, 1990a; Molecke, 1989; Lappin & Slezak, 1990). Molecke argues that the only credible ignition source proposed for the gases within the bins is the potential for spontaneous combustion due to organic-matrix waste.

Lappin & Slezak (1990) calculate that the temperature in a bin would have to increase to more than 450°C to initiate spontaneous combustion. That estimate is consistent with the autoignition temperatures listed in Table 1.

In addition to temperature monitoring, the safety mitigation measures include electrical grounding, oxygen monitoring, and gas monitoring. "The oxygen, hydrogen, methane, and other gas concentrations within the bins will be periodically sampled, analyzed by GC-MS, and closely monitored so that any approach to a potentially explosible gas level will be quite evident (Molecke, 1990a, p. 167)." Molecke further notes that it is indeed "the bin-scale test which will provide the best available data for WIPP PA (performance assessment) purposes, concerning the reality of potentially flammable and/or explosible gas mixtures during the full-scale waste emplacements at the WIPP."

The bin-scale tests have been modified and will not include leachate sampling. Leachate sampling will be done in "drum-scale" and "liter-scale" experiments (Lappin, 1990). Those

experiments should include analyses for dissolved organic compounds as discussed in Molecke's original bin-scale test plan (1990a, p. 121).

The issue of explosibility is also addressed in the In-Situ Alcove Test Plan (Molecke, 1990b). The plan notes that there is no credible possibility of generating an explosible gas in four of the alcoves because the alcoves will be continuously purged of oxygen with a chemical getter-reactant system. For the alcove containing "as is" waste, Molecke calculates and argues that the potential for an explosion is minimal given the nature of the experiment and the safety measures incorporated into the experimental plan. The safety measures described for the "alcove-scale" tests are similar to the measures described for the "bin-scale" tests.

4. EXPLOSIBILITY OF ACETONE

4.1 Explosibility of Acetone

Clearly, a responsible calculation of the explosibility of acetone or any other volatile organic compound requires an accurate estimate of the composition of the vapor for each waste form: a number that can only be obtained from actual vapor composition measurements. As noted in the previous section, the "bin-scale," "drum-scale," and "liter-scale" tests will provide an estimate of the amount of acetone in each waste form. Once the concentration of acetone is known, then the potential for an explosion can be determined.

The key word acetone and key syllables explo-, were used in a data base search of the recent literature. The search yielded fifty nine titles: seven of which have titles that directly address the issue of the explosibility of acetone. Unfortunately, all of the articles with promising titles are written in languages other than English. The titles of those articles are listed here (for future reference) should the analytical effort indicate substantial amounts of acetone in the mixed-hazardous TRU waste.

4.2 Potential References an Acetone Explosibility

Mitsui, Toshiyuki and Fujimura, Yoshikazu, 1987. Calculation of flammability limits with a personal computer. Anzen Kogaku, 26, p. 161-5. (Japanese)

Baratov, A.N., Smolin, I.M. and Vogman, L.P., 1985. Formation of local vapor-air explodable regions in rooms. Mosk. Khim, Tekhnol. Inst. Im. D.I. Mendeleeva, 138, p. 63-5. (Russian)

Baratov, A.N., and Korotkikh, N.I., 1980. Study of explosion pressures in the combustion of mixtures of acetone vapors with air in a local volume. Khim, Prom, St, p. 97-8. (Russian)

Rietz, Gerhard, 1989. Classification of gases, vapors and dusts according to explosion action. Brandschutz, Explosionsschutz Forsch. Prax, 1, p. 99-116. (German)

Pilc, Aleksander, 1979. Mutual relations of the lower flammability limit (VD) with the maximum experimental safe gap (MSAG) and comparative caloric effect (Q) of flammable mixtures with air. Przem, Chem, 58, p. 476-80. (Polish)

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5. SUMMARY OF CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Many of the volatile organic compounds, specifically the halogenated organic compounds, used in various machining and cleaning activities are nonflammable and are not considered highly explosive under expected repository conditions.

Efforts to measure the quantity of acetone in liquids taken from tanks at the Rocky Flats Plant and the quantity of acetone in sludge samples taken from drums of TRU waste generated at the Rocky Flats Plant are largely inconclusive. Acetone was not detected in the headspace gas analyses on several drums of CH-TRU waste. There were very small, but detectable, amounts of acetone in some inorganic sludge samples. But similar amounts were detected in blank samples as well, leaving those analyses inconclusive. Detectable quantities of acetone appeared in liquid samples taken directly from some process tanks at the Rocky Flats Plant. However, there remains some question as to how much of the volatile organic components present in the process tanks, particularly acetone, will persist in the final TRU sludge after vacuum filtration.

Compliance with the WIPP Waste Acceptance Criteria (WIPP WAC) and the TRUPACT Authorized Methods for Payload Control (TRAMPAC) bans shipping explosives and compressed gases to WIPP and specifies that potentially flammable organic compounds shall be limited to 500 ppm in the headspace gas—a concentration well below the lower limit of flammability or explosibility for organic compounds that may be present.

The bin experiments (Molecke, 1990a) are designed to determine gas generation rates for various waste forms. Scheduled analyses of the headspace gas includes monitoring the amount of hydrogen, methane, and oxygen and potentially flammable compounds including acetone in addition to other non-flammable organic compounds. Analyses of leachate samples from the "drum scale" and "liter scale" experiments described by Lappin (1990) can provide an estimate of the organic compounds dissolved in the leachate. In addition to evaluating the role of organic compounds in promoting radionuclide solubilities, results of the above analyses are needed to make a responsible assessment of the potential for an explosion due to the accumulation of flammable organic components.

In the bin-scale and alcove-scale test plans, Molecke (1990a & 1990b) has described precautions that will be taken to minimize the possibility of an explosion during the test phase. While the presence of volatile organic compounds will be monitored throughout the test phase, the precautions were primarily intended to address more immediate concerns regarding the generation of hydrogen and methane. The precautions include temperature monitoring, electrical grounding, oxygen monitoring, gas monitoring, and nitrogen purging.

5.2 Recommendations

Adhere to the WIPP WAC and TRAMPAC, which are intended to minimize the risk of explosion during transportation.

Implement the measures outlined by Molecke (1990a & 1990b) to mitigate the risk of explosion during the bin-scale and alcove-scale experiments.

Use the analyses from the scheduled liter-scale, drum-scale, bin-scale, and alcove-scale experiments to determine the amount of volatile flammable organic compounds in the CH-TRU waste forms that can be sent to WIPP. If flammable components are present, then use that information to calculate the potential for explosibility during the operational and long term repository conditions and to estimate the possible consequences of such an explosion.

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7. APPENDICES

7.1 <u>Appendix A</u> - From Brush, 1989, "Organic Compounds Identified in the Preliminary Inventory of Nonradioactive Waste Constituents to be Emplaced in the WIPP."

FROM BRUSH, 1989

TABLE 7.2 ORGANIC COMPOUNDS IDENTIFIED IN THE PRELIMINARY INVENTORY OF NONRADIOACTIVE WASTE CONSTITUENTS TO BE EMPLACED IN THE WIPP[1, 2]

Acids, Organic

- Acetic acid
- Ascorbic acid
- Citric acid
- DHP[3]
- α-hydroxyisobutyric acid
- Lactic acid
- Oxalic acid

Alcohols and Glycols

- Butanol
- Ethanol
- 2-ethyl-1-hexanol
- Glycerin
- Isopropanol
- Methanol
- Polyethylene glycol

Aldehydes

- Formaldehyde

Amides

- Acetamide

Amines, Aliphatic and Aromatic

- Adogen-364-hp(tri-laurylamine)
- Hydroxylamine

Azo Compounds, Diazo Compounds, and Hydrazines

- Hydrazine
- Hydrazine mononitrate

Esters

- Amyl acetate

TABLE 7.2 ORGANIC COMPOUNDS IDENTIFIED IN THE PRELIMINARY INVENTORY OF NONRADIOACTIVE WASTE CONSTITUENTS TO BE EMPLACED IN THE WIPP (cont.)

Halogenated Organics

- Bromoform
- Carbon tetrachloride
- Chloroform
- Dichloroethane
- Methylene chloride
- Tetrachloroethylene
- Trichloroethane
- 1,1,1-trichloroethane
- Trichloroethylene
- 1,1,2-trichloro-1,2,2-trifluoroethane

Hydrocarbons, Aliphatic, Saturated

- Decane
- N-dodecane
- Hexane
- Kerosene
- Nonane
- Pentane
- Petroleum ether
- Octane
- Oils (C6 to C20)

Hydrocarbons, Aliphatic, Unsaturated

- Butadiene
- Styrene

Hydrocarbons, Aromatic

- Diethyl benzene
- Diisopropylbenzene
- Ethyl benzene
- Toluene
- Xylene

Isocyanates

- Ammonium thiocyanate

TABLE 7.2 ORGANIC COMPOUNDS IDENTIFIED IN THE PRELIMINARY INVENTORY OF NONRADIOACTIVE WASTE CONSTITUENTS TO BE EMPLACED IN THE WIPP (cont.)

Ketones

- Acetone
- 2-5-di-tert-butyl-hydroquinone
- Methyl acetone
- Methyl ethyl ketone
- Methyl isobutyl ketone
- Thenoylfluoroacetone

Nitro Compounds

- Nitrocellulose
- Urea nitrate

Organophosphates, Phosphothioates, Phosphodithioates

- TBP[4]
- TOPO[5]

Phenols, Cresols

- Picric acid

Polymerizable Compounds

- Epoxy

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1. From Drez and James-Lipponer (1989).
2. Most of these organic present in trace amounts only.
3. Di(2-ethylhexyl)-phosphoric acid.
4. Tributyl phosphate.
5. Tri-n-octylphosphine oxide.

7.2 <u>Appendix B</u> - From Molecke, 1990a,"WIPP Test Gases to be Quantified."

FROM MOLECKE, 1990a

Table 11.1 WIPP Test Gases To Be Quantified

Hydrogen *	VOCs:
Oxygen *	Freons
Carbon Dioxide *	Xylenes, Mixed
Carbon Monoxide *	Cyclohexane
Methane *	Carbon Tetrachloride
Water Vapor *	Dichloromethane
(for humidity, 100 ppm)	Trichloroethylene
Neon (Tracer) *	1,1,1-Trichloroethane
Other Tracer Gases *	1,2-Dichloroethane
(and isotopic ratios)	1,1,1-Trichloro-
Argon (mostly alcoves)	1,2,2-Trifluoroethane
Nitrogen (mostly bins)	Perchloroethane
Hydrogen Sulfide	Methyl Alcohol
Nitrogen Oxides	Butyl Alcohol
Ammonia	Acetone
Hydrogen Chloride	Others, as detectable
Radon	(at > 1 ppm)

[* = major gas, generated or other]

7.3 <u>Appendix C</u> - From Molecke, 1990b, "WIPP Test Gases to be Quantified."

FROM MOLECKE, 1990b

Table 12.2 WIPP Test Gases To Be Quantified

Hydrogen *	VOCs:
Oxygen *	Carbon Tetrachloride
Carbon Dioxide *	1,1,1-Trichloroethane
Carbon Monoxide *	Dichloromethane
Methane *	Freon 113 (& others)
Water Vapor *	Trichloroethylene
(for humidity, 100 ppm)	1,2-Dichloroethane
Neon (Tracer) *	1,1,1-Trichloro-
Other Tracer Gases *	1,2,2-Trifluoroethane
(and isotopic ratios)	Perchloroethane
Argon (mostly alcoves)	Xylenes, Mixed
Nitrogen (mostly bins)	Cyclohexane
Hydrogen Sulfide	Methyl Alcohol
Nitrogen Oxides	Butyl Alcohol
Ammonia	Acetone
Hydrogen Chloride	Others, as detectable
Radon	(at > 1 ppm)

[* = major gas, generated or other]

7.4 <u>Appendix D</u> - From FSEIS, 1990, "Hazardous chemical constituents reported in CH-TRU mixed waste for which no estimates on concentrations are available."

FROM FSEIS, 1990

TABLE 5.32 Hazardous chemical constituents reported in CH TRU mixed waste for which no estimates on concentrations are available[a]

Metals[b]	Organics[b]
Arsenic	Tetrachloroethylene
Barium	Acetone
Chromium	
Mercury	
Selenium	
Silver	
Beryllium	

[a] Information obtained from the "Radioactive Mixed Waste Compliance Manual," (WEC, 1989).

[b] Based on knowledge of the waste and/or the processes that generate it.

7.5 Appendix E - From FSEIS, 1990, "Estimated concentrations of hazardous constituents in TRU mixed waste from the Rocky Flats Plant."

FROM FSEIS, 1990

TABLE 5.31 Estimated concentrations of hazardous constituents in TRU mixed waste from the Rocky Flats Plant [a]

Hazardous constituent	Minimum	Maximum
	mg/kg	
1,1,1-trichloroethane	15	150,000
Trichloroethylene[b]	15	150,000
Carbon tetrachloride	25	50,000
1,1,2-trichloro-1,2,2-trifluoroethane	75	50,000
Methylene chloride	50	750
Methyl alcohol	0	25
Xylene	0	50
Butyl alcohol	0	10
Cadmium	0	10
Lead	0	1×10^6

[a] Rockwell International, 1988.

[b] No estimates were available on the total concentration of trichloroethylene. Based on knowledge of past industry practice, the concentration was assumed to be equivalent to that of 1,1,1-trichloroethane.

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