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(a) Author (Print/Sign): J. E. Meacham	J E Meacham	Date: 5/23/2006
(b) Responsible Manager (Print/Sign): S. M. MacKay	S MacKay	Date: 5/25/2006
(c) Reviewer (Optional, Print/Sign): T. J. Anderson	Thomas Anderson	Date: 5/23/2006
(d) Reviewer (Optional, Print/Sign):		Date:

(12) Distribution:

(a) Name	(b) MSIN	(a) Name	(b) MSIN
J. O. Honeyman		S. J. Eberlein	
J. E. Meacham		S. M. MacKay	
J. L. Huckaby		M. L. Zabel	
D. F. Farler		D. J. Washenfelder	

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INDUSTRIAL HYGIENE CHEMICAL VAPOR TECHNICAL BASIS

J.E. Meacham
CH2M HILL Hanford Group, Inc.
Richland, WA 99352
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Abstract: This document updates and consolidates technical information related to the Industrial Hygiene Chemical Vapor Program at the Hanford Site. Technical studies and evaluations are summarized and sampling results from potential vapor sources are examined to produce a list of Chemicals of Potential Concern (COPC).

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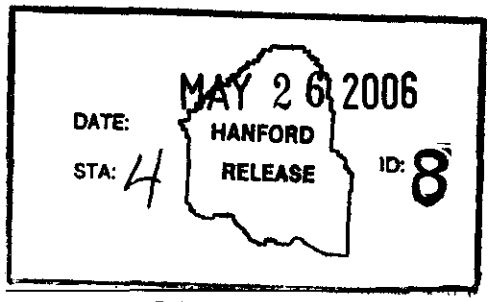

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INDUSTRIAL HYGIENE CHEMICAL VAPOR TECHNICAL BASIS

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
Office of River Protection under Contract DE-AC27-99RL14047

CH2MHILL
Hanford Group, Inc.
P.O. Box 1500
Richland, Washington

RPP-22491
Revision 1

INDUSTRIAL HYGIENE CHEMICAL VAPOR TECHNICAL BASIS

J. E. Meacham
J. O. Honeyman
T. J. Anderson
M. L. Zabel
CH2M HILL Hanford Group, Inc.

J. L. Huckaby
Pacific Northwest National Laboratory

Date Published
May 2006

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Office of River Protection under Contract DE-AC27-99RL14047

CH2MHILL
Hanford Group, Inc.
P.O. Box 1500
Richland, Washington

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EXECUTIVE SUMMARY

The Industrial Hygiene Technical Basis purpose is to identify all chemicals within a waste vapor source (i.e., tank headspaces, ventilation stacks and the 242-A Evaporator) that are potentially hazardous and might be released into worker breathing zones. It provides the Industrial Hygiene program with the basis to make decisions and set controls that ensure worker protection.

The approach assesses gases and vapors generated by ongoing waste decomposition, release mechanisms from the waste to tank headspaces, behavior of gases and vapors in tank headspaces, discharges of the headspace atmosphere through breather filters and stacks to the environment, and environmental effects on chemical vapor concentrations. CH2M HILL Hanford Group, Inc. technical expertise was augmented with tank chemistry and toxicology experts. An Independent Toxicological Panel of nationally recognized toxicology and industrial hygiene experts reviewed and validated the methodology used and particularly, the toxicological basis for preparation of the Chemicals of Potential Concern (COPC) list.

Headspace gas and vapor origins are understood and can be related back to chemicals placed into tanks and their degradation chemistry. Concentrations are determined by dynamic competition between evolution from the waste and removal by ventilation or other means. Absent waste-disturbing activities, changes are slow, and there are no large, rapid changes in headspace concentrations. Headspace concentrations do vary over months and years, but sampling results indicate that 95% of the chemicals in a passively-ventilated single-shell tank (SST) vary by less than a factor of three. Most SST headspaces have been sampled (118 of 149), and similarities between sampled tanks suggest that the non-sampled SSTs have similar compositions.

Headspace characterization provides a large body of information about the identities and concentrations of the waste gases and vapors. Sampling and analyses have progressed sufficiently to identify and evaluate a broad range of chemicals. Characterization data maintained in the Tank Characterization Database (TCD) are based on appropriate sampling and analytical methods, and these data were used to identify chemical species and estimate concentrations to be expected in tank headspaces. Headspace gases are released via breather filters and other penetrations in tanks and might enter worker breathing zones.

Dispersion modeling indicates that SST headspace and double-shell tank stack chemical concentrations would be diluted up to several orders of magnitude after traveling five or more feet from the source. Worker breathing zone data (area samples and personal monitoring) indicate that gas and vapor concentrations are orders of magnitude lower than concentrations found in tank headspaces, consistent with the dispersion modeling results. Most tank headspace chemicals present in the worker breathing zones are below sampling and analytical detection limits and those chemicals that have been detected are well below occupational exposure limits. Sampling and analytical detection limits are established by evaluating the Occupational Exposure Limits for those chemicals that might be present in the workplace to provide assurance that all hazardous or potentially hazardous chemicals would be detected if present.

Volatile waste chemicals were evaluated for their potential hazard to workers. The evaluation was comprehensive and addressed all chemicals reported in tank headspace and ventilation system samples, volatile chemicals reported in liquid and solid waste samples, and chemicals identified as potentially present in the tank headspaces but not reported because of sampling and/or analytical limitations. Forty-eight chemicals have been detected at tank farm sources at greater than 10% of the Occupational Safety & Health Administration Permissible Exposure Limits, American Conference of Governmental Industrial Hygienists Threshold Limit Values, or Hanford Site Tank Farms Acceptable Occupational Exposure Levels were placed on the COPC list.

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LIST OF TERMS

Abbreviations and Acronyms

ACGIH	American Conference of Governmental Industrial Hygienists
ACLs	Administrative Control Limits
AIHA	American Industrial Hygiene Association
AOEL	Acceptable Occupational Exposure Level
BDGRE	Buoyant Displacement Gas Release Event
CAS	Chemical Abstracts Service
CH2M HILL	CH2M HILL Hanford Group, Inc.
CNFE	Chemicals Needing Further Evaluation
COPC	Chemicals of Potential Concern
CSF	Cancer slope factor
DOE	U.S. Department of Energy
DRI	Direct Reading Instrument
DST	Double-Shell Tank
EAS	Exposure Assessment Strategy
EASRG	Exposure Assessment Strategy Review Group
EPA	U.S. Environmental Protection Agency
GC	Gas chromatograph
GRE	Gas Release Event
IARC	International Agency for Research on Cancer
ICP	Induced coupled plasma
ICP-MS	Induced coupled plasma mass spectroscopy
IH	Industrial Hygiene
ISS	In situ sampling
ISVS	In situ vapor sampling
ITP	Independent Toxicological Panel
LFL	Lower Flammability Limit
LOEG	Lowest Occupational Exposure Guideline
LOEL	lowest-observed-effect-level
MF	Modifying factor
MS	Mass spectrometer
NAS	National Academy of Sciences
NOEL	No-observed-effect-level
NEVS	Non-Electrical Vapor Sampling
NIOSH	National Institute for Occupational Safety and Health
NPH	Normal Paraffin Hydrocarbon
OA	U.S. Department of Energy Office of Independent Oversight and Performance
OEL	Occupational Exposure Limit
OSHA	Occupational Safety and Health Administration
PEL	Permissible Exposure Limit
PNNL	Pacific Northwest National Laboratory
POD	Point of Departure

PUREX	Plutonium Uranium Extraction
REDOX	Reduction-Oxidation
REL	Recommended Exposure Limit
RfC	Reference concentration
SST	Single-Shell Tank
STEL	Short-Term Exposure Limit
TBP	Tributyl phosphate
TCD	Tank Characterization Database
TEEL	Temporary Emergency Exposure Limit
TIC	Tentatively identified compound
TLV	Threshold Limit Value
TWA	Time-Weighted Average
TWINS	Tank Waste Information Network System
UF	Uncertainty Factor
VOA	Volatile Organic Analyte
VOC	Volatile Organic Compound
VSS	Vapor Sampling System
WEEL	Workplace Environmental Exposure Level

Units

cm	centimeters
ft	feet
ft^2	square feet
ft^3	cubic feet
°C	degrees Celsius
g/mol	grams per mole
hr	hour
kg	kilograms
L	liters
m	meters
m^3	cubic meters
mg	milligrams
min	minute
mm	millimeters
µg	microgram
ppbv	parts per billion by volume
ppmv	parts per million by volume
pptv	parts per trillion by volume
s	second
yr	year

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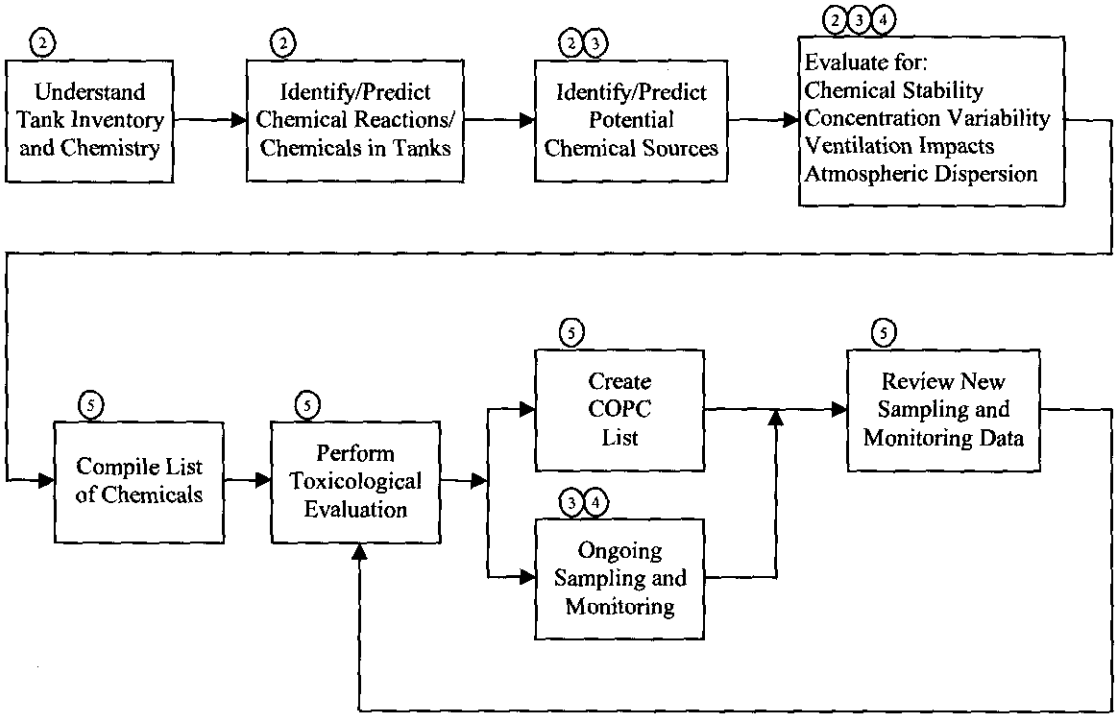
1.0 INTRODUCTION

1.1 PURPOSE

The primary purpose of the Industrial Hygiene Technical Basis is to identify all tank vapor chemicals that are hazardous or might be hazardous in tank headspaces and could reasonably be postulated to be released into worker breathing zones. Given this information, the CH2M HILL Hanford Group Inc. (CH2M HILL) Industrial Hygiene organization has identified what must be sampled or monitored in the workplace; and can confidently answer the question "have you looked for everything that might be harmful in the workplace?" This document summarizes results of several technical studies and evaluations to update the Industrial Hygiene Technical Basis. Conclusions were evaluated and applied to enhance the Industrial Hygiene (IH) program hazard communication and worker training. Periodic updates will occur as more evaluations are conducted and field experience is gained. Figure 1-1 summarizes the IH technical basis approach.

Figure 1-1. Industrial Hygiene Technical Basis Approach



Note: Numbers above the boxes in the chart refer to the section relevant to that topic.

1.2 BACKGROUND

A comprehensive effort began in September 2003 to improve the technical basis supporting the IH program. Improvements focused on limiting tank farm worker exposures to as low as reasonably achievable and evaluation of the following:

- Selection and implementation of engineering controls,
- Improvements to the IH Exposure Assessment Strategy (EAS),
- Improvements to training, and
- Improvements to worker communications.

In February 2004, a decision was reached to produce this document to accomplish the following goals:

- Consolidate and update, as necessary, technical information needed by IH personnel that had not been readily available or user friendly;
- Provide a better correlation between technical data and rationale for exposure assessment strategies;
- Provide a greater degree of confidence in the characterization data used for the IH program;
- Develop and document a technically sound basis for selecting a list of chemicals of potential concern (COPC) to the IH program, demonstrating conservatism, compliance with U.S. Department of Energy (DOE) orders, regulations, and industry standards; and to using technically sound standards where no established guidelines existed;
- Improve worker confidence in the EAS basis; and
- Document key information for use in worker training and hazard communications.

This need was reinforced during discussions with the DOE Office of Independent Oversight and Performance Assurance (OA) during a management assessment of the IH program conducted by OA from February to April 2004. The OA assessment team identified the need for a technical basis as an important part of improving the IH program. In Section C.2.1 (page 24) of its April 2004 "Investigation of Worker Vapor Exposure and Occupational Medicine Programs at the Hanford Site" (OA 2004), OA stated:

During April 2004, CH2M HILL recognized the value of developing a technical basis for the tank vapor source, and initiated the development of an ongoing program for headspace vapor characterization.

This document was initially completed in October 2004, and this is the first revision. The following was done to prepare and revise this document:

- Developed a team of workers, engineers, industrial hygienists, and managers to identify, evaluate, and document all key aspects of the technical basis needing revision;
- Engaged Pacific Northwest National Laboratory (PNNL) to perform toxicological evaluation of chemicals and provide technical support in the area of tank chemistry;
- Engaged Dr. Leon Stock (see biography in Appendix A), outside consultant, to provide expert advice in the area of tank waste chemistry (i.e., nuclear and organic chemistry);
- Engaged Dr. Carl Mackerer (see biography in Appendix A) to evaluate hydrocarbon mixture synergistic effects and establish appropriate occupational exposure levels.
- Continued use of an independent panel (see panel biographies in Appendix A) of nationally recognized experts in toxicology and IH to (1) review and validate methodologies used to screen chemicals and develop Acceptable Occupational Exposure Levels (AOELs), and (2) review sampling/monitoring plans and results.

Completion of this document met the established objectives and OA commitments. Control and future updates of this document are under the purview of the CH2M HILL Industrial Hygiene organization and its successors.

1.3 CONCLUSIONS

"Conclusions" are results of technical studies which form the basis for establishing IH program controls. Each section includes conclusions resulting from that section while overall conclusions are presented in Section 6.

2.0 GAS AND VAPOR SOURCES AND DYNAMICS

Hanford Site processes associated with chemical separation of plutonium from uranium and other fission products produced a variety of volatile, semi-volatile, and nonvolatile organic and inorganic waste chemicals that were sent to the waste tanks. These chemicals have undergone and continue to undergo radiolytically and thermally induced chemical reactions in the tanks, producing a wide variety of degradation reaction products. Many of the degradation products are nonvolatile and remain in the solid and liquid waste phases, but others are volatile and may be released from the waste into the tank headspaces and eventually into the tank farm atmosphere and possibly worker breathing zone as gases and vapors.

This section provides an overview of the origin of volatile waste species, transport in the waste and release into the tank headspaces, dynamics within the headspaces, and potential releases from the 242-A Evaporator. Understanding the types of chemicals and mechanisms for gases and vapors to enter the worker breathing zone is critical for defining and maintaining an IH program.

2.1 GAS AND VAPOR SOURCES

Volatile and semi-volatile gases and vapors evolve continuously from tank wastes. Headspace gas and vapor concentrations are a function of waste chemistry, temperature, tank ventilation, and waste-disturbing operations. The following sections describe the process wastes, the ongoing chemical reactions that occur in the waste that produce gases and vapors, and some compounds that cannot be definitively tied to process wastes or their degradation products.

2.1.1 Process Wastes

Several waste-generating processes were operated at the Hanford Site, including the following:

- Bismuth phosphate,
- Uranium recovery process,
- Reduction-oxidation (REDOX),
- Waste fractionation,
- Plutonium-uranium extraction (PUREX), and
- Processes conducted at the Plutonium Finishing Plant.

The primary goal of these processes was to extract and/or process plutonium or separate other selected radionuclides from the waste (strontium, cesium, cerium, neptunium, and americium, among others). Each of the waste-generating processes had a variety of waste streams (at least 49 different types have been identified). Of those streams, the following broad categories can be established:

- Cladding (or coating) waste from the removal of the fuel element cladding,

- Metal waste from the processing of the fuel itself to remove the plutonium or other fissile material,
- Decontamination waste from systems cleanout (e.g., from N Reactor), and
- Other miscellaneous waste (e.g., laboratory waste).

After initial storage in the tanks, various other operations were performed on the waste in the tanks, including removal/recovery of various materials (e.g., uranium, strontium, and cesium); evaporation; solidification; and settling. The principal organic compounds sent to the waste tanks can be divided into two classes: (1) complexants (for chelating divalent, trivalent, and tetravalent cations), and (2) extractants and their associated diluents.

The principal organic complexants were glycolic acid, citric acid, hydroxyethylethylenediaminetriacetic acid, and ethylenediaminetetraacetic acid. Besides these complexants, others including nitrilotriacetic acid and oxalic acid were used, but the quantities were relatively small and were not well-documented. RPP-21854 provides a review of these complexants and the quantities used.

Tributyl phosphate (TBP) mixed with diluents was the principal organic extractant used to separate plutonium and uranium from spent nuclear fuels. Bis(2-ethylhexyl) phosphate was also used as an extractant and is found in the solid waste but not in tank vapors (RPP-21854). Diluents included Shell E-2342, Soltrol-170, and normal paraffin hydrocarbon (NPH). During normal operations in the PUREX Plant, the TBP/diluent mixture was washed to remove contaminants and recycled. The aqueous wash solution, which contained entrained organic diluent and dissolved degradation products (e.g., butanol and dibutyl phosphate), was sent to the Tank Farms.

Operations (e.g., tank-to-tank waste transfers, evaporator campaigns) have spread organic complexants and solvents throughout the single-shell tank (SST) and double-shell tank (DST) farms, and nearly all tank headspaces have some organic compounds present. These organic compounds and their degradation products are the primary sources of gases and vapors. See Section 2.1.2 for details about the organic compounds and their degradation products.

2.1.2 Chemical Generation and Storage

Gases and vapors found in the tank headspaces can be traced back to the following sources (RPP-21854):

- Chemicals used during large-scale plant operations,
- Support activities to the large-scale plant operations, and
- Ongoing chemical and radiolytic reactions.

Fragments of the original organics, including the homologous series of several classes of organic chemicals, remain in the waste. Identified compounds and compound families include the following:

- Alkanes,
- Alkenes and alkadienes,
- Cyclic hydrocarbons,
- Benzene and benzene derivatives,
- Alcohols and ethers,
- Aldehydes and ketones,
- Acids and esters,
- Amines and amides,
- Other nitrogen compounds (e.g., nitroso and nitro compounds),
- Heterocycles,
- Halogen-containing compounds,
- Metals and organometals, and
- Sulfur and silicon containing organic compounds.

Oxidation is initiated by radioactive decay processes involving free radicals, radiation assisted thermal chemical reactions, and thermally induced chemical reactions that do not involve free radicals. The decay processes produce ammonia, hydrogen atoms, hydroxyl radicals, nitric oxide, and nitrogen dioxide. Similar radical reagents are also obtained by thermal reactions. These reactive substances transform the organic constituents into organic radicals. The radicals react with oxygen and other radicals to give organic intermediates and products that, in turn, react with ionic reagents to yield different products. These reactions occur in parallel, and many different products are obtained. Generally, the organic intermediates formed in the initial reactions are more reactive than the compounds from which they were formed. Volatile organic compounds are obtained in both the beginning and later stages of the chemistry.

Many substances like formaldehyde are continuously formed and destroyed, resulting in small but non-zero quasi-steady state concentrations. Even though formaldehyde is almost completely converted to a much less volatile hydrate, it appears in the headspaces of some tanks. This phenomenon can be explained by recognizing that the constituents in the waste tanks are not in thermodynamic equilibrium. Even when rapidly converted into nonvolatile forms, the volatile intermediate forms can evaporate from the aqueous solution, micelles, or organic films into the headspace.

Chemical reactions produce one- and two-carbon compounds that might not have been well characterized by past sampling and analytical methods. Appendix B presents plausible compounds and evaluates the compounds to determine if any should be added to the COPC list. Evaluations indicated that source sampling should be conducted for only three compounds, methylamine, dimethylamine, and ethylamine. All others were either amenable to past/current sampling and analytical methodologies, or judged too unstable to exist at significant levels in the worker breathing zone.

Metal species that might be present in addition to mercury and dimethyl mercury were evaluated. A focus group of senior chemists postulated what four types of volatile inorganic compounds could be evolved by the wastes, alkyl, carbonyl, halide, and nitroso metal compounds (TWS05.019 - Letter). Sulfides and hydrides had already been reported in tank headspaces (e.g.,

hydrogen sulfide), so these were included in the evaluation. A list of possible volatile metal compounds was produced by reviewing constituents found in tank waste and then examining thermodynamic chemical electronic databases and other thermodynamic literature. The list included arsenic, antimony, lead, molybdenum, ruthenium, selenium, tin, tellurium, and tungsten (TWS05.019 - Letter).

2.1.3 Other Chemicals

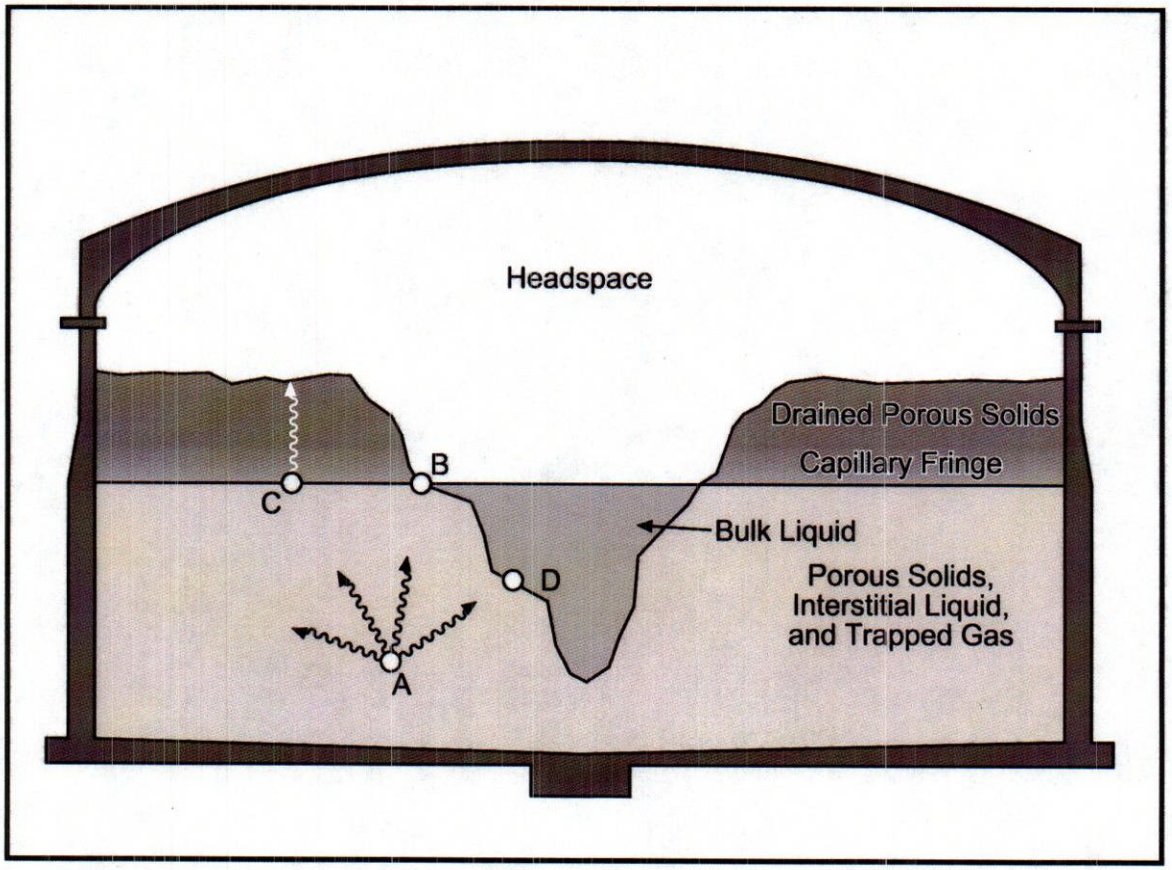
Not all of the gases and vapors detected in headspace samples have direct or established associations to the Hanford Site separations processes or their degradation products. There are a variety of freons and other halogenated compounds whose origins are not well-established, as well as a small number of specialized organic chemicals associated with specific commercial operations. Some, such as Freon 11 (trichlorofluoromethane), are very commonly observed; Freon 11 has been unambiguously identified (at low concentrations) in most passively-ventilated tank headspaces.

2.2 TRANSPORT AND RELEASE MECHANISMS

Volatile compounds stored or generated in the tank wastes must first be transported through any overlaying waste before they are released into the headspace. The transport rate of any given volatile waste chemical to the headspace depends on (1) its location in the waste, and (2) the configuration of waste it must pass through to reach the headspace. The transport rate also depends on the chemical nature of the volatile species (e.g., its solubility in waste liquids), because this generally dictates the transport mechanism for a given waste configuration.

An overview of the mass transfer of volatile waste species to the headspace is depicted in Figure 2-1. Figure 2-1 shows that volatile waste species stored or generated in a region of settled solids at Point A may migrate to the headspace through different paths. Migration through the settled solids region may take the species directly to the surface of the waste (Point B), to a drained region of solids (Point C), or to a region of bulk liquid (Point D).

Figure 2-1. Schematic of Tank Waste and Possible Mass Transfer Paths



While thermally-induced convection of the interstitial liquid in the porous solids is possible (TWS02.074 - Letter), the dominant mechanism of transport through the settled solids is thought to be either liquid-phase diffusion or bubble migration (PNNL-14831). Chemicals that are soluble in the interstitial liquid tend to be transported via diffusion through the liquid. Chemicals that are highly insoluble in the interstitial liquid tend to diffuse through it very slowly, and insoluble gases (e.g., hydrogen, nitrogen) are typically transported more by bubble migration than by diffusion. The release of these gases also enables the simultaneous release of volatile and semi-volatile organic compounds.

Whether via diffusion or bubble migration, the transfer of a volatile species through the interstitial liquid in the settled solids region tends to be the rate-limiting step in the process of releasing the chemicals into the headspace. Diffusion through the drained porous solids (between Point C and the headspace in Figure 2-1) is relatively fast, because gas-phase diffusion through the pores is generally much faster than liquid-phase diffusion. Chemical transport within a bulk liquid waste (between Point D and the headspace) also tends to be faster than the transfer through interstitial liquid, because bulk waste liquids are generally convectively mixed by thermal gradients.

Note that because of their differing solubilities in the interstitial liquid, nonpolar organic waste chemicals are not transported through the settled solids as readily as polar waste chemicals. Therefore, the quiescent headspace concentrations of nonpolar chemicals may not be representative of the inventory of those chemicals in the waste. Waste-disturbing activities, in particular waste retrieval, can be expected to significantly alter the headspace composition, both the absolute concentrations and the ratios of one chemical to another.

Tanks with settled solids and liquid supernatant layers can accumulate significant amounts of trapped gas. The trapped gas bubbles are primarily composed of hydrogen, nitrogen, and nitrous oxide, with lower levels of ammonia, methane, and carbon dioxide, along with trace levels of organic vapors (PNNL-13000). Under certain conditions, large amounts of this trapped gas can be spontaneously released, temporarily raising the concentrations of the bubbles' constituents in the headspace (PNNL-13781). From the perspective of the potential impact on the worker breathing zone, it is important to note that large gases release events do not occur in the passively-ventilated SSTs. A physical criterion for the large spontaneous gas releases is a significant layer of supernatant liquid, and the supernatant liquids have been drained from the passively-ventilated SSTs. Gas release events in the DSTs were extensively studied in the 1990s for their potential to reach flammable conditions in the headspaces, and controls are now in place to preclude the waste configurations and conditions that can lead to large gas release events.

2.3 HEADSPACE DYNAMICS

Air in the waste tank headspaces tends to be relatively well-mixed by convection. Temperature differences between the waste surface and tank dome produce a corresponding difference in the density of the air, which in turn induces convection within the headspace. The temperature differences are inherent to almost all of the tanks; the waste itself is heated by radioactive decay and its surface is warmer than the tank dome. Air near the waste surface is warmed by the waste and rises, displaced by air that has been cooled by contact with the tank dome. This thermally induced convection mixes the gases and vapors vertically and horizontally throughout the convective zone.

Studies employing numerical modeling and semi-empirical relationships have concluded that transport and mixing of gases and vapors in the convection zone are rapid compared with their release from the waste surface, making concentration gradients within the convection zone negligible (WHC-SD-WM-ER-344; WHC-SD-WM-SARR-001; FAI/95-63; PNNL-11640). The conclusions of those studies are supported by tests performed in tanks 241-C-103 and 241-C-111 (WHC-EP-0780; WHC-SD-WM-TP-254); a tracer gas experiment conducted to evaluate the speed of mixing (PNNL-11683); and a series of multi-riser, multi-level headspace samples collected from three relatively cool tanks (PNNL-13029).

Convective mixing of the headspace air ensures that samples collected from the bulk region of the headspace will be representative (assuming samples are not collected in a downdraft of incoming air). Convective mixing also ensures that small episodic gas releases from the waste will be quickly diluted within the headspace.

Temperature differences between different regions of the headspace may also induce the condensation of vapors in the warmer, wetter tanks (PNNL-14831). Air warmed and humidified by contact with a wet waste surface rises as it is displaced by cool air from the region near the tank dome. The rising moist air is itself cooled by contact with the tank dome, and if it is cooled below its dew point temperature, some of the water vapor will condense on the dome. Condensate accumulates and drains off the curved dome to the walls or risers, or may drip directly from the dome itself, and eventually return to the waste. While this phenomenon is probably limited to water vapor and that in and of itself is of no concern in the worker breathing zone, the condensate tends to absorb water-soluble species and may significantly reduce the headspace concentrations of such species (e.g., ammonia).

Convective mixing can also occur within a tank riser, but under certain conditions, the riser might be warmer than the tank headspace air. Mixing would then be primarily through molecular diffusion. Depending on riser length, changes in headspace concentrations would take a few days to three weeks for diffusion to equilibrate concentrations found in the headspace and riser (RPP-19013). There is also the possibility of air leakage into a riser, because it is difficult to hermetically seal a riser. To ensure representative headspace samples, sampling must occur away from air inlets and within the bulk headspace, rather than at existing riser sample ports.

2.4 242-A EVAPORATOR

In the 242-A Evaporator, liquid waste is pumped into a recirculation loop and then passed though a heat exchanger where the waste is warmed before being passed into a vapor-liquid separator. The liquid-vapor separator operates at a temperature of 50 to 60 °C and at a pressure of approximately 60 torr. The evaporator removes the volatile constituents from the liquid waste (e.g., water, ammonia, organic vapors, gases) in proportion to their volatility, and increases the degradation rate of the residual complexants, phosphate esters, and the hydrocarbon diluents because of the temperature increase.

Retained gas sampling indicates that liquid wastes usually retained less than 1% by volume of gas. This retained gas will be promptly released in the evaporator and will have the same composition as the gas in the feed (RPP-21854). The chemical reactions that fragment and oxidize organic constituents will accelerate slightly in the evaporator in proportion with the difference between the temperature in the feed tank and the evaporator. The difference in temperature is too small to cause the onset of unusual chemical reactions, and the slow degradation reactions that occur in the waste tanks will simply increase in the evaporator. The amount of a chemical that is retained in a waste generally exceeds the amount that can be made during an evaporator campaign (RPP-21854).

RPP-21926 evaluated potential vapor emissions from a 242-A Evaporator campaign using evaporator condensate analysis data and the Environmental Simulation Program™ (OLI Systems, Morris Plains, New Jersey) thermodynamic chemical equilibrium model. The modeling suggested several organic and inorganic species could be released at significant concentrations. However, emissions measured during the 242-A Evaporator Campaign 05-01 in March 2005 indicated the earlier model predictions were more than an order of magnitude higher

than actual emissions (RPP-RPT-27963). Sampling and analysis (as described in Section 3.1) was conducted in the feed stack (241-AW), evaporator stack, and receiver stack (241-AP). Only 16 chemicals were detected in the 242-A Evaporator stack. Table 2-1 shows the maximum measured concentrations during the campaign. Ammonia and N-nitrosodimethylamine peak concentrations exceeded their respective Occupational Exposure Limit (OEL)/AOEL in the 242-A Evaporator Stack. Mercury peak concentration exceeded 50% of its OEL.

Table 2-1. Maximum Chemical Concentrations During Evaporator Campaign 05-01

CAS #	Chemical	OEL (ppmv)	Maximum Measured Concentration (ppmv)*		
			241-AW Stack	242-A Stack	241-AP Stack
COPC					
7664-41-7	Ammonia	25	200	275	100
75-07-0	Acetaldehyde	25	1.2	0.098	0.19
123-72-8	Butanal	25	0.34	0.059	<0.01
593-74-8	Dimethyl Mercury	0.00122	<0.00000009	0.00000071	0.00000027
7439-97-6	Mercury	0.0030	0.000026	0.0017	0.000065
50-00-0	Formaldehyde	0.30	0.008	0.002	0.025
67-56-1	Methanol	200	3.9	0.22	2.0
10024-97-2	Nitrous Oxide	50	7.4	3.2	7.9
71-36-3	1-Butanol	20	4.0	0.076	0.71
62-75-9	N-Nitrosodimethylamine	0.00030	0.0023	0.0040	0.0062
Non-COPC					
1333-74-0	Hydrogen	n.a.	38	6.0	240
107-87-9	2-Pentanone	200	0.20	0.021	0.27
64-17-5	Ethanol	1000	0.71	0.069	0.96
71-23-8	n-Propanol	200	0.32	0.022	0.022
1120-21-4	Undecane	n.a.	0.061	0.006	0.036
112-40-3	Dodecane	n.a.	0.092	0.020	ND

Notes: CAS = Chemical Abstracts Service
ND = not detected
n.a. = not available
* Data from RPP-RPT-27963.

2.5 CONCLUSIONS

Headspace gas and vapor origins are understood and can be related back to original chemicals placed into tanks and their degradation chemistry. There are a few chemicals that cannot be directly tied to process wastes or their degradation products.

Concentrations are determined by a dynamic competition between the evolution of chemicals by the waste and their removal by ventilation or other means. Changes tend to be relatively slow, significant changes requiring days or weeks, because the headspaces are large compared to changes in the rates of release from the waste and removal by ventilation. Gases and vapors are released into the tank headspaces at slow rates compared to the rates at which they are convectively mixed within the headspaces. There is no basis for expecting large, rapid changes in the headspace concentrations in any of the passively-ventilated SSTs in the absence of significant waste-disturbing activities (see Section 3.5).

Chemistry occurring within the 242-A Evaporator is comparable to that occurring in the DSTs and emissions from the 242-A stack are similar to that coming from DST stacks. The most recent evaporator campaign indicated that only ammonia, mercury, and dimethyl mercury were at slightly higher concentrations than the concentrations found in the feed and evaporator bottoms stacks.

3.0 MEASURED AND PROJECTED HEADSPACE COMPOSITIONS

Headspace gas and vapor characterization was systematically conducted in the 1990s on those SSTs thought to have the highest concentrations of noxious gases and vapors (WHC-EP-0562). Samples were collected from a majority of the SSTs and analyzed using robust methods that allowed the quantification of the major volatile waste species (e.g., hydrogen, nitrous oxide, ammonia) and the identification of a broad array of trace organic vapors to provide source term data to the IH program (WHC-SD-WM-ER-514). Vapor headspace sampling has continued through the present, and over 2,000 headspace samples have been collected and analyzed since 1994, and over 1,200 organic vapors have been identified in the waste tank headspaces (PNNL-13366). These headspace characterization data indicate the following:

- Which chemicals may be released into the worker breathing zone,
- Identification of tanks from which chemicals may be released, and
- Approximate maximum chemical concentrations at the point of release.

This section provides overviews of vapor sampling basics, sampling media and analytical methods, the characterization data, the observed variability in headspace compositions with time, and a discussion of the effects of waste-disturbing activities.

3.1 VAPOR SAMPLING BASICS

Vapor source characterization is best done by sampling the air inside the headspaces of the passively-ventilated tanks and at the exhaust stacks of the actively-ventilated tanks. Tank headspace air from passively-ventilated tanks should be collected from the headspace itself; far enough below the end of the riser to avoid air drifting down the riser. Samples collected directly from a riser may not be representative of the headspace. Source samples collected at likely points in the worker breathing zone (e.g., at the breather filter) should be accompanied by vapor monitoring (e.g., an ammonia monitor) to demonstrate that tank air was being emitted by the source.

As a general rule, it is desirable to minimize the tubing, valves, filters, etc. between the sampling devices (e.g. sorbent traps, SUMMA[1] canisters, bubblers) and the air being sampled. This reduces the loss of analytes via adsorption onto tubing walls, the filter, etc., and the potential for condensation of water vapor. Sampling manifold components that must be upstream of the sampling devices should be free of contaminants (such as plasticizers, perfluroalkoxy, polyurethane foam; tubing is plasticizer-free) and chosen to minimize adsorption of analytes (e.g., C-Flex® and Tygon® are known to aggressively adsorb many analytes and should not be used). Cleaning of the manifold should be done with consideration of the analytes being sampled and any previous uses of the manifold. To ensure cleaning solvents do not get trapped in valves and at tubing connections, it is advisable to completely dismantle all manifold components before cleaning, and thoroughly dry all components before reassembly.

[1] SUMMA is a trademark of Moletrics, Inc., Cleveland, Ohio.

It is also generally desirable to purge any part of the manifold upstream of the sampling devices with the air being sampled prior to collecting the sample. This serves to replace the air in the manifold with the air being sampled, and conditions the inner surfaces of the manifold so adsorption of analytes from the air being sampled is reduced. The total air volume and duration of the purge depend on the manifold, but should ensure several air-turnovers of the upstream manifold volume and sufficient time for the components in the air to equilibrate with the inner manifold surfaces. Consideration should also be given to potentially deleterious effects of long purges, such as the accumulation of water vapor condensate when sampling humid air.

Quality assurance "blank" samples should be collected based on consideration of the potential contamination of the samples. It is generally advisable to collect ambient air blank samples upwind of source and area samples for each type of sample being collected. When a new or extensive sampling manifold is used between the sampling devices and the air being sampled, upwind ambient air blank samples should also be collected using the complete sampling manifold. (This should be done before actual samples are collected to ensure the blank samples are not affected by fresh contamination of the manifold.) Trip blanks, samples that are carried with the actual samples but not exposed to the air being sampled, should be used periodically to demonstrate that handling and shipment have not altered the samples. Trip blanks can be pre-spiked with analyte (to demonstrate likely losses) or not spiked (to demonstrate contamination was not appreciable).

3.2 SAMPLING MEDIA AND ANALYSIS METHODS

Sampling and analytical methods were chosen to provide the identification and estimation of concentrations for a very broad array of gases and vapors. Using gas chromatography to separate the species and mass spectroscopy to identify and quantify individual analytes allows potentially millions of different organic vapors to be identified from the samples. However, no single sampling device is appropriate for all volatile compounds, and no single analytical system can address all species. The majority of headspace characterization data have been obtained by collecting gas and vapor samples from the tank headspaces, transporting the samples to an established analytical laboratory, and conducting suitable analyses to identify and quantify the species collected. This section discusses the sampling systems, sampling devices, and analyses conducted.

Tank headspace samples have generally been collected using two types of sampling systems. The first type transferred a stream of air from the tank headspace via heated transfer lines to various sampling devices outside of the tank. Only one such system, the Vapor Sampling System (VSS), was deployed. The second type of sampling system avoided the need for heated transfer lines by lowering some of the sampling devices directly into the tank headspace. Several such systems have been deployed including the In Situ Sampling (ISS), In Situ Vapor Sampling (ISVS), and Non-Electrical Vapor Sampling (NEVS) systems. A comparison of sample collection systems conducted on three SSTs over several sampling dates concluded that they gave very similar results (PNNL-11186). The sampling systems deployed at the Hanford Site tanks provide the means for collection of air samples using two types of sampling devices:

SUMMA® canister – A "whole air" sampling device with specially passivated interior surfaces. SUMMA canisters are good for gases and volatile compounds and poor for species that tend to be highly soluble in water (e.g., ammonia).

Sorbent trap – A device that adsorbs gases and vapors of interest onto solid sorbent media as sample air is passed through the device. Sorbent traps are not good for permanent gases, but a wide variety of sorbent traps are available to address specific analytes, and many organic vapors can be addressed with a single multi-sorbent trap.

Volatile metals required a third type of sampling device, a bubbler. Bubblers are common for some applications but have not been commonly used to sample tank vapors. A sampling train was built consisting of tubing and small bubblers containing acidic oxidizing solutions. Air drawn through the train is bubbled through the acidic solution, which absorbs the vapors of interest.

3.2.1 SUMMA Canister Samples

SUMMA canisters are reusable stainless steel vessels that are cleaned and evacuated before each use. Because of their size (the most common size, 6-L, is about 22 cm in diameter), SUMMA canisters are not lowered into the tank headspaces. To collect a headspace air sample, the canister is connected to a tube that extends into the headspace, and a valve on the canister is opened to allow sample air to fill the evacuated canister. To ensure the SUMMA canister is not contaminated with radioactive particulates, the sample air is generally filtered. The effect of the filter was evaluated by PNNL-11186 and determined to be minor. Both the air transfer tubing and the particulate filter are purged before collection of the sample to reduce dilution of sample by the existing air in the system and to reduce the active adsorption sites on the inner walls of the tubing and filter. The sample air flowrate through small diameter tubing to fill the canister is rapid, which limits the loss of analytes by adsorption on the walls of the tubing and filter.

SUMMA canister samples are sent to an analytical laboratory, where small aliquots of the sample air can be withdrawn for analyses by different instruments. Analyses are generally conducted using a gas chromatograph that separates the constituents of the sample and a detection system that indicates the amount of the analyte present. Organic vapors are usually analyzed using a mass spectrometer detector that allows positive identification of any species that have been previously introduced as a standard, and the tentative identification of a large number of other organic vapors using a published library of mass spectral data. Confidence that any given tentatively identified compound has been properly identified tends to go down as its concentration goes down and as the number of possible chemical isomers goes up. Concentrations of targeted analytes are based on a multi-point calibration curve. Concentrations of tentatively identified compounds are estimated by comparing their instrument response to that of chromatographically adjacent internal standards, and generally should be considered only accurate to a factor of two (PNNL-13366).

3.2.2 Sorbent Trap Samples

Sorbent taps are typically one-time use sampling devices that remove and collect the analytes of interest from a stream of sample air. They are typically glass or stainless steel tubes about 0.25-inches in diameter and several inches long, packed with a granular solid sorbent. Variations of this basis design have been used, such as the polyurethane foam sorbent trap used for semi-volatile organic vapors. Specific sorbent traps are deployed to collect ammonia, volatile organic analytes (VOAs), semi-VOAs, dimethylmercury, mercury, formaldehyde, amines, nitrosamines, SO_X, and methylisocyanate.

A measured quantity of sample air is drawn through the sorbent trap, which collects essentially all of the target analyte on the sorbent by physical adsorption, chemisorption, or derivatization. The flowrate of air through the trap must also be limited to ensure essentially all of the analyte is adsorbed, and much of the design of the sampling systems (e.g., VSS, ISVS) is associated with the control and measurement of the sample air flowrate. Many sorbent traps are equipped with two beds of sorbent media, with the second bed being analyzed to demonstrate that the first bed had collected essentially all of the analyte.

The analytes collected on a sorbent trap may be extracted either by solvent (e.g., water is used to extract ammonia from the ammonia traps) or by air (e.g., organic vapors may be extracted by rapidly heating the sorbent traps while ultra clean air is blown backwards through the trap). Analyses of the recovered analyte are then conducted according to standard procedures. The concentration of the analyte is calculated by dividing the mass of analyte collected by the volume of sample air drawn through the trap, so the reported concentration is only as accurate as the measurement of sample air volume.

As with the analysis of organic vapors from SUMMA canister samples, organic vapors extracted from sorbent traps are typically analyzed with a gas chromatograph equipped with a mass spectrometer detector, giving the ability to tentatively identify many organic vapors.

3.2.3 Metals Sampling

Metal and organometallic sampling was performed using a slightly modified U.S. Environmental Protection Agency (EPA) Method 29, *Determination of Metals Emissions from Stationary Sources*. Sixty liters of air exiting the tank risers immediately next to the breather filters were bubbled through two oxidizing acid solutions; the first was an aqueous mixture of 5% HNO_3/10% H_2O_2 and the second was an aqueous mixture of 4% $KMnO_4$/10% H_2SO_4. The oxidizing acid solutions were analyzed for metals using induced coupled plasma mass spectroscopy (ICP-MS), and also subjected to a broad spectrum induced coupled plasma (ICP) analysis.

3.3 SOURCE SAMPLING DATA SUMMARY

Characterization of the waste gases and vapors in the tank headspaces was initiated in the early 1990s to identify noxious species that might be emitted into the worker breathing zone (WHC-EP-0562). Data on noxious species collected before 1993 were from isolated efforts or using sampling systems under development. Headspace characterization data from August 1993 through the present are maintained in the Tank Characterization Database (TCD) and available via the Tank Waste Information Network System (TWINS) network website. The TCD includes headspace data for 118 of the 149 SSTs (see Table 3-1), 20 of the 28 DSTs, as well as multiple sampling events from all five DST ventilation systems.

The highest concentration gases and vapors are inorganic compounds. Hydrogen, ammonia, and nitrous oxide concentrations are generally in the parts per million by volume (ppmv) range, typically higher in the passively-ventilated SSTs and lower in the actively-ventilated DSTs. Organic gases and vapors are present in virtually all of the tanks, though generally at much lower levels than the inorganic waste species. Headspace sampling and analysis has typically targeted about 50 to 65 organic compounds for positive identification and quantitative measurement of their concentrations. Non-target organic compounds were tentatively identified by comparing their observed mass spectra with those in a mass spectral library, and applying both automatic search methods and professional judgment to identify the best match. Experience indicates this method for identification of organic compounds is reasonably reliable for many compounds.

Among the over 1,200 identified organic vapors are roughly 350 alkanes and cycloalkanes; 170 alkenes and alkadienes; 120 alcohols, phenols, and ethers; 120 ketones; 100 heterocyclic compounds (ring compounds containing non-carbon atoms in the ring); 60 halocarbons; over 50 esters; over 40 aldehydes; and over 20 nitriles (PNNL-13366). Results since renewed interest in characterizing tank headspaces in 2004 are consistent with expectations; the measured levels of organic vapors, ammonia, and nitrous oxide were similar to the levels measured in the mid-1990s.

Mercury and dimethyl mercury vapors are prevalent at the evaporators and in the high-level waste tanks at the Savannah River Site (SRS). Experiments performed there showed that dimethyl mercury can be produced at temperatures as low as 40 °C. This prompted sampling for these volatile species at the Hanford Site, despite the general expectation that the small inventory of mercury in the Hanford Site tanks and the chemistry of the waste would be unfavorable to the formation of volatile mercury species. Since 2005, headspace samples have been analyzed for both mercury and dimethyl mercury, using methods identical to those deployed at SRS. Low levels of mercury and dimethyl mercury have been detected in many tank headspace samples. Mercury vapors have been measured in five SST headspaces above OEL concentrations (tanks 241-C-102, 103, 104, 107, and 109). No dimethylmercury source samples have exceeded 10% of its OEL (0.01 mg/m^3), and the maximum ever measured was only about 3% of the OEL (tank 241-U-105).

Table 3-1. Single-Shell Tank Headspace Sampling

Tank #	A Farm	AX Farm	B Farm	BX Farm	BY Farm	C Farm	S Farm	SX Farm	T Farm	TX Farm	TY Farm	U Farm
101	2	2	NA	NA	1	1	2	1	1	1	2	1
102	1	1	1	1	1	3	9	1	NA	1	1	1
103	1	1	2	1	2	10	1	1	NA	1	3	1
104	1	1	NA	6	2	4	1	1	1	1	2	1
105	1	---	1	2	3	3	1	1	NA	1	1	1
106	1	---	NA	2	3	3	1	1	NA	1	NA	2
107	---	---	1	2	2	9	2	1	1	NA	---	2
108	---	---	NA	NA	8	2	1	2	NA	1	---	2
109	---	---	NA	NA	1	3	1	1	NA	NA	---	1
110	---	---	NA	1	1	1	1	2	1	1	---	1
111	---	---	NA	1	2	4	2	1	1	1	---	2
112	---	---	NA	NA	1	2	2	1	NA	1	---	2
113	---	---	---	---	---	---	---	NA	---	1	---	---
114	---	---	---	---	---	---	---	2	---	1	---	---
115	---	---	---	---	---	---	---	NA	---	1	---	---
116	---	---	---	---	---	---	---	---	---	1	---	---
117	---	---	---	---	---	---	---	---	---	1	---	---
118	---	---	---	---	---	---	---	---	---	3	---	---
201	---	---	NA	---	---	1	---	---	NA	---	---	1
202	---	---	1	---	---	1	---	---	NA	---	---	1
203	---	---	NA	---	---	1	---	---	NA	---	---	2
204	---	---	NA	---	---	2	---	---	NA	---	---	2
Total	6 of 6	4 of 4	5 of 16	8 of 12	12 of 12	16 of 16	12 of 12	13 of 15	5 of 16	16 of 18	5 of 6	16 of 16

Note: NA = Not Available.

Special samples have been collected to address selected chemicals that may not be properly measured with SUMMA canister or thermal desorption sorbent trap samples. A sampling effort to determine whether formaldehyde was at measurable levels in the headspaces (despite similar expectations that the chemistry was unfavorable for its release into the headspaces) indicated that formaldehyde was present at average headspace concentrations of 3.3 to 68 ppbv in four 241-C farm tanks. Source sampling for the low-molecular weight amines have thus far shown only methylamine above its OEL (see Section 5 and Appendix C). Nitrosamines have been detected above OEL concentrations also. Source sampling for sulfur oxides (SO_X) have thus far shown concentrations at least two orders of magnitude lower than the OEL. Sorbent traps deployed for methylisocyanate have not detected that compound.

Sampling for metals and organometals was performed on 14 tanks (all six A Farm tanks, all four AX Farm tanks, and tanks 241-C-104, 241-S-101, -102, and -103). Blank corrected results showed near or less than detection limit concentrations (~0.0006 mg/m^3) for the metals analyzed by inductively coupled plasma mass spectroscopy. All samples (including the field blanks) contained small concentrations of calcium, boron, silica, and sodium, common components of the glass containers holding the oxidizing acid solutions. Based on these results, no more metals sampling is planned.

3.4 HEADSPACE VARIABILITY

The applicability of headspace composition data obtained from a given sampling event to estimate what is present in the headspace at any other point in time depends on how much the headspace composition varies with time. The concentration of any given gas or vapor in the headspace of a tank is determined by a competition between the rate that it is generated and evolved by the waste and the rate that it is removed by ventilation. Other potentially important factors may also affect the headspace concentration:

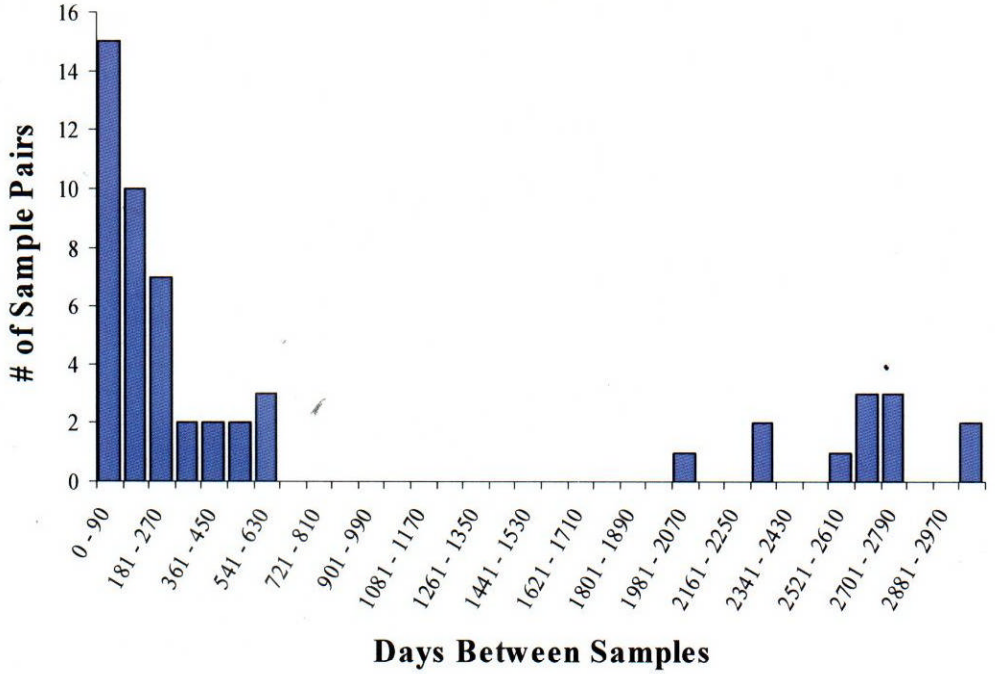
- Absorption of a species by condensate in the headspace (e.g., ammonia vapor is absorbed by water vapor condensate);
- Introduction of waste gases and vapors when air from a connected tank flows into the headspace (e.g., air exchange via a cascade line); and
- Waste-disturbing activities.

Given day-to-day variations in the ventilation rates of the passively-ventilated tanks and the gradually changing waste conditions, it is thought that the compositions of most headspaces are continuously changing. Evidence from tanks that have been sampled on multiple occasions supports this, but does indicate that the variability in composition is limited (PNNL-14831).

Statistical analyses of multiple headspace vapor concentrations taken over time indicate less than an order of magnitude change (RPP-21972). RPP-21972 considered the data from 42 SSTs that had been sampled on more than one occasion and estimated the 95th percentile relative standard deviation for organic vapors, ammonia, hydrogen, and nitrous oxide. Figure 3-1 shows a histogram of days between sampling events.

As indicated in Figure 3-1, roughly half of the sampling event comparisons are less than six months apart, and 12 sampling events are more than five years apart. The overall average organic vapor variability was 126% for triple sorbent traps and 113% for SUMMAs. That is, 95% of the organic chemical maximum measured concentrations would be within a factor of two of the average when measured on different dates. The highest temporal variability was about a factor of three (265% for tank 241-C-107 triple sorbent trap samples). Temporal variabilities for ammonia, hydrogen, and nitrous oxide were even lower: 36, 35, and 49%, respectively. Sorbent trap analytical and sampling variabilities were small (12 and 48%, respectively) compared to temporal variability. SUMMA analytical and sampling variabilities were also small (13 and 37%, respectively) compared to temporal variability.

Figure 3-1. Days Between Sampling Events



Headspace monitoring data collected in the 1990s to verify the headspaces did not spontaneously reach flammable conditions indicate that spontaneous gas release events occurred in certain tanks (HNF-SD-WM-TI-797). Monitoring data suggest that gas releases detected in the passively-ventilated SSTs typically increase the headspace concentration of hydrogen by less than a factor of ten, and much less than a factor of ten when the initial (steady state) concentration of hydrogen was more than 100 ppmv. As was discussed in Section 2.2, these gas releases should have the greatest effect on the headspace concentrations of gases and vapors that are insoluble in the aqueous waste (e.g., hydrogen), so the factor of ten should represent an upper bound on the increases in concentrations of other gases and vapors from small gas releases in SSTs. Large gas releases are not plausible in the passively-ventilated SSTs (PNNL-11391).

Spontaneous buoyant displacement gas release events (BDGREs) in the actively-ventilated DSTs have been extensively studied and controls have been established to prevent the formation of new BDGRE tanks (HNF-SD-WM-TSR-006). The volume of gas released during a BDGRE is small relative to tank headspace volumes. Release volumes were higher in the early 1990s and historical releases (PNNL-11391) averaged less than 27 m^3 for the five (241-SY-101 was remediated) BDGRE tanks (241-AN-103, -104, and -105, 241-AW-101, and 241-SY-103). Headspace volumes in the BDGRE tanks all exceed 1000 m^3 (RPP-10006), which would result in a substantial initial dilution. Any COPC released would be further diluted by roughly a factor of three to seven because all DSTs within a tank farm share the same ventilation system. There is a further dilution of two to three orders of magnitude from the DST stack concentration before any COPC could hypothetically reach the worker breathing zone (see dispersion discussion in Section 4.3).

3.5 EFFECTS OF WASTE-DISTURBING ACTIVITIES

Waste-disturbing activities are defined in the *Documented Safety Analysis* (RPP-13033) and include waste transfers (both into and out of a tank), sluicing, dissolution, and mixer pump operation. Waste-disturbing activities can have a profound temporary effect on headspace concentrations. PNNL-13781 examines the effects of waste-disturbing activities on gas generation, retention, and release. Sluicing of waste with water jets, dissolution, and mixer pump operations were postulated to have the highest potential to release a large fraction of retained gas over a brief time period. Compounds known or expected to exist in the waste but that have not been detected in headspace samples may be released at much higher rates during waste-disturbing activities. Measurements taken during salt well pumping (RPP-7249) indicate that gas releases were proportional to the pumping rate. No large releases were observed during salt well pumping.

When organic liquid wastes such as the extractants and their diluents are retained in the solid layers, their volatile decomposition products may be trapped within the solid matrix. This is important because intrusive operations (e.g., sluicing, mixer pump operation) that disturb the solids can release significant quantities of these trapped volatile species. This phenomenon was demonstrated in the sluicing operations of tank 241-C-106.

Waste retrieval by sluicing was observed to cause organic vapor concentrations in tank 241-C-106 to increase several orders of magnitude (HNF-4261). Tank 241-C-106 contained sludge waste that had contacted organic wash waste. Organic vapor concentrations in the actively-ventilated tank were low before sluicing; however, measurements made during sluicing showed increases up to four orders of magnitude (e.g., undecane was measured at 0.003 mg/m^3 [0.47 ppbv] before sluicing and measured up to 41 mg/m^3 [~6.4 ppmv] while sluicing).

By contrast, flammability data taken during tank 241-S-112 saltcake waste dissolution showed only small increases during waste retrieval. The tank was actively ventilated and flammability levels were mostly below 1% of the lower flammability limit (LFL); peak measurements were only a couple of percent of the LFL.

Organic concentrations during initial waste retrieval in tank 241-C-103 were considerably different than in the pre-retrieval quiescent headspace. Table 3-2 shows a comparison between SUMMA headspace sample results from September 2004 and stack sample results during waste retrieval in November 2005. Tank 241-C-103 was actively ventilated with a portable exhauster at about 780 ft^3/min when the stack samples were taken. Chemicals were at lower concentration in the stack during retrieval with the exception of 2-nitropropane and carbon disulfide.

Table 3-2. Comparison between Ambient Headspace Samples and Stack Samples during Initial Retrieval of Tank 241-C-103

Chemical	Chemical ID	Headspace Concentration (ppmv)	Stack Concentration (ppmv)
1-Butanol	71-36-3	6.5	0.71
2-Hexanone	591-78-6	0.34	0.039
2-Nitropropane	79-46-9	<0.010	0.11
3-Buten-2-one	78-94-4	0.064	0.030
3-Hexanone	589-38-8	0.051	0.009
Butanal	123-72-8	1.8	0.13
Butanenitrile	109-74-0	0.90	0.068
Carbon disulfide	75-15-0	ND	0.013
Methyl benzene	108-88-3	<0.010	0.004
Nitrous oxide	10024-97-2	175	20
Pentanenitrile	110-59-8	0.195	0.068
Propanenitrile	107-12-0	2.1	0.11

Note: ND = not detected.

3.6 CONCLUSIONS

Headspace characterization from the early 1990s to the present provides a large body of information about the identities and concentrations of the waste gases and vapors. Sampling and analyses have addressed a broad range of chemicals that might be present at significant concentrations. Characterization data maintained in the TCD are based on appropriate sampling and analytical methods, and these data can be used to identify chemical species and estimate the concentrations to be expected in tank headspaces.

Although headspace concentrations vary with time, sampling results indicate that 95% of the chemicals in a passively-ventilated SST vary by less than a factor of three. Because most SST waste compositions have changed little over time, it is concluded that the existing headspace characterization data are indicative of the probable identities and approximate concentrations of the tank headspace constituents. Similarities in the compositions of many passively-ventilated headspaces can be used as evidence that the uncharacterized SSTs will have similar compositions.

Waste-disturbing activities can temporarily increase toxic vapor concentrations by exposing/disturbing organic liquid below the waste surface (e.g., as was observed during tank 241-C-106 sluicing). Sampling and monitoring of tanks 241-S-112 and 241-C-103 during retrieval showed a smaller impact on the concentrations of released organic vapors than that observed for tank 241-C-106.

4.0 WASTE GASES AND VAPORS IN THE WORKER BREATHING ZONE

Gases and vapors that accumulate in tank headspaces are released to the atmosphere and the worker breathing zone by ventilation. The DSTs are actively ventilated with mechanical exhausters that ensure waste gases and vapors are released at a defined point well above the worker breathing zone. The inactive SSTs are each passively ventilated to the atmosphere via filtered ventilation risers at rates that vary with local meteorological conditions, while portable exhausters are added to SSTs before and during waste retrieval. This section discusses the mechanisms by which waste gases and vapors are released to the atmosphere and how they are dispersed and diluted within the worker breathing zone.

4.1 ACTIVE VENTILATION

Active ventilation is applied to the headspaces of all DSTs and any SST that are undergoing waste retrieval operations. When active ventilation is lost due to exhauster problems, the affected tanks are passively ventilated via their filtered air inlets. Without the exhauster to provide a slight negative pressure in the headspace, fugitive emissions may occur from other points. However, both the filtered and fugitive emissions will initially be at the low headspace concentrations associated with active ventilation. Concentrations in DSTs tied to this shutdown exhauster will increase until it reaches equilibrium concentrations expected to be similar to SST headspaces. This process would take several months.

The release points (stacks) of the actively-ventilated waste tanks are elevated to reduce the amount of noxious gases and vapors in the worker breathing zone, and the velocity of the exhaust air does enhance mixing and dilution in the atmosphere. Because the rates that noxious gases and vapors are released from the waste are usually independent of their headspace concentrations, active ventilation also ensures their continuous dilution within the headspaces.

It should also be recognized that not all DST ventilation systems perform all of the same functions. In some farms, substantial dilution is achieved by inlet of ambient air and exhaust from forced ventilation stacks. In the combined AY/AZ system (701-AZ), a substantial portion of the ventilation air is recycled, with a small purge volume discharged for a forced ventilation stack. Headspace and discharged concentrations should be proportionally higher due to the smaller dilution air.

4.2 PASSIVE VENTILATION

Each of the 149 SSTs is equipped with a filtered ventilation riser to allow air exchange between the tank headspace and the atmosphere. First, this ensures that the tanks do not pressurize, and second, the passive air exchange effectively purges the headspaces and limits the concentrations of flammable waste gases in the headspaces. In addition to the filtered ventilation riser, most SSTs are connected via underground pipes to other SSTs. These connections are typically 3- or 4-inch-diameter cascade lines, but there are also large underground ventilation systems that greatly facilitate air exchanges between tanks (e.g., SSTs in 241-A tank farm are each connected

to a 20-inch-diameter underground ventilation manifold). Thus, air exchanges occur between one tank headspace and another as well as between the headspace and the atmosphere.

Passive ventilation of the tank headspaces is the result of three general driving forces (PNNL-14831):

- Barometric pressure changes – Changes in barometric pressures create slight, transient pressure imbalances that either push air into the tank or draw it out (ARH-CD-256; WHC-EP-0651). The magnitude of this effect is easily estimated, and it is the best understood of the identified passive ventilation motive forces.
- Buoyancy forces – Air that is colder than the headspace can cause a convective transport of the cold, dense air down into the headspace, and the warm, less dense headspace air out into the atmosphere. This "chimney effect" depends on the number and configuration of ventilation pathways and is less easily calculated than barometric pressure-driven air exchange.
- Wind – Wind in the tank farm can induce pressure differences between connected tanks and between individual tanks and the atmosphere, which in turn induce air exchanges between tanks and the atmosphere. Wind can also induce a pressure change at an open riser. When the vent is leeward, a venturi effect can draw air out of the tank. When the vent is windward, the air will tend to be compressed into the tank. The pressure drop downwind of an obstruction can also induce flow though a riser from a tank. Largely because of the complex interactions with ambient winds, these are the least well understood and most difficult to evaluate.

It is important to note that these three influences act in interdependent ways to drive, or impede, the ventilation of the tanks. Depending on the ambient conditions, they may be acting together or in opposing ways, causing each tank to alternately inhale and exhale air, or inducing continuous airflows among two or more tanks. Note also that barometric pressure fluctuations cannot by themselves sustain a flow of air in or out of the tank because the barometric pressure does not rise or fall for long. However, given two independent air pathways into a headspace (e.g., the filtered ventilation riser and an open cascade line to another tank headspace), the chimney effect can sustain simultaneous airflows in and out of the headspace as long as the ambient air is cooler than the headspace.

Passive ventilation rates have not been measured directly because air flowrates tend to be too low for existing field-appropriate instrumentation[2] and because some air flow occurs via inaccessible pathways (e.g., buried cascade lines that connect the tank headspaces). The best current estimates of passive ventilation rates are based on an indirect method that relates measured changes in the concentration of a headspace gas to the ventilation rate. This technique has been applied to headspace gases that are sporadically released by the waste

[2] Very low gas flowrates are routinely measured with great accuracy in laboratory settings with inexpensive instruments. However, these instruments require the air flow to pass through small-diameter tubing within the instrument, and introduce a resistance to flow that would effectively alter the measurement of passive ventilation rates.

(HNF-SD-WM-TI-797; PNNL-11926) and to tracer gases injected into the headspace for the purpose of estimating ventilation rates (PNNL-11683; PNNL-13029).

Table 4-1 lists the measured average ventilation rates calculated using the tracer gas method. Consistent with analyses of the exponential hydrogen concentration decreases after gas release events (GREs) (PNNL-11926), 241-A, 241-AX, and 241-BY tank farms were found to have relatively high passive ventilation rates. Also consistent with the analyses of GREs (HNF-SD-WM-TI-797; PNNL-11926), measured ventilation rates are significantly higher than those expected from barometric pressure fluctuations alone.

Table 4-1. Passive Ventilation Rates Measured with Tracer Gas Method

Tank	Tracer Gas	Time Period	Reference	Ventilation Rate	
				(m^3/hr)	(ft^3/min)
241-A-101	He	07/09/97 – 07/15/97	(2)	17	10
241-AX-102	He	08/08/97 – 09/08/97	(2)	28	16
241-AX-103[1]	He	02/25/97 – 03/03/97	(2)	42	25
241-BY-105	He	04/17/97 – 04/23/97	(2)	36	21
	SF_6	04/17/97 – 05/08/97	(2)	26	15
241-C-107[1]	He	02/21/97 – 03/21/97	(2)	1.9	1.1
241-S-102	He	09/24/96 – 10/11/96	(2)	3.3	1.9
	SF_6	09/24/96 – 02/11/97	(2)	3.8	2.2
241-S-106	He	04/16/99 – 05/06/99	(4)	17	9.9
		05/19/99 – 0613/99	(4)	15	8.6
241-TX-104	He	01/14/98 – 02/12/98	(3)	5.9	3.5
241-U-102	He	01/09/98 – 03/24/98	(3)	3.5	2.1
241-U-103	He	02/27/97 – 04/09/97	(2)	4.3	2.5
		07/15/97 – 08/13/97	(2)	2.6	1.5
		11/18/97 – 01/08/98	(3)	4.0	2.3
	SF_6	02/27/97 – 07/22/97	(2)	2.9	1.7
241-U-105	He	07/18/97 – 08/15/97	(2)	8.6	5.1
241-U-106	He	01/09/98 – 03/24/98	(3)	2.2	1.3
241-U-111	He	01/09/98 – 03/24/98	(3)	3.2	1.9

Notes: [1] Ventilation rates calculated from SF_6 data for tanks 241-AX-103 and 241-C-107 are not included because of apparent absorption and chemical degradation of SF_6.
[2] PNNL-11683
[3] PNNL-11925.
[4] PNNL-13029.

4.3 ATMOSPHERIC DISPERSION OF RELEASES

PNNL-14767 used modeling to estimate potential dilution of hypothetical vapor releases from actively- and passively-ventilated tanks. The study examined the effects of distance from vent source, meteorological conditions, local tank farm surface roughness, and topography. Concentrations at the vent source (i.e., at the breather filter for passively-ventilated SSTs and at the stack for actively-ventilated tanks) were assumed to be at the same concentration as the headspace. Calculations indicated that the plume would essentially travel at, or slightly lower than, the initial release height. Plume rise was based on the volumes of air released and ambient-to-plume density differences. The wake downwash effect dominated in most cases, resulting in a

slight lowering of the plume height. Concentrations were expressed as a fraction of the headspace concentration as a function of distance.

Scenarios evaluated included seven meteorological stability classes wind speeds from 1 to 20 m/s, and ventilation rates from 1 m^3/hr (a well-sealed passively-ventilated tank) to 3,400 m^3/hr (241-AW Tank Farm forced ventilation at high flow). The bounding case was for a near-surface vent under stable meteorological conditions, low-wind (1 m/s), and a high-passive ventilation rate (100 m^3/hr). Concentrations at one meter from the vent were near headspace concentrations but dropped an order of magnitude at about ten meters. This case represents an upper limit where an individual's intake follows the small meandering plume centerline for an extended time. The average exposure would be much lower for this and other conditions because of natural plume meandering and individual movements. Results suggest that headspace concentrations are possible near a tank vent for short durations (i.e., several seconds). Scenarios at higher wind speeds and less meteorological stability generally produce a factor of ten drop in concentration at one meter and more than a factor of 100 at ten meters (PNNL-14767).

Stacks on passively-ventilated tanks (i.e., vent release points more than ten feet above ground) had a significant effect on modeling results. Stack extensions lowered vapor concentrations by an order of magnitude for all scenarios. Modeling indicates that stacks are an effective means for reducing potential gas and vapor concentrations in the worker breathing zone.

Tanks are located in farms, and several tanks are in proximity of each other. PNNL-14767 indicated that exhaust plumes from multiple tanks could hypothetically intersect for brief periods of time under specific meteorological conditions. Appendix D shows the combined influences of tank-farm specific emissions from vents/stacks on potential worker breathing zones around the A prefix tanks and C Farm tanks. Source-specific ammonia and nitrous oxide data were combined with topographical and meteorological data to estimate an annual peak concentration. Results indicate that peak ammonia and nitrous oxide concentrations might be found within A and C Farms and south/southwest of the AN Stack. Peak concentrations were more than an order of magnitude less than the 25 ppmv ammonia/nitrous oxide OELs. Parametric modeling showed that 242-A Evaporator and AN and AP stacks influenced the largest areas within the A Tank Farm Complex, but that peak concentrations within the worker breathing zones were several orders of magnitude lower than plume centerline concentrations.

Ground level concentrations near the stacks for the 241-AN, 241-AP, 241-AW, 241-AY/AZ, and 241-SY tank farms, and the 242-A Evaporator were at least two orders of magnitude lower than headspace concentrations for all scenarios. Although higher ventilation rates caused less dilution at the plume centerline (i.e., horizontally downwind of the stack exit), concentrations at ground level (the worker breathing zone) were always reduced by at least two orders of magnitude.

4.4 CORRELATION BETWEEN VAPOR INCIDENTS AND METEOROLOGICAL CONDITIONS

A study on potential meteorological influences on reported vapor incidents examined whether Tank Farms shift log vapor incident entries (for calendar years 2001 through 2004) could be correlated with meteorological and weather information (RPP-RPT-22914). Vapor entries were separated into events associated with intrusive work and transient work (i.e., walkdowns, surveys, and other work that did not require working directly with the tanks, pits, or transfer lines), and plotted against observed barometric pressure and wind speed and direction. Vapor entries were also assessed against whether the 242-A Evaporator was running when the vapor entry was made.

The study concluded that barometric pressure decreases, wind velocity, and direction can cause or exacerbate a vapor release within the SST and DST farms. Transient work related vapor entries were correlated with wind direction and velocity, and a decrease in barometric pressure could result in increased rate of vapor emissions. There was no definitive correlation between evaporator operation and vapor incidents. Only 16 of the 144 vapor entries corresponded with 242-A Evaporator operations, and only eight of these incidents were downwind from the evaporator.

4.5 INDUSTRIAL HYGIENE SOURCE, AREA AND PERSONAL DATA

In addition to the headspace and ventilation system characterization data discussed in Section 3, Tank Farms IH has conducted emission source sampling and monitoring at breather filter outlets, above ground riser penetrations, pit covers, etc. This was done to:

- identify the locations of emission sources for establishment of buffer zones,
- confirm tank headspace and ventilation system characterization data did indeed represent maximum source concentrations, and
- test for selected source chemicals without conducting full headspace characterization.

The IH source data with headspace characterization data can be used to identify what chemicals are likely to be present in the worker breathing zone and estimate their maximum concentrations, but worker protection must be based on actual workplace data. Workplace data can come from monitoring or sampling the worker breathing zone. Monitoring is conducted with direct reading instruments (DRI) and colorimetric devices (e.g., Draeger tubes) that provide essentially real-time field measurements. Sampling, which entails subsequent laboratory analysis of the samples, is conducted to identify and measure chemicals not specifically addressed by monitoring methods and/or to obtain time weighted average (TWA) workplace concentrations.

A further distinction of importance is that between personal exposure and area characterization data. Personal exposure data are usually collected with sampling devices worn by the worker, typically with the sampling device (or tubing connected to the sampling device) being attached to the worker's lapel. Personal samples are collected to establish the TWA concentration of vapors

to which the worker has been exposed. Area characterization data are also usually from sampling devices, though area monitoring can be used for some of the COPC. Area characterization data are typically collected from several fixed locations considered representative of the worker breathing zone (not at sources such as the breather filter of an SST).

This section briefly summarizes IH source, area, and personal data. It is divided roughly into the periods before and after the 2004 reassessment of Tank Farms vapor hazards.

4.5.1 Data from 1992 through 2003

IH monitoring in the Tank Farms began in March 1992 when area vapor monitoring was instituted (WHC-SD-TWR-RPT-001). Local surveys using organic vapor monitors recorded volatile organic compound (VOC) concentrations in work areas and worker breathing zones. In addition to VOCs, ammonia and nitrous oxide were also measured. Surveys were used to locate potential sources. Surveys were taken at about 2,000 locations, and the IH technicians attempted to identify the source of any non-zero breathing zone readings. The highest measured VOC source concentration was 100 ppmv and the highest measured ammonia source concentration was 500 ppmv. Work area and worker breathing zone monitoring indicated VOC concentrations less than 2 ppmv and ammonia concentrations less than 25 ppmv.

Over 350 personal samples were collected from January 1993 to June 1996, including samples for hydrogen cyanide, acetone, butanol, ammonia, and nitrous oxide. Personal samples varied in length from 20 minutes to over five hours. Ammonia, nitrous oxide, and butanol samples indicated the highest eight-hour TWA concentrations: 2.6, 3.9, and 0.4 ppmv, respectively (WHC-SD-TWR-RPT-001).

DRI surveys taken between 1996 and 2003 were focused primarily on ammonia. At that time, it was believed that ammonia was consistently found at much higher concentrations than other potential contaminants and that ammonia could be used as an indicator for tank vapors. More recent work, as discussed in this document, suggests acceptable ammonia levels in the worker breathing zone are not necessarily indicative of acceptable levels of all COPC.

During the period from 1997 to 2003, periodic personal and area sampling continued for operations where increased emissions were anticipated to assess exposures and confirm controls were adequate. Samples were analyzed for ammonia, nitrous oxide, and VOCs. No personal or area sample concentrations exceeded Tank Farms OELs.

Personal and area sampling was performed during the startup of the tank C-106 sluicing operation to characterize exposures. This was a major waste-disturbing operation both at the source tank and the receiver tank. Prior to operational startup, 11 area and seven personal samples were collected to establish a baseline, and all results were less than analytical detection limits. Between November 1998 and April 1999, 128 area samples, 22 personal samples and 180 source exhaust stack samples were collected and analyzed. The maximum eight-hour TWA concentrations for personal and area samples were less than 1 ppmv for ammonia and targeted VOCs, and 2 ppmv for nitrous oxide; well below OELs. Maximum source exhaust stack sample

concentrations were 368 ppmv for VOCs, 34 ppmv for ammonia, and 760 ppmv for nitrous oxide. This characterization effort demonstrated the exhaust stack configuration was effective in controlling exposures at the ground level (HNF-4261).

4.5.2 Data from 2004 through 2006

In 2004, 430 passive nitrous oxide samples were collected at and near the SST breather filters to evaluate concentrations near likely SST sources (RPP-21448). Most (343) were collected directly at breather filters and the remaining (87) were taken 1.5 to 5 feet from the breather filter. The majority of samples collected at the breather filters (307 of the 343) indicated 12 to 24-hour TWA concentrations to be less than 1 ppmv. Thirty measured between 1 and 10 ppmv, and six were between 10 and 40 ppmv. All 87 nitrous oxide samples taken 1.5 to 5 feet away from the breather filters showed 24-hour time weighted average concentrations less than 1 ppmv.

Between April and July 2004, personal sample sets were collected on 153 employees. Sample sets included ammonia, nitrous oxide, and VOCs. Table 4-2 summarizes ammonia and nitrous oxide results. Maximum measured ammonia concentration for an eight-hour TWA was 0.03 ppmv. Sample durations ranged from 11 to 203 minutes, with the median duration being 57 minutes. Only 14 of the 195 samples showed concentrations above the detection limit for the sampling method. The maximum nitrous oxide concentration for an eight-hour TWA was 2.1 ppmv. Median sample duration was 69 minutes. About half of the personal samples (122 of 245) showed concentrations above the detection limit for the sampling method.

Table 4-2. Personal Sample Results Between April and July 2004

Description	Total Number of Samples	Maximum Measured Concentration (ppmv, 8-hr TWA)	OEL (ppmv)
Ammonia	195	0.03	25 (TLV)
Nitrous Oxide	245	2.1	50 (TLV)

Notes: REL = Recommended Exposure Limit
TLV = Threshold Limit Value
TWA = Time Weighted Average
Source: Personal communication from J. W. Jabara.

The A complex area was intensely sampled and monitored between May 24 and September 6, 2005. Sampling was conducted in 34 locations outside work areas, in the AN, AP, AW, and 702-AZ DST stacks, at all the A and AX SST breather filters, and at five feet surrounding the A and AX SST breather filters (see Figure 4-1). Sampling deployed all the media and analysis methods summarized in Section 3.2 (7X700-OMC-05-033 – Letter), and results are documented in RPP-RPT-29262. About 900 samples were taken and only the DST stack and SST breather filter source samples showed significant COPC concentrations (i.e., > 10% of an OEL/AOEL). Eight chemicals exceeded 10% of their OEL at the source. These are listed in Table 4-3 along with their maximum measured concentrations.

Figure 4-1. A Complex Area and Source Sampling

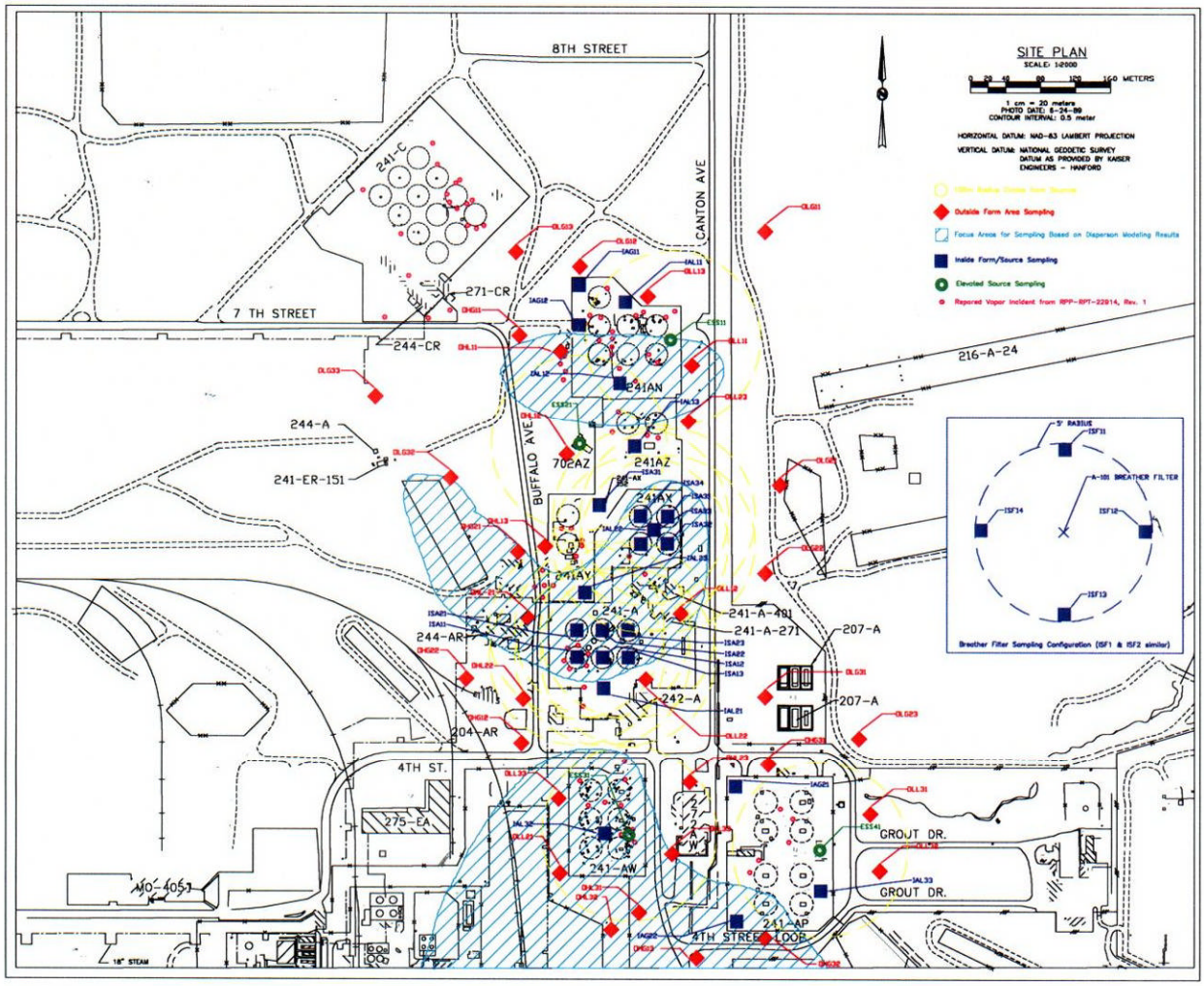


Table 4-3. COPC with Source Concentrations Above 10% of OEL in A Complex

Chemical	Maximum Concentration	OEL	Location*
Ammonia	104 ppmv	25 ppmv	AN Stack
Formaldehyde	0.03 ppmv	0.1 ppmv	241-A-105 Breather Filter
Ethylamine	0.83 ppmv	5 ppmv	AP Stack
Mercury	0.016 mg/m^3	0.025 mg/m^3	241-A-105 Breather Filter
Nitrous oxide	120 ppmv	50 ppmv	241-A-105 Breather Filter
N-Nitrosodimethylamine	0.042 ppmv	0.0003 ppmv	AN Stack
N-Nitrosomethylethylamine	0.0007 ppmv	0.0003 ppmv	AN Stack
N-Nitrosomorpholine	0.0004 ppmv	0.0006 ppmv	AN Stack

Area samples taken from five feet or further away from a source showed negligible chemical concentrations. Table 4-4 shows the seven COPC found above method detection limits in area samples. The chemical nearest its OEL was acetonitrile, which had a maximum measured concentration of less than 3% of its OEL. The six other chemicals detected were all less than

0.3% of their respective OELs. Results suggest that although chemicals can be found above OEL concentrations at the sources, atmospheric dispersion (see Section 4.3) keeps concentrations low when more than five feet from the source.

Table 4-4. COPC Detected in A Complex Area Samples

Chemical	Maximum Concentration (ppmv)	OEL (ppmv)	Location*
1-Butanol	0.047	20	OLL22 – North of 242-A Evaporator
2-Hexanone	0.009	5	OHG31 – AP Farm Change Trailer
Acetaldehyde	0.044	20	IAL12 – AN Farm South Fence
Acetonitrile	0.544	20	ISF21 – 5 ft North of 241-A-103
Ammonia	0.215	25	OHG21 – Across from AY Change Trailer
Butanal	0.026	25	OHG31 – AP Farm Change Trailer
Nitrous Oxide	0.017	50	ISF11 – 5 ft North of 241-A-105

Note: *Locations shown in Figure 4-1.

From May 2005, to April 2006, 1,500 personal sample sets were collected on workers in the A-Prefix, SY, and C tank farms. Sets included samples for ammonia, nitrous oxide, mercury, formaldehyde, nitrosamines, volatile organic compounds, and semivolatile organic compounds. Only one of the 327 ammonia samples showed concentrations above the detection limit (~0.50 μg). The maximum eight-hour TWA concentration for ammonia was 0.02 ppmv. Less than half of the nitrous oxide personal samples (124 of 271) had concentrations above the detection limit (~2.0 μg). The maximum nitrous oxide concentration for an eight-hour TWA was 2 ppmv. Only 33 of the 348 mercury samples returned values above the detection limit (~0.01 μg), and the maximum TWA concentration was 0.018 mg/m^3. All seven formaldehyde samples were above the detection limit (~0.03μg); however, the maximum TWA concentration was only 0.005 ppmv. None of the six nitrosamine samples were above the detection limit (~0.02 μg). Six VOC thermal desorption unit (TDU) samples were taken, and no chemicals on the COPC list were detected. Eight semi-VOC TDU samples were taken, and no chemicals on the COPC list were detected.

4.6 CONCLUSIONS

Theory and tank headspace measurements show that natural convection in the tanks keep the headspace gases and vapors well mixed. Passive ventilation rates in the SSTs vary, but are relatively small compared to the actively-ventilated tanks. Headspace gases are released via breather filters and other penetrations in tanks. For the majority of atmospheric stability conditions, these releases are diluted with ambient air by at least a factor of ten within one meter of a tank vent, and often much more. Although concentrations near a passive vent can be near headspace concentrations, the small volumes released (a direct result of the low ventilation rate) ensure that the exposure area is localized and that duration would likely last only seconds. In combination with the substantial variability in individuals to detect a given odor, this concentration variability near passive vents is why it is possible for one person to smell an odor while another standing near by does not.

Headspace characterization data show that properly maintained and operating active ventilation systems will significantly reduce. However, headspace concentrations would increase over several months and are expected to be similar to that found in the passively-ventilated tanks if active ventilation were to be shut down.

Modeling indicates that vent stacks (i.e., vent release points more than ten feet above ground) for both passively- and actively-ventilated tanks are an effective means for reducing potential gas and vapor concentrations in the worker breathing zone. For the actively-ventilated stacks, concentrations at ground level should be at least two orders of magnitude lower than headspace concentrations under the least favorable conditions (i.e., stable low-wind). For the passively-ventilated stacks, concentrations at ground level should be at least three orders of magnitude lower than headspace concentrations under stable low-wind conditions.

Worker breathing zone data (area samples and monitor and personal sampling) indicate that gas and vapor concentrations are orders of magnitude lower than concentrations found in tank headspaces, consistent with the dispersion modeling results. Most COPC are below sampling and analytical detection limits, and those that have been detected are well below OEL concentrations.

5.0 TOXICOLOGICAL EVALUATION

Tank waste and headspace characterization data have been reviewed to identify volatile chemicals that could be emitted into the worker breathing zones. Waste chemistry and the limitations of the characterization methods have also been examined to hypothesize what other potentially hazardous chemicals might be present. The reported and hypothesized chemicals were then individually evaluated against toxicological criteria to identify those that could be present at levels of concern in the worker breathing zone.

All chemicals known or thought to be present in the tank headspaces at levels of concern have been evaluated for their potential to harm workers, and those chemicals deemed to be of potential concern have been identified. The COPC are the only chemicals that could, based on the available data, exceed their administrative control limits (ACLs) at the sources. Actual workplace concentrations are to be determined by workplace sampling and environmental assessments.

5.1 VOLATILE TANK WASTE CHEMICALS

Some 1,826 chemicals were previously identified in an initial listing of volatile tank waste chemicals. That document also described an initial evaluation of the chemicals, and divided them into the following three categories in order of decreasing importance:

52	COPC;
1,538	Chemicals Needing Further Evaluation (CNFE); and
236	Chemicals with Low Probability of Exposure.

The 52 COPC were deemed to be of high importance and were the focus of source, area, and personal sampling in Tank Farms. Changes to the original list (both additions and removals) have been made for various reasons as the knowledge of tank chemicals and their potential toxicity were evaluated (see Appendix C).

The list of 1,538 CNFE was revised to eliminate certain identification errors and duplications and to add recently identified chemicals. The revised list included 1,576 chemicals (revisions are described in Section C2.1 of Appendix C).

The 236 chemicals previously identified as having low probability of exposure have been removed from further consideration and are not listed in this report. None of these non-carcinogenic chemicals had been identified in tank headspace samples nor were there reasons to expect them to be present in the tank headspaces at levels of concern.

5.2 CHEMICALS

Evaluations of the chemicals on both the CNFE and COPC lists were conducted with the goal of determining whether each chemical was indeed a tank headspace constituent or not. All

analytical vapor characterization data available in TCD as of January 2006 were retrieved and reviewed for selected chemicals to ensure they had been correctly identified, and suspicious analytical results concerning possible sample and analytical laboratory contamination were investigated.

5.2.1 Misidentified Chemicals

Most volatile waste tank chemicals were originally identified in tank headspace samples using an analytical chemistry technique that only provided "tentative identification" of the chemicals. The technique compares the mass spectrum of each analyte to a published library containing millions of known mass spectra. Confidence in the matching of unknown and library spectra is affected by complications such as the spectra of two analytes being combined, nondescript spectra, background issues, and weak spectra (from low analyte concentrations). Though computers do much of the work, the identification of an analyte as a specific chemical is ultimately based on criteria that may vary between laboratories and the analyst's judgment.

To reduce errors in the identification of potentially important chemicals, archived analytical data for selected headspace chemicals were retrieved and independently reviewed by experienced mass spectroscopists (TWSS05.008 - Letter; TWS05.016 - Letter; PNNL-15673; 7FA00-05-SJE-005). The reviews and findings were documented and were themselves independently reviewed, with all recommended changes recorded in the TCD. Appendix C discusses and lists the misidentified chemicals.

5.2.2 Contaminants

Despite considerable effort to ensure vapor samples collected from the waste tank headspaces would not be affected by contaminants, there is strong evidence that several identified vapor compounds were actually plasticizers associated with sampling manifold components (PNNL-15646). Several halogenated compounds reported in vapor samples were also determined to be from a standards handling problem within one of the analytical laboratories (PNNL-15646). Data associated with these problems have been flagged and comments added to the TCD. Appendix C discusses and lists those chemicals determined to be erroneously reported.

5.2.3 Hypothetical Tank Vapors

Sampling and analysis methodologies used for tank headspace characterization in the past did not address all gases and vapors. Specifically, low molecular weight organic compounds and some inorganic vapors were not addressed by the methodologies.

Mass spectroscopy is the primary analytical technique for identification of organic vapors, but this has generally been conducted with scans that precluded the detection of low molecular weight compounds (see Appendix C, Section C2.2). To address this issue, a list of plausible one- and two-carbon compounds was developed, and an evaluation was conducted to determine if any

of these compounds should be added to the COPC list. The evaluation, described in Appendix B, found that three amines on the one- and two-carbon compounds list warranted the collection of special samples. Initial sample results from the A-prefix region of 200 East Area have indicated ethylamine to be present in the headspaces and ventilation systems at levels of concern. Ethylamine has been added to the COPC list, and sampling for amines will be conducted in other tank farms until they are deemed to be appropriately characterized.

The discovery in 2004 of mercury and dimethylmercury vapors at measurable levels in the tank headspaces was not expected and contrary to the collective wisdom of various chemists who had considered the issue (External Letter, "Summary of Regulated Toxic Air Pollutants Identified in 102 Hanford Site High-Level Radioactive Waste Tanks"). The implication that there may be other unexpected inorganic vapors present that could impact the quality of air in the worker breathing zone has been addressed by (1) conducting a thermodynamics study to identify species that are plausible in the tank headspaces, and then (2) collecting and analyzing air samples that would allow the identification of the thermodynamically plausible species. Sampling results indicated no other volatile metals present and further sampling is not warranted (see Section C3.2 in Appendix C).

5.3 TOXICOLOGY

A chemical is of potential concern if its maximum reported concentration is above its ACL. DOE G 440.1-3 Implementation Guide for DOE Order 440.1A (a contract requirement of CH2M HILL) provides guidance on the establishment of ACLs using occupational exposure limits. Section 4.4.6.2 of the implementation guide states

> "The function of the ACL ... is to designate an exposure level at which monitoring procedures become appropriate.
>
> Usually, an ACL is set to one-tenth or possibly one-fourth the OEL when monitoring is initiated or when there are not yet sufficient data to generate a statistically valid exposure profile."

Based on this guidance and consideration of the inherent uncertainties in the concentrations of volatile waste chemicals, it was determined that any chemical present at or above 10% of its OEL at a tank farm source (e.g., a breather filter or exhaust stack) should be evaluated for addition to the COPC list.

The same DOE implementation guide also provides guidance on OELs, specifying compliance with 29 CFR 1910, Occupational Safety and Health Standards [i.e., Occupational Safety and Health Administration (OSHA) permissible exposure limits (PELs)] and with Threshold Limit Values (TLVs) established by the American Conference of Governmental Industrial Hygienists (ACGIH). Thus DOE Order 440.1A guidance is to use the more restrictive of the OSHA PEL and the ACGIH TLV as the OEL.

Of more than 1,600 chemicals identified, there are only 131 that have U.S. OELs (e.g., PEL or TLV). For chemicals not having U.S. OELs, a process was developed to evaluate potential occupational exposure hazards using alternative occupational exposure standards and toxicological data. The process results in each chemical being either determined to pose no significant risk to workers, or a COPC with a Tank Farms-approved AOEL. The process is depicted in Figure 5-1 and discussed in the following subsections.

5.3.1 Established U.S. Occupational Exposure Limits (OELs)

As depicted in Figure 5-1, the first step in the evaluation of a CNFE was to determine whether it had an established U.S. OEL. For evaluation purposes, OELs established by a U.S. governmental agency or national professional organization were considered equivalent to the OSHA PEL and ACGIH TLV (i.e., when neither a PEL nor a TLV had been established for the chemical). While OELs were sought from other U.S. sources, the only OELs actually used for this step were the American Industrial Hygiene Association (AIHA) Workplace Environmental Exposure Level (WEEL) and the National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limit (REL).

Chemicals having maximum reported concentrations below 10% of an established U.S. OEL were considered to not pose a significant risk to tank farm workers. Those chemicals reported at concentrations at or above 10% of their OELs were subjected to further toxicological review as described in Section 5.3.4.

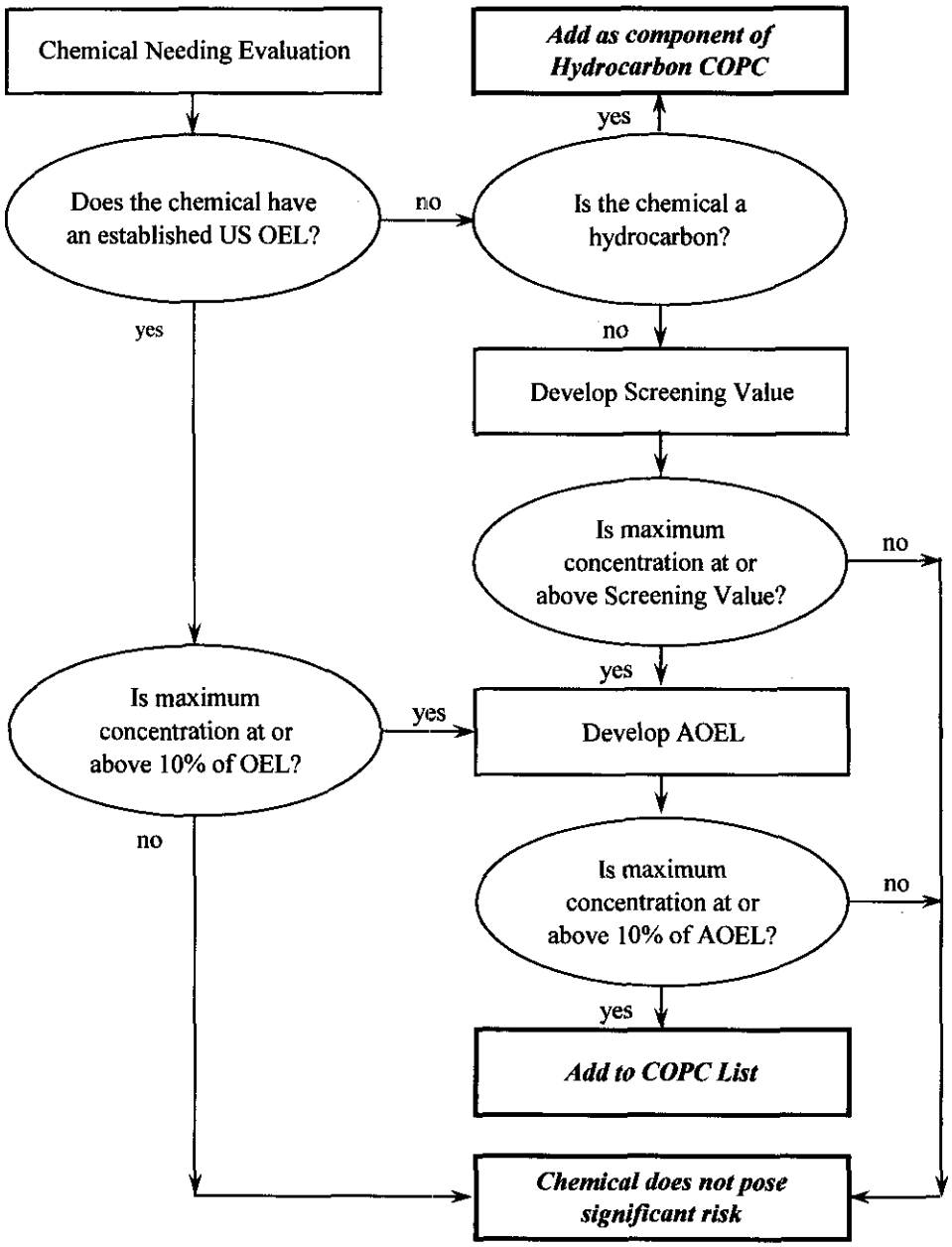
5.3.2 Hydrocarbons

Hydrocarbons that did not have established U.S. OELs were evaluated as a mixture. This was done on the advice of the Independent Toxicology Panel (ITP) and with support from a petroleum industry toxicologist, Dr. Carl R. Mackerer (a curriculum vitae for Dr. Mackerer is given in Appendix A). RPP-RPT-29404 determined that the hydrocarbon mixtures found in the tank headspaces were similar in composition and toxicology to the standard petroleum industry fuel streams (i.e., gasoline, kerosene, diesel, etc.). He noted that the tank headspace hydrocarbon mixtures have relatively low aromaticity and would, therefore, tend to be less toxic than standard fuel streams. Mackerer recommended that the ACGIH TLV for kerosene (200 mg/m^3) be applied as the Tank Farms OEL for hydrocarbons measured as a mixture. The recommendation to use the 200 mg/m^3 ACGIH TLV for kerosene as the AOEL for Tank Farms hydrocarbon mixtures was adopted by the Exposure Assessment Strategy Review Group (EASRG) on December 7, 2005 (EASRG meeting minutes are shown in Appendix E). Individual chemicals that have an established PEL or TLV were evaluated using that existing exposure limit by itself, as well as considering it a part of the larger hydrocarbon mixture.

5.3.3 Screening Values

It was recognized that many of the relatively non-toxic chemicals had only been reported at very low concentrations, and that these did not warrant in-depth toxicological assessments. The first step of the evaluation of non-hydrocarbon chemicals was to conduct a screening to identify those chemicals needing in-depth toxicological assessments.

Figure 5-1. Toxicological Evaluation Logic Diagram



Screening was performed by comparing the maximum average headspace concentration to a conservatively established screening value. The screening values were based on occupational exposure data and guidelines (e.g., non-U.S. OELs); on available toxicological data; and in lieu of adequate information on the specific chemical, on information for toxicologically similar chemicals (surrogates). PNNL-15640 describes the procedure used to develop screening values and list all chemicals screened, their screening values, and the bases of each screening value.

Chemicals with maximum reported concentrations less than their screening values were considered to not pose significant risks to workers. More in-depth toxicological analyses were conducted on the chemicals having maximum reported concentrations above their screening values.

5.3.4 Acceptable Occupational Exposure Levels (AOELs)

Additional toxicological analyses were performed on the chemicals reported above 10% of their established U.S. OELs or above their screening values. Analyses were conducted by toxicologists using approved procedures, and if warranted, draft AOELs were developed (PNNL-15736). AOELs were based on established OELs when available and deemed appropriate for Tank Farms, and developed according to procedures otherwise. Appendix F gives the AOEL development procedure for non-carcinogens, and Appendix G gives the procedure for carcinogens. Both AOEL development procedures are based on standard toxicological practices and were reviewed extensively by the ITP.

Draft AOELs were presented to the EASRG for review and approval; EASRG meeting minutes are attached as Appendix E. Chemicals with maximum reported concentrations at or above 10% of their approved AOELs were added to the COPC list, and chemicals below 10% of their approved AOELs were judged to be not of significant risk to workers. Approved AOELs were developed for each chemical that did not have either an OSHA PEL or an ACGIH TLV.

5.4 CHEMICALS OF POTENTIAL CONCERN

All chemicals identified in tank headspace samples and volatile chemicals identified or hypothesized to be in the waste have been considered. The original list of 52 COPC was modified by both removals and additions based on the chemical and toxicological evaluations described previously. Appendix C describes the bases for the modifications.

Removals from the COPC list include seven misidentified chemicals; four sample manifold and analytical laboratory contaminants; eleven chemicals with maximum reported concentrations below 10% of their PEL, TLV, or AOEL; and two chemicals that had neither been reported nor estimated to be potentially present at levels of concern. Three other chemicals, CO, CO_2, and NO_2, were removed after an IH analysis indicated these to be addressed by existing worker protection policies and management (7B600-MLZ-05-005 - Letter). Two others, Aroclor-1242 and Aroclor-1254, were removed from the COPC list and replaced by the more comprehensive "chlorinated biphenyls" entry.

Additions to the COPC list include three chemicals with maximum concentrations above 10% of their ACGIH TLVs; hydrocarbons (as a mixture of all hydrocarbons present); 19 chemicals with maximum concentrations above 10% of their AOELs; and a class of chemicals, "substituted furans," which includes seven reported and an indefinite number of possible furan ring-containing molecules.

The evaluation process established AOELs for seven individual chemicals that had been on the original COPC list, and an AOEL for "chlorinated biphenyls." The resulting COPC list of 48 chemicals is given in Table 5-1, along with the Tank Farms OEL and its source. Additional modifications to the COPC list will be made as warranted by the IH organization as additional data or improved toxicological information becomes available.

5.5 CONCLUSIONS

All volatile waste chemicals have been evaluated for their potential hazard to workers. The evaluation was as comprehensive as reasonably possible, addressing all chemicals reported in tank headspace and ventilation system samples, volatile chemicals reported in liquid and solid waste samples, and chemicals identified as potentially present in the tank headspaces but not reported because of sampling and/or analytical limitations.

A procedure was developed and applied to systematically identify chemicals of likely concern amongst the hundreds of chemicals present at trace levels in the headspaces. Further toxicological evaluations were conducted on those chemicals identified by the initial screening process as being potential hazards. AOELs for these chemicals were developed using thoroughly reviewed procedures, and reviewed and approved by the EASRG. Chemicals present at a tank farm source at greater than 10% of the OSHA PEL, ACGIH TLV, or Hanford Site Tank Farms AOEL have been placed on the COPC list.

Adjustments to the COPC list were made based on reviews of analytical laboratory data and the OELs of the carcinogens. The analyses described in Appendix C constitute the technical basis for the current COPC list. Based on those analyses, the 48 chemicals on the COPC list (Table 5-1) are the only chemicals emitted by the tanks that are of potential concern to worker health.

The primary purpose for this COPC list is to describe the chemicals present in tank headspaces that may pose a significant workplace risk. The list provides guidance to the IH organization as to which chemicals must be characterized in the workplace to ensure that sampling and monitoring methods will detect all chemicals emitted from tanks that are present in tanks at a significant concentration that might pose a potential risk to the worker.

Table 5-1. Chemicals of Potential Concern

	Chemical	Chemical Identification Number	Tank Farms OEL	
			Value	Source
1	1,1'-Biphenyl	92-52-4	0.2 ppmv	ACGIH TLV
2	1,3-Butadiene	106-99-0	1 ppmv	OSHA PEL
3	1,3-Dinitrate-1,2,3-propantriol	623-87-0	0.05 ppmv	AOEL
4	1,4-Butanediol dinitrate	3457-91-8	0.05 ppmv	AOEL
5	1-Butanol	71-36-3	20 ppmv	ACGIH TLV
6	2,4-Dimethylpyridine	108-47-4	0.5 ppmv	AOEL
7	2,4-Pentadienenitrile	1615-70-9	0.3 ppmv	AOEL
8	2-Ethylhex-2-enal	645-62-5	0.1 ppmv	AOEL
9	2-Fluoropropene	1184-60-7	0.1 ppmv	AOEL
10	2-Hexanone	591-78-6	5 ppmv	ACGIH TLV
11	2-Methylbut-2-enal	1115-11-3	0.03 ppmv	AOEL
12	2-Methylene butanenitrile	1647-11-6	0.3 ppmv	AOEL
13	2-Nitro-2-methylpropane	594-70-7	0.3 ppmv	AOEL
14	3-Buten-2-one	78-94-4	0.2 ppmv	ACGIH ceiling
15	3-Methyl-3-buten-2-one	814-78-8	0.02 ppmv	AOEL
16	4-Methyl-2-hexanone	105-42-0	0.5 ppmv	AOEL
17	6-Methyl-2-heptanone	928-68-7	8 ppmv	AOEL
18	Acetaldehyde	75-07-0	25 ppmv	ACGIH ceiling
19	Acetonitrile	75-05-8	20 ppmv	ACGIH TLV
20	Ammonia	7664-41-7	25 ppmv	ACGIH TLV
21	Benzene	71-43-2	0.5 ppmv	ACGIH TLV
22	Butanal	123-72-8	25 ppmv	AOEL
23	Butanenitrile	109-74-0	8 ppmv	AOEL
24	Butyl nitrate	928-45-0	8 ppmv	AOEL
25	Butyl nitrite	544-16-1	0.1 ppmv	AOEL
26	Chlorinated biphenyls	---	0.03 mg/m^3	AOEL
27	Dibutyl butylphosphonate	78-46-6	0.007 ppmv	AOEL
28	Diethyl phthalate	84-66-2	5 mg/m^3	ACGIH TLV
29	Dimethylmercury	593-74-8	0.01 mg/m^3	ACGIH TLV
30	Ethylamine	75-04-7	5 ppmv	ACGIH TLV
31	Formaldehyde	50-00-0	0.3 ppmv	ACGIH Ceiling
32	Furan	110-00-9	0.001 ppmv	AOEL
33	Substituted furans	---	0.001 ppmv	AOEL
34	Heptanenitrile	629-08-3	6 ppmv	AOEL
35	Hexanenitrile	628-73-9	6 ppmv	AOEL
36	Hydrocarbons	---	200 mg/m^3	AOEL
37	Mercury	7439-97-6	0.025 mg/m^3	ACGIH TLV
38	Methanol	67-56-1	200 ppmv	ACGIH TLV
39	Methyl isocyanate	624-83-9	0.02 ppmv	ACGIH TLV
40	Methyl nitrite	624-91-9	0.1 ppmv	AOEL
41	Nitrous oxide (N_2O)	10024-97-2	50 ppmv	ACGIH TLV
42	N-Nitrosodimethylamine	62-75-9	0.0003 ppmv	AOEL
43	N-Nitrosomethylethylamine	10595-95-6	0.0003 ppmv	AOEL
44	N-Nitrosomorpholine	59-89-2	0.0006 ppmv	AOEL
45	Pentanenitrile	110-59-8	6 ppmv	AOEL
46	Propanenitrile	107-12-0	6 ppmv	AOEL
47	Pyridine	110-86-1	1 ppmv	ACGIH TLV
48	Tributyl phosphate	126-73-8	0.2 ppmv	ACGIH TLV

6.0 CONCLUSIONS

Headspace gas and vapor origins are understood and can be related back to original chemicals placed into tanks and their degradation chemistry. Concentrations are determined by a dynamic competition between evolution from the waste and removal by ventilation or other means. Absent waste-disturbing activities, changes are slow, and there are no large, rapid changes in headspace concentrations. Headspace concentrations do vary some over months and years, but sampling results indicate that 95% of the chemicals in a passively-ventilated SST vary by less than a factor of three. Most SST headspaces have been sampled (118 of 149), and similarities between sampled tanks and waste types suggest that the non-sampled SSTs will also have similar compositions.

Headspace characterization provides a large body of information about the identities and concentrations of the waste gases and vapors. Sampling and analyses were selected to identify a broad range of chemicals. Characterization data maintained in the TCD are based on appropriate sampling and analytical methods, and these data can be used to identify chemical species and estimate the concentrations to be expected in tank headspaces. Headspace gases are released via breather filters and other penetrations in tanks and might enter worker breathing zones.

Modeling indicates that SST headspace and DST stack chemical concentrations would be diluted up to several orders of magnitude after leaving the source. Worker breathing zone data (area samples and personal monitoring) indicate that gas and vapor concentrations are orders of magnitude lower than concentrations found in tank headspaces, consistent with the dispersion modeling results. Most tank headspace chemicals in the worker breathing zones are below sampling and analytical detection limits, and those chemicals that have been detected are well below OEL concentrations.

Volatile waste chemicals were evaluated for their potential hazard to workers. The evaluation was comprehensive and addressed all chemicals reported in tank headspace and ventilation system samples, volatile chemicals reported in liquid and solid waste samples, and chemicals identified as potentially present in the tank headspaces but not reported because of sampling and/or analytical limitations. Forty-eight chemicals present at tank farm sources at greater than 10% of the OSHA PEL, ACGIH TLV, or Hanford Site Tank Farms AOEL were placed on the COPC list.

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APPENDIX A

CONSULTANT BIOGRAPHICAL SUMMARIES

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Carl R. Mackerer, Ph.D.

EMPLOYER: C&C, Consulting in Toxicology
5 Blue Spruce Dr.
Pennington, NJ 08534
T: 609-737-9689
F: 609-737-9226
crmack@rcn.com

TITLE: Principal

EDUCATION:

1958-1963	Rutgers, The State University of New Jersey (Newark College of Arts and Sciences) Biology, Chemistry, (B.A.)
1966-1968	Rutgers, The State University of New Jersey, Newark & New Brunswick, NJ (The Graduate School) Biochemistry
1969-1971	University of Nebraska, College of Medicine, Omaha, NE (The Graduate School) Medical Biochemistry, (Ph.D.)

PROFESSIONAL ASSOCIATIONS:
American Society for Pharmacology and Experimental Therapeutics
American Chemical Society
Society of Experimental Biology and Medicine
Society of Toxicology

PROFESSIONAL EXPERIENCE:

2000-2004 Principal, C&C, Consulting in Toxicology

Provide a wide range of toxicology support services including preparing literature reviews, writing technical papers and reports, giving advice and direction for toxicology research and testing programs, interpreting research/testing results, acting as company representative to trade organizations, government agencies, etc..

1996-2000 Principal Toxicologist, Mobil Business Resources Corporation

Technical oversight for all toxicological and ecotoxicological research and testing performed for Mobil Oil Corporation. Responsible for a team of consulting toxicologists who develop Mobil positions on specific issues of interest to Business Units and on major health effects issues of importance to Mobil Corporation. Staff consists of nine senior toxicologists and three technicians. Performs special consulting activities in covering major health related issues for Mobil Corporation. Operating budget for supporting staff and conducting research and testing is $5,400,000/year.

1993-1999 President, Stonybrook Laboratories Inc.

President and CEO of Stonybrook Laboratories Inc. (a wholly owned subsidiary of Mobil Oil Corporation), which conducts toxicology and environmental research, testing and consultative work on a contractual basis for Mobil and third parties. Responsible for directing and managing all business and marketing efforts, testing and research activities, support functions (administration, computers, information services), and facility operations. The facility consisted of a 130, 000 ft^2 building containing individual laboratories, offices, work rooms, animals rooms, etc. Staff consisted of ~75 scientists and support personnel; the 1995 operating budget was $12,700,000. Stonybrook successfully entered the contract business in 1994, and maintained an excellent reputation for high quality work. Stonybrook Labs was closed in December 1996 when the Mobil Technical Center was sold and vacated, and the corporation is now inactive. The Stonybrook Dun and Bradstreet ID number is 84-801-0765.

Rutgers University, External Advisory Committee, Joint Graduate Program in Toxicology.

1989-1993 Manager, Environmental and Health Sciences Laboratory (EHSL). Mobil Oil Corporation, Environmental Health and Safety Department, Princeton, NJ

Responsible for directing and managing: Research and testing programs in toxicology, environmental science and related disciplines; support groups (Word Processing, Computer Services, Quality Assurance and the Library); and the operation, maintenance, etc. of the Mobil Environmental and Health Science Laboratory. Staff included 68 Mobil scientists and support staff, temporary agency technicians and office workers. Annual budget was $12,000,000. Duties included developing EHSL policy, program/budget planning and study design; managing scientific activities and staff; representing Mobil interests to regulatory agencies, trade and scientific organizations, and academic institutions; recommending and

administering Mobil Foundation grants in toxicology and environmental sciences; discovering and developing safer products; assisting Mobil Corporation Legal, Medical and other departments by supplying scientific expertise as required; establishing a high degree of credibility for Mobil Corporation in the areas of toxicology and environmental health; and participating in setting corporate policies and goals in areas related to human health and environmental protection.

1987-1989 Assistant Director of Toxicology/Manager of Toxicology Services
Mobil Oil Corporation, Toxicology Division, Princeton, NJ

Responsible for directing and managing all research and testing activities, of the Toxicology Division, conducted by 64 scientists and support staff including 18 with Ph.D. degrees and one with an MD degree. Activities were divided between standard testing (60%) and research (40%). The research program emphasized genetic toxicology, pharmacokinetics/metabolism, ecotoxicology and environmental chemistry. The laboratory was also actively involved in new product development. Duties included budget administration, planning and participation in new product development.

1978-1987 Manager of Biochemical Toxicology
Mobil Oil Corporation, Toxicology Division, Princeton, NJ

Responsible for directing and managing the Biochemical Toxicology Section of the Toxicology Division. The Biochemical Section was primarily concerned with work performed in the areas of genetic toxicology, pharmacology, metabolism, in vitro toxicology, pharmacokinetics, clinical biochemistry, enzymology, environmental chemistry, aquatic toxicology, biodegradation, cytology and analytical chemistry. In addition, the Chemical Repository Unit was in the Biochemical Toxicology Section. Responsibilities included work performed in-house and at contract facilities. (Supervised a staff of 19 professional scientists, eight technicians and two secretaries). Was also responsible for designing and coordinating the overall toxicology testing program for Mobil Chemical Company's pesticide business. Served as worldwide technical representative for obtaining USA and Foreign pesticide registrations.

1975-1978 Research Scientist and Senior Research Scientist
Searle Laboratories, Pharmacology Department Chicago, IL

1972-1975 Research Investigator and Senior Research Investigator.
Searle Laboratories, Pathology/Toxicology Department, Chicago, IL

SELECTED PROFESSIONAL ACTIVITIES:

American Society for Testing and Materials (ASTM) Committee E34.5 on Occupational Health and Safety (1988-2000).

AIHC Scientific Committee (1990-1992).

The Oil Companies European Organization for Environmental and Health Protection (CONCAWE). Health Management Group -Toxicology Subcommittee (1987-1992, 1997 - 2000).

The American Petroleum Institute (API). White Oil and Wax Technical Group (1997-2000).

Chemical Industry Institute of Toxicology (CIIT). Scientific Research Committee (1999-2000).

Asphalt Institute. Toxicology Committee (Chairman; 1990-1992).

American College of Toxicology. (Finance Committee, 1991-1994)
Health Effects Institute. Mobile Air Toxics Workshop, Benzene Working Group, invited participant, Monterey, California (December 1992). Workshop on complex mixtures.

Rutgers University, External Advisory Committee, Joint Graduate Program in Toxicology (1993-2000)

EDITORIAL RESPONSIBILITIES:

Journal of Toxicology and Environmental Health - Editorial Board (1975-1980) (1993-2000)
Journal of Toxicology and Environmental Health, Part A – Special Issue, The Toxicology of Nine Light Petroleum Hydrocarbons, C.R. Mackerer and J.B. Galvin, eds., Taylor and Frances, Phila, 1999.
Journal of Environmental Pathology and Toxicology - Editorial Board (1977-1982)
Toxicology and Industrial Health - Section Editor (1985-1989)

PATENTS: (17 to Date)

PUBLICATIONS: (Numerous pages – not listed)

LEON M. STOCK, Consultant

EDUCATION

Institution	Degree	Year	Field of Study
University of Michigan	B. S.	1952	Chemistry
Purdue University	Ph.D.	1959	Chemistry

PROFESSIONAL POSITIONS

1958-61	Instructor, Department of Chemistry, University of Chicago
1961-65	Assistant Professor, Department of Chemistry, University of Chicago
1965-70	Associate Professor, Department of Chemistry, University of Chicago
1970-96	Professor, Department of Chemistry, University of Chicago
1976-81	Master, Physical Sciences Collegiate Division, University of Chicago
1976-81	Associate Dean, Division of Physical Sciences, University of Chicago
1976-81	Associate Dean, The College of the University of Chicago
1984-87	Faculty Associate, Argonne National Laboratory
1985-87	Joint Appointment, Chemistry Division, Argonne National Laboratory
1985-88	Chairman, Department of Chemistry, University of Chicago
1988-95	Director, Chemistry Division, Argonne National Laboratory
1988-95	Senior Chemist, Chemistry Division, Argonne National Laboratory
1996-	Professor Emeritus, Department of Chemistry, University of Chicago
1996-97	Visiting Senior Chemist, Chemistry Division, Argonne National Laboratory
1995-03	Consultant to Safety Issue Resolution Teams, Hanford Site, Richland, Washington
1996-00	Faculty Associate, Washington State University
2003-	Consultant to Research and Technology Department, WTP, Richland, Washington

HONORS AND APPOINTMENTS

1971	Rosetta Briegel Barton Lecture, University of Oklahoma
1974	L. J. and N. M. Quantrell Prize
1981-86	Editorial Board, Journal of Organic Chemistry
1982	Member, FASAC Panel on Soviet Fast Reaction Chemistry Research
1983	Chairman, Gordon Conference on Fuel Science
1983-86	Member, Council of the Gordon Research Conferences
1984	Member, National Research Council Panel on Cooperative Research in Fossil Energy
1984-90	Member, Energy Engineering Board, National Research Council, National Academy of Sciences
1985	Member, National Research Council Panel on the Strategic Petroleum Reserve
1986-89	Member, Program Panel, Illinois Coal Board
1986-96	Member, Editorial Board, Energy and Fuel
1987	H. H. Storch Award of the American Chemical Society
1987	Member, National Research Council Panel on Future Directions in Fossil Energy Research

1988	Energy Lecturer, University of Utah
1988-90	Exploratory Research Associate, Electric Power Research Institute
1989	Member, National Research Council Panel on Liquid Fuels Production Technologies
1990-95	Scientific Advisory Committee, Center for Imaging Science, University of Chicago
1990-95	Advisory Board, Center for Applied Research, University of Kentucky
1990-95	Member, Coal and Energy Advisory Committee, Illinois Coal Association
1990-92	Member, American Chemical Society Joint Board, Council Committee on Science
1992	Brown Lecturer, Purdue University
1992-93	Member, National Research Council Panel on Research Needs of Advanced Process Technology Program
1992-95	Member, Tank Waste Science Panel, Pacific Northwest National Laboratory
1994-95	Editorial Advisory Panel, Coal: Resources, Properties, Utilization, Pollution.
1995	Peter Given Award of Pennsylvania State University
1995	Member, Department of Energy Panel on Research Opportunities at Synchrotron Facilities
1996-97	Member, Panel on New Strategy for Resolution of Hanford Waste Tank Safety Issues, Pacific Northwest National Laboratory
1998	Member, Department of Energy Panel on Research Needs in Radiation Chemistry

CONSULTANT

1964-95	Phillips Petroleum Company
1966	Mondolfo Associates, Inc.
1972	Judge Abraham L. Marovitz
1975	Dow Chemical Company
1978-80	Lankanau, Kovner, and Bickner, Inc.
1978-88	Peoples Gas Company, Chicago, Illinois
1990-95	AMOCO Oil Company
1991-92	Helene Curtis, Inc.
1993	Imperial Oil Company, Canada
1994	Advanced Fuel Research
1995-03	Contractor Groups, Hanford Facility, Richland Washington
1996	Resin Technology, Inc.
1995-	Pacific Northwest National Laboratory
2000-	InterTox, Inc.
2003-	Bechtel, Waste Treatment Plant Facility, Richland Washington

Address
6695 SW 86th Avenue
Portland, Oregon 97223
1-503-768-4642
lmstock6695@aol.com

Professor Stock has written over 220 articles and paper

INDEPENDENT TOXICOLOGICAL PANEL MEMBERS

Dr. Kenneth R. Still, Chair

Dr. Still has just retired from his position as Senior Director, Safety and Occupational Health for the U.S. Navy's Pacific Fleet, and is currently the principal of his own consulting firm, Occupational Toxicology Associates. He has held senior positions involving toxicology, industrial hygiene, occupational safety and health, research and major program development. During this time, he also held adjunct faculty professorships at several universities including the University of Hawaii John Burns School of Medicine; Johns Hopkins University School of Public Health; Wright State University School of Medicine; Uniform Services University of Health Sciences; Eastern Virginia Medical School; Wright State University Institute of Environmental Quality; and the Air Force Institute of Technology School of Engineering and Environmental Management.

Dr. Still's expertise and experience includes toxicology research program development; toxicology and occupational health program development and management; interpretation of toxicological data; hazard identification; human health and ecological risk assessment; exposure control and prevention; communication and interpretation of occupational health, environmental, preventive medicine and toxicological data; exposure assessment characterization; toxicology, occupational health, risk assessment training; research laboratory management and organization; Chemical/Biological/Radiological/Nuclear defense vulnerability assessments; and confined space characterization.

Dr. Still's research interests are in biochemical toxicology, occupational exposure level development, human health risk assessment, ecological risk assessment, reproductive/developmental effects of depleted uranium, health effects of jet propulsion fuels, submarine atmosphere contaminants and escape mechanisms, PCB control and health effects, chemical hormesis, chemical warfare agent exposure effects, and occupational toxicology. He has over 240 publications to his credit and is currently working on his third book. .

Dr. Still is a National Research Council Post Graduate Advisor in biochemical and occupational toxicology. He has served or is serving on over 25 government and industry committees related to toxicology, occupational health and industrial hygiene, including seven different subcommittees of the National Academy of Sciences, National Research Council, Committee on Toxicology; National Advisory Committee, U.S. Environmental Protection Agency, on Acute Exposure Guidelines; American Industrial Hygiene Association (AIHA), current Chair of Toxicology Committee; AIHA Emergency Response Planning Guidelines Committee; AIHA Workplace Environmental Exposure Level Committee; American Conference of Governmental Industrial Hygienists (ACGIH), past Board Member; Permanent Conference Committee ACGIH/AIHA, Chair; Bureau of Medicine and Surgery Closed Living and Working Space Environmental Working Group and Industrial Hygiene Officer Advisory Board; Navy, Army, Air Force Tri-Service Toxicology Consortium Executive Management Council Chair; and Department of Defense Committee on Low Dose Exposure to Chemical Warfare Agents. He is a Certified Industrial Hygienist; Certified Environmental Auditor; Certified Safety Professional;

Certified Hazardous Materials Manager, Master Level; Registered Environmental Manager; and Registered Environmental Property Assessor.

Dr. Still holds a PhD in Chemical/Physiological Ecology from Oklahoma State University and has received advanced training in toxicology and risk assessment from Harvard, Johns Hopkins, MIT, and University of Cincinnati.

Dr. Donald E. Gardner

Dr. Gardner has over forty years of experience in the field of toxicology. He received a B.S. and M.S. degree from Creighton University with majors in biology, chemistry and medical microbiology, and holds a PhD in Environmental Health from the University of Cincinnati.

Dr. Gardner's past employment includes 20 years at the U.S. Environmental Protection Agency/U.S. Public Health Service. While at the EPA he served as the Director, Inhalation Toxicology Division, where he was responsible for both the animal and human toxicology program that addressed the potential health risks associated with exposure to environmental chemicals. Following retirement from the EPA, Dr. Gardner joined Northrop/ManTech Corporation as Vice-President and Chief Scientist. At the present time he is President of Inhalation Toxicology Associates, Inc., a company that provides consulting services to several government agencies and private industry including U.S. EPA, NIEHS, NIH, NASA, WHO, and private law firms.

Dr. Gardner has served on numerous advisory panels in the area of environmental health and toxicology. He has been on the National Academy of Science, National Research Council since 1989 and has been Vice-Chairman of the Committee on Toxicology. Dr. Gardner has served as Chairman for eight NAS/NRC COT subcommittees, including the subcommittee on Guidelines for Space Maximum Allowable Concentration for Space Station Contaminants and Acute Exposure Guideline Levels for Selected Airborne Chemicals. He is presently on the Editorial Board of Toxic Substances Journal, the Environmental and Nutritional Interactions Journal, the Journal of Immunotoxicology, Toxicology Mechanisms and Methods, and New Perspectives: Toxicology. He is co- Editor of the Target Organ Toxicology Series (15 volumes) and Toxicology of the Lung (four editions). Throughout his career he has published over 250 manuscripts. He is the founding Editor and Editor-in-Chief of the Journal of Inhalation Toxicology.

He has been designated Lifetime National Associate Member of the National Academy of Sciences in "recognition as advisor to the Nation in matters of science, engineering, and health." He has received the lifetime outstanding achievement award from the Society of Toxicology Specialty Sections in both inhalation toxicology and in immunotoxicology, several EPA Scientific and Technological Achievement Awards and the Meritorious Service Award from the U.S. Public Health Service. Dr. Gardner was awarded the NASA Outstanding Public Service Award in recognition for guiding NASA toward a safer environment to enhance future exploration of space. He has held numerous elected positions in toxicology organizations, including President and Vice-president of three Society of Toxicology Specialty Sections

including Metals, Inhalation Toxicology, and Immunology. He also served as President of the North Carolina Chapter of the Society of Toxicology and as President of the Academy of Toxicological Sciences.

Dr. Gardner is a Board Certified Fellow of the Academy of Toxicological Sciences and has served as adjunct professor at seven academic institutions including Duke University, North Carolina State University and the University of Massachusetts.

Dr. Gardner's fields of specialization include occupational and environmental health, toxicology of confined space, U.S. EPA Programs and Policies, assessment of health effects associated with tobacco smoke, and NASA's ISS Program.

Dr. Robert Snyder

Dr. Snyder is Professor of Pharmacology and Toxicology, Rutgers Ernest Mario School of Pharmacy, Professor of Toxicology, Rutgers, The State University of New Jersey and has 40 years of academic experience in toxicology and pharmacology. He also holds visiting professorships at various European universities including Nueherberg, Germany and University of Tubingen. Dr. Snyder was the Director, Joint Graduate Program in Toxicology and Robert Wood Johnson Medical School, University of Medicine and Dentistry of New Jersey; Chairman, Department of Pharmacology and Toxicology, Rutgers Ernest Mario School of Pharmacy; Director, Division of Toxicology, Environmental and Occupational Health Sciences Institute; Acting Director, Environmental and Occupational Health Sciences Institute; and, Associate Director for Research, Ernest Mario School of Pharmacy.

He has conducted numerous seminars and lectures on toxicology at over 100 national and international universities, seminars, conferences, and industries. He has edited, reviewed, or written chapters on over 25 books and co-authored over 70 research reports related to toxicology.

He received Rutgers University Board of Trustees Award for Excellence in Research and twice received Humboldt Research Award for U.S. Scientists. He is or has been a member of the National Academy of Sciences Committee on Toxicology and six different subcommittees of this committee; Board of Toxicology, National Academy of Sciences; Chairman, NAS-NRC Committee on Alkylbenzenes; and witness on several OSHA Hearings on Benzene. He has been a member of the editorial board of Toxicology and Applied Pharmacology Journal and is currently on the editorial board of Journal of Applied Toxicology and the International Journal of Toxicology.

Dr. Snyder currently serves as the President of the American College of Toxicology.

Dr. Snyder's research involves solvent toxicology, chemically induced bone marrow depression, liver toxicity, chemical carcinogenesis, drug metabolism, mixed function oxidase, cytochrome P-450, biological reactive intermediates, enzyme isolation and purification, and biomarkers for exposure to chemicals.

Dr. Snyder is board certified by the Academy of Toxicological Sciences. He holds a PhD in Biochemistry from State University of New York.

Dr. Jorge C. Olguin

Dr. Olguin has 35 years of experience with DuPont Company in several facets of industrial hygiene, including regulatory compliance; development of corporate safety and health guidelines; coordination of occupational health programs; and acting as company's regulatory resource on TSCA and OSHA regulations. Dr. Olguin is the Principal Consultant for DuPont Safety Resources and previously was the Principal Occupational Health Consultant and Senior Occupational Health Fellow for the DuPont Nylon Strategic Business Unit.

Dr. Olguin is a past Diplomate of the American Board of Industrial Hygiene and received certification in the Comprehensive Practice of Industrial Hygiene.

Dr. Olguin holds a PhD in Analytical Chemistry from Kansas State University.

APPENDIX B

ONE- AND TWO-CARBON COMPOUNDS

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B1.0 INTRODUCTION

Sampling and analysis methodologies historically used for tank headspace characterization did not address all organic gases and vapors. Mass spectroscopy is the primary analytical technique for identification of organic vapors, and it does allow a vast number of volatile compounds to be identified. However, it has generally been conducted with scans that precluded the detection of low molecular weight compounds. There have also been limitations to the sampling devices and the quantitative recovery of small, highly polar organic compounds. To address these issues, a list of plausible one- and two-carbon compounds was developed and evaluated to determine whether there are compounds that should be added to the Chemicals of Potential Concern list. The one- and two-carbon compound list developed is given in Table B-1.

Evaluations were based on the efficacy of past and current sampling methods to detect the compounds at levels of concern, and on the potential for formation, release, and emission of the compounds.

Table B-1. One- and Two-Carbon Compounds Evaluated (2 Sheets)

Chemical	CAS Number	Formula	Molecular Weight (g/mol)
Ethane	74-84-0	CH_3CH_3	30.070
Ethene	74-85-1	CH_2CH_2	28.054
Ethyne	74-86-2	CHCH	26.038
Hydrogen cyanide	74-90-8	HCN	27.026
Isocyanic acid	75-13-8	HNCO	43.025
Formic acid	64-18-6	HCO_2H	46.026
Acetic acid	64-19-7	CH_3CO_2H	60.053
Glyoxylic acid	298-12-4	$OHCCO_2H$	74.036
Glycine	56-40-6	$H_2NCH_2CO_2H$	75.067
Glycolic acid	79-14-1	$HOCH_2CO_2H$	76.052
Oxalic acid	144-62-7	HO_2CO_2H	90.035
Formamide	75-12-7	$HCONH_2$	45.041
Acetamide	60-35-5	CH_3CONH_2	59.068
N-Methylformamide	123-39-7	$HCONHCH_3$	59.068
Nitromethane	75-52-5	CH_3NO_2	61.041
Dinitromethane	625-76-3	$CH_2(NO_2)_2$	106.038
Trinitromethane	517-25-9	$CH(NO_2)_3$	151.035
Nitroethane	79-24-3	$CH_3CH_2NO_2$	75.067
1,1-Dinitroethane	600-40-8	$CH_3CH(NO_2)_2$	120.065
Methyl nitrite	624-91-9	CH_3ONO	61.041
Ethyl nitrite	109-95-5	CH_3CH_2ONO	75.067
Methyl nitrate	598-58-3	CH_3ONO_2	77.040
Ethyl nitrate	625-58-1	$CH_3CH_2ONO_2$	91.067
Methylamine	74-89-5	CH_3NH_2	31.057
Dimethylamine	124-40-3	CH_3NHCH_3	45.084
Ethylamine	75-04-7	$CH_3CH_2NH_2$	45.084
Carbon disulfide	75-15-0	CS_2	76.139
Carbonyl sulfide	463-58-1	OCS	60.075
Hydrazine	302-01-2	H_2NNH_2	32.045
Methyl hydrazine	60-34-4	CH_3NHNH_2	46.072
1,1-Dimethylhydrazine	57-14-7	$(CH_3)_2NNH_2$	60.099

Table B-1. One- and Two-Carbon Compounds Evaluated (2 Sheets)

Chemical	CAS Number	Formula	Molecular Weight (g/mol)
1,2-Dimethylhydrazine	540-73-8	$(CH_3)NHNHCH_3$	60.099
Methyl hydroperoxide	3031-73-0	CH_3OOH	48.041
Ethyl hydroperoxide	3031-74-1	$CH_3CH2OOH$	62.068
Methyl peroxynitrite	484678-32-2	CH_3OONO	77.040
Ethyl peroxynitrite	215229-01-9	CH_3CH_2OONO	91.066
Methyl peroxynitrate	42829-59-4	CH_3OONO_2	93.039
Ethyl peroxynitrate	64160-40-3	$CH_3CH_2OONO_2$	107.066
Nitrosomethane	865-40-7	CH_3NO	45.041
Nitrosoethane	925-91-7	CH_3CH_2NO	59.068
Methanal oxime	75-17-2	CH_2NOH	45.041
Ethanal oxime	107-29-9	CH_3CHNOH	59.068
Aziridine (Ethyleneimine)	151-56-4	cyclic-CH_2CH_2NH	43.068

Note: CAS = Chemical Abstracts Service.

B2.0 HYDROCARBONS

Three low molecular weight hydrocarbons would generally not have been detected by the analytical methods: Ethane, ethene, and ethyne. These simple molecules are undoubtedly produced by degradation of organic wastes and would be readily released into the headspaces. The observed headspace concentrations of other low molecular weight hydrocarbons that are routinely detected (methane, propane, propene, butane, etc.) suggest that the waste chemistry does not produce large quantities of the short-chained hydrocarbons. Table B-2 lists the three species of interest along with the four other smallest hydrocarbons (in italics), their Occupational Exposure Limits (OELs), and their maximum reported headspace concentrations. These chemicals are considered simple asphyxiants by the ACGIH and have correspondingly high OELs. Considering the relatively low concentrations of other hydrocarbons, there is no basis for expecting the headspace concentrations of ethane, ethene, or ethyne to be at or above 10% of their OELs.

Table B-2. Low Molecular Weight Hydrocarbons

Chemical	CAS[1] Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Methane	*74-82-8*	*16.043*	*ACGIH TLV = 1000 ppmv*	*17*
Ethane[2]	74-84-0	30.070	ACGIH TLV = 1000 ppmv	0.089
Ethene	74-85-1	28.054	ACGIH TLV = 200 ppmv	ND[3]
Ethyne	74-86-2	26.038	NIOSH REL = 2500 ppmv	ND
Propane	*74-98-6*	*44.097*	*OSHA PEL = 1000 ppmv*	*4.7*
Propene	*115-07-1*	*42.081*	*ACGIH TLV = 1000 ppmv*	*4.4*
Propyne	*74-99-7*	*40.065*	*OSHA PEL = 1000 ppmv*	*0.34*

Notes: [1] CAS = Chemical Abstract Service
[2] Ethane has been reported in samples from tanks 241-TX-111 and 241-S-110, apparently because mass spectral scans had been adjusted to allow their detection. The majority of organic vapor samples were not analyzed in that fashion.
[3] ND = not detected

B3.0 ACIDS

Oxidation reactions of organic wastes result in the production of organic acids and their sodium salts. Release of the low molecular weight organic acids into the tank headspaces is deterred by both their high water solubility and their tendency to exist in ionic form in basic aqueous solution. Table B-3 lists seven organic acids identified as potentially present in the headspaces but not reported due to sampling or analytical limitations, along with one observed organic acid (acetic acid) and its maximum reported headspace concentration.

Table B-3. Low Molecular Weight Organic Acids

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Hydrogen cyanide	74-90-8	27.026	ACGIH TLV = 4.7 ppmv	ND
Isocyanic acid	75-13-8	43.025	Screening Value = 0.13 ppmv	ND
Formic acid	64-18-6	46.026	ACGIH TLV = 5 ppmv	ND
Acetic acid	64-19-7	60.053	OSHA PEL = 10 ppmv	0.26
Glyoxylic acid	298-12-4	74.036	Screening Value = 12 ppmv	ND
Glycine	56-40-6	75.067	Screening Value = 100 ppmv	ND
Glycolic acid	79-14-1	76.052	Screening Value = 1.2 ppmv	ND
Oxalic acid	144-62-7	90.035	ACGIH TLV = 0.5 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

To evaluate the potential headspace concentrations of formic acid, thermodynamic modeling of the partial pressures of formic and acetic acids were conducted for six tanks with measured formate and acetate liquid concentrations, and two additional worst-case scenarios. Modeling was done using the Environmental Simulation Program® (ESP) Water Analyzer module. Results indicated much lower acetic acid vapor concentrations than the maximum reported and are presented in Table B-4.[3] The model consistently predicts a partial pressure of acetic acid higher than that of formic acid, even at a very low waste pH of 9.5. Given this result, the maximum formic acid vapor concentration is expected to be lower than the maximum reported concentration of acetic acid vapor, 0.26 ppmv, and below 10% of its OEL of 5 ppmv.

[3] ESP Water Analyzer runs to estimate the partial pressure of other acids were attempted but the library of thermodynamic data used did not include the necessary parameters to model the partial pressure of oxalic or glycolic acids. Glycine and glyoxylic acid (or glyoxylate) have not been detected in the waste, so ESP analyses of these was not attempted.

Table B-4. Estimated Partial Pressures of Formic and Acetic Acids

Tank	Partial Pressure (mmHg)		Sample Description
	Acetic Acid	Formic Acid	
241- AY-102	5.2E-11	6.9E-13	241-AY-102 Core 312:15; Riser 67 Segment Lower Half; Centrifuged Liquid
241-BY-105	1.4E-13	6.3E-15	241-BY-105 Core 251:2; Riser 7 Drainable Liquid; Total
241-AW-101	6.7E-14	4.1E-15	241-AW-101 Core 306; CentLiquid; Riser 13 Core Composite; Centrifuged Liquid
241-BY-105	3.8E-11	2.1E-12	241-BY-105 Core 246R: 2R; Riser 11B Drainable Liquid; Total
241-U-109	1.9E-13	2.6E-14	241-U-109 Core 238: 1; Riser 8 Drainable Liquid; Total
241-AN-107	9.3E-13	5.9E-13	241-AN-107 7AN-02-01A; Riser 19 Grab Sample; Supernatant Liquid
Low pH (9.8)	1.5E-08	1.4E-08	High CN, low pH, others roughly consistent
Lowest pH (9.5)	2.9E-08	2.7E-08	High CN, lowest pH, others roughly consistent

In the high pH, high sodium content aqueous waste, dissolved oxalic acid is expected to exist primarily in ionic forms that are non-volatile (oxalate, monosodium oxalate, etc.). High concentrations of oxalic acid are prohibited by high sodium waste content and the fact that sodium oxalate has a low solubility. By contrast, the sodium salt of acetic acid is relatively soluble, and acetate ions are much more soluble in the aqueous waste. These considerations suggest the oxalic acid vapor concentration in the tanks is very low compared to the acetic acid concentration, and well below levels of concern.

Glycine and glyoxylic and glycolic acids are also not expected to be present in the tank headspaces at levels of concern. Like the other organic acids, these are expected to exist in primarily their ionic, non-volatile forms, and have been judged to be below levels of concern.

Headspace sampling for hydrogen cyanide was conducted at ten ferrocyanide waste-bearing tanks in 1994. None of the 35 samples collected indicated detectable levels of hydrogen cyanide. Detection limits for these samples ranged from 0.04 to 19 ppbv, all well below 10% of the 4.7 ppmv established OEL for hydrogen cyanide. Given these data, hydrogen cyanide was judged to not be at levels of concern.

Isocyanic acid was considered with its tautomer, cyanic acid. In the high pH waste liquids, they would be expected to exist in their ionic form, cyanate. Cyanate has been hypothesized to exist as a short-lived intermediate in the decomposition of certain wastes (RPP-21854). Based on the low expected steady state concentrations of cyanate ion and the even lower concentrations of either acidic form, isocyanic acid was judged to be below levels of concern.

B4.0 AMIDES

Table B-5 lists the three low molecular weight amides considered to be of potential concern along with applicable toxicological guidelines and reported headspace concentrations. Laboratory tests conducted on these compounds indicated that each would have higher detection limits than less polar organic vapors (i.e., > 0.010 ppmv), but that existing thermal desorption trap methods would allow its detection if it were present at high concentrations (Sears 2005).

Table B-5. Low Molecular Weight Amides

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Formamide	75-12-7	45.041	ACGIH TLV = 10 ppmv	0.050
Acetamide	60-35-5	59.068	Screening Value = 0.01 ppmv	0.003
N-Methylformamide	123-39-7	59.068	Screening Value = 0.4 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

Formamide has been reported in sorbent trap samples from tanks 241-AX-102, 241-BY-112, 241-U-103, and the AN Farm exhaust stack, with the highest concentration about 0.050 ppmv. Reported levels of formamide are well below 10% of its TLV, and it is not considered a potential risk. Thermal desorption trap methods would easily indicate the presence of formamide if it occurred at concentrations approaching 1 ppmv (10% of its TLV).

Acetamide has been reported in two tanks, 241-AX-102 and 241-AX-103, at the maximum concentration of about 0.003 ppmv. The reported levels of acetamide are below the established screening value (PNNL-15640), but given the poor recovery of this chemical in laboratory studies, it could have been present above the established 0.01 ppmv screening value. However, the 0.01 ppmv screening value includes a factor of ten for the potential carcinogenicity of acetamide, which on subsequent analysis was deemed to be inappropriate (PNNL-15736). The reported maximum 0.003 ppmv of acetamide is well below an adjusted screening value of 0.1 ppmv and, therefore, is concluded to not be present at a level of concern.

N-Methylformamide has not been reported in any headspace samples, but the laboratory studies indicate that the thermal desorption trap methods would have detected it had it been at its screening value of 0.4 ppmv. On this basis, it is concluded that N-methylformamide is not present at a level of concern.

B5.0 NITRO- COMPOUNDS

Five low molecular weight nitro- compounds have been identified as potentially present at levels of concern in the tank headspaces. Table B-6 lists these with available toxicological guidelines and reported headspace concentrations. Laboratory studies found both the SUMMA and thermal desorption trap characterization methods to allow identification and quantitation of both nitromethane and nitroethane (Sears 2005).

Table B-6. Low Molecular Weight Nitro- Compounds

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Nitromethane	75-52-5	61.041	ACGIH TLV = 20 ppmv	0.036
Dinitromethane	625-76-3	106.038	Screening Value = 0.2 ppmv	ND
Trinitromethane	517-25-9	151.035	Screening Value = 0.2 ppmv	ND
Nitroethane	79-24-3	75.067	ACGIH TLV = 100 ppmv	ND
1,1-Dinitroethane	600-40-8	120.065	ACGIH TLV = 100 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

The only nitro- compound to have been reported in the headspaces, nitromethane, has been reported in tanks 241-AX-103, 241-TX-118, and 241-U-112. The maximum reported concentration, 0.036 ppmv, is less than 0.2% of its TLV. Based on laboratory tests that indicated this chemical to be amenable to past and current methods (Sears 2005), there is no reason to expect this chemical is above 10% of its TLV in any headspace. A similar argument applies to the nitroethane, and it is concluded here that nitroethane is not present at a level of concern.

Increased polarity has the potential to complicate the recovery and analysis of the dinitro- and trinitro- compounds in Table B-6. Laboratory tests similar to those conducted on nitromethane and nitroethane were not conducted for the dinitro- and trinitro- compounds because standards were not available. However, there is no reason to think that the dinitro- and trinitro- compounds are so much more difficult to analyze that the past and current methods would not be able to detect them if they were present above the screening value of 0.2 ppmv (detection limits for tentative identification of many organic vapors range from 0.001 to 0.01 ppmv in headspace sample analyses). It is judged that none of the nitro- compounds are likely to be present in the headspaces above their Screening Values or 10% of their OELs.

B6.0 ORGANIC NITRITES AND NITRATES

Four low molecular weight organic nitrite and nitrate compounds have been identified as potentially present at levels of concern in the tank headspaces. Table B-7 lists these with their established Hanford Site Acceptable Occupational Exposure Levels (AOELs) and maximum reported headspace concentrations. Laboratory tests to evaluate the recovery and analysis of these chemicals from thermal desorption traps and SUMMA canister samples were limited by the availability of standards, and only ethyl nitrite was tested (Sears 2005). The tests indicated ethyl nitrite to be easily detected and analyzed using SUMMA canisters and the EPA TO-15 method, but problems were experienced with the thermal desorption traps and EPA TO-17 method. Methyl nitrite, methyl nitrate, ethyl nitrate, and several other organic nitrites and nitrates have frequently been detected in both SUMMA and thermal desorption trap samples, indicating these methods capable of detecting these analytes. Because the SUMMA TO-15 method has been routinely deployed to characterize the tank headspaces, and over 400 EPA TO-15 results for these and other organic nitrite and nitrate vapors exist in the TCD, the existing data on these chemicals is considered sufficient to evaluate their presence.

Table B-7. Low Molecular Weight Organic Nitrites and Nitrates

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Methyl nitrite	624-91-9	61.041	Hanford AOEL = 0.1 ppmv	0.32
Ethyl nitrite	109-95-5	75.067	Hanford AOEL = 0.1 ppmv	ND
Methyl nitrate	598-58-3	77.040	Hanford AOEL = 8 ppmv	0.33
Ethyl nitrate	625-58-1	91.067	Hanford AOEL = 8 ppmv	0.40

Note: CAS = Chemical Abstract Service
ND = not detected.

Methyl nitrite has been reported above its screening value, an AOEL has been developed for it, and it has been added to the COPC list. None of the other three in Table B-6 have been reported above their screening values and are, therefore, not considered to present a significant risk to tank farm workers.

B7.0 AMINES

Three low molecular weight amines were identified as potentially not being properly addressed by past or existing vapor sampling methods. These are listed in Table B-8 with their ACGIH TLVs. None have been detected in the tank headspaces. Laboratory tests conducted with these three chemicals indicated neither the SUMMA TO-15 method nor the thermal desorption trap TO-17 method was appropriate for measurement of low levels of these chemicals (Sears 2005).

Table B-8. Low Molecular Weight Amines

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Methylamine	74-89-5	31.057	5 ppmv	ND
Dimethylamine	124-40-3	45.084	5 ppmv	ND
Ethylamine	75-04-7	45.084	5 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

Subsequent to the laboratory testing, a campaign to survey tank farm sources for these amines was initiated, and ethylamine has been detected above 10% of its TLV in the exhaust stacks for AN, AP, and AW farms, as well as at the breather filter of tank 241-A-105. Methylamine and dimethylamine have not been found to be at levels of concern. The survey of sources for these low molecular weight amines will be extended to other farms as warranted.

B8.0 SULFIDES

Two sulfides, listed in Table B-9, were identified as being potentially not addressed by past or existing sampling and analysis methods. Both have been reported in headspace samples, with the maximum reported concentrations given in Table B-9. Laboratory studies indicated the SUMMA EPA TO-15 method to be easily capable of detection limits of less than 0.010 ppmv. Carbon disulfide was also found to be amenable to analysis by the thermal desorption trap EPA TO-17 method. Both carbon disulfide and carbonyl sulfide are listed target analytes of the EPA TO-15 methodology. Because the sampling and analytical methods should adequately address these sulfides, and their reported maximum concentrations are below levels of concern, they were determined to require no further evaluation.

Table B-9. Low Molecular Weight Amines

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Carbon disulfide	75-15-0	76.139	ACGIH TLV = 10 ppmv	0.79
Carbonyl sulfide	463-58-1	60.075	Screening Value = 1 ppmv	0.026

Note: CAS = Chemical Abstract Service
ND = not detected.

B9.0 HYDRAZINES

The four hydrazines listed in Table B-10 were considered as potential tank headspace constituents. Hydrazines are highly reactive and good reducing agents, and are not expected to be present at significant concentrations in the waste or headspaces. RPP-21854 considered the formation of hydrazines possible but did not identify plausible reactions for formation of hydrazines. They were included on the 1- and 2-carbon potential chemicals list because methyl hydrazine and 1,1-dimethyl hydrazine had been reported in headspace samples. However, review of the analytical data indicated the analytes were not correctly identified (TWS05.008 - Letter), and there is no evidence that any of the hydrazines in Table B-10 are present at levels of concern.

Table B-10. Hydrazines

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Hydrazine	302-01-2	32.045	ACGIH TLV = 0.010 ppmv	ND
Methyl hydrazine	60-34-4	46.072	ACGIH TLV = 0.010 ppmv	ND
1,1-Dimethylhydrazine	57-14-7	60.099	ACGIH TLV = 0.010 ppmv	ND
1,2-Dimethylhydrazine	540-73-8	60.099	IARC 2A carcinogen	ND

Note: CAS = Chemical Abstract Service
IARC = International Agency for Research on Cancer
ND = not detected.

B10.0 HYDROPEROXIDES, PEROXYNITRITES, AND PEROXYNITRATES

Table B-11 lists the hydroperoxides, peroxynitrites, and peroxynitrates considered. These highly reactive compounds are unstable in water, and have consequently not been measured in either waste or headspace samples. They are presumed to exist as reaction intermediates in the waste (RPP-21854) and some fraction of the intermediates must escape into the headspace. However, they continue to react with ventilation system condensates and surfaces such as the high efficiency particulate air filters before being released into the worker breathing zone. On these bases, the hydroperoxides, peroxynitrites, and peroxynitrates are judged to be at levels far below levels of concern in the worker breathing zone and are not expected to be present at appreciable concentrations in the tank headspaces.

Table B-11. Hydroperoxides

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Methyl hydroperoxide	3031-73-0	48.041	Screening Value = 0.1 ppmv	ND
Ethyl hydroperoxide	3031-74-1	62.068	Screening Value = 0.1 ppmv	ND
Methyl peroxynitrite	484678-32-2	77.040	Screening Value = 0.1 ppmv	ND
Ethyl peroxynitrite	215229-01-9	91.066	Screening Value = 0.1 ppmv	ND
Methyl peroxynitrate	42829-59-4	93.039	Screening Value = 0.3 ppmv	ND
Ethyl peroxynitrate	64160-40-3	107.066	Screening Value = 0.3 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

B11.0 NITROSO COMPOUNDS AND OXIMES

Table B-12 lists two low molecular weight nitroso compounds and their corresponding oximes that were considered here. While expected as waste reaction intermediates, neither the nitroso compounds nor the oximes are stable under waste conditions. RPP-21854 points out that nitroso compounds are spontaneously converted to aldehydes via the hydrolysis of oxime intermediates in the waste:

$$RCH_2N{=}O \rightarrow RCH{=}NOH$$

$$RCH{=}NOH + H_2O \rightarrow RCHO + NH_2OH$$

The aldehydes are also thermodynamically unstable in the waste and can be considered reaction intermediates in the production of other waste species. However, they are expected to be significantly more stable than either the corresponding nitroso compounds or oximes. Furthermore, there are other reaction pathways for the production of aldehydes than via the nitroso compound – oxime pathway (RPP-21854). These considerations suggest, given comparable volatility, the headspace concentrations of the aldehydes would be much (probably many orders of magnitude) higher than either the corresponding nitroso compound or oxime. Given the highest reported concentration of formaldehyde (the aldehyde associated with nitrosomethane and methanal oxime) in the tank headspaces is 0.064 ppmv, and that for acetaldehyde (associated with nitrosoethane and ethanal oxime) was 12 ppmv, the likely concentrations of the nitroso compounds and oximes listed in Table B-12 are judged to be well below their Screening Values.

Table B-12. Nitroso Compounds and Oximes

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Nitrosomethane	865-40-7	45.041	Screening Value = 0.2 ppmv	ND
Nitrosoethane	925-91-7	59.068	Screening Value = 0.2 ppmv	ND
Methanal oxime	75-17-2	45.041	Screening Value = 0.1 ppmv	ND
Ethanal oxime	107-29-9	59.068	Screening Value = 0.1 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

B12.0 AZIRIDINE

Aziridine was identified as a two-carbon molecule that past and current methods might not adequately characterize. However, aziridine is a listed target analyte for the EPA TO-15 air sampling and analysis methodology (EPA 1999), the method currently used for SUMMA canister samples. Hanford Site tank headspace samples collected before the introduction of EPA TO-15 were analyzed using the EPA TO-14 method, modified to allow characterization of polar compounds (the essential difference between the methods). The required detection limit for aziridine, based on the need to detect at 10% of the Tank Farms OEL, is 0.050 ppmv (Table B-13), well above the expected detection limits of the EPA TO-15 methodology. It is judged that appropriate methods have been and are being used to detect and quantify aziridine in Tank Farms vapor samples, and its absence in past samples is evidence that it is not present at levels of concern.

Table B-13. Aziridine

Chemical	CAS Number	Molecular Weight (g/mol)	Exposure Guideline	Maximum Headspace Concentration (ppmv)
Aziridine (Ethyleneimine)	151-56-4	43.068	ACGIH TLV = 0.5 ppmv	ND

Note: CAS = Chemical Abstract Service
ND = not detected.

B13.0 SUMMARY

The evaluations indicated that source sampling should be conducted for three compounds, methylamine, dimethylamine, and ethylamine. All other compounds listed in Table B-1 were deemed to either (1) be amenable to past and current sampling and analytical methodologies and the fact that they were not reported at levels of concern taken as evidence they were not present at levels of concern, or (2) be highly unlikely to exist at levels of concern in the worker breathing zone on the bases of their waste and headspace chemistry.

B14.0 REFERENCES

EPA, 1999, *Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air: Compendium Method TO-15*, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, EPA/625/R-96/010b.

PNNL-15640, 2006, *Screening Values for Non-Carcinogenic Hanford Waste Tank Vapor Chemicals that Lack Established Occupational Exposure Limits*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15736, 2006, *Proposed Occupational Exposure Limits for Non-Carcinogenic Hanford Waste Tank Vapor Chemicals*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

RPP-21854, 2004, *Occurrence and Chemistry of Organic Compounds in Hanford Site Waste Tanks*, Rev. 0, CH2M HILL Hanford Group, Inc., Richland, Washington.

Sears, J., 2005, *27 Organic Compounds Method Development Report for 222-S Analytical Process Group, CH2M HILL utilizing TO-15 and TO-17 methods for Vapor Studies*, RJ Lee Group, Inc. Center for Laboratory Sciences, Pasco, Washington.

TWS05.008, 2005, "Review of ORNL Mass Spectrometry Data from Waste Tank Headspace Analyses," (external letter from D. S. Sklarew and A. Mitroshkov to J. O. Honeyman, CH2M HILL, Hanford Group, Inc., January 25), Pacific Northwest National Laboratory, Richland, Washington.

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APPENDIX C

TECHNICAL BASES FOR LIST OF CHEMICALS OF POTENTIAL CONCERN

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C1.0 INTRODUCTION

This appendix is an update of the toxicological assessment in the previous revision of this report. That revision considered 1,826 chemicals that had been proposed as being potential hazards to tank farm workers, applied established criteria and identified 52 chemicals of potential concern (COPC), 1,538 chemicals needing further evaluation (CNFE), and 236 chemicals with low probabilities of exposure. A concerted effort was conducted to verify the COPC bases and evaluate risks associated with the 1,538 chemicals designated as needing further evaluation. The evaluations are complete, and all chemicals have been either placed on the COPC list or the determined to pose a significant risk to tank farm workers.

C2.0 CHEMICALS NEEDING FURTHER EVALUATION (CNFE)

The 1,538 CNFE were evaluated to determine which should be added to the COPC list and which do not pose a significant risk to tank farm workers. The evaluation process involved revising the CNFE list to address errors, omissions, duplications, and the addition of newly reported chemicals. Evaluations were aimed at (1) verifying (or refuting) the evidence that each chemical was indeed a detected or plausible tank headspace constituent, and (2) establishing reasonable toxicological bases for the inclusion (or exclusion) of each chemical on the COPC list.

C2.1 CNFE LIST CORRECTIONS AND ADDITIONS

The CNFE list was revised to correct several errors and duplicate entries. It was also updated; the original list was based on the characterization data considered final as of September 22, 2004, and much headspace and ventilation system characterization data has subsequently been obtained.

Duplicate entries in the CNFE list were from several sources. Most duplications were from different laboratories reporting partially identified species by different names, such as "Unknown C13 Ketone" and "C13-Alkanone" that are assumed here to be equivalent. Others were associated with there being a limited number of positional isomers; the partially identified "C5-Alkane," for example, was considered a duplicate because all three possible C5-alkanes (n-pentane, 2-methylbutane, and 2,2-dimethylpropane) have been detected in the headspaces and are included individually on the CNFE list. The 62 duplicate entries removed from the CNFE list are included in Table C-1.

Five chemicals were incorrectly included and counted as CNFE when in fact their chemical names (assigned by the analytical laboratories) are ambiguous and do not allow specification of molecular weight. These did not meet the CNFE criteria. Two acid anhydrides were also included as CNFE. These are very improbable headspace constituents because they would hydrolyze to form the corresponding acids. (The corresponding acids of both of these anhydrides have been reported in other headspace samples and are included as CNFE.) Two additional CNFE were apparently misnamed by the analytical laboratories, the errors probably

being typographical. Because the likely correct names for these two chemicals are already on the CNFE list, both of these have been removed. The five errors, two acid anhydrides, and two misnamed chemicals removed from the CNFE list are included, as noted, in Table C-1.

New chemicals detected in the headspaces and added to the Tank Characterization Database (TCD) have been added to the CNFE list. This increased the CNFE list by 89 chemicals. An additional 20 low-molecular weight organic chemicals were added to the CNFE list on the basis of a preliminary review that indicated (1) they were potential waste degradation products, and (2) past and current vapor sampling methods may not be capable of detecting them. The result of the CNFE list corrections described above and these additions was a list of 1,576 chemicals.

C2.2 VERIFICATION THAT CNFE ARE PRESENT IN HEADSPACES

One aspect of CNFE evaluation was a verification that the chemical either was properly identified and was a real headspace constituent, or could reasonably be expected to be present at a level of concern. This addresses chemicals that have not been detected in the headspaces, errors in the analytical reporting, and the group of low-molecular weight organic compounds that a preliminary review suggested may be of importance.

CNFE that are expected to be amenable to past and current vapor sampling methods, but that have not been detected in any tank headspace or ventilation system sample, are listed in Table C-2. Because none have been detected, these 91 chemicals were deemed to be present below levels of concern. None of these are known or probable carcinogens.

At various stages in the evaluation process, the archived analytical data associated with selected CNFE were reviewed for accuracy by qualified analytical chemists. Most CNFE were originally identified in samples using a gas chromatograph (GC) with a mass spectrometer (MS) detector. The GC chromatographically separates the different vapors from each other, and the MS provides mass spectra that are then compared to a library of known spectra. Vapors separation is not always complete and low analyte concentrations can give weak mass spectra. These and other factors can result in difficult and sometimes erroneous identifications. Though computers do much of the work, the identification of an analyte as a specific chemical is ultimately based on the analyst's judgment and criteria that may vary between laboratories and analysts. While a complete review of the 100,000+ analytical vapor data in the TCD was unwarranted, many CNFE considered to be unlikely headspace constituents based on known waste chemistry and all CNFE identified as being potentially present at levels of concern (see Section C2.3) were subjected to analytical review. Reviews and findings were documented and independently reviewed, with all recommended changes recorded in the TCD. Table C-3 lists the 70 misidentified CNFE (TWS05.008; TWS05.016; PNNL-15673).

Two chemicals, cis- and trans-1,3-dichloropropene, were erroneously reported as headspace sample constituents. All reported instances of these two chemicals were found to be associated with the laboratory contamination (from a gas standard) introduced during sample analysis (PNNL-15673). These two chemicals are listed in Table C-3 and were excluded from further consideration.

There were 41 low-molecular weight organic vapors included on the CNFE list that were thought to *not* be addressed by past and current sampling methods. Preliminary assessments suggested that each was a plausible waste degradation product. Several CNFE were included because the analytical GC/MS procedures employed did not collect mass spectral information for molecules of less than 33 atomic mass units (vapors with molecular weights less than 33 were categorically not detected). These 41 CNFE either do not have measured headspace concentrations with which to judge occupational exposure risk, or their measured headspace concentrations were considered potentially skewed. At issue for each of these chemicals is

- Would the sampling and analytical methods allow its detection and a meaningful estimate of its concentrations to be made?
- Is the CNFE plausibly present at levels of concern where it is released into the worker breathing zone?

The evaluation of these 41 chemicals is described in Appendix B, and results are summarized in Table C-4. Three compounds were determined to be inadequately addressed by past and current sampling and analytical methods, and potentially present at levels of concern: Methylamine, ethylamine, and dimethylamine. Further efforts to evaluate these three amines are described in Section C3.0. The remaining 38 chemicals were judged not to pose a significant risk to tank farm workers. Table C-4 gives brief summaries of the bases for these conclusions.

C2.3 EVALUATION OF OCCUPATIONAL EXPOSURE RISK

The remaining 1,372 CNFE have each been detected in a tank headspace and/or ventilation system, their existence considered reasonable (or verified by review of the analytical data), and their reported concentrations are assumed to be unbiased. The criterion for determining whether a reported chemical belongs on the COPC list is that its maximum reported source (headspace or ventilation system) concentration[4] be greater than or equal to 10% of its OSHA PEL or ACGIH TLV. When neither an OSHA PEL nor an ACGIH TLV was available, the same criterion was applied using the lowest OEL established by a U.S. governmental agency (e.g., NIOSH REL) or professional organization (e.g., AIHA WEEL).

About 10% of the 1,372 CNFE do have established U.S. OELs, and their evaluation was straightforward. The evaluation of CNFE that do not have established U.S. OELs was conducted by first separating these into their various chemical classes. Hydrocarbons (i.e., compounds composed only of carbon and hydrogen), which constituted over half of the CNFE, were evaluated as a class. Non-hydrocarbons were evaluated using a multi-step process described in Section C2.3.3.

[4] Maximum source concentrations were calculated as described in PNNL-15640. Analytical results for each analyte were averaged by laboratory, sample type, and sampling event (e.g., the three results for acetone reported by PNNL in SUMMA canisters for the June 8, 1995 tank 241-A-101 sampling event were averaged), then the highest chosen as the maximum source concentration.

There were 18 chlorinated biphenyls that were effectively added to the COPC list without individual evaluations. This occurred in July 2005 when the two COPC chlorinated biphenyl mixtures (Arochlor-1254 and Arochlor-1242) were combined and re-listed as a class of compounds, "chlorinated biphenyls," that includes any and all mono-, di- and poly-chlorinated biphenyls. This is discussed in Section C2.4.3.

C2.3.1 CNFE with Established U.S. OELs

There were 131 CNFE for which U.S. OELs were available. The maximum source concentration of each was calculated and compared to 10% of the corresponding OEL. Two CNFE, pyridine and 3-buten-2-one, were identified as having been reported in headspace samples above 10% of their OELs and were added to the COPC list on July 6, 2005 (7F800-05-JOH-006 – Letter). The 129 CNFE for which the maximum source concentration was below 10% of the OEL are listed in Table C-5 with their OELs and maximum source concentrations.

C2.3.2 Hydrocarbon CNFE

On advice from the Independent Toxicology Panel (ITP), the hydrocarbons were evaluated as a mixture. RPP-RPT-29404 determined that the hydrocarbon mixtures found in the tank headspaces were similar in composition and toxicology to the standard petroleum industry fuel stream mixtures (i.e., gasoline, kerosene, diesel, etc.). RPP-RPT-29404 noted that the tank headspace hydrocarbon mixtures have relatively low aromaticity, and recommended that the ACGIH TLV for kerosene (200 mg/m^3) be applied as the Tank Farms OEL for hydrocarbons measured as a mixture. Note that this does not obviate or supersede any existing OELs for individual hydrocarbons (e.g., benzene and 1,3-butadiene). Any OELs applicable to individual hydrocarbons still apply and must be considered apart from the treatment of hydrocarbons as a mixture. The recommendation to use the 200 mg/m^3 ACGIH TLV for kerosene as the AOEL for Tank Farms hydrocarbon mixtures was adopted by the EASRG on December 7, 2005 (see Appendix E). Table C-6 lists the 701 hydrocarbons that were addressed.

C2.3.3 Other CNFE

Those 522 CNFE not having established U.S. OELs or addressed as hydrocarbons were subjected to an evaluation process to determine whether they should be added to the COPC list. It was recognized that many of the relatively non-toxic chemicals had been detected only at very low concentrations, and that these did not warrant in-depth toxicological assessments. The first step of the evaluation process, therefore, was to conduct a screening to identify those CNFE needing in-depth toxicological assessments, and those below levels of concern.

Screening was performed by comparing the maximum average headspace concentration of each chemical to a conservatively established screening value. The screening values were based on

occupational exposure data and guidelines (e.g., non-U.S. OELs), on available toxicological data, and on information for toxicologically similar chemicals (surrogates) if no specific toxicological data were available. PNNL-15640 describes the procedure used to develop screening values and list all chemicals screened, their screening values, and the bases of each screening value. This process identified 51 chemicals as needing in-depth evaluations.[5] Additionally, PNNL-15640 considered potentially carcinogenic chemicals separately, and recommended that acetamide and five additional substituted furans be further evaluated to address their carcinogenic potential. Those with maximum headspace concentrations less than their screening values (and not considered potential carcinogens) are considered to not pose significant risks to tank farm workers.

The 57 chemicals identified as needing in-depth evaluations are listed in Table C-7. Six of the 57 chemicals identified by the screening process for further work were ambiguously identified by the reporting analytical laboratory, and it was determined that their identification was too vague to warrant further attention. Three of the 57 are common plasticizers and thought to be associated with contamination of the vapor sampling manifold (PNNL-15646). One other, SO_X, is thought to be based on questionable analytical data, and a sampling campaign to verify or refute its existence at levels of concern was conducted (see Section C3.3.2).

Toxicologists evaluated the remaining 47 chemicals using established procedures. AOELs were proposed for 41 of the 47 chemicals, the remaining six were determined to not warrant further attention.[6] The proposed AOELs and their bases were peer reviewed and presented to the EASRG. Accepted values for these AOELs are listed in Table C-8. Also listed are the corresponding maximum reported headspace concentrations. Those chemicals for which the maximum headspace concentration equals or exceeds 10% of the AOEL are noted in the final column as belonging on the COPC list. Those chemicals not identified as belonging on the COPC list were judged to not pose significant risks to tank farm workers.

[5] PNNL-15640 lists 72 non-carcinogens (Table 3). Of these, 18 were subsequently determined to be misidentified or laboratory contaminants (see Table B-3 of this appendix), and three were COPCs without established OELs (not CNFEs). These 21 chemicals are not counted in the 522 CNFEs discussed in this section.

[6] The six determined to not warrant further attention include the potential carcinogen (acetamide) which evidence suggest is not carcinogenic to humans, four fatty acid esters and one 18-carbon alcohol which are safe enough to be used as emollients in hand lotions and cosmetics (PNNL-15673).

C2.4 COPC VERIFICATION

The original COPC list was composed of chemicals meeting one of the following three criteria:

(1) The chemical was a known or probable carcinogen as determined by the International Agency for Research on Cancer Carcinogen (IARC) (IARC group 1 and 2A), the U.S. Environmental Protection Agency (EPA) (EPA group A, B1, and B2), or the American Conference of Governmental Industrial Hygienists (ACGIH) (ACGIH group A1 or A2);

(2) The chemical had a maximum reported tank headspace concentration equal to or greater than 10% of the lowest occupational exposure guideline (LOEG) available; and

(3) The chemical was identified by the contracted ITP as warranting special consideration as a COPC.

The resulting list included 51 chemicals with (when the criteria were applied in the order above) 24 selected by criterion 1, 23 selected by criterion 2, and four selected by criterion 3. One chemical, dimethyl mercury, was added to the COPC list because it had recently been detected for the first time in the tanks, and its maximum headspace concentration was considered too uncertain to omit it from the COPC list.

Four chemicals were included that had been reported in waste (condensed phase) samples, but never in a tank headspace. Some chemicals had no recognizable origin as process waste or degradation products, several were more likely to be present in the worker breathing zone from non-tank sources, and several carcinogens were present at very low levels compared to their OELs. Reviews were conducted to determine whether they are indeed present at levels of concern in the tanks. Table C-9 shows chemicals that have subsequently been removed from the COPC list. The following subsections explain the bases for these changes.

C2.4.1 Misidentified Chemicals

As described in Section C2.2, many headspace chemicals, including most of the COPC list, were originally identified using GC/MS techniques that entail a degree of subjective interpretation of mass spectra. To ensure that these identifications were reasonable, a peer review of the archived analytical data for selected chemicals was conducted (TWS05.008). Findings were in turn reviewed (7FA00-05-SJE-005), and there was concurrence that seven of the chemicals had been misidentified by the original laboratory. These are noted in Table C-9.

C2.4.2 NO_2, CO and CO_2

Tank Farms IH conducted a risk comparison and determined that three chemicals (nitrogen dioxide, carbon monoxide, and carbon dioxide) were more likely to be present in the worker breathing zone from non-tank sources (e.g., exhaust from internal combustion engines) (7B600-MLZ-05-005 - Letter) and needed to be addressed in the workplace regardless of contributions from in tank sources. Because these are addressed by an existing worker safety

program, these three chemicals were removed from the COPC list in July 2005 (7F800-05-JOH-006 - Letter).

C2.4.3 Aroclor-1242 and Aroclor-1254

Two commercial carcinogenic polychlorinated biphenyl (PCB) mixtures, Aroclor-1242 and Aroclor-1254, were reported in (condensed phase) waste samples (WTP-RPT-008, PNWD-2461). Though neither of these PCB mixtures had been detected in any tank headspace, based on the first criterion these two chemicals were included on the original COPC list. Vapor samples from several tanks indicated the presence of individual PCBs. Given that EPA guidance has been to assume all chlorinated biphenyls (mono-, di- and polychlorinated) are carcinogenic and it is reasonable that other chlorinated biphenyls besides those specifically identified in samples may be present, it was decided that all chlorinated biphenyls properly belong on the COPC list. A class of chemicals "chlorinated biphenyls" was added, and the two Aroclor mixtures were simultaneously removed from the COPC list because all their constituents are included in the "chlorinated biphenyl" category.

C2.4.4 Estimated DDE and 1-Naphthylamine Headspace Concentrations

Two chemicals, p,p'-dichlorodiphenyldichloroethylene (DDE) and 1-naphthylamine, were included on the previous COPC list because they had been detected in waste (condensed phase) samples and are carcinogens.[7] Neither had been reported in headspace samples, but initial assessments of their potential concentrations in the tank headspaces considered only their (pure-component) vapor pressures, which would be sufficient to present health hazards. However, when the measured concentrations of these chemicals in the waste (in the tanks where they were detected) were used to estimate potential headspace concentrations (PNNL-15648), the evidence indicated these would not be at levels of concern in the tank headspaces.

DDE was found only in solid waste samples from tank 241-C-104 (WPT-RPT-008), evidently coating solid particles. Mass transfer of DDE from this region to the tank headspace, because it has very low solubility in the aqueous waste, is very slow. PNNL-15632 estimated the steady-state concentration of DDE in the passively-ventilated tank 241-C-104 to be on the order of 5×10^{-5} ppbv, well below its established AOEL of 3.7 ppbv and not a plausible hazard to tank farm workers. DDE was removed from the COPC list by EASRG consensus on February 15, 2006 (see Appendix E).

1-Naphthylamine was detected in solid waste samples in tanks 241-AN-107 and 241-AW-107, but below detection limits in the aqueous waste above the solids (PNWD-2461). Using the detection limit reported for the aqueous phase samples and Henry's Law, PNNL-15632 estimated the equilibrium concentration of 1-naphthylamine above the aqueous waste would be about 0.23 ppbv. This value represents an upper bound because it assumed 1-naphthylamine was actually present at the detection limit (and indeed it was not detected in the aqueous waste

[7] DDE is classified as a possible human carcinogen by IARC (group 2B); 1-naphthylamine has been identified by OSHA as a known carcinogen.

samples), and would be decreased by active ventilation maintained on these tanks, and by the dilution of air from other tanks connected to the exhausters. When compared to the AOEL of 0.2 ppbv, the EASRG recommended on February 15, 2006, that 1-naphthylamine be removed from the COPC list (see Appendix E).

C2.4.5 Analytical Laboratory Contaminants

Three chemicals on the COPC list (chloroethene, 1,2-dichloroethene, and 1,2-dibromoethane) were determined to be erroneously reported in headspace samples. These three chemicals had been reported by only one of the analytical laboratories, and only in the SUMMA canister samples – not in sorbent trap samples collected at the same times that provided equivalent detection capabilities for these vapors. Review of the analytical data clearly showed that these three chemicals were associated with the laboratory gas standard, and the reported results were suspect (PNNL-15648). The analytical results have been flagged as suspect in the TCD. The EASRG determined by consensus that these should be removed from the COPC on January 26, 2006 (see Appendix E).

C2.4.6 Sampling Manifold Contaminant

Analytical results for 2,6-bis(1,1-dimethylethyl)-4-methylphenol (BHT) were determined to be suspect because there was evidence that it was off-gassed by a component of the sample collection manifold. BHT is a common antioxidant and plasticizer that is believed to have been released by the glass-fiber particulate air filters used in a specific vapor sampling manifold (PNNL-15646). Analytical data for this chemical, as well as others thought to be of similar origins, have been flagged suspect in the TCD. BHT was removed from the COPC list on February 15, 2006 (see Appendix E).

C2.4.7 Carcinogens Reported at Less Than 10% of Tank Farms OEL

As described earlier, the first COPC criterion was whether the chemical was a known or probable human carcinogen. This selection criterion took precedence over the other criteria, so eight carcinogenic chemicals were added to the COPC despite the fact that their maximum reported headspace concentrations were less than 10% of their established OELs. This was deemed necessary to allow time to evaluate whether or not the OELs included and properly addressed the carcinogenicity of each chemical.[8] An evaluation indicated that the OELs did adequately address carcinogenicity (7M500-MLZ-06-008). Based on these findings, the EASRG decided to remove these eight chemicals from the COPC list (see Appendix E). These are noted in Table C-9.

[8] Some OELs were developed before their carcinogenicity had been established.

C2.4.8 Carbon Disulfide

Carbon disulfide was included on the COPC list because its maximum average headspace concentration, 0.86 ppmv, was above 10% of the 1 ppmv NIOSH REL. The Tank Farms OEL and Action Limit for carbon disulfide, however, are based on the OSHA PEL value of 10 ppmv, and using the OSHA PEL as the guideline, carbon disulfide would not be on the COPC list. Given that carbon disulfide is not a commonly detected vapor and that it can be detected and estimated by both SUMMA and thermal desorption sorbent traps, the EASRG decided to remove carbon disulfide from the COPC list on January 26, 2006 (see Appendix E) to make the COPC list consistently based on the Tank Farms 10% OEL criterion.

C2.4.9 2-Ethyl-1-hexanol and 3-Hexanone

Four non-carcinogenic chemicals were on the original COPC list based on ITP recommendations. Exposure and toxicological data on these four chemicals were evaluated, and AOELs were developed (PNNL-15736), reviewed, and accepted by the EASRG (January 16, 2006 EASRG meeting minutes). Two chemicals (2-ethyl-1-hexanol and 3-hexanone) were determined to have maximum Tank Farms concentrations less than 10% of their established AOELs, and were removed from the COPC list by consensus of the EASRG on January 26, 2006 (see Appendix E).

C3.0 FIELD SCREENING FOR SELECTED CHEMICALS

Two general types of chemicals were considered plausibly present at levels of concern and warranting field studies to determine concentrations. The first type includes organic vapors that are too polar to be quantitatively retrieved from the sampling devices used in Tank Farms or too small to be detected by the mass spectrometric analytical techniques. Consideration of these small organic molecules (see Appendix B) led to a sampling campaign to measure concentrations of several small amines at tank farm sources. The second type includes inorganic vapors that would not have been detected using any past or existing sampling methods. This section discusses these sampling campaigns and their results.

C3.1 AMINES

A laboratory study indicated that past vapor sampling methods were inadequate for the quantitative recovery of low-molecular weight amines (Sears 2005). Given that amines are chemically reasonable products of waste degradation reactions, particularly from the degradation of certain complexants (RPP-21854), a special sampling campaign was conducted to evaluate the concentrations of methylamine, dimethylamine, and ethylamine at sources in the 200-East Area.

An appropriate sampling and analysis method was selected (OSHA Organic Method #36) and 22 samples collected from the AN, AP, AW, and the AZ-702 primary exhaust stacks, as well as the breather filters of tanks 241-A-101, 241-A-103, and 241-A-105. Ethylamine concentrations

were reported above 10% of its Tank Farms OEL (ACGIH TLV of 5 ppmv) in ten of the samples, and this chemical was added to the COPC list (see Table C-10). Neither methylamine nor dimethylamine were reported at or above 10% of their Tank Farms OELs (both have an ACGIH TLV of 5 ppmv) in the A-complex.

C3.2 METALS

Inorganic species that might be present in addition to mercury and dimethyl mercury were evaluated. A focus group of senior chemists postulated what inorganic species are thermodynamically possible, and four species types were identified, alkyl, carbonyl, halide, and nitroso metal compounds (TWS05.019). In addition, some inorganic species had already been measured in tank headspaces (e.g., hydrogen sulfide), so sulfides and hydrides were included in the evaluation. A chemical species list was produced by reviewing chemicals found in tank waste and then examining thermodynamic chemical electronic databases and other thermodynamic literature. The list included arsenic, antimony, lead, molybdenum, ruthenium, selenium, tin, tellurium, and tungsten (TWS05.019).

Metals and organometallic sampling was performed on 14 tanks (all six A Farm tanks, all four AX Farm tanks, 241-C-104, 241-S-101, -102, and -103) using a slightly modified EPA Method 29 (*Determination of Metals Emissions from Stationary Sources*). Sixty liters of air exiting the tank risers immediately next to the tank breather filter were pulled through two oxidizing acid solutions; the first was an aqueous mixture of 5% HNO_3/10% H_2O_2 and the second was an aqueous mixture of 4% $KMnO_4$/10% H_2SO_4. The oxidizing acid solutions were analyzed specifically for the metals identified above using induced coupled plasma mass spectroscopy, and also subjected to a broad spectrum induced coupled plasma analysis for any other metals. Blank corrected results showed near or less than detection limit concentrations (~0.0006 mg/m^3) for most specific analytes. All samples (including blanks) contained small concentrations of calcium, boron, silica, and sodium, common components of the glass containers holding the oxidizing acid solutions. Based on these results, further metals sampling was judged to be not warranted.

C4.0 CHEMICALS OF POTENTIAL CONCERN

The COPC list was modified to remove chemicals for various reasons and add others as described in the previous sections. The resulting 48 chemicals are listed in Table C-10 along with their Tank Farms OEL, the source of the OEL, and the date the chemical was added. Seven "substituted furans" are listed under that entry in Table C-10; these are the only substituted furans that have been detected in tank headspace samples. The chemicals listed all meet the following single criterion:

The measured concentration exceeds 10% of its Tank Farms OEL.

Three COPC list entries refer to classes of chemicals. For clarification, they are defined here.

Chlorinated biphenyls – any of the 209 congeners of chlorinated biphenyls, including mono-, di-, and poly-chlorinated biphenyls. If more than one chlorinated biphenyl is present, the concentrations of all chlorinated biphenyls are to be added when determining the exposure level.

Hydrocarbons – the summation of all chemicals composed only of carbon and hydrogen.

Substituted furans – any chemically substituted form of furan that includes the five-member oxygen-containing ring moiety of furan and contains at least one carbon-carbon double bond in the furan ring. If more than one substituted furan and/or furan itself is present, the concentrations of all substituted furans and furan are to be added when determining the exposure level.

C6.0 REFERENCES

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Table C-1. Duplicate CNFE List Entries (2 Sheets)

Chemical Identification Number	Chemical Name
106-31-0	Butanoic acid, anhydride
122-39-4	Benzenamine, N-phenyl-
UAE000-04b	C16-Alkene (or C15 alkene) mixture
UAK000-02a	C12-Alkane (or C13 alkane) mixture
UAK000-02b	C13-Alkane (or C12-alkane) mixture
UAK000-04a	C14-Alkane (or C15-alkane) mixture
UAK000-04b	C15-Alkane (or C14-alkane) mixture
USI000-06	Tetramethylcyclotrisiloxane
USI000-09	Octamethylcyclotrisiloxane
1336-36-3	Polychlorinated biphenyls
14898-79-4	2-Butanol
1565-80-6	1-Butanol, 2-methyl-, (S)-
18936-17-9	Butanenitrile, 2-methyl-
2051-49-2	Hexanoic acid, anhydride
4254-15-3	1,2-Propanediol, (S)-
542-75-6	1,3-Dichloropropene
54676-39-0	Cyclohexane, 2-butyl-1,1,3-trimethyl-
MAMUAR0-01b	n-Phenyl benzenamine mixture
MARUAK0-01b	C11-Alkane mixture
MAYUAE0-02a	1-Pentyne mixture
MCYCY00-01a	Cyclobutane, 1,2-diethyl-, trans mixture
MCYKE00-01a	Cyclohexane, 1,2-diethyl-1-methyl- mixture
MCYKE00-01b	Ethanone,1-phenyl mixture
MKEUAR0-03a	3-Decanone mixture
MNIUAK0-01b	C6-Alkane mixture
MOHUAR0-01a	3-Ethyl-2-methyl-2-pentanol mixture
MU00UAR-01b	Dimethyl benzene mixture
MUAEUAR-02a	C12-Alkene mixture
MUAEUAY-01a	Pentene mixture
MUAEUAY-01b	Pentyne mixture
UAE006-01M	C6-Alkene and others
UAE007-02	Heptene
UAE007-03b	C7-Cycloalkane (or C7-alkene) mixture
UAE010-02b	C10-Cycloalkane(or C10-alkene) mixture
UAE011-03b	C11-Cycloalkane (or C11-alkene) mixture
UAE011-04a	C11-Diene (or C11 cycloalkene) mixture
UAE012-02b	C12-Cycloalkane (or C12-alkene) mixture
UAE013-02b	C13-Cycloalkane (or C13-alkene) mixture
UAE013-03a	C13-Diene (or C13-cycloalkene) mixture
UAE015-01b	C15-Cycloalkane (or C15-alkene) mixture
UAK005-01	C5-Alkane
UAK008-02	Pentane, trimethyl-, isomer
UAK009-02	Hexane, trimethyl-, isomer
UAK010-01M	C10-Alkane and others
UAK010-02	Heptane, trimethyl-, isomer
UAK013-01	C13-Alkane
UAR000-03M	Dimethylnaphthalenes
UAR000-12M	C4-Benzene & others
UAR000-17	C3-Benzene

Table C-1. Duplicate CNFE List Entries (2 Sheets)

Chemical Identification Number	Chemical Name
UCY007-02	C4-Cyclopropane
UCY008-03	Dimethylcyclohexane
UCY009-01M	C3-Cyclohexane and others
UCY009-03	Trimethylcyclohexane (coeluent)
UCY010-03	Tetramethylcyclohexane
UCY012-06	dimethyl-decahydronaphthalene
UCY012-06M	Dimethyl-decahydronaphthalene + others
UCY012-07	Unknown C2 Alkyl Decahydronaphthalene
UCY013-05	Trimethyldecahydronaphthalene
UCY014-05	Unknown C4-Decahydronaphthalene
UHC000-09M	Methyl pyridine and others or mixture containing methyl pyridine
UKE006-01	C6-Ketone
UKE007-02	C7-Ketone
UKE008-01	C8-Alkanone
UKE008-02	Octanone
UKE008-03	Unknown C8-Ketone
UKE009-01	C9-Ketone
UKE011-01	C11-Ketone
UKE012-01	C12-Ketone
UKE013-01	Tridecanone
UKE013-03	Unknown C13 Ketone
UKE014-02	Tetradecanone

Table C-2. CNFE with Concentrations Below Analytical Reporting Limits (2 Sheets)

Chemical Identification Number	Chemical Name
106-44-5	4-Methylphenol (p-Cresol)
1319-77-3	Cresol (all isomers)
616-40-0	Hydrazine, 1,1-diethyl-
101-83-7	Cyclohexylamine, N-cyclohexyl- (Dicyclohexylamine)
1024-57-3	Heptachlor epoxide
106-94-5	Propane,1-bromo-
107-10-8	1-Propanamine
1071-26-7	2,2-Dimethylheptane
107-31-1	Butanal, 3-hydroxy-
108-21-4	1-Methylethyl acetate
108-64-5	Ethyl 3-methylbutanoate
11096-82-5	Arochlor-1260
1116-54-7	Ethanol, 2,2'-(nitrosoimino)bis-
112-37-8	Undecanoic acid
119-33-5	4-Methyl-2-nitrophenol
12672-29-6	Arochlor-1248
12674-11-2	Arochlor-1016
129-00-0	Pyrene
13952-84-6	2-Butanamine
140-79-4	Piperazine, 1,4-dinitroso-
15104-03-7	Piperidine, 4-methyl-1-nitroso-
1526-17-6	2-Fluoro-6-nitrophenol
156-87-6	1-Propanol, 3-amino-
16536-57-5	cis-2-Bromocyclohexanol
16747-32-3	Pentane, 3-ethyl-2,2-dimethyl-
1721-93-3	Isoquinoline, 1-methyl-
1825-61-2	Methoxytrimethylsilane
1825-65-6	Butoxytrimethylsilane
18720-66-6	3-Heptanol, 6-methyl-
19549-83-8	3-Heptanone, 2,6-dimethyl-
19689-18-0	4-Decene
2110-78-3	Methyl 2-hydroxy-2-isobutyrate
21571-34-6	2-Fluoro-4-nitrophenol
22967-92-6	Methylmercury
2562-37-0	1-Nitrocyclohexene
2581-34-2	3-Methyl-4-nitrophenol
286-18-0	7-Azabicyclo[4.1.0]heptane
3034-41-1	1-Methyl-4-nitro-1H-imidazole
309-00-2	Aldrin
319-84-6	alpha-BHC
319-85-7	beta-BHC
319-86-8	delta-BHC
3404-58-8	3-Ethyl-1-hexene
34075-28-0	Butane, 2,3-dimethy-2-nitro-
34419-76-6	1-Propanamine, N,2-dimethyl-
37324-23-5	Arochlor-1262
394-41-2	3-Fluoro-4-nitrophenol
3970-62-5	3-Pentanol, 2,2-dimethyl-
3973-27-1	p-Dioxin, 2,3-dihydro-2,5,6-trimethyl-

Table C-2. CNFE with Concentrations Below Analytical Reporting Limits (2 Sheets)

Chemical Identification Number	Chemical Name
39884-53-2	N-nitroso-2-methyl-oxazolidine
403-19-0	2-Fluoro-4-nitrophenol
4245-37-8	2-Propenoic acid, 2-methyl-, ethenyl-
497-56-3	2-Methyl-3,5-dinitrophenol
504-20-1	2,5-Heptadien-4-one, 2,6-dimethyl-
50623-57-9	Butyl nonanoate
5103-71-9	alpha-Chlordane
5343-96-4	2-Butanol, 3-methyl-, acetate
53778-73-7	2-Butanol, 1-methoxy-
54166-32-4	2,6,6-Trimethyloctane
553-97-9	p-Benzoquinone, 2-methyl-
55556-86-0	Pyrrolidine, 2,5-dimethyl-1-nitroso-
55556-93-9	4-Piperidinol, 1-nitroso-
58-89-9	Lindane (isomeric mix)
59-50-7	4-Chloro-3-methylphenol
608-33-3	2,6-Dibromophenol
62016-37-9	2,4,6-Trimethyloctane
62108-23-0	2,5,6-Trimethyldecane
625-50-3	Acetamide, N-ethyl-
638-10-8	2-Butenoic acid, 3-methyl-, ethyl
700-38-9	5-Methyl-2-nitrophenol
7247-89-4	Piperidine, 2-methyl-1-nitroso-
73583-56-9	2,6-Dimethyl-6-nitro-2-hepten-4-one
7421-93-4	Endrin Aldehyde
75-25-2	Bromoform (Tribromomethane)
758-21-4	Silane, ethyldimethyl-
75-98-9	Propanoic acid, 2,2-dimethyl
76-44-8	Heptachlor
78-42-2	Tri(2-ethylhexyl)phosphate
79-05-0	Propanamide
79-77-6	2,6,6-Trimethylcyclohexen-1-yl-3-buten-2-one
83-32-9	Acenaphthene
91-63-4	Quinoline, 2-methyl-
922-64-5	Propanedinitrile, methylene
924-46-9	1-Propanamine, N-methyl-N-nitroso-
96-69-5	bis(3-tert-Butyl-4-hydroxy-6-methylphenyl) sulfide
98060-52-7	2,2,6-Trimethyloctane
98060-54-9	2,2,8-Trimethyldecane
99-28-5	2,6-Dibromo-4-nitrophenol
994-05-8	Butane, 2-methoxy-2-methyl-
99-66-1	Valproic acid
Not available	Phosphonic acid, dioctadecyl ester

Table C-3. CNFE with Concentrations Below Analytical Reporting Limits (2 Sheets)

Chemical Identification Number	Chemical Name	Note
110-60-1	1,4-Butanediamine	4
123-75-1	Pyrrolidine	4
1453-58-3	1H-Pyrazole, 3-methyl-	4
16339-12-1	Methanamine, N-methoxy-N-nitroso-	4
16778-70-4	1H-1,2,4-Triazole, 1-ethyl-	4
18294-04-7	Ethanedioic acid, bis(trimethylsilyl) ester	4
1886-75-5	Propane, 2-[(1,1-dimethylethyl)sulfonyl]-2-methyl-	4
2432-55-5	Butanethioic acid, S-decyl ester	4
27750-45-4	Benzenepropanoic acid, .alpha.-[(trimethylsilyl)oxy]-, trimethylsilyl ester	4
29052-10-6	Butyric acid, ester with p-hydroxybenzonitrile	4
33342-89-1	1-Propanone, 1-[4-[(trimethylsilyl)oxy]phenyl]-	4
3518-07-8M	Benz[a]acridine, 8,10-diethyl- and others	4
37148-64-4	Benzeneacetic acid, .alpha.,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	4
38165-93-4	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	4
39251-86-0M	2-Furancarboxylic acid, hexyl ester and others	4
421-50-1	2-Propanone, 1,1,1-trifluoro-	4
4342-25-0	3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-	4
505-57-7	2-Hexenal	4
541-01-5	Heptasiloxane, hexadecamethyl-	4
55334-40-2	Benzeneacetic acid, .alpha.,4-bis[(trimethylsilyl)oxy]-, methyl ester	4
55471-01-7	Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-[2-[(trimethylsilyl)oxy]-2-[4-[(trimethylsilyl)oxy]phenyl]ethyl]-	4
55494-10-5	2-Hexenedioic acid, bis(trimethylsilyl) ester, (E)	4
599-70-2	Benzene, (ethylsulfonyl)-	4
637-64-9	2-Furanmethanol, tetrahydro-, acetate	4
75268-01-8	1H-Azepin-1-amine, N-ethylidenehexahydro-	4
75-55-8	1,2-Propylenimine (2-Methyl aziridine)	4
75-77-4	Silane, chlorotrimethyl-	4
883-93-2	Benzothiazole, 2-phenyl-	4
930-22-3	Oxirane, ethenyl-	4
993-07-7	Silane, trimethyl-	4
MAYHC00-01a	2-Decyne mixture	4
MAYHC00-01b	6-Methyl-8,9-(7H)-dihydro-1,2,4-triazolo[4,3-B]-1,2,4-triazepin-8-one	4
UES010-02	Formic acid, 2,6-dimethyl-5-hepten-2-ol ester	4
UHC000-03	C1-Hydroxyquinoline	4
UHC000-04	C2-Hydroxyquinoline	4
UHC000-08M	C1-Acridine and others	4
UHC000-11	6-Amino-2,3-diphenyl(1H)pyrrolo[2,3-b]pyridine	4
USI000-04	p-Trimethylsilyloxyphenyl-bis(trimethylsilyloxy)ethane	4
101300-62-3	Silane, (4,5-dimethyl-1,4-cyclohexadiene-1,2-diyl)	2
107-16-4	Acetonitrile, hydroxy-	2
1115-07-7	Borane, diethylmethyl-	2
22058-71-5	Methylamine, N-(1-methylhexylidene)-	2
31053-55-1	Thiophene, 2-methoxy-5-methyl-	2
311-89-7	1-Butanamine, 1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis	2
430-51-3M	2-Propanone, 1-fluoro- and others	2
512-85-6	2,3-Dioxabicyclo[2.2.2]oct-5-ene, 1-methyl-4-(1-methylethyl)-	2
694-87-1	Bicyclo[4.2.0]octa-1,3,5-triene	2
710-04-3	2H-Pyran-2-one, 6-hexyltetrahydro-	2

Table C-3. CNFE with Concentrations Below Analytical Reporting Limits (2 Sheets)

Chemical Identification Number	Chemical Name	Note
1192-51-4	2,4(3H,5H)-Furandione, 3-methyl-	5
1708-29-8	Furan, 2,5-dihydro-	5
1795-48-8	Propane, 2-isocyanato-	5
1838-59-1	Formic acid, 2-propenyl ester	5
20474-93-5	2-Butenoic acid, 2-propenyl ester	5
22431-09-0	Methanamine, N-(1-methylbutylidene)-	5
2549-67-9	Aziridine, 2-ethyl-	5
31681-26-2	2-Furanacetaldehyde, .alpha.-propyl-	5
34314-82-4	Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	5
3457-92-9	1,5-Pentanediol, dinitrate	5
3777-71-7	Furan, 2-heptyl-	5
4179-38-8	Furan, 2-octyl-	5
4229-91-8	Furan, 2-propyl-	5
56052-94-9	Oxirane, 2-ethyl-3-propyl-, cis-	5
616-45-5	2-Pyrrolidinone	5
627-27-0	3-Buten-1-ol	5
694-05-3	Pyridine, 1,2,3,6-tetrahydro-	5
717-21-5	2-Propen-1-one, 3-(2-furanyl)-1-phenyl-	5
78-76-2	Butane, 2-bromo-	5
96-41-3	Cyclopentanol	5
UAD010-01	Decadienal	5
1072-85-1	Benzene, 1-bromo-2-fluoro-	3
10061-01-5	cis-1,3-Dichloro-1-propene	1
10061-02-6	trans-1,3-Dichloro-1-propene	1

Notes: [1] Determined to be an analytical laboratory contaminant (PNNL-15648).
[2] Misidentified by reporting analytical laboratory (TWS05.008).
[3] Personal email communication from M Stauffer to J.L. Huckaby, September 9, 2004.
[4] Misidentified by reporting analytical laboratory (TWS05.016).
[5] Misidentified by reporting analytical laboratory (PNNL-15673).

Table C-4. Low Molecular Weight Organic Vapors With Potential Characterization Problems

Chemical Identification Number	Name	Formula	Molecular Weight (g/mol)	Exposure Guideline	Exposure Guideline Source*
107-29-9	Ethanal oxime	CH_3CHNOH	59.068	0.1	Screening Value
109-95-5	Ethyl nitrite	$CH_3CH2ONO$	75.067	0.2	Screening Value
123-39-7	N-Methylformamide	$HCONHCH_3$	59.068	0.4	Screening Value
124-40-3	Dimethylamine	CH_3NHCH_3	45.084	5	TLV
144-62-7	Oxalic acid	HO_2CO_2H	90.035	0.5	TLV
151-56-4	Aziridine	cyclic-CH_2CH_2NH	43.068	0.5	TLV
215229-01-9	Ethyl peroxynitrite	CH_3CH_2OONO	91.066	0.01	Screening Value
298-12-4	Glyoxylic acid	$OHCCO_2H$	74.036	12	Screening Value
302-01-2	Hydrazine	H_2NNH_2	32.045	0.01	TLV
3031-73-0	Methyl hydroperoxide	CH_3OOH	48.041	0.01	Screening Value
3031-74-1	Ethyl hydroperoxide	CH_3CH_2OOH	62.068	0.01	Screening Value
42829-59-4	Methyl peroxynitrate	CH_3OONO_2	93.039	0.03	Screening Value
463-58-1	Carbonyl sulfide	OCS	60.075	1	Screening Value
484678-32-2	Methyl peroxynitrite	CH_3OONO	77.040	0.01	Screening Value
517-25-9	Trinitromethane	$CH(NO_2)_3$	151.035	0.2	Screening Value
540-73-8	1,2-Dimethylhydrazine	$(CH_3)NHNHCH_3$	60.099	carcinogen	IARC 2A
56-40-6	Glycine	$H_2NCH_2CO_2H$	75.067	100	Screening Value
57-14-7	1,1-Dimethylhydrazine	$(CH_3)_2NNH_2$	60.099	0.01	TLV
598-58-3	Methyl nitrate	CH_3ONO_2	77.040	1.3	Screening Value
600-40-8	1,1-Dinitroethane	$CH_3CH(NO_2)_2$	120.065	100	TLV
60-34-4	Methyl hydrazine	CH_3NHNH_2	46.072	0.01	TLV
625-58-1	Ethyl nitrate	$CH_3CH_2ONO_2$	91.067	1.3	Screening Value
625-76-3	Dinitromethane	$CH_2(NO_2)_2$	106.038	0.2	Screening Value
64160-40-3	Ethyl peroxynitrate	$CH_3CH_2OONO_2$	107.066	0.03	Screening Value
64-18-6	Formic acid	HCO_2H	46.026	5	TLV
64-19-7	Acetic acid	CH_3CO_2H	60.053	10	PEL
74-84-0	Ethane	CH_3CH_3	30.070	1000	TLV
74-85-1	Ethene	CH_2CH_2	28.054	200	TLV
74-86-2	Ethyne	CHCH	26.038	2500	REL
74-89-5	Methylamine	CH_3NH_2	31.057	5	TLV
74-90-8	Hydrogen cyanide	HCN	27.026	4.7	TLV
75-04-7	Ethylamine	$CH_3CH_2NH_2$	45.084	5	TLV
75-12-7	Formamide	$HCONH_2$	45.041	10	TLV
75-13-8	Isocyanic acid	HNCO	43.025	0.13	Screening Value
75-15-0	Carbon disulfide	CS_2	76.139	10	TLV
75-17-2	Methanal oxime	CH_2NOH	45.041	0.1	Screening Value
75-52-5	Nitromethane	CH_3NO_2	61.041	20	TLV
79-14-1	Glycolic acid	$HOCH_2CO_2H$	76.052	1.2	Screening Value
79-24-3	Nitroethane	$CH_3CH_2NO_2$	75.067	100	TLV
865-40-7	Nitrosomethane	CH_3NO	45.041	0.2	Screening Value
925-91-7	Nitrosoethane	CH_3CH_2NO	59.068	0.2	Screening Value

Notes: * Screening Values are from PNNL-15640
IARC = International Agency for Research on Cancer
PEL = OSHA Permissible Exposure Limit
REL = NIOSH Recommended Exposure Limit.
TLV = ACGIH Threshold Limit Value

Table C-5. CNFE with Established U.S. OELs (3 Sheets)

Chemical Identification Number	Chemical Name	OEL		Maximum Source Concentration	
		Type	(ppmv)	(ppmv)	% of OEL
100-00-5	1-Chloro-4-nitrobenzene	TLV	0.1	0.00076	0.8%
100-41-4	Ethylbenzene	PEL	100	0.14	0.1%
100-42-5	Styrene (Ethenylbenzene)	TLV	20	0.28	1%
100-51-6	Benzenemethanol	WEEL	10	0.010	0.1%
100-52-7	Benzaldehyde	WEEL	4	0.0068	0.2%
100-61-8	Benzenamine, N-methyl-	TLV	0.5	0.0036	0.7%
10102-43-9	Nitric oxide (NO)	PEL	25	1.6	7%
101-84-8	Benzene, 1,1`-oxybis-	PEL	1	0.024	2%
106-35-4	3-Heptanone	PEL	50	1.8	4%
106-46-7	1,4-Dichlorobenzene	TLV	10	0.0033	0.03%
106-68-3	3-Octanone	PEL	25	0.44	2%
106-88-7	1,2-Epoxybutane	WEEL	2	0.084	4%
106-97-8	n-Butane	TLV	800	7.7	1%
107-02-8	Acrolein (2-Propenal)	PEL	0.1	0.0060	6%
107-05-1	3-Chloropropene (Allyl chloride)	PEL	1	0.0064	0.6%
107-13-1	Acrylonitrile (2-Propenenitrile)	REL	1	0.011	1%
107-15-3	Ethylenediamine	PEL	10	0.23	2%
107-18-6	2-Propen-1-ol	TLV	0.5	0.0037	0.7%
107-31-3	Formic acid, methyl ester	PEL	100	0.024	0.02%
107-39-1	1-Pentene, 2,4,4-trimethyl-	WEEL	300	0.046	0.02%
107-87-9	2-Pentanone	REL	150	1.2	0.8%
108-03-2	1-Nitropropane	PEL	25	0.034	0.1%
108-05-4	Vinyl acetate (Ethenyl ethanoate)	TLV	10	0.00078	0.008%
108-10-1	Hexone (Methyl isobutyl ketone)	TLV	50	0.94	2%
108-20-3	Propane, 2,2`-oxybis-	TLV	25	0.097	0.4%
108-39-4	3-Methylphenol (m-Cresol)	REL	2	0.0021	0.1%
108-67-8	1,3,5-Trimethylbenzene	REL	25	0.015	0.06%
108-87-2	Methylcyclohexane	PEL	300	0.38	0.1%
108-88-3	Toluene	TLV	50	1.2	2%
108-89-4	Pyridine, 4-methyl-	WEEL	2	0.057	3%
108-90-7	Chlorobenzene	TLV	10	0.015	0.2%
108-93-0	Cyclohexanol	PEL	50	0.00049	0.001%
108-94-1	Cyclohexanone	TLV	25	0.085	0.3%
108-95-2	Phenol	PEL	5	0.27	5%
108-99-6	Pyridine, 3-methyl-	WEEL	2	0.036	2%
109-06-8	Pyridine, 2-methyl-	WEEL	2	0.062	3%
109-66-0	n-Pentane	REL	120	5.7	5%
109-99-9	Tetrahydrofuran	PEL	200	4.9	2%
110-12-3	5-Methyl-2-hexanone	TLV	50	0.038	0.08%
110-43-0	2-Heptanone	TLV	50	0.60	1%
110-54-3	n-Hexane	TLV	50	2.2	4%
110-62-3	Pentanal	TLV	50	0.24	0.5%
110-82-7	Cyclohexane	TLV	100	1.1	1%
110-83-8	Cyclohexene	PEL	300	0.0027	0.001%
110-89-4	Piperidine	WEEL	1	0.0072	0.7%
111-65-9	n-Octane	REL	75	0.35	0.5%
111-76-2	2-Butoxyethanol	TLV	25	0.061	0.2%
111-84-2	n-Nonane	TLV	200	0.30	0.1%

Table C-5. CNFE with Established U.S. OELs (3 Sheets)

Chemical Identification Number	Chemical Name	OEL		Maximum Source Concentration	
		Type	(ppmv)	(ppmv)	% of OEL
111-87-5	1-Octanol	WEEL	50	0.061	0.1%
115-10-6	Methane, oxybis-	WEEL	1000	2.0	0.2%
120-82-1	1,2,4-Trichlorobenzene	TLV	5	0.016	0.3%
122-39-4	Benzamine, N-phenyl	TLV	1.45	0.030	2%
123-19-3	4-Heptanone	TLV	50	0.44	0.9%
123-38-6	Propionaldehyde	TLV	20	0.26	1%
123-51-3	3-Methyl-1-butanol	PEL	100	0.027	0.03%
123-73-9	trans-2-Butenal	TLV Ceiling	0.3	0.0031	1%
123-86-4	Acetic acid, butyl ester	PEL	150	3.4	2%
126-98-7	2-Propenenitrile, 2-methyl-	TLV	1	0.037	4%
127-19-5	Acetamide, N,N-dimethyl-	PEL	10	0.013	0.1%
1330-20-7	Xylene (all isomers)	PEL	100	0.33	0.3%
1333-74-0	Hydrogen	n.a.[1]	n.a.	n.a.	n.a.
138-86-3	Cyclohexene, 1-methyl-4-(1-methylethenyl)-	WEEL	30	0.022	0.07%
141-78-6	Acetic acid ethyl ester	PEL	400	12	3%
141-79-7	3-Penten-2-one, 4-methyl-	REL	10	0.020	0.2%
142-82-5	n-Heptane	REL	85	0.98	1%
149-57-5	Hexanoic acid, 2-ethyl-	TLV	0.848	0.00031	0.04%
156-59-2	cis-1,2-Dichloroethene	TLV	200	0.0098	0.005%
1717-00-6	Ethane, 1,1-dichloro-1-fluoro-	WEEL	500	0.18	0.04%
287-92-3	Cyclopentane	TLV	600	0.21	0.03%
4170-30-3	2-Butenal	TLV	0.3	0.023	8%
463-82-1	Propane, 2,2-dimethyl-	TLV	600	0.054	0.009%
541-85-5	5-Methyl-3-heptanone	TLV	25	0.043	0.2%
542-56-3	2-Methyl-1-propyl nitrite	TLV	1	0.025	3%
563-80-4	2-Butanone, 3-methyl-	TLV	200	1.8	0.9%
57-55-6	1,2-Propanediol	WEEL	50	0.15	0.3%
592-45-0	1,4-Hexadiene	WEEL	10	0.042	0.4%
6032-29-7	2-Pentanol	PEL	100	0.14	0.1%
627-13-4	Nitric acid, propyl ester	PEL	25	1.2	5%
637-92-3	Propane, 2-ethoxy-2-methyl-	TLV	5	0.00024	0.005%
64-17-5	Ethanol	PEL	1000	21	2%
67-63-0	2-Propanol	PEL	400	2.0	0.5%
67-64-1	Acetone	REL	250	19	8%
71-23-8	1-Propanol	PEL	200	5	3%
71-55-6	1,1,1-Trichloroethane	PEL	350	0.011	0.003%
7440-37-1	Argon	n.a.[1]	n.a.	n.a.	n.a.
74-83-9	Bromomethane	TLV	1	0.014	1%
74-87-3	Chloromethane	TLV	50	0.10	0.2%
74-98-6	Propane	PEL	998	4.7	0.5%
74-99-7	1-Propyne	PEL	1000	0.34	0.03%
75-00-3	Chloroethane	TLV	100	0.039	0.04%
75-28-5	2-Methylpropane	REL	800	0.65	0.08%
75-34-3	1,1-Dichloroethane	PEL	100	0.011	0.01%
75-35-4	1,1-Dichloroethene	TLV	5	0.021	0.4%
75-43-4	Methane, dichlorofluoro-	TLV	10	0.054	0.5%
75-45-6	Chlorodifluoromethane (Freon 22)	TLV	1000	1.7	0.2%
75-65-0	2-Propanol, 2-methyl-	PEL	100	0.13	0.1%
75-68-3	Ethane, 1-chloro-1,1-difluoro-	WEEL	1000	0.73	0.07%

Table C-5. CNFE with Established U.S. OELs (3 Sheets)

Chemical Identification Number	Chemical Name	OEL		Maximum Source Concentration	
		Type	(ppmv)	(ppmv)	% of OEL
75-69-4	Trichlorofluoromethane (Freon 11)	PEL	1000	3.7	0.4%
75-71-8	Dichlorodifluoromethane (Freon 12)	PEL	1000	0.020	0.002%
76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane (Freon 113)	PEL	1000	0.21	0.02%
76-14-2	1,2-Dichloro-1,1,2,2-tetrafluoroethane	PEL	1000	0.012	0.001%
78-78-4	Butane, 2-methyl-	TLV	600	2.5	0.4%
78-79-5	1,3-Butadiene, 2-methyl-	WEEL	50	0.052	0.1%
78-82-0	2-Methylpropanenitrile	REL	8	0.019	0.2%
78-83-1	2-Methyl-1-propanol	TLV	50	0.018	0.04%
78-84-2	Propanal, 2-methyl-	WEEL	25	0.004	0.01%
78-87-5	1,2-Dichloropropane	PEL	75	0.0099	0.01%
78-92-2	2-Butanol	TLV	100	0.21	0.2%
78-93-3	2-Butanone	PEL	200	13	7%
79-00-5	1,1,2-Trichloroethane	TLV	10	0.034	0.3%
79-09-4	Propanoic acid	TLV	10	0.0051	0.05%
79-20-9	Acetic acid, methyl ester	PEL	200	0.043	0.02%
79-34-5	1,1,2,2-Tetrachloroethane	TLV	1	0.021	2%
84-74-2	Dibutylphthalate	PEL	0.4	0.00048	0.1%
872-50-4	2-Pyrrolidinone, 1-methyl-	WEEL	10	0.024	0.2%
88-72-2	1-Methyl-2-nitrobenzene	TLV	2	0.0014	0.07%
91-20-3	Naphthalene	PEL	10	0.014	0.1%
95-48-7	2-Methylphenol (o-Cresol)	REL	2	0.012	0.6%
95-50-1	1,2-Dichlorobenzene	TLV	25	0.0081	0.03%
95-63-6	1,2,4-Trimethylbenzene	TLV	25	0.015	0.06%
96-22-0	3-Pentanone	TLV	200	0.062	0.03%
97-99-4	2-Furanmethanol, tetrahydro-	WEEL	2	0.016	0.8%
98-82-8	Cumene (Isopropylbenzene)	PEL	50	0.088	0.2%
98-83-9	Benzene, (1-methylethenyl)-	TLV	50	0.031	0.06%
98-86-2	Acetophenone	TLV	10	0.44	4%
98-95-3	Nitrobenzene	PEL	1	0.0027	0.3%
99-08-1	Benzene, 1-methyl-3-nitro-	TLV	2	0.00019	0.01%
99-82-1	Cyclohexane, 1-methyl-4-(1-methylethyl)-	WEEL	30	0.047	0.2%
99-99-0	Benzene, 1-methyl-4-nitro-	TLV	2	0.00033	0.02%

Note: [1] Hydrogen and argon are both simple asphyxiants and do not have OELs.

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
1002-17-1	Decane, 2,9-dimethyl-
1002-43-3	Undecane, 3-methyl-
1002-68-2	3-Undecene, (E)-
1008-80-6	Naphthalene, decahydro-2,3-dimethyl-
101-81-5	Benzene, 1,1`-methylenebis-
103-65-1	Benzene, propyl-
10374-74-0	7-Tetradecene
106-42-3	1,4-Dimethylbenzene
1068-19-5	4,4-Dimethylheptane
1069-53-0	Hexane, 2,3,5-trimethyl-
106-98-9	1-Butene
107-00-6	1-Butyne
107-01-7	2-Butene
1071-81-4	Hexane, 2,2,5,5-tetramethyl-
1072-05-5	Heptane, 2,6-dimethyl-
1074-17-5	Benzene, 1-methyl-2-propyl-
107-83-5	2-Methylpentane
108-08-7	Pentane, 2,4-dimethyl-
1083-56-3	Benzene, 1,1`-(1,4-butanediyl)bis-
108-38-3	1,3-Dimethylbenzene
109-67-1	1-Pentene
109-68-2	2-Pentene
1113-56-0	1,3-Pentadiene, 2,3-dimethyl-
111-66-0	1-Octene
111-67-1	2-Octene
1116-90-1	1,4-Hexadiene, 4-methyl-
1118-58-7	1,3-Pentadiene, 2-methyl-
1120-21-4	n-Undecane
1120-36-1	1-Tetradecene
112-40-3	n-Dodecane
112-41-4	1-Dodecene
112-88-9	1-Octadecene
112-95-8	Eicosane
115-07-1	1-Propene
115-11-7	1-Propene, 2-methyl-
1191-96-4	Cyclopropane, ethyl-
1192-18-3	cis-1,2-Dimethylcyclopentane
124-11-8	1-Nonene
124-18-5	n-Decane
13049-35-9	1,1`-Biphenyl, 2,2`-diethyl-
13151-04-7	1-Heptene, 5-methyl-
13151-06-9	1-Octene, 7-methyl-
13151-29-6	1-Decene, 4-methyl-
13151-34-3	Decane, 3-methyl-
13151-35-4	Decane, 5-methyl-
13151-74-1	Decane 3-cyclohexyl-, 3-cyclohexyl-
13151-75-2	Decane 4-cyclohexyl-, 4-cyclohexyl-
13151-99-0	Cyclooctane, 1,4-dimethyl-, cis-
13286-73-2	Tridecane, 3-ethyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
13287-21-3	Tridecane, 6-methyl-
13287-23-5	Heptadecane, 8-methyl-
13287-24-6	Nonadecane, 9-methyl-
1331-43-7	Cyclohexane, diethyl-
13360-61-7	1-Pentadecene
13475-75-7	Pentadecane, 8-hexyl-
13475-78-0	Heptane, 5-ethyl-2-methyl-
13475-82-6	Heptane, 2,2,4,6,6-pentamethyl-
135-98-8	Benzene, (1-methylpropyl)-
13828-31-4	Cyclohexene, 1-methyl-3-(1-methylethyl)-
14255-23-3	2-Hexene, 2,4-dimethyl-
1453-24-3	Cyclohexene, 1-ethyl-
14676-29-0	Heptane, 3-ethyl-2-methyl-
14686-13-6	2-Heptene, (E)-
14686-14-7	3-Heptene, (E)-
14720-74-2	Heptane, 2,2,4-trimethyl-
1472-09-9	Cyclopropane, octyl-
14850-23-8	4-Octene, (E)-
14905-56-7	Tetradecane, 2,6,10-trimethyl-
14919-01-8	3-Octene, (E)-
15232-85-6	Cyclohexene, 1-pentyl-
1560-88-9	Octadecane, 2-methyl-
1560-92-5	Hexadecane, 2-methyl-
1560-93-6	Pentadecane, 2-methyl-
1560-96-9	Tridecane, 2-methyl-
1560-97-0	Dodecane, 2-methyl-
1574-41-0	1,3-Pentadiene, (Z)-
15869-80-4	Heptane, 3-ethyl-
15869-86-0	Octane, 4-ethyl-
15869-89-3	Octane, 2,5-dimethyl-
15869-92-8	Octane, 3,4-dimethyl-
15869-93-9	Octane, 3,5-dimethyl-
15869-94-0	3,6-Dimethyloctane
15890-40-1	cis-1,2-trans-3-Trimethylcyclopentane
15918-07-7	4-Nonene, 5-methyl-
16106-59-5	1-Hexene, 4,5-dimethyl-
1618-22-0	Naphthalene, decahydro-2,6-dimethyl-
1630-94-0	Cyclopropane, 1,1-dimethyl-
1632-16-2	2-Ethyl-1-hexene
1632-70-8	Undecane, 5-methyl-
1638-26-2	1,1-Dimethylcyclopentane
1640-89-7	Cyclopentane, ethyl-
16538-89-9	Cyclooctane, (1-methylpropyl)
16538-93-5	Cyclooctane, butyl-
16580-24-8	Cyclohexane, 1-methyl-3-(1-methylethyl)-
16580-26-0	1-Methyl-1-(1-methylethyl)cyclohexane
16745-94-1	1-Hexene, 3,4-dimethyl-
16746-85-3	1-Hexene, 4-ethyl-
16747-25-4	Hexane, 2,2,3-trimethyl-
16747-26-5	Hexane, 2,2,4-trimethyl-
16747-28-7	Hexane, 2,3,3-trimethyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
1678-81-5	cis, trans,cis-1,2,3-trimethylcyclohexane
1678-91-7	Cyclohexane, ethyl-
1678-92-8	Cyclohexane, propyl-
1678-93-9	Cyclohexane, butyl-
1678-97-3	Cyclohexane, 1,2,3-trimethyl-
1678-98-4	Cyclohexane, (2-methylpropyl)-
17301-22-3	Undecane, 2,5-dimethyl-
17301-23-4	Undecane, 2,6-dimethyl-
17301-24-5	Undecane, 2,7-dimethyl-
17301-25-6	Undecane, 2,8-dimethyl-
17301-26-7	Undecane, 2,9-dimethyl-
17301-27-8	Undecane, 2,10-dimethyl-
17301-28-9	Undecane, 3,6-dimethyl-
17301-29-0	Undecane, 3,7-dimethyl-
17301-30-3	Undecane, 3,8-dimethyl-
17301-31-4	Undecane, 3,9-dimethyl-
17301-32-5	Undecane, 4,7-dimethyl-
17301-33-6	Undecane, 4,8-dimethyl-
17301-94-9	Nonane, 4-methyl-
17302-23-7	Nonane, 4,5-dimethyl-
17302-28-2	Nonane, 2,6-dimethyl-
17302-32-8	Nonane, 3,7-dimethyl-
17302-33-9	Undecane, 6-methyl-
17302-37-3	2,2-Dimethyldecane
17312-50-4	Decane, 2,5-dimethyl-
17312-54-8	3,7-Diemthyldecane
17312-55-9	Decane, 3,8-dimethyl-
17312-57-1	Dodecane, 3-methyl-
17312-58-2	Undecane, 3-ethyl-
17312-60-6	Undecane, 6-ethyl-
17312-62-8	Decane, 5-propyl-
17312-63-9	Nonane, 5-butyl-
17312-64-0	Undecane, 2,2-dimethyl-
17312-68-4	Undecane, 4,4-dimethyl-
17312-73-1	Undecane, 5,5-dimethyl-
17312-74-2	Decane, 5-ethyl-5-methyl-
17312-76-4	Undecane, 6,6-dimethyl-
17312-77-5	Undecane, 2,3-dimethyl-
17312-78-6	Undecane, 3,4-dimethyl-
17312-80-0	Undecane, 2,4-dimethyl-
17312-81-1	Undecane, 3,5-dimethyl-
17312-82-2	Undecane, 4,6-dimethyl-
17312-83-3	Undecane, 5,7-dimethyl-
17453-93-9	Dodecane, 5-methyl-
17453-94-0	Undecane, 5-ethyl-
1750-51-2	Naphthalene, decahydro-1,6-dimethyl-
1759-58-6	trans-1,3-Dimethylcyclopentane
1795-15-9	Cyclohexane, octyl-
1795-16-0	Cyclohexane, decyl-
1795-21-7	Cyclopentane, decyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
1795-27-3	Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,
18344-37-1	Heptadecane, 2,6,10,14-tetramethyl-
1839-63-0	Cyclohexane, 1,3,5-trimethyl-
18435-22-8	Tetradecane, 3-methyl-
18435-45-5	1-Nonadecene
18476-57-8	2,6-Octadiene, 4,5-dimethyl-
18669-52-8	1,4-Hexadiene, 2,3-dimethyl-
1921-70-6	Pentadecane, 2,6,10,14-tetramethyl-
19341-98-1	Cyclobutane, 1,2-diethyl-, trans-
19398-37-9	3-Decene
19549-87-2	1-Heptene, 2,4-dimethyl-
19689-19-1	5-Decene
20063-97-2	2-Decene, (E)-
20184-89-8	3-Nonyne
20184-91-2	4-Nonyne
20278-85-7	Heptane, 2,3,5-trimethyl-
2030-84-4	4-Dodecene
2049-95-8	Benzene, (1,1-dimethylpropyl)-
2051-30-1	Octane, 2,6-dimethyl-
2090-38-2	Cyclohexane, 1,2,4,5-tetramethyl-
20959-33-5	Heptadecane, 7-methyl-
21164-95-4	Hexadecane, 7,9-dimethyl-
2132-84-5	Benzene, (1-methylhexyl)-
21328-57-4	Cyclooctane, 1,5-dimethyl-
21964-48-7	1,12-Tridecadiene
219783-06-9	1,3,4-Trimethyl-1-(1-methylethyl)cyclohexane
2213-23-2	Heptane, 2,4-dimethyl-
2216-30-0	Heptane, 2,5-dimethyl-
2216-33-3	Octane, 3-methyl-
2216-34-4	Octane, 4-methyl-
2223-52-1	Cyclohexane, 1,1,4,4-tetramethyl-
22808-06-6	3-Hexene, 2,2,5,5-tetramethyl-
23609-46-3	1,2-Diethylcyclooctene
2384-85-2	3-Decyne
2402-06-4	Cyclopropane, 1,2-dimethyl-, trans-
2415-72-7	Cyclopropane, propyl-
24251-86-3	Dodecane, 5,8-diethyl-
2437-56-1	1-Tridecene
2452-99-5	Cyclopentane, 1,2-dimethyl-
2453-00-1	1,3-Dimethylcyclopentane
24949-38-0	6-Tridecene
24949-42-6	6-Tridecene, 7-methyl-
25117-24-2	Tetradecane, 4-methyl-
25117-31-1	Tridecane, 5-methyl-
25117-32-2	Tetradecane, 5-methyl-
2511-91-3	Cyclopropane, pentyl-
2532-58-3	Cyclopentane, 1,3-dimethyl-, cis-
2613-66-3	Cyclopentane, 1-ethyl-3-methyl-, cis-
26730-12-1	Tridecane, 4-methyl-
26730-14-3	Tridecane, 7-methyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
2719-61-1	Benzene, (1-methylundecyl)-
2719-62-2	Benzene, (1-pentylheptyl)-
2719-63-3	Benzene, (1-butyloctyl)-
2719-64-4	Benzene, (1-propylnonyl)-
279-23-2	Bicyclo[2.2.1]heptane
2801-84-5	Decane, 2,4-dimethyl-
280-65-9	Bicyclo[3.3.1]nonane
2815-57-8	Cyclopentane, 1,2,3-trimethyl-
2815-58-9	Cyclopentane, 1,2,4-trimethyl-
2847-72-5	Decane, 4-methyl-
286-08-8	Bicyclo[4.1.0]heptane
287-23-0	Cyclobutane
2882-96-4	Pentadecane, 3-methyl-
2883-05-8	Octane, 2-cyclohexyl-
28981-49-9	Cyclododecane, ethyl-
29053-04-1	Cyclopentane, 1-methyl-3-(2-methylpropyl)-
29212-09-7	2-Methyl-2,3-hexadiene
292-64-8	Cyclooctane
294-62-2	Cyclododecane
295-17-0	Cyclotetradecane
295-65-8	Cyclohexadecane
2958-75-0	1-Methyldecahydronaphthalene
2958-76-1	Naphthalene, decahydro-2-methyl-
29799-19-7	Cyclohexane, 1-(1,5-dimethylhexyl)-4-methyl-
2980-69-0	Undecane, 4-methyl-
300-57-2	Benzene, 2-propenyl-
3054-63-5	Dodecane, 4,9-dipropyl-
3073-66-3	Cyclohexane, 1,1,3-trimethyl-
3074-71-3	Heptane, 2,3-dimethyl-
31081-17-1	Nonane, 2-methyl-5-propyl-
31081-18-2	Nonane, 3-methyl-5-propyl-
31295-56-4	Dodecane, 2,6,11-trimethyl-
3178-29-8	Heptane, 4-propyl-
3221-61-2	Octane, 2-methyl-
32281-85-9	Cyclopentane, 1,3-dimethyl-2-(1-methylethyl)-
32669-86-6	Cyclohexane, cyclopropyl-
3290-53-7	Benzene, (2-methyl-2-propenyl)-
3404-75-9	2-Heptene, 3-methyl-
34303-81-6	3-Hexadecene, (Z)-
3452-09-3	1-Nonyne
3522-94-9	Hexane, 2,2,5-trimethyl-
3524-73-0	1-Hexene, 5-methyl-
35507-09-6	7-Hexadecene, (Z)-
3604-14-6	Naphthalene, decahydro-1,2-dimethyl-
3638-35-5	Cyclopropane, (1-methylethyl)-
37050-03-6	3,4-Nonadiene
3769-23-1	1-Hexene, 4-methyl-
3788-32-7	Cyclopentane, (2-methylpropyl)-
38851-69-3	cis-1-Butyl-2-methylcyclopropane
38851-70-6	Cyclopropane, 1-butyl-2-methyl-, trans-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
3891-98-3	Dodecane, 2,6,10-trimethyl-
3892-00-0	Pentadecane, 2,6,10-trimethyl-
4032-86-4	Heptane, 3,3-dimethyl-
4032-93-3	Heptane, 2,3,6-trimethyl-
4050-45-7	2-Hexene, (E)-
41446-60-0	7-Tetradecene, (Z)-
41446-61-1	6-Tetradecene, (Z)-
41446-66-6	5-Tetradecene, (E)-
41446-67-7	3-Tetradecene, (Z)-
41446-68-8	3-Tetradecene, (E)-
41977-32-6	Cyclopropane, 1,2-dibutyl-
41977-33-7	Cyclopropane, 1-pentyl-2-propyl-
41977-34-8	Cyclopropane, 1-butyl-1-methyl-2-propyl-
41977-43-9	Cyclopropane, 1,1,2-trimethyl-3-(2-methylpropyl)-
41977-48-4	Bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-
4259-00-1	1,1,2-Trimethylcyclopentane
4291-79-6	Cyclohexane, 1-methyl-2-propyl-
4291-80-9	Cyclohexane, 1-methyl-3-propyl-
4292-75-5	Cyclohexane, hexyl-
4292-92-6	Cyclohexane, pentyl-
4316-65-8	1-Hexene, 3,5,5-trimethyl-
4390-04-9	Nonane, 2,2,4,4,6,8,8-heptamethyl-
4413-16-5M	Benzene, (1-cyclohexylethyl)- and others
4461-48-7M	2-Pentene, 4-methyl- and others
4485-13-6	3-Heptene, 4-propyl-
4516-69-2	Cyclopentane, 1,1,3-trimethyl-
4536-87-2	Benzene, (1-ethylnonyl)-
4536-88-3	Benzene, (1-methyldecyl)-
4537-15-9	Benzene, (1-butylheptyl)-
4551-51-3	1H-Indene, octahydro-, cis-
463-49-0	Propadiene
464-06-2	Butane, 2,2,3-trimethyl-
4683-94-7	trans-2-Methyldecahydronaphthalene
4737-43-3	Cyclopentane, (1-methylbutyl)-
4795-86-2	2,2,6-Trimethylbicyclo[3.1.1]heptane
4806-61-5	Cyclobutane, ethyl-
4810-09-7	1-Heptene, 3-methyl-
4850-28-6	Cyclopentane, 1,2,4-trimethyl-, (1.alpha.,2.alpha.
4866-55-1	Cyclopropane, 1,2-dimethyl-3-methylene-, cis-
489-20-3	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-
4923-77-7	Cyclohexane, 1-ethyl-2-methyl-, cis-
4926-78-7	Cyclohexane, 1-ethyl-4-methyl-, cis-
493-02-7	Naphthalene, decahydro-, trans-
4941-53-1	5-Undecene
49622-16-4	2-Undecene, 2,5-dimethyl-
5026-76-6	1-Heptene, 6-methyl-
504-60-9	1,3-Pentadiene
50746-53-7	Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-
50871-03-9	1-Decene, 3,4-dimethyl-
50876-31-8	Cyclohexane, 1,1,3,5-tetramethyl-, trans-
50876-32-9	Cyclohexane, 1,1,3,5-tetramethyl-, cis-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
50915-91-8	Cyclopropene, 1-butyl-2-ethyl-
50991-08-7	1,1`-Bicyclohexyl, 2-methyl-, cis-
50991-09-8	1,1`-Bicyclohexyl, 2-methyl-, trans-
51284-29-8	Cyclohexane, (1,2-dimethylpropyl)-
513-35-9	2-Butene, 2-methyl-
513-81-5	1,3-Butadiene, 2,3-dimethyl-
5171-86-8	Hexane, 3,3,4,4-tetraethyl-
526-73-8	1,2,3-Trimethylbenzene
527-84-4	1-Isopropyl-2-methylbenzene
52896-87-4	Heptane, 4-(1-methylethyl)-
52896-90-9	Heptane, 3-ethyl-5-methyl-
53366-38-4	Cyclopentane, (2-methylbutyl)-
535-77-3	Benzene, 1-methyl-3-(1-methylethyl)-
5364-83-0	Cyclohexane, 1-propenyl-
538-68-1	Benzene, pentyl-
53907-60-1	Cyclopentane, 1,1,3,4-tetramethyl-, cis-
540-84-1	2,2,4-Trimethylpentane
54105-66-7M	Cyclohexane, undecyl- and others
54244-79-0	1-Decene, 5-methyl-
54299-96-6	1,2-Dimethylcyclooctene
54411-00-6	Cyclohexane, 1-methyl-4-(1-methylbutyl)-
54411-01-7	Cyclohexane, 1-methyl-2-pentyl-
54411-02-8	Cyclohexane, 1-methyl-3-pentyl-
544-76-3	Hexadecane
54549-80-3	Cyclopentane, 2-ethyl-1,1-dimethyl-
5458-16-2	Pentane, 2-cyclopropyl-
54823-94-8	Cyclohexane, 1-(cyclohexylmethyl)-2-methyl-, trans
54823-98-2	Cyclohexane, 1-(cyclohexylmethyl)-4-methyl-, trans
54824-04-3	Cyclohexane, 1-(cyclohexylmethyl)-2-methyl-, cis-
54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, tran
54833-48-6	Heptadecane, 2,6,10,15-tetramethyl-
54845-26-0	3-Heptene, 2,2,3,5,5,6,6-heptamethyl-
54934-90-6	Cyclohexane, 1,1`-(1-methylethylidene)bis-
54934-93-9	Cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-, cis-
54934-95-1	Cyclohexane, 1-(cyclohexylmethyl)-4-ethyl-, cis-
54965-05-8	Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-
55030-62-1	Tridecane, 4,8-dimethyl-
55045-07-3	Dodecane, 2-methyl-8-propyl-
55045-08-4	Dodecane, 2-methyl-6-propyl-
55045-11-9	Tridecane, 5-propyl-
55045-12-0	Tetradecane, 4,11-dimethyl-
55045-13-1	Tetradecane, 6,9-dimethyl-
55045-14-2	Tetradecane, 4-ethyl-
55170-92-8	2-Undecene, 4,5-dimethyl-, (E)-
55282-34-3	Cyclohexane, 1,3,5-trimethyl-2-octadecyl-
55373-86-9	Docosane, 7-hexyl-
55702-61-9	2-Hexene, 4,4,5-trimethyl-
558-37-2	1-Butene, 3,3-dimethyl-
55937-92-3	Bicyclo[4.1.0]heptane, 2-methyl-7-pentyl-
560-21-4	2,3,3-Trimethylpentane

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
562-49-2	Pentane, 3,3-dimethyl-
56292-65-0	Dodecane, 2,5-dimethyl-
56292-66-1	Tridecane, 2,5-dimethyl-
56292-69-4	Tetradecane, 2,5-dimethyl-
563-16-6	3,3-Dimethylhexane
563-45-1	1-Butene, 3-methyl-
563-46-2	1-Butene, 2-methyl-
563-78-0	1-Butene, 2,3-dimethyl-
563-79-1	2-Butene, 2,3-dimethyl-
564-02-3	2,2,3-Trimethylpentane
565-59-3	Pentane, 2,3-dimethyl-
565-75-3	Pentane, 2,3,4-trimethyl-
56728-10-0	1-Hexene, 3,4,5-trimethyl-
56851-45-7	2-Dodecene, 4-methyl-
571-61-9M	Naphthalene, 1,5-dimethyl- and others
575-37-1	Naphthalene, 1,7-dimethyl-
57905-86-9	Cyclobutane, 1,1,2,3,3-pentamethyl-
581-40-8	Naphthalene, 2,3-dimethyl-
583-48-2	3,4-Dimethylhexane
583-48-2M	Hexane, 3,4-dimethyl- and others
583-57-3	Cyclohexane, 1,2-dimethyl-
58462-32-1	trans,trans-3-Ethyldecahydronaphthalene
584-94-1	Hexane, 2,3-dimethyl-
5876-87-9	1,11-Dodecadiene
589-34-4	3-Methyl-Hexane
589-43-5	Hexane, 2,4-dimethyl-
589-53-7	Heptane, 4-methyl-
589-81-1	Heptane, 3-methyl-
589-90-2	Cyclohexane, 1,4-dimethyl-
590-18-1	2-Butene, (Z)-
590-35-2	Pentane, 2,2-dimethyl-
590-66-9	Cyclohexane, 1,1-dimethyl-
590-73-8	2,2-Dimethylhexane
5911-04-6	Nonane, 3-methyl-
591-76-4	Hexane, 2-methyl-
591-95-7	1,2-Pentadiene
592-13-2	Hexane, 2,5-dimethyl-
592-27-8	Heptane, 2-methyl-
592-41-6	1-Hexene
592-42-7	1,5-Hexadiene
592-43-8	2-Hexene
592-48-3	1,3-Hexadiene
592-76-7	1-Heptene
592-77-8	2-Heptene
592-78-9	3-Heptene
592-98-3	3-Octene
593-45-3	Octadecane
594-11-6	Cyclopropane, methyl-
594-82-1	Butane, 2,2,3,3-tetramethyl-
59681-06-0	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,19,23-pen
598-61-8	Cyclobutane, methyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
5989-27-5	Cyclohexene, 1-methyl-4-(1-methylethenyl)
6031-02-3	Benzene, (1-methylpentyl)-
6044-71-9	Dodecane, 6-methyl-
60643-93-8	3-Hexene, 2,3,4,5-tetramethyl-, (Z)-
6069-98-3	Cyclohexane, 1-methyl-4-(1-methylethyl)-, cis-
609-26-7	Pentane, 3-ethyl-2-methyl-
6094-02-6	1-Hexene, 2-methyl-
611-14-3	Benzene, 1-ethyl-2-methyl-
61141-57-9	Cyclohexene, 1-ethyl-6-ethylidene-
61141-72-8	Dodecane, 4,6-dimethyl-
61141-79-5	Cyclohexane, 1,2-diethyl-1-methyl-
61141-80-8	Cyclohexane, 1,2-diethyl-3-methyl-
61142-20-9	Cyclohexane, (4-methylpentyl)-
61142-23-2	Cyclohexane, (2,2-dimethylcyclopentyl)-
61142-24-3	Cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alph
61142-37-8	Cyclohexane, (1,2-dimethylbutyl)-
61142-38-9	Cyclohexane, (3-methylpentyl)-
61142-40-3	4-Undecene, 4-methyl-
61142-41-4	Cyclooctane, ethenyl-
61142-47-0	2-Pentene, 2-methoxy-
61142-65-2	Cyclopentane, 3-hexyl-1,1-dimethyl-
61142-66-3	Cyclopentene, 5-hexyl-3,3-dimethyl-
61142-68-5	Cyclopentane, 1-hexyl-3-methyl-
61142-70-9	Cyclohexane, 2,4-diethyl-1-methyl-
6117-97-1	Dodecane, 4-methyl-
617-78-7	3-Ethylpentane
61886-62-2	3-Hexadecyne
620-00-8	3-Ethyl-2-hexene
620-14-4	3-Methylethylbenzene
62016-14-2	Octane, 2,5,6-trimethyl-
62016-18-6	Octane, 5-ethyl-2-methyl-
62016-19-7	Octane, 6-ethyl-2-methyl-
62016-30-2	Octane, 2,3,3-trimethyl-
62016-34-6	Octane, 2,3,7-trimethyl-
62108-21-8	Decane, 6-ethyl-2-methyl-
62108-22-9	Decane, 2,5,9-trimethyl-
62108-25-2	Decane, 2,6,7-trimethyl-
62108-26-3	Decane, 2,6,8-trimethyl-
62108-27-4	Decane, 2,4,6-trimethyl-
62108-31-0	Heptane, 4-ethyl-2,2,6,6-tetramethyl-
62108-32-1	Heptane, 2,2,3,4,6,6-hexamethyl-
62183-55-5	Octane, 3-ethyl-2,7-dimethyl-
62185-21-1	3,4,5,6-Tetramethyloctane
62185-53-9	Nonane, 5-(2-methylpropyl)-
62199-50-2	Cyclopentane, 1-butyl-2-propyl-
62199-51-3	Cyclopentane, 1-pentyl-2-propyl-
62237-97-2	Decane, 2,2,6-trimethyl-
62238-01-1	Decane, 2,2,8-trimethyl-
62238-08-8	Cyclopropane, 1-ethyl-2-pentyl-
62238-11-3	Decane, 2,3,5-trimethyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
62238-12-4	Decane, 2,3,6-trimethyl-
62238-13-5	Decane, 2,3,7-trimethyl-
62238-14-6	Decane, 2,3,8-trimethyl-
62238-33-9	Cyclohexane, 1-ethyl-2-propyl-
622-96-8	Benzene, 1-ethyl-4-methyl-
62338-08-3	3-Hexene, 3-ethyl-2,5-dimethyl-
62338-09-4	Decane, 2,2,3-trimethyl-
62338-40-3M	Cyclohexane, decylidene- and others
62338-45-8	Bicyclo[2.2.2]octane, 1,2,3,6-tetramethyl-
62338-47-0	4-Decene, 3-methyl-, (E)-
62338-52-7M	Cyclobutane, 3-hexyl-1,1,2-trimethyl- and others
6236-88-0	Cyclohexane, 1-ethyl-4-methyl-, trans-
62376-15-2	Cycloundecane, 1,1,2-trimethyl-
624-64-6	2-Butene, (E)-
625-65-0	2-Pentene, 2,4-dimethyl-
627-20-3	2-Pentene, (Z)-
629-50-5	n-Tridecane
629-59-4	n-Tetradecane
629-62-9	Pentadecane
629-73-2	1-Hexadecene
629-78-7	Heptadecane
629-89-0	1-Octadecyne
629-92-5	Nonadecane
629-94-7	Heneicosane
630-01-3	Hexacosane
630-02-4	Octacosane
6304-50-3	Dodecane, 2,2,4,9,11,11-hexamethyl-
6305-52-8	Naphthalene, 2-butyldecahydro-
637-50-3	Benzene, 1-propenyl-
638-04-0	Cyclohexane, 1,3-dimethyl-, cis-
63830-68-2	4-Nonene, 2,3,3-trimethyl-, (Z)-
638-36-8	Hexadecane, 2,6,10,14-tetramethyl-
6418-41-3	Tridecane, 3-methyl-
6418-43-5	Hexadecane, 3-methyl-
6418-44-6	Heptadecane, 3-methyl-
6434-78-2	2-Nonene, (E)-
643-58-3	1,1`-Biphenyl, 2-methyl-
645-10-3	1,7-Dimethyl-4-(1-methylethyl)cyclodecane
646-04-8	2-Pentene, (E)-
66552-62-3	Naphthalene, decahydro-1,5-dimethyl-
66553-50-2	Cyclopentane, 1-methyl-2-(4-methylpentyl)-, trans-
66660-41-1	cis,trans-3-Ethyldecahydronaphthalene
66660-42-2	cis, cis-3-Ethylbicyclo[4.4.0]decane
66660-43-3	trans, cis-3-Ethylbicyclo[4.4.0]decane
66826-95-7	Cyclohexane, 1-(cyclohexylmethyl)-4-methyl-
674-76-0	2-Pentene, 4-methyl-, (E)-
6765-39-5	1-Heptadecene
67730-63-6	4,6-Decadiene, 3,8-dimethyl-, (E,E)-
6783-92-2	Cyclohexane, 1,1,2,3-tetramethyl-
67975-92-2	1-Cyclohexyl-1-hexene
690-08-4M	2-Pentene, 4,4-dimethyl-, (E)- and others

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
691-37-2	1-Pentene, 4-methyl-
692-47-7M	3-Hexene, 2,2,5,5-tetramethyl-, (Z)- and others
693-61-8	E-2-Undecene
693-62-9	4-Undecene, (E)-
696-29-7	Cyclohexane, (1-methylethyl)-
6975-98-0	Decane, 2-methyl-
7045-71-8	Undecane, 2-methyl-
7058-01-7	Cyclohexane, (1-methylpropyl)-
7094-26-0	Cyclohexane, 1,1,2-trimethyl-
7116-86-1	1-Hexene, 5,5-dimethyl-
71186-27-1	trans-2-ethyl-1,1,3-trimethylcyclohexane
7154-80-5	Heptane, 3,3,5-trimethyl-
72014-90-5M	1,4-Pentadiene, 2,3,4-trimethyl- and others
7206-14-6	3-Dodecene, (E)-
7206-15-7	4-Dodecene, (E)-
7206-17-9	6-Dodecene, (E)-
7206-28-2	5-Dodecene, (Z)-
7225-64-1	Heptadecane, 9-octyl-
7239-23-8	3-Dodecene, (Z)-
72993-32-9	Cyclopentane, 1-butyl-2-ethyl-
7300-03-0	3-Methyl-3-heptene
7367-38-6	4-Nonene, 5-butyl-
7385-78-6	1-Pentene, 3,4-dimethyl-
74054-92-5	1,1,6,6-Tetramethylspiro[4,4]nonane
7433-56-9	5-Decene, (E)-
74421-09-3	Cyclopentane, 1,1,3-trimethyl-3-(2-methyl-2-propen
74630-08-3	1-Octene, 3-ethyl-
74630-30-1	2-Decene, 4-methyl-, (Z)-
74630-39-0	1-Undecene, 4-methyl-
74630-40-3	1-Undecene, 8-methyl-
74630-42-5	1-Undecene, 7-methyl-
74630-44-7	2-Undecene, 8-methyl-, (Z)-
74630-48-1	3-Undecene, 2-methyl-, (Z)-
74630-61-8	2-Undecene, 6-methyl-, (E)-
74630-62-9	5-Undecene, 7-methyl-, (Z)-
74630-66-3	5-Undecene, 7-methyl-, (E)-
74630-69-6	4-Undecene, 5-methyl-, (Z)-
74645-98-0	Dodecane, 2,7,10-trimethyl-
74663-66-4	Cyclohexane, 1,5-diethyl-2,3-dimethyl-
74663-86-8	Cyclopropane, 1-ethyl-2-heptyl-
74663-91-5	Cyclopropane, 1-heptyl-2-methyl-
74685-30-6	5-Eicosene, (E)-
74752-97-9	1,3-Hexadiene, 3-ethyl-2-methyl-, (Z)-
74764-46-8M	3-Heptene, 3-ethyl and others
74810-41-6	Cyclohexane, (2-ethyl-1-methylbutylidene)-
74810-42-7	Cyclohexane, (2-ethyl-1-methyl-1-butenyl)-
74-82-8	Methane
75163-97-2	Octadecane, 2,6-dimethyl-
75-19-4	Cyclopropane
75-83-2	Butane, 2,2-dimethyl-
758-86-1	1,4-Pentadiene, 2,3-dimethyl-

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
762-62-9	1-Pentene, 4,4-dimethyl-
763-29-1	1-Pentene, 2-methyl-
7642-09-3	3-Hexene, (Z)-
7642-15-1	Z-4-Octene
764-96-5	5-Undecene, (Z)-
764-97-6	5-Undecene, (E)-
7667-60-9	Cyclohexane, 1,2,4-trimethyl-, (1.alpha.,2.beta.,4
7683-64-9	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-
7688-21-3	2-Hexene, (Z)-
777-22-0	Benzene, (1-methylheptyl)-
79-29-8	Butane, 2,3-dimethyl-
816-79-5	2-Pentene, 3-ethyl-
81983-71-3	Cyclohexane, 1,1-dimethyl-2-propyl-
82085-14-1	2,4-Dimethyl-3-hexene
821-74-9	4,5-Nonadiene
821-95-4	1-Undecene
821-96-5	2-Undecene, (Z)-
821-98-7	Z-4-Undecene
822-50-4	Cyclopentane, 1,2-dimethyl-, trans-
86-73-7	9H-Fluorene
871-83-0	Nonane, 2-methyl-
872-05-9	1-Decene
872-56-0	Cyclobutane, (1-methylethyl)-
90-12-0	1-Methylnaphthalene
91-17-8	Naphthalene, decahydro-
91-57-6	Naphthalene, 2-methyl-
91695-32-8	2-Undecene, 4-methyl-
921-47-1	2,3,4-Trimethylhexane
922-28-1	3,4-Dimethylheptane
92-51-3	1,1`-Bicyclohexyl
926-82-9	Heptane, 3,5-dimethyl-
930-18-7	Cyclopropane, 1,2-dimethyl-, cis-
930-57-4	Cyclopropane, butyl-
95-47-6	1,2-Dimethylbenzene
96-14-0	Pentane, 3-methyl-
96-37-7	Cyclopentane, methyl-
98-06-6	Benzene, (1,1-dimethylethyl)-
998-35-6	Nonane, 5-propyl-
CYCY00-01	cis-1,2-Diethylcyclobutane
MAEUAE0-01a	1,3-Pentadiene, (E)- mixture
MAEUCY0-01a	2,4-Hexadiene, 3-methyl- mixture
MARUAK0-01a	Benzene, butyl mixture
MARUPH0-01a	9H-Fluorene, 3-methyl- mixture
MAYUAE0-01a	1-Pentyne mixture
MCYCY00-01b	Cyclobutane, 1,2-diethyl-, cis- mixture
MCYNT00-01b	Cyclohexane, 2-butyl- mixture
MUAEUAR-03a	Methyl fluorene mixture
MUAEUAY-02b	C5-Alkyne mixture
U00005-01	Branched C5 hydrocarbon
U00013-01	C13 Aliphatic hydrocarbon
UAE003-01	C3-Alkene/Cycloalkane

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
UAE003-01a	C3-Alkene (or C3 cycloalkane) mixture
UAE004-01	C4-Alkene
UAE004-02	C4-Alkene/Cycloalkane
UAE005-01	C5-Alkene
UAE005-02	C5-Alkene/Cycloalkane
UAE005-02b	C5-Cycloalkane (or C5 alkene) mixture
UAE006-01	C6-Alkene
UAE007-01	C7-Alkene
UAE007-03	C7-Alkene/Cycloalkane
UAE007-03a	C7-Alkene (or C7-cycloalkane) mixture
UAE008-01	C8-Alkene
UAE008-02	C8-Alkene/Cycloalkane
UAE008-02b	C8-Cycloalkane (or C8-alkene) mixture
UAE009-01	C9-Alkene
UAE009-02	C9-Alkene/Cycloalkane
UAE009-02b	C9-Cycloalkane (or C9-alkene) mixture
UAE010-01	C10-Alkene
UAE010-02	C10-Alkene/Cycloalkane
UAE010-02a	C10-Alkene (or C10-cycloalkane) mixture
UAE011-01	C11-alkene
UAE011-02	c4-heptadiene
UAE011-03	C11-Alkene/Cycloalkane
UAE011-03a	C11-Alkene (or C11-cycloalkane) mixture
UAE011-04	C11-Diene/Cycloalkene
UAE011-04b	C11-Cycloalkene (or C11 diene) mixture
UAE011-05	4-Decene, 7-methyl-
UAE012-01	C12-Alkene
UAE012-02	C12-Alkene/Cycloalkane
UAE012-02a	C12-Alkene (or C12-cycloalkane) mixture
UAE012-03	2-undecene, 7-methyl-, cis=trans
UAE012-04	3-Undecene, 8-methyl
UAE012-05	4-undecene, 6-methyl
UAE012-06	3-Undecene, 5-methyl-
UAE013-01	c13-alkene
UAE013-02	C13-Alkene/Cycloalkane
UAE013-02a	C13-Alkene (or C13-cycloalkane) mixture
UAE013-03	C13-Diene/Cycloalkene
UAE013-03b	C13-Cycloalkene (of C13 diene) mixture
UAE014-01	C14-Alkene
UAE014-02	C14-Alkene/Cycloalkane
UAE014-02b	C14-Cycloalkane (or C14-alkene) mixture
UAE015-01	C15-Alkene/Cycloalkane
UAE015-01a	C15-Alkene (or C15-Cycloalkane) mixture
UAE015-02	C15-Alkene
UAK004-01	C4-Alkane
UAK006-01	C6-Alkane
UAK006-02M	C6-Alkane (coeluent)
UAK007-01	C7-Alkane
UAK008-01	C8-Alkane
UAK009-01	C9-Alkane
UAK010-01	C10-Alkane
UAK011-01	C11-Alkane

Table C-6. Hydrocarbons (14 Sheets)

Chemical Identification Number	Chemical Name
UAK012-01	C12-Alkane
UAK014-01	C14-alkane
UAK014-02	Decane, 2,3,5,8-tetramethyl
UAK015-01	C15-alkane
UAK016-01	C16-alkane
UAK017-01	C17-Alkane
UAK018-01	C18-Alkane
UAK020-01	Unknown C20-Alkane
UAR000-02	C4-Dihydronaphthalene
UAR000-03	Dimethyl-naphthalene
UAR000-11	C2-Benzene
UAR000-12	C4 substituted benzene
UAR000-15	Benzene, ethyl-methyl-, isomer
UAR000-16	Benzene, -trimethyl-, isomer
UAY013-01	C5-Octyne
UCY006-01	C3-Cyclopropane
UCY007-01	C2-Cyclopentane
UCY008-01	C2-Cyclohexane
UCY008-02	C3-Cyclopentane
UCY009-01	C3-Cyclohexane
UCY009-02	C3-Cyclohexene
UCY009-04	C4-Cyclopentane
UCY010-01	C4-Cyclohexane
UCY010-02	C5-cyclopentane
UCY011-01	C5-Cyclohexane
UCY011-02	C6-Alkenyl-cyclopentane
UCY011-03	C6-Cyclopentane
UCY011-04	1-ethyl-2,2,6-trimethylcyclohexane
UCY011-05	Methyldecahydronaphthalene
UCY011-06	C5-Cyclohexene
UCY012-02	C6-Cyclohexane
UCY012-03	C7-Cyclopentane
UCY012-04	2-Propyl-1,1,3-trimethylcyclohexane
UCY012-05	C2-Decahydro-naphthalene
UCY012-08	Cyclopropane, 1-(2-butyl)-1-(2-methylbutyl)-
UCY013-01	C7-Cyclohexane
UCY013-02	C8-Cyclopentane
UCY013-03	Cyclohexane, 1,2-dimethyl-3-pentyl-
UCY013-04	C3-Decahydronaphthalene
UCY014-01	C8-Cyclohexane
UCY014-02	C8-Cyclohexene
UCY014-03	C9-Cyclopentane
UCY014-04	Unknown C4 Alkyl Decahydronaphthalene
UCY015-01	C9-Cyclohexane

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
1002-16-0	Nitric acid, pentyl ester	0.25	0.16	No
1002-84-2	Pentadecanoic acid	1.0	0.23	No
1004-29-1	2-Butyltetrahydrofuran	0.50	0.037	No
100-47-0	Benzonitrile	1.0	0.016	No
100-71-0	Pyridine, 2-ethyl-	0.050	0.0023	No
100-73-2	2H-Pyran-2-carboxaldehyde, 3,4-dihydro-	1.9	0.0016	No
1009-61-6	Ethanone, 1,1'-(1,4-phenylene)bis-	0.10	0.0004	No
100-97-0	1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane	0.052	0.0051	No
10203-30-2	3-Dodecanol	0.015	0.0010	No
10264-17-2	Butanamide, N-hexyl-	0.10	0.0001	No
103-23-1	Hexanedioic acid, bis(2-ethylhexyl) ester	0.15	0.0039	No
10374-14-8	Cyclobutanone, 2-ethyl-	0.067	0.0050	No
104-50-7	2(3H)-Furanone, 5-butyldihydro-	5.0	0.00087	No
104-61-0	2(3H)-Furanone, dihydro-5-pentyl-	0.50	0.0025	No
104-67-6	2(3H)-Furanone, 5-heptyldihydro-	15	0.00069	No
10486-19-8	Tridecanal	0.50	0.00023	No
104-90-5	Pyridine, 5-ethyl-2-methyl-	0.020	0.0026	No
105-21-5	2(3H)-Furanone, dihydro-5-propyl-	5.0	0.0019	No
105-42-0	2-Hexanone, 4-methyl-	0.050	1.1	**Yes**
105-66-8	Propyl butanoate	15.00	0.042	No
10599-75-4	N-(Pentylidene)methanamine	0.05	0.022	No
10599-77-6	1-Butanamine, N-pentylidene-	0.010	0.00063	No
1066-40-6	Silanol, trimethyl-	5.0	0.056	No
106-72-9	5-Heptenal, 2,6-dimethyl-	25	0.067	No
1072-44-2	1-Methylaziridine	0.020	0.065	**Yes**
1073-11-6	2(3H)-Furanone, 5-ethenyldihydro-5-methyl-	0.50	0.00044	No
107-75-5	Octanal, 7-hydroxy-3,7-dimethyl-	0.50	0.00013	No
107-89-1	3-Hydroxybutanal	0.20	0.019	No
107-92-6	Butyric Acid (Butanoic acid)	1.0	0.85	No
108-29-2	2(3H)-Furanone, dihydro-5-methyl-	75	0.0098	No
108-30-5	2,5-Furandione, dihydro-	0.0025	0.0020	No
108-47-4	Pyridine, 2,4-dimethyl-	0.020	0.10	**Yes**
108-48-5	Pyridine, 2,6-dimethyl-	0.020	0.0025	No
109-08-0	Pyrazine, methyl-	1.0	0.0055	No
109-21-7	Butanoic acid, butyl ester	1.5	0.40	No
109-69-3	Butane, 1-chloro-	0.75	0.15	No
109-75-1	3-Butenenitrile	0.020	0.021	**Yes**
109-93-3	Ethene, 1,1`-oxybis-	2.0	0.031	No
109-97-7	1H-Pyrrole	0.030	0.011	No
110-00-9	Furan	0.010	3.2	**Yes**
110-13-4	2,5-Hexanedione	0.0050	0.0015	No
110-27-0	Tetradecanoic acid, 1-methylethyl ester	0.0035	0.17	**Yes**
110-36-1	Tetradecanoic acid, butyl ester	0.0035	0.20	**Yes**
110-71-4	Ethane, 1,2-dimethoxy-	100	0.0025	No
110-74-7	Propyl formate	1.00	0.054	No
110-93-0	5-Hepten-2-one, 6-methyl-	0.15	0.0012	No
111-06-8	Hexadecanoic acid, butyl ester	0.0035	0.00019	No
111-13-7	2-Octanone	0.50	0.32	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
1112-39-6	Silane, dimethoxydimethyl-	5.0	0.011	No
111-27-3	1-Hexanol	1.0	0.073	No
1115-11-3	2-Butenal, 2-methyl-	0.0030	0.013	**Yes**
111-70-6	1-Heptanol	0.50	0.40	No
111-71-7	Heptanal	0.50	0.12	No
1117-59-5	Pentanoic acid, hexyl ester	1.5	0.0021	No
1120-06-5	2-Decanol	0.015	0.00068	No
1120-07-6	Nonanamide	5.0	0.0011	No
1120-64-5	Oxazole, 4,5-dihydro-2-methyl-	0.50	0.016	No
1121-05-7	2-Cyclopenten-1-one, 2,3-dimethyl-	0.050	0.0013	No
1121-07-9	2,5-Pyrrolidinedione, 1-methyl-	10	0.0055	No
112-12-9	2-Undecanone	0.50	0.37	No
1121-33-1	Cyclopentanone, 2,4-dimethyl-	0.20	0.0052	No
112-30-1	1-Decanol	0.15	0.0011	No
112-31-2	Decanal	0.50	0.042	No
1123-28-0	1-Hydroxycyclohexanecarboxylic acid	0.30	0.018	No
112-42-5	1-Undecanol	0.015	0.00069	No
112-44-7	Undecanal	0.50	0.00053	No
112-53-8	1-Dodecanol	0.015	0.00096	No
112-54-9	Dodecanal	0.50	0.00067	No
112-72-1	1-Tetradecanol	0.015	0.0010	No
112-80-1	9-Octadecenoic acid (Z)-	1.0	0.0055	No
112-92-5	1-Octadecanol	0.015	0.96	**Yes**
1184-60-7	1-Propene, 2-fluoro-	0.010	0.53	**Yes**
1191-95-3	Cyclobutanone	0.067	0.048	No
1191-99-7	Furan, 2,3-dihydro-	0.50	0.025	**Yes**
1192-33-2	Cyclobutanone, 3,3-dimethyl-	0.067	0.0011	No
1196-92-5	Phenol, 4-(aminomethyl)-2-methoxy-	0.050	0.0031	No
121-00-6	Phenol, 2-(1,1-dimethylethyl)-4-methoxy-	0.050	0.00050	No
123-05-7	Hexanal, 2-ethyl-	0.50	0.033	No
123-15-9	Pentanal, 2-methyl-	0.50	0.051	No
123-25-1	Butanedioic acid, diethyl ester	1.5	0.67	No
123-32-0	Pyrazine, 2,5-dimethyl-	1.0	0.00038	No
123-56-8	2,5-Pyrrolidinedione	10	0.0025	No
123-79-5	Hexanedioic acid, dioctyl ester	0.15	0.099	No
123-95-5	Octadecanoic acid, butyl ester	0.0035	0.0019	No
123-96-6	2-Octanol	0.50	0.070	No
124-12-9	Octanenitrile	0.080	0.49	**Yes**
124-13-0	Octanal	0.50	0.46	No
124-19-6	Nonanal	5.0	1.0	No
124-28-7	1-Octadecanamine, N,N-dimethyl-	0.10	0.00030	No
13040-03-4	Bicyclo[3.1.1]hept-3-en-2-ol, 4,6,6-trimethyl	0.50	0.00088	No
136-77-6	1,3-Benzenediol, 4-hexyl-	0.20	0.00063	No
137-32-6	1-Butanol, 2-methyl-	1.0	0.041	No
13861-97-7	2(3H)-Furanone, dihydro-4,4-dimethyl-	0.50	0.0012	No
13925-00-3	Pyrazine, ethyl-	0.10	0.0065	No
14128-61-1	5-Methyl-5-phenyl-2-hexanone	0.50	0.0072	No
14129-48-7	4-Octen-3-one	0.15	0.0036	No
141-62-8	Tetrasiloxane, decamethyl-	3.0	0.0027	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
142-30-3	3-Hexyne-2,5-diol, 2,5-dimethyl-	0.10	0.00036	No
142-60-9	Propanoic acid, octyl ester	1.5	0.0036	No
142-62-1	Caprioc Acid (Hexanoic acid)	1.0	0.00077	No
142-78-9	Dodecanamide, N-(2-hydroxyethyl)-	5.0	0.00072	No
142-91-6	Hexadecanoic acid, 1-methylethyl ester	0.0035	0.033	**Yes**
142-96-1	Butane, 1,1`-oxybis-	1.0	0.39	No
143-07-7	Dodecanoic acid	1.0	0.034	No
143-08-8	1-Nonanol	0.070	0.0037	No
143-28-2	9-Octadecen-1-ol, (Z)-	1.0	0.00042	No
14476-37-0	4-Undecanone	0.50	0.011	No
1454-84-8	1-Nonadecanol	0.015	0.00071	No
1454-85-9	1-Heptadecanol	0.015	0.0020	No
1462-84-6	Pyridine, 2,3,6-trimethyl-	0.020	0.00012	No
1467-79-4	Cyanamide, dimethyl-	8.0	0.042	No
1482-15-1	1-Pentyn-3-ol, 3,4-dimethyl-	1.0	0.00054	No
1506-02-1	Ethanone, 1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-)	0.10	0.00009	No
151-18-8	Propanenitrile, 3-amino-	0.060	0.00075	No
1534-26-5	3-Tridecanone	0.50	0.61	**Yes**
1534-27-6	3-Dodecanone	0.50	1.1	**Yes**
1565-81-7	3-Decanol	0.015	0.0026	No
1568-20-3	1H-Pyrazole, 4,5-dihydro-5-methyl-	0.020	0.018	No
1569-50-2	3-Penten-2-ol	0.020	0.0016	No
15726-15-5	4-Heptanone, 3-methyl-	0.50	0.0035	No
15877-57-3	Pentanal, 3-methyl-	0.17	0.042	No
15932-80-6	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-	0.20	0.043	No
1604-34-8	2-Undecanone, 6,10-dimethyl-	0.50	0.040	No
1615-70-9	2,4-Pentadienenitrile	0.020	0.041	**Yes**
1626-09-1	2,7-Octanedione	0.050	0.0070	No
1647-11-6	2-Methylene butanenitrile	0.02	0.043	**Yes**
16519-68-9	Cyclohexanone, 2,6-diethyl-	0.20	0.00058	No
1653-30-1	2-Undecanol	0.015	0.00046	No
1653-31-2	2-Tridecanol	0.015	0.00056	No
16624-06-9	Cyclooctanemethanol, .alpha.,.alpha.-dimethyl-	0.015	0.0023	No
1669-44-9	3-Octen-2-one	0.15	0.047	No
16778-26-0	2(3H)-Benzofuranone, 3a,4,5,6-tetrahydro-3a,6,6-tr	0.50	0.090	No
1679-08-9	1-Propanethiol, 2,2-dimethyl-	7.3	0.066	No
1703-52-2	Furan, 2-ethyl-5-methyl-	0.010	0.010	**Yes**
1712-64-7	Nitric acid, 1-methylethyl ester	1.0	0.091	No
1713-33-3	7-Oxabicyclo[4.1.0]heptane, 1-methyl-	0.050	0.0021	No
17351-34-7	14-Pentadecenoic acid	1.0	0.0039	No
17429-02-6	Cyclohexanone, 4-hydroxy-4-methyl-	0.20	0.00035	No
1757-42-2	Cyclopentanone, 3-methyl-	0.20	0.022	No
1759-53-1	Cyclopropanecarboxylic acid	0.10	0.054	No
17622-46-7	2-Cyclohexen-1-one, 4-ethyl-3,4-dimethyl-	0.020	0.00048	No
1779-19-7	1,3,6-Trioxocane	0.20	0.0016	No
17851-53-5	1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl	0.0055	0.00085	No
1840-42-2	Methane, fluorotrinitro-	10	0.015	No
18433-98-2	Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-	0.020	0.0013	No
18521-07-8	3-Octen-2-ol, 2-methyl-, (Z)-	1.0	0.058	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
18829-55-5	2-Heptenal, (E)-	0.0030	0.0016	No
18829-56-6	2-Nonenal, (E)-	0.0030	0.0029	No
1888-57-9	3-Hexanone, 2,5-dimethyl-	0.50	0.0057	No
19269-28-4	Hexanal, 3-methyl-	1.0	0.14	No
1927-69-1	2H-Pyran, 2-(1,1-dimethylethoxy)tetrahydro-	0.19	0.023	No
1932-92-9	2-Propyn-1-ol, propanoate	1.5	0.0012	No
1937-62-8	9-Octadecenoic acid, methyl ester, (E)-	0.0035	0.00064	No
19549-80-5	2-Heptanone, 4,6-dimethyl-	0.50	0.00096	No
19550-03-9	2-Hexanol, 2,3-dimethyl-	0.50	0.00012	No
19550-46-0	1,3-Dimethylcyclopentanol	0.50	0.025	No
19550-73-3	Cyclopentanone, 3,4-dimethyl-, trans-	0.20	0.00012	No
1975-78-6	Decanenitrile	0.080	0.16	**Yes**
19780-10-0	5-Dodecanone	0.50	0.024	No
19780-59-7	2-Heptanol, 3-ethyl-2-methyl-	0.50	0.00097	No
19780-63-3	2-Pentanol, 3-ethyl-2-methyl-	0.25	0.00017	No
19781-07-8	2,7-Octanediol, 2,7-dimethyl-	0.50	0.0027	No
19781-27-2	3-Octanol, 6-ethyl-	0.50	0.0013	No
20192-66-9	1,3-Benzodioxol-2-one, hexahydro-, trans-	0.020	0.00037	No
2040-07-5	Ethanone, 1-(2,4,5-trimethylphenyl)-	0.10	0.0023	No
2050-78-4	Nitric acid, decyl ester	0.25	0.00095	No
20633-11-8	Nitric acid, hexyl ester	0.25	0.10	No
20633-12-9	Nitric acid, heptyl ester	0.25	0.10	No
20633-13-0	Nitric acid, nonyl ester	0.25	0.00017	No
20691-89-8	4-Piperidinemethanol, 1-methyl-	0.010	0.0075	No
20698-91-3	Benzeneacetic acid, .alpha.-hydroxy-, methyl ester	0.0035	0.0011	No
20743-95-7	Benzene, 1-butoxy-4-methoxy-	0.010	0.00050	No
20754-04-5	4-Octanone, 3-methyl-	0.50	0.0029	No
2091-29-4	9-Hexadecenoic acid	1.0	0.33	No
21078-65-9	1-Decanol, 2-ethyl-	0.015	0.00012	No
2136-70-1	Ethanol, 2-(tetradecyloxy)-	0.20	0.18	No
22026-12-6	6-Tridecanone	0.50	0.099	No
2216-87-7	3-Undecanone	0.50	0.11	No
22319-25-1	3-Hepten-2-one, 4-methyl-	0.15	0.0071	No
22319-29-5	4-Hepten-3-one, 5-ethyl-2,4-dimethyl-	0.15	0.031	No
2243-27-8	Nonanenitrile	0.080	0.16	**Yes**
2244-07-7	Undecanenitrile	0.080	0.00029	No
2345-27-9	2-Tetradecanone	0.50	0.011	No
23462-75-1	2H-Pyran-3(4H)-one, dihydro-	1.0	0.0010	No
2371-19-9	2-Heptanone, 3-methyl-	0.50	0.0086	No
2407-94-5	Cyclohexanol, 1,1`-dioxybis-	0.50	0.00019	No
2408-37-9	Cyclohexanone, 2,2,6-trimethyl-	0.20	0.030	No
2425-77-6	2-Hexyl-1-decanol	0.20	0.025	No
24405-16-1	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	1.0	0.21	No
2456-28-2	Decane, 1,1`-oxybis-	1.0	0.073	No
2490-48-4	1-Hexadecanol, 2-methyl-	0.0015	0.00039	No
25013-16-5	Phenol, (1,1-dimethylethyl)-4-methoxy-	0.050	0.00037	No
2508-29-4	1-Pentanol, 5-amino-	0.050	0.00065	No
2548-87-0	2-Octenal, (E)-	0.0030	0.0016	No
25564-22-1	2-Pentyl-2-cyclopenten-1-one	0.05	0.040	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
2610-95-9	2H-Pyran-2-one, tetrahydro-6,6-dimethyl-	1.0	0.00052	No
26215-90-7	4-Tridecanone	0.50	0.019	No
26248-42-0	Tridecanol	0.0015	0.0011	No
2639-63-6	Butanoic acid, hexyl ester	1.5	0.00013	No
26465-81-6	1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl-	0.010	0.00042	No
26496-20-8	4-Tetradecanone	0.50	0.0014	No
26537-19-9	Benzoic acid, 4-(1,1-dimethylethyl)-, methyl ester	0.00055	0.00052	No
27392-16-1	Cyclohexanecarboxylic acid, 2-(1,1-dimethylethyl)-	0.00066	0.00024	No
27675-36-1	1-Propene, 1-nitro-, (Z)-	0.25	0.0021	No
2799-17-9	2-Propanol, 1-amino-	0.20	0.19	No
28019-94-5	1H-Pyrazole, 4,5-dihydro-4,5-dimethyl-	0.020	0.0055	No
28290-01-9	Cyclobutanone, 2,3,3-trimethyl-	0.067	0.0021	No
28473-21-4	1-Nonanol	0.070	0.0032	No
2865-82-9	2(3H)-Furanone, 5-ethyldihydro-5-methyl-	0.50	0.0014	No
288-16-4	Isothiazole	0.010	0.00079	No
288-47-1	Thiazole	0.10	0.0024	No
288-88-0	1H-1,2,4-Triazole	1.0	0.0087	No
289-95-2	Pyrimidine	3.0	0.029	No
29006-00-6	2-Hexanone, 6-methoxy-	2.0	0.00011	No
2902-96-7	2-Nitro-1-propanol	0.10	0.43	**Yes**
290-37-9	Pyrazine	2.0	0.12	No
2919-23-5	Cyclobutanol	0.50	0.0055	No
2922-51-2	2-Heptadecanone	0.50	0.00009	No
29354-98-1	Hexadecanol	0.0015	0.00009	No
29366-35-6	4-Dodecanone, 11-methyl-	0.50	0.0029	No
29887-79-4	Cycloheptane, 1,3-dimethoxy-, trans-	0.20	0.00028	No
3054-92-0	3-Pentanol, 2,3,4-trimethyl-	0.25	0.0017	No
30692-16-1	5-Tridecanone	0.50	0.0034	No
30951-17-8	1-Naphthalenol, decahydro-4a-methyl-8-methylene-2-(1-methylethyl)	0.50	0.00071	No
32064-72-5	2-Nonen-4-one	0.15	0.010	No
33083-83-9	5-Undecanone	0.50	0.016	No
334-48-5	Decanoic acid	1.0	0.00039	No
33933-82-3	2-Decanone, 5,9-dimethyl-	0.50	0.0029	No
34379-54-9	Furan, 2,3-dihydro-4-(1-methylpropyl)-	0.50	0.00098	**Yes**
3438-46-8	Pyrimidine, 4-methyl-	0.30	0.0091	No
34386-42-0	Benzenemethanol, 4-(1,1-dimethylethyl)-.alpha.-methyl-	0.010	0.0031	No
3457-90-7	1,3-Propanediol, dinitrate	0.00050	0.018	**Yes**
3457-91-8	1,4-Butanediol, dinitrate	0.00050	0.26	**Yes**
35194-30-0	9-Decen-2-one	0.15	0.00048	No
35468-97-4	1-Hepten-1-ol, acetate	1.5	0.0034	No
35996-97-5	Pentadecanoic acid, butyl ester	0.0035	0.00062	No
3622-84-2	Benzenesulfonamide, N-butyl-	0.015	0.16	**Yes**
3664-60-6	7-Octen-2-one	0.15	0.0012	No
36653-82-4	1-Hexadecanol	0.015	1.1	**Yes**
3682-42-6	Pentanoic acid, 3-methyl-2-oxo-, methyl ester	1.5	0.0036	No
3760-54-1	1-Pyrrolidinecarboxaldehyde	0.10	0.00014	No
3760-63-2	1-Butanone, 4-(dimethylamino)-1-phenyl-	0.010	0.0019	No
3761-94-2	Cycloheptanol, 1-methyl-	0.50	0.00017	No
3777-69-3	Furan, 2-pentyl-	0.010	0.0025	**Yes**

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
3789-85-3	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyls	0.25	0.017	No
3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	0.15	0.00008	No
38447-22-2	Hexanedioic acid, bis(1-methylpropyl) ester	0.15	0.00017	No
3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	0.15	0.00077	No
3913-02-8	1-Octanol, 2-butyl-	0.50	0.042	No
3913-81-3	2-Decenal, (E)-	0.0030	0.00062	No
39161-19-8	3-Penten-1-ol	0.020	0.0069	No
39168-02-0	Furan, tetrahydro-2,4-dimethyl-, trans-	0.50	0.0032	No
3944-36-3	2-Propanol, 1-(1-methylethoxy)-	0.20	0.0063	No
39515-51-0	Benzaldehyde, 3-phenoxy-	0.0023	0.00023	No
39899-08-6	3-Hepten-2-one, 3-methyl-	0.15	0.026	No
40649-36-3	4-Propylcyclohexanone	0.20	0.034	No
40702-26-9	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	0.0030	0.00074	No
4088-60-2	2-Buten-1-ol, (Z)-	0.070	0.037	No
41239-48-9	Furan, 2,5-diethyltetrahydro-	0.50	0.019	No
41744-75-6	1-Heptadecanol, 16-methyl-	0.0015	0.00033	No
4176-04-9	Bicyclo[4.1.0]heptan-3-one, 4,7,7-trimethyl	0.020	0.086	**Yes**
420-56-4	Silane, fluorotrimethyl-	0.050	0.00049	No
42565-49-1	10-Undecen-4-one, 2,2,6,6-tetramethyl-	0.15	0.0014	No
42604-04-6	Cycloheptane, methoxy-	0.20	0.019	No
4272-06-4	4-Undecanol	0.015	0.00030	No
42786-06-1	4H-1,2,4-Triazol-3-amine, 4-ethyl-	1.0	0.0019	No
4312-99-6	1-Octen-3-one	0.15	0.0060	No
4337-65-9	Hexanedioic acid, mono(2-ethylhexyl) ester	0.15	0.0026	No
4457-62-9	Furan, tetrahydro-2,5-dipropyl-	0.50	0.00097	No
4485-09-0	4-Nonanone	0.50	0.12	No
4562-27-0	4(1H)-Pyrimidinone	0.10	0.0016	No
4573-09-5	Cyclopentanone, 2,2,5-trimethyl-	0.20	0.0026	No
460-13-9	Propane, 1-fluoro-	0.75	0.057	No
4631-98-5	Cyclohexanol, 4-(1,1,3,3-tetramethylbutyl)-	0.50	0.00045	No
470-65-5	Cyclohexanol, 4-methyl-1-(1-methylethyl)-	0.50	0.00018	No
4786-20-3	2-Butenenitrile	0.020	0.0057	No
4799-62-6	1-Pentanol, 5-methoxy-	1.0	0.0021	No
4826-62-4	2-Dodecenal	0.0030	0.00049	No
486-25-9	9H-Fluoren-9-one	0.010	0.0021	No
4911-70-0	2-Pentanol, 2,3-dimethyl-	0.25	0.0012	No
502-56-7	5-Nonanone	0.0050	0.0024	No
502-69-2	2-Pentadecanone, 6,10,14-trimethyl-	0.50	0.00047	No
503-30-0	Trimethylene oxide	2.5	0.56	No
5057-99-8	1,2-Cyclopentanediol, trans-	0.10	0.0018	No
50639-02-6	5-Undecanone, 2-methyl-	0.50	0.20	No
507-55-1	1,3-Dichloro-1,1,2,2,3-pentafluoropropane	1.67	1.0	No
5115-98-0	3-Piperidinecarboxamide, N-methyl-	1.0	0.0015	No
51411-24-6	6,10-Dodecadien-1-ol, 3,7,11-trimethyl-	1.0	0.26	No
5145-01-7	2(3H)-Furanone, dihydro-3,5-dimethyl-	0.50	0.14	No
51595-87-0	2-Heptanone, 6-(2-furanyl)-6-methyl-	0.010	0.00052	**Yes**
5166-53-0	3-Hexen-2-one, 5-methyl-	0.15	0.0034	No
51756-19-5	1-Nonen-3-one, 2-methyl-	0.15	0.00087	No
51953-17-4	4(3H)-Pyrimidinone	0.10	0.0051	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
5204-80-8	4-Pentenal, 2-ethyl-	5.0	0.014	No
5205-34-5	5-Decanol	0.015	0.0035	No
52588-78-0	3,4-Undecadiene-2,10-dione, 6,6-dimethyl-	0.015	0.00022	No
53229-39-3	Oxirane, (1-methylbutyl)-	0.020	0.00046	No
53398-83-7	Butanoic acid, 2-hexenyl ester, (E)-	1.5	0.0053	No
534-22-5	Furan, 2-methyl-	0.010	1.0	**Yes**
53535-33-4	Heptanol	0.50	0.059	No
53833-32-2	Oxazole, 4,5-dimethyl-2-propyl-	0.50	0.0075	No
53907-75-8	Oxirane, 2-methyl-2-pentyl-	0.020	0.0028	No
54004-41-0	1-Pentanol, 4-methyl-2-propyl-	0.25	0.0055	No
541-05-9	Cyclotrisiloxane, hexamethyl-	4.4	0.63	No
541-35-5	Butanamide	0.10	0.020	No
541-73-1	Benzene, 1,3-dichloro-	0.25	0.010	No
542-44-9	Hexadecanoic acid, 2,3-dihydroxypropyl ester	0.0035	0.00027	No
542-54-1	4-Methylpentanenitrile	0.08	0.024	No
542-55-2	Formic acid, 2-methylpropyl ester	1.0	0.066	No
543-29-3	Nitric acid, 2-methylpropyl ester	0.25	0.070	No
543-49-7	2-Heptanol	0.50	0.052	No
543-87-3	1-Butanol, 3-methyl-, nitrate	0.25	0.15	No
544-16-1	Nitrous acid, butyl ester	0.40	0.49	**Yes**
544-63-8	Tetradecanoic acid	1.0	0.39	No
5454-28-4	Heptanoic acid, butyl ester	0.15	0.0011	No
54658-01-4	Hexane, 3-methoxy-	0.050	0.045	No
54774-28-6	2-Furanmethanol, tetrahydro-5-methyl-, trans-	0.020	0.00065	No
54845-28-2	2-Hexenoic acid, 2-hexenyl ester, (E,E)-	0.15	0.035	No
5500-21-0	Cyclopropanecarbonitrile	0.060	0.0073	No
55429-85-1	Benzeneethanamine, N-[(pentafluorophenyl)methylene	1.0	0.0039	No
556-67-2	Cyclotetrasiloxane, octamethyl	3.0	0.41	No
55956-20-2	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	0.50	0.011	No
56052-85-8	2-Pentene, 5-(pentyloxy)-, (E)-	1.0	0.0034	No
56554-96-2	2-Octadecenal	0.0030	0.0020	No
565-61-7	2-Pentanone, 3-methyl-	0.50	0.036	No
565-67-3	3-Pentanol, 2-methyl-	0.25	0.073	No
565-68-4	1-Pentyn-3-ol, 4-methyl-	1.0	0.0098	No
565-69-5	3-Pentanone, 2-methyl-	0.50	0.013	No
565-80-0	3-Pentanone, 2,4-dimethyl-	0.50	0.061	No
5675-51-4	1,12-Dodecanediol	0.0015	0.00011	No
57-10-3	Hexadecanoic acid	1.0	0.37	No
57-11-4	Octadecanoic acid	1.0	0.00032	No
5715-25-3	2-Cyclohexen-1-one, 4,5-dimethyl-	0.020	0.0044	No
5746-58-7	Tetradecanoic acid, 12-methyl-, (S)-	1.0	0.00088	No
5756-43-4	Hexane, 1-ethoxy-	0.050	0.019	No
57706-88-4	3-Octanol, 3,7-dimethyl-, (.+-.)-	0.50	0.0012	No
5775-96-2	1H-Pyrazole, 4,5-dihydro-1,5-dimethyl-	0.20	0.0071	No
578-54-1	Benzenamine, 2-ethyl-	0.0050	0.0015	No
583-58-4	Pyridine, 3,4-dimethyl-	0.020	0.0015	No
58467-28-0	2,5-Pyrrolidinedione, 3-ethyl-3-hydroxy-	10	0.0011	No
5857-36-3	3-Pentanone, 2,2,4-trimethyl-	0.50	0.012	No
585-74-0	Ethanone, 1-(3-methylphenyl)-	0.10	0.00033	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
589-63-9	4-Octanone	0.50	0.47	No
589-82-2	3-Heptanol	0.50	0.065	No
589-93-5	Pyridine, 2,5-dimethyl-	0.020	0.019	No
590-01-2	Propanoic acid, butyl ester	1.5	0.20	No
590-36-3	2-Pentanol, 2-methyl-	0.25	0.051	No
590-50-1	2-Pentanone, 4,4-dimethyl-	0.50	0.11	No
590-86-3	Butanal, 3-methyl-	0.50	0.085	No
5910-87-2	2,4-Nonadienal, (E,E)-	0.0030	0.00087	No
5910-89-4	Pyrazine, 2,3-dimethyl-	0.50	0.0089	No
591-22-0	Pyridine, 3,5-dimethyl-	0.020	0.0021	No
591-23-1	Cyclohexanol, 3-methyl-	0.50	0.00059	No
591-24-2	Cyclohexanone, 3-methyl-	0.20	0.029	No
591-87-7	Acetic acid, 2-propenyl ester	5.0	1.0	No
592-84-7	Formic acid, butyl ester	1.0	0.72	No
593-08-8	2-Tridecanone	0.50	0.24	No
594-70-7	Propane, 2-methyl-2-nitro-	0.10	0.23	**Yes**
598-32-3	3-Buten-2-ol	5.0	0.026	No
59-89-2	N-Nitrosomorpholine	0.0050	0.0097	**Yes**
59983-39-0	1-Pyrrolidinamine, 2-(methoxymethyl)-, (S)-	0.10	0.00031	No
600-14-6	2,3-Pentanedione	0.20	0.016	No
600-24-8	Butane, 2-nitro-	0.10	0.0012	No
60-35-5	Acetamide	0.0100	0.0032	**Yes**
6064-27-3	C6-Dodecanone	0.50	0.090	No
608-25-3	1,3-Benzenediol, 2-methyl-	10	0.00099	No
6137-06-0	2-Heptanone, 4-methyl-	0.50	0.017	No
6137-12-8	3-Hexanone, 4-ethyl-	0.50	0.00059	No
6137-26-4	4-Dodecanone	0.50	0.026	No
613-93-4	Benzamide, N-methyl-	0.0050	0.00033	No
617-29-8	3-Hexanol, 2-methyl-	0.060	0.018	No
6175-49-1	2-Dodecanone	0.50	0.018	No
617-94-7	Benzenemethanol, .alpha.,.alpha.-dimethyl-	0.10	2.2	**Yes**
623-37-0	3-Hexanol	0.060	0.0081	No
623-56-3	3-Hexanone, 5-methyl-	0.50	0.0017	No
623-87-0	1,3-Dinitrate-1,2,3-propanetriol	0.00050	0.010	**Yes**
624-16-8	4-Decanone	0.50	0.0026	No
624-42-0	3-Heptanone, 6-methyl-	0.25	0.0052	No
624-43-1	1,2,3-Propanetriol, 1-nitrate	0.00050	0.026	**Yes**
624-91-9	Nitrous acid, methyl ester	0.20	0.32	**Yes**
624-95-3	1-Butanol, 3,3-dimethyl-	1.0	0.018	No
625-25-2	2-Heptanol, 2-methyl-	0.50	0.00069	No
625-74-1	Propane, 2-methyl-1-nitro-	0.10	0.0020	No
625-84-3	1H-Pyrrole, 2,5-dimethyl-	0.010	0.0027	No
625-86-5	Furan, 2,5-dimethyl-	0.010	0.0093	**Yes**
627-05-4	Butane, 1-nitro-	0.25	0.39	**Yes**
627-59-8	2-Hexanol, 5-methyl-	0.50	0.00051	No
6281-96-5	Formamide, N-(2-methylpropyl)-	0.10	0.0058	No
628-28-4	Butane, 1-methoxy-	0.050	0.43	**Yes**
628-44-4	2-Octanol, 2-methyl-	0.50	0.0056	No
628-61-5	Octane, 2-chloro-	0.010	0.00071	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
628-80-8	Pentane, 1-methoxy-	0.20	0.0077	No
629-08-3	Heptanenitrile	0.080	0.64	**Yes**
629-23-2	3-Tetradecanone	0.50	0.14	No
6295-06-3	Acetic acid, oxo-, butyl ester	1.5	0.00025	No
629-54-9	Hexadecanamide	5.0	0.00026	No
629-60-7	Tridecanenitrile	0.080	0.052	No
629-70-9	1-Hexadecanol, acetate	1.5	0.0043	No
629-76-5	1-Pentadecanol	0.015	0.0021	No
629-80-1	Hexadecanal	0.50	0.00044	No
630-18-2	Propanenitrile, 2,2-dimethyl-	0.080	0.021	No
630-19-3	Propanal, 2,2-dimethyl-	0.25	0.020	No
637-88-7	1,4-Cyclohexanedione	0.067	0.0034	No
645-56-7	Phenol, 4-propyl-	0.050	0.00051	No
645-62-5	2-Hexenal, 2-ethyl-	0.0030	0.028	**Yes**
66-25-1	Hexanal	5.0	1.3	No
6711-26-8	Cyclohexanone, 2,5-dimethyl-2-(1-methylethenyl)-	0.020	0.00040	No
6728-26-3	2-Hexenal, (E)-	0.0030	0.00030	No
6728-31-0	4-Heptenal, (Z)-	5.0	0.0020	No
6789-80-6	3-Hexenal, (Z)-	5.0	0.0047	No
6836-38-0	6-Dodecanol	0.015	0.0017	No
68443-63-0	Hexanoic acid, 2-ethyl-, butyl ester	0.15	0.0012	No
68820-35-9	4-Undecenal, (E)-	5.0	0.0024	No
6898-69-7	N-(Butylidene)methanamine	0.05	0.029	No
6898-74-4	1-Butanamine, N-ethylidene-	0.010	0.0079	No
693-54-9	2-Decanone	0.50	0.086	No
693-98-1	1H-Imidazole, 2-methyl-	0.10	0.00043	No
695-06-7	2(3H)-Furanone, 5-ethyldihydro-	5.0	0.017	No
69687-91-8	2-Hexenoic acid, 4-methylphenyl ester	0.15	0.0014	No
69770-96-3	Cyclopentanone, 2-methyl-4-(2-methylpropyl)-	0.20	0.068	No
699-22-9	1H-Pyrrole, 1-pentyl-	0.10	0.016	No
705-15-7	1-(2-Hydroxy-5-methoxyphenyl)ethanone	0.10	0.013	No
706-14-9	2(3H)-Furanone, 5-hexyldihydro-	5.0	0.00079	No
7112-02-9	Octanamide, N-(2-hydroxyethyl)-	0.50	0.0034	No
71-41-0	1-Pentanol	0.20	0.12	No
719-22-2	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethyl	0.010	0.0029	No
7250-80-8	Benzenesulfonamide, N-hexyl-	0.0015	0.00043	No
7379-12-6	2-Methyl-3-hexanone	0.50	0.064	No
74367-34-3	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimeth	0.15	0.00052	No
74381-40-1	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2	0.10	0.45	**Yes**
74646-36-9	1-Dodecyn-4-ol	1.0	0.0051	No
74646-37-0	1-Tridecyn-4-ol	1.0	0.00065	No
74793-02-5	2,2`-Bioxepane	0.050	0.045	No
75011-90-4	1H-Pyrazole, 4,5-dihydro-5-propyl-	0.020	0.0045	No
753-89-9	Propane, 1-chloro-2,2-dimethyl-	0.75	0.0037	No
75-84-3	1-Propanol, 2,2-dimethyl-	0.50	0.036	No
75-85-4	2-Butanol, 2-methyl-	10	0.018	No
75-97-8	2-Butanone, 3,3-dimethyl-	2.0	0.034	No
76-09-5	2,3-Butanediol, 2,3-dimethyl-	0.10	0.0017	No
763-93-9	3-Hexen-2-one	0.15	0.011	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
766-15-4	1,3-Dioxane, 4,4-dimethyl-	0.020	0.0017	No
7726-08-1	Decanamide, N-(2-hydroxyethyl)-	5.0	0.00057	No
774-40-3	Benzeneacetic acid, .alpha.-hydroxy-, ethyl ester	0.0035	0.0017	No
78-46-6	Phosphonic acid, butyl-, dibutyl ester	0.0020	0.070	**Yes**
78-85-3	2-Propenal, 2-methyl-	0.20	0.026	No
79-16-3	Acetamide, N-methyl-	0.10	0.00037	No
79-31-2	2-Methylpropionic acid	1.00	0.010	No
80-39-7	Benzenesulfonamide, N-ethyl-4-methyl-	0.0015	0.0014	No
814-78-8	3-Buten-2-one, 3-methyl-	0.0020	0.021	**Yes**
819-97-6	Butanoic acid, 1-methylpropyl ester	1.5	0.00016	No
820-29-1	5-Decanone	0.50	0.0061	No
821-41-0	5-Hexen-1-ol	0.020	0.016	No
821-55-6	2-Nonanone	0.50	1.6	**Yes**
83321-16-8	3-Cyclopenten-1-one, 2,3,4-trimethyl-	0.15	0.00081	No
84-64-0	1,2-Benzenedicarboxylic acid, butyl cyclohexyl est	0.055	0.0059	No
85-69-8	1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl e	0.0055	0.00060	No
871-71-6	Formamide, N-butyl-	0.10	0.013	No
873-94-9	Cyclohexanone, 3,3,5-trimethyl-	0.20	0.034	No
89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)	0.20	0.37	**Yes**
91894-15-4	4-Methoxy-6-methyl-6,7-dihydro-4H-furo[3,2-c]pyran	1.00	0.078	No
922-63-4	2-Methylenebutanal	0.20	0.012	No
922-65-6	1,4-Pentadien-3-ol	0.020	0.0073	No
925-54-2	2-Methylhexanal	1.00	0.053	No
925-78-0	3-Nonanone	0.50	0.14	No
926-42-1	1-Propanol, 2,2-dimethyl-, nitrate	0.25	0.078	No
928-45-0	Nitric acid, butyl ester	0.25	0.36	**Yes**
928-68-7	2-Heptanone, 6-methyl-	0.50	2.1	**Yes**
928-80-3	3-Decanone	0.50	0.0049	No
930-02-9	1-Ethenyloxyoctadecane	0.50	0.044	No
930-36-9	1H-Pyrazole, 1-methyl-	0.020	0.0018	No
93-55-0	1-Propanone, 1-phenyl-	0.10	0.047	No
948-65-2	1H-Indole, 2-phenyl-	0.10	0.00065	No
95-16-9	Benzothiazole	1.0	0.0099	No
96-17-3	Butanal, 2-methyl-	0.50	0.021	No
96-47-9	2-Methyltetrahydrofuran	0.50	0.039	No
96-48-0	2(3H)-Furanone, dihydro-	75	0.91	No
97-87-0	Propanoic acid, 2-methyl-, butyl ester	1.5	0.0040	No
97-95-0	1-Butanol, 2-ethyl-	1.0	0.012	No
98-54-4	Phenol, 4-(1,1-dimethylethyl)-	0.050	0.0013	No
MADUAK0-01b	Benzaldehyde, 4-hydroxy- mixture	0.0046	0.0013	No
MADUAR0-01a	Undecanal, 2-methyl- mixture	0.50	0.0048	No
MARSI00-01a	Trisiloxane, octamethyl- mixture	3.0	0.0068	No
MARUPH0-01b	di-t-Butyl-ethylphenol mixture	0.050	0.00041	No
MKEUAE0-01b	Acetophenone, 2`-hydroxy-5`methoxy- mixture	0.10	0.013	No
MOHOH00-01a	Benzenemethanol, alpha, methyl- mixture	0.010	0.0047	No
MUPHUSI-01a	Nonylphenol isomer mixture	0.050	0.00010	No
OHUES0-01	1-Heptadecanyl acetate	1.50	0.00008	No
UAD012-01	(7E,9E)-Dodecadienal	5.0	0.067	No
UCA014-01	C14-Alkanoic Acid	1.0	0.11	No

Table C-7. CNFE with Screening Values (11 Sheets)

Chemical Identification Number	Chemical Name	Screening Value (ppmv)	Maximum Conc (ppmv)	Need In-Depth Analysis?
UCA016-01	C16-Alkanoic acid	1.0	1.1	**Yes**
UES010-01	C6 Ester of butanoic acid	0.15	0.00013	No
UES013-01	1-ethylpropyl octanoate	0.0035	0.00007	No
UET005-01	Unknown C5 ether	2.0	0.014	No
UHC000-05	C3-Pyridine	0.050	0.0015	No
UHC000-06	C4-2-Pyrrolidinone	1.0	0.00059	No
UHC000-07	C4-Piperidine	0.010	0.00069	No
UHC000-09	Methyl pyridine	0.020	0.52	**Yes**
UHC000-10	C2-Pyrrolidine	0.40	0.29	No
UHC000-13	C2-Pyridine	0.050	0.19	**Yes**
UIN000-01	Sulfur oxides (SO_X)	0.020	0.37	**Yes**
UKE006-02	C6-Alkenone	0.15	0.0021	No
UKE006-03	4-Hydroxy-4-methylpentanone	0.050	0.0034	No
UKE006-04	C6-Alkanone	0.050	0.021	No
UKE007-01	C7-Alkanone	0.50	0.071	No
UKE008-01	C8-Alkanone	0.50	1.2	**Yes**
UKE009-02	C9-Alkenone	0.15	0.13	No
UKE009-03	C9-Alkanone	0.50	1.1	**Yes**
UKE010-01	C10-Alkanone	0.50	0.027	No
UKE010-02	3-t-Pentylcyclopentanone	0.067	0.0016	No
UKE011-02	C11-Alkanone	0.50	0.013	No
UKE012-02	C12-Alkanone	0.50	0.41	No
UKE013-02	C13-Alkanone	0.50	1.1	**Yes**
UKE014-01	C14-Alkanone	0.50	0.050	No
UKE014-03	2-Hexanone, 3-cyclohexyliden-4-ethyl	0.050	0.029	No
UKE015-01	2-Pentanone, 4-cyclohexyliden-3,3-diethyl	0.15	0.017	No
UNA003-01	Unknown C3-Nitrate	0.25	0.019	No
UNI000-02M	2-Butanenitrile and others	0.080	0.040	No
UNI007-01	C7-Alkyl nitrile	0.080	0.011	No
UNI008-01	C8-Alkyl nitrile	0.080	0.018	No
UOH010-01	1-Cyclopentyl-2,2-dimethyl-1-propanol	0.50	0.017	No
UPH000-01	Octyl phenol isomer	0.050	0.00011	No
USI000-05	Trimethylsilylester of methoxy benzoic acid	0.25	0.0015	No

Note: Conc = Concentration

Table C-8. Chemicals Given In-Depth Analysis (2 Sheets)

Chemical Identification Number	Chemical Name	AOEL (ppmv)	Max Conc (ppmv)	COPC?
105-42-0	2-Hexanone, 4-methyl-	0.50	1.1	**Yes**
1072-44-2	1-Methylaziridine	0.050	0.065	No
108-47-4	Pyridine, 2,4-dimethyl-	0.50	0.10	**Yes**
109-75-1	3-Butenenitrile	1.0	0.021	No
110-00-9	Furan	0.0010	3.2	No
110-27-0	Tetradecanoic acid, 1-methylethyl ester	not needed	0.17	No
110-36-1	Tetradecanoic acid, butyl ester	not needed	0.20	No
1115-11-3	2-Butenal, 2-methyl-	0.030	0.013	No
112-92-5	1-Octadecanol	not needed	0.96	No
1184-60-7	1-Propene, 2-fluoro-	0.10	0.53	**Yes**
1191-99-7	Furan, 2,3-dihydro-	0.0010	0.025	No
124-12-9	Octanenitrile	6.0	0.49	No
142-91-6	Hexadecanoic acid, 1-methylethyl ester	not needed	0.033	No
1534-26-5	3-Tridecanone	17	0.61	No
1534-27-6	3-Dodecanone	17	1.1	No
1615-70-9	2,4-Pentadienenitrile	0.30	0.041	**Yes**
1647-11-6	2-Methylene butanenitrile	0.30	0.043	**Yes**
1703-52-2	Furan, 2-ethyl-5-methyl-	0.0010	0.010	No
1975-78-6	Decanenitrile	6.0	0.16	No
2243-27-8	Nonanenitrile	6.0	0.16	No
2902-96-7	2-Nitro-1-propanol	8.0	0.43	No
34379-54-9	Furan, 2,3-dihydro-4-(1-methylpropyl)-	0.0010	0.00098	No
3457-90-7	1,3-Propanediol, dinitrate	0.050	0.018	No
3457-91-8	1,4-Butanediol, dinitrate	0.050	0.26	No
3622-84-2	Benzenesulfonamide, N-butyl-	contaminant	0.16	No
36653-82-4	1-Hexadecanol	not needed	1.1	No
3777-69-3	Furan, 2-pentyl-	0.0010	0.0025	No
4176-04-9	Bicyclo[4.1.0]heptan-3-one, 4,7,7-trimethyl	0.70	0.086	**Yes**
51595-87-0	2-Heptanone, 6-(2-furanyl)-6-methyl-	0.0010	0.00052	No
534-22-5	Furan, 2-methyl-	0.0010	1.0	No
544-16-1	Nitrous acid, butyl ester	0.10	0.49	**Yes**
594-70-7	Propane, 2-methyl-2-nitro-	0.30	0.23	**Yes**
59-89-2	N-Nitrosomorpholine	Intertox	0.010	**Yes**
60-35-5	Acetamide	not needed	0.0032	No
617-94-7	Benzenemethanol, .alpha.,.alpha.-dimethyl-	contaminant	2.2	No
623-87-0	1,3-Dinitrate-1,2,3-propanetriol	0.050	0.010	No
624-43-1	1,2,3-Propanetriol, 1-nitrate	8.0	0.026	No
624-91-9	Nitrous acid, methyl ester	0.10	0.32	**Yes**
625-86-5	Furan, 2,5-dimethyl-	0.0010	0.0093	No
627-05-4	Butane, 1-nitro-	2.5	0.39	**Yes**
628-28-4	Butane, 1-methoxy-	17	0.43	No
629-08-3	Heptanenitrile	6.0	0.64	**Yes**
645-62-5	2-Hexenal, 2-ethyl-	0.10	0.028	**Yes**
74381-40-1	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3- propanediyl ester	contaminant	0.45	No
78-46-6	Phosphonic acid, butyl-, dibutyl ester	0.0070	0.070	No
814-78-8	3-Buten-2-one, 3-methyl-	0.020	0.021	No
821-55-6	2-Nonanone	17	1.6	No

Table C-8. Chemicals Given In-Depth Analysis (2 Sheets)

Chemical Identification Number	Chemical Name	AOEL (ppmv)	Max Conc (ppmv)	COPC?
89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)	2.5	0.37	**Yes**
928-45-0	Nitric acid, butyl ester	8.0	0.36	No
928-68-7	2-Heptanone, 6-methyl-	8.0	2.1	**Yes**
UCA016-01	C16-Alkanoic acid	Ambiguous	1.1	No
UHC000-09	Methyl pyridine	Ambiguous	0.52	No
UHC000-13	C2-Pyridine	Ambiguous	0.19	No
UIN000-01	Sulfur oxides (SO_X)		0.37	No
UKE008-01	C8-Alkanone	Ambiguous	1.2	No
UKE009-03	C9-Alkanone	Ambiguous	1.1	No
UKE013-02	C13-Alkanone	Ambiguous	1.1	No

Table C-9. Chemicals Removed from the COPC List

Chemical Identification Number	Chemical Name	Basis for Removal	Removal Date	Notes
100-40-3	4-Ethenylcyclohexene	Misidentified	6-Jul-05	1, 2
10102-44-0	Nitrogen dioxide	Non-tank source	6-Jul-05	2, 3
104-76-7	2-Ethyl-1-hexanol	Below 10% of AOEL	26-Jan-06	4, 5
106-93-4	1,2-Dibromoethane	Analytical contaminant	26-Jan-06	5, 6
107-06-2	1,2-Dichloroethane	Analytical contaminant	26-Jan-06	5, 6
11097-69-1	Aroclor-1254	Chlorinated biphenyls	6-Jul-05	2
117-81-7	bis(2-Ethylhexyl)phthalate	Below 10% of TLV	26-Jan-06	5, 7
123-91-1	1,4-Dioxane	Below 10% of TLV	26-Jan-06	5, 7
124-38-9	Carbon dioxide	Removed by IH	6-Jul-05	2, 3
127-18-4	Tetrachloroethylene	Below 10% of TLV	26-Jan-06	5, 7
128-37-0	2,6-bis(1,1-Dimethylethyl)-4-methylphenol [BHT]	Sampling contaminant	15-Feb-06	8, 10
134-32-7	1-Napthylamine	Low concentration	15-Feb-06	8, 9
53469-21-9	Aroclor-1242	Chlorinated biphenyls	6-Jul-05	2
56-23-5	Carbon tetrachloride	Below 10% of TLV	26-Jan-06	5, 7
57-14-7	1.1-Dimethylhydrazine	Misidentified	6-Jul-05	1, 2
589-38-8	3-Hexanone	Below 10% of AOEL	26-Jan-06	4, 5
60-34-4	Methyl hydrazine	Misidentified	6-Jul-05	1, 2
630-08-0	Carbon monoxide	Non-tank source	6-Jul-05	2, 3
67-66-3	Chloroform	Below 10% of TLV	26-Jan-06	5, 7
72-55-9	Dichlorodiphenyldichloroethylene (DDE)	Low concentration	15-Feb-06	8, 9
75-01-4	Chloroethene	Analytical contaminant	26-Jan-06	5, 7
75-02-5	Fluoroethene	Misidentified	6-Jul-05	1, 2
75-09-2	Dichloromethane	Below 10% of PEL	15-Feb-06	7, 8
75-15-0	Carbon disulfide	Below 10% of TLV	26-Jan-06	5
75-21-8	Ethylene oxide	Misidentified	6-Jul-05	1, 2
75-50-3	N,N-Dimethylmethanamine	Misidentified	6-Jul-05	1, 2
79-01-6	Trichloroethylene	Below 10% of TLV	26-Jan-06	5, 7
79-10-7	Acrylic acid	Misidentified	6-Jul-05	1, 2
79-46-9	2-Nitropropane	Below 10% of TLV	26-Jan-06	5, 7

Notes: [1] TWS05.008
[2] Interoffice Memo 7F800-05-JOH-006
[3] Interoffice Memo 7B600-MLZ-05-005
[4] PNNL-15736
[5] EASRG meeting minutes 1/26/2006 (Appendix E)
[6] PNNL-15648
[7] EASRG meeting minutes 12/7/2005 (Appendix E)
[8] EASRG meeting minutes 2/15/2006 (Appendix E)
[9] PNNL-15632
[10] PNNL-15640

Table C-10. Chemicals of Potential Concern

Chemical Identification Number	Chemical Name	Tank Farms OEL		Date Added to COPC List
		Value	Source	
92-52-4	1,1'-Biphenyl	0.2 ppmv	ACGIH TLV	7-Oct-04
106-99-0	1,3-Butadiene	1 ppmv	OSHA PEL	7-Oct-04
623-87-0	1,3-Dinitrate-1,2,3-propantriol	0.05 ppmv	AOEL	26-Jan-06
3457-91-8	1,4-Butanediol dinitrate	0.05 ppmv	AOEL	26-Jan-06
71-36-3	1-Butanol	20 ppmv	ACGIH TLV	7-Oct-04
108-47-4	2,4-Dimethylpyridine	0.5 ppmv	AOEL	26-Jan-06
1615-70-9	2,4-Pentadienenitrile	0.3 ppmv	AOEL	15-Feb-06
645-62-5	2-Ethylhex-2-enal	0.1 ppmv	AOEL	15-Feb-06
1184-60-7	2-Fluoropropene	0.1 ppmv	AOEL	26-Jan-06
591-78-6	2-Hexanone	5 ppmv	ACGIH TLV	7-Oct-04
1115-11-3	2-Methylbut-2-enal	0.03 ppmv	AOEL	26-Jan-06
1647-11-6	2-Methylene butanenitrile	0.3 ppmv	AOEL	15-Feb-06
594-70-7	2-Nitro-2-methylpropane	0.3 ppmv	AOEL	15-Feb-06
78-94-4	3-Buten-2-one	0.2 ppmv	ACGIH ceiling	6-Jul-05
814-78-8	3-Methyl-3-buten-2-one	0.02 ppmv	AOEL	26-Jan-06
105-42-0	4-Methyl-2-hexanone	0.5 ppmv	AOEL	26-Jan-06
928-68-7	6-Methyl-2-heptanone	8 ppmv	AOEL	26-Jan-06
75-07-0	Acetaldehyde	25 ppmv	ACGIH ceiling	7-Oct-04
75-05-8	Acetonitrile	20 ppmv	ACGIH TLV	7-Oct-04
7664-41-7	Ammonia	25 ppmv	ACGIH TLV	7-Oct-04
71-43-2	Benzene	0.5 ppmv	ACGIH TLV	7-Oct-04
123-72-8	Butanal	25 ppmv	AOEL	7-Oct-04
109-74-0	Butanenitrile	8 ppmv	AOEL	7-Oct-04
928-45-0	Butyl nitrate	8 ppmv	AOEL	26-Jan-06
544-16-1	Butyl nitrite	0.1 ppmv	AOEL	26-Jan-06
	Chlorinated biphenyls	0.03 mg/m^3	AOEL	6-Jul-05
78-46-6	Dibutyl butylphosphonate	0.007 ppmv	AOEL	26-Jan-06
84-66-2	Diethyl phthalate	5 mg/m^3	ACGIH TLV	7-Oct-04
593-74-8	Dimethylmercury	0.01 mg/m^3	ACGIH TLV	7-Oct-04
75-04-7	Ethylamine	5 ppmv	ACGIH TLV	14-May-06
50-00-0	Formaldehyde	0.3 ppmv	ACGIH ceiling	7-Oct-04
110-00-9	Furan	0.001 ppmv	AOEL	26-Jan-06
---	Substituted furans	0.001 ppmv	AOEL	26-Jan-06
1191-99-7	*2,3-Dihydrofuran*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
51595-87-0	*2-(2-Methyl-6-oxoheptyl)furan*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
625-86-5	*2,5-Dimethylfuran*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
1703-52-2	*2-Ethyl-5-methylfuran*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
534-22-5	*2-Methylfuran*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
3777-69-3	*2-Pentylfuran*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
34379-54-9	*4-(1-Methylpropyl)-2,3-dihydrofuran*	*0.001 ppmv*	*AOEL*	*26-Jan-06*
629-08-3	Heptanenitrile	6 ppmv	AOEL	26-Jan-06
628-73-9	Hexanenitrile	6 ppmv	AOEL	7-Oct-04
---	Hydrocarbons	200 mg/m^3	AOEL	7-Dec-05
7439-97-6	Mercury	0.003 ppmv	ACGIH TLV	7-Oct-04
67-56-1	Methanol	200 ppmv	ACGIH TLV	7-Oct-04
624-83-9	Methyl isocyanate	0.02 ppmv	ACGIH TLV	7-Oct-04
624-91-9	Methyl nitrite	0.1 ppmv	AOEL	26-Jan-06
10024-97-2	Nitrous oxide (N_2O)	50 ppmv	ACGIH TLV	7-Oct-04
62-75-9	N-Nitrosodimethylamine	0.0003 ppmv	AOEL	7-Oct-04
10595-95-6	N-Nitrosomethylethylamine	0.0003 ppmv	AOEL	7-Oct-04
59-89-2	N-Nitrosomorpholine	0.0006 ppmv	AOEL	26-Jan-06
110-59-8	Pentanenitrile	6 ppmv	AOEL	7-Oct-04
107-12-0	Propanenitrile	6 ppmv	AOEL	7-Oct-04
110-86-1	Pyridine	1 ppmv	ACGIH TLV	6-Jul-05
126-73-8	Tributyl phosphate	0.2 ppmv	ACGIH TLV	7-Oct-04

APPENDIX D

PREDICTED PEAK VAPOR CONCENTRATIONS FROM DISPERSION MODELING

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D1.0 BACKGROUND

This analysis uses standard air-quality dispersion models to complement the parameterized computations reported in PNNL-14767. In that report, tank exhaust processes from a single stack/vent were modeled to provide estimates of the normalized (15 minute average) peak vapor concentrations in the immediate vicinity (i.e., closer than 100 m from the vent/stack). Unit emission factors were used to determine potential impact from a single isolated vent/stack located on level ground over a matrix of potential meteorological conditions. These "close-to-the-source" estimates addressed potential worker exposures for the near-surface releases from passively-vented tanks as well as from elevated stack/vent releases. Background information for these parameterized computations of near-source air concentrations for the various Hanford Site underground tank venting mechanisms is described in PNNL-14767.

This appendix expands that earlier analysis to a consideration of the combined influences of estimated tank-farm specific emissions from vents/stacks on potential worker breathing zones around the A-prefix tanks.

D2.0 ANALYSIS

The potential combination of plumes from the multiple stacks and vents in the A-prefix tank farm area is addressed by modeling the hourly fate of plumes for one year. To provide site-specific results, emission rates were estimated for each of the vents/stacks in the area. The modeling also accounted for the specific characteristics of each release point (location, height, exit velocity, exit temperature, exit area). Terrain and building wake effects were included along with actual tank-specific emission estimates for nitrous oxide and ammonia. Figure D-1 shows the topography used by the model. Computations were made for the 2003 annual cycle of hourly meteorological data (PNNL-14616). Wind speeds and directions were taken at telemetry observation station number 6 in the 200 East Area, and the rest of the surface observations were taken at the Hanford Site Meteorological Station (Figure D-2). Because the stack heights were on the same order as the local terrain features, inclusion of the terrain was critical for conducting these plume simulations. Figure D-3 shows relative location and elevation of the vapor sources.

At near-field distances, it was assumed that the maximum concentration can be no larger than the concentrations coming out of the vents (i.e., headspace concentrations). Near the vent, that initial concentration will be representative of the air concentration in the plume with the computed average value representing mainly the spatial movement of that plume. Thus at near-field distances, it is reasonable to experience short-duration, undiluted pockets of that initial concentration. As the plume moves away from the vent, ambient turbulence will diffuse the plume, and the average will be a combination of the spatial movement and the dilution of the air.

Of the applicable air-dispersion models currently recommended by the U.S. Environmental Protection Agency (EPA 2004), the Industrial Source Complex (ISC3) model series was selected as appropriate for this analysis (EPA 454/B-95-003a; EPA 454/B-95-003b). A model was needed that emphasized the processes resulting in the peak exposures in the immediate vicinity of the release. The ISC Short-Term version was developed for detailed studies of maximum air

quality impacts. The Short-Term version uses hourly meteorological data to compute short-term concentrations and/or deposition values from multiple sources on specified receptors. A short-term version of ISC with improved building wake algorithms, ISC-Prime (ISC3P), was used to account for the influence of buildings located near the current release stacks. The ISC3P version has advanced building wake algorithms for the influences of building orientation, length, widths, and heights of multiple buildings and provides estimates of concentrations at locations close to the source. Also, the ISC rural option used in these analyses employs the same dispersion rate parameterization that was used in the previous study of single vent/stack emissions.

A revised version of the EPA preprocessor program called BPIP (Building Profile Input Program) was used to prepare the input files for ISC3P. Also, the ISC3P model is one of very few such models recommended by the EPA that provide concentrations at distances relatively close to the release areas. The general ISC3 and specific ISC3P model information and documentation are available at the EPA website for regulatory air models (EPA 2004).

Figure D-1. Topographical Map

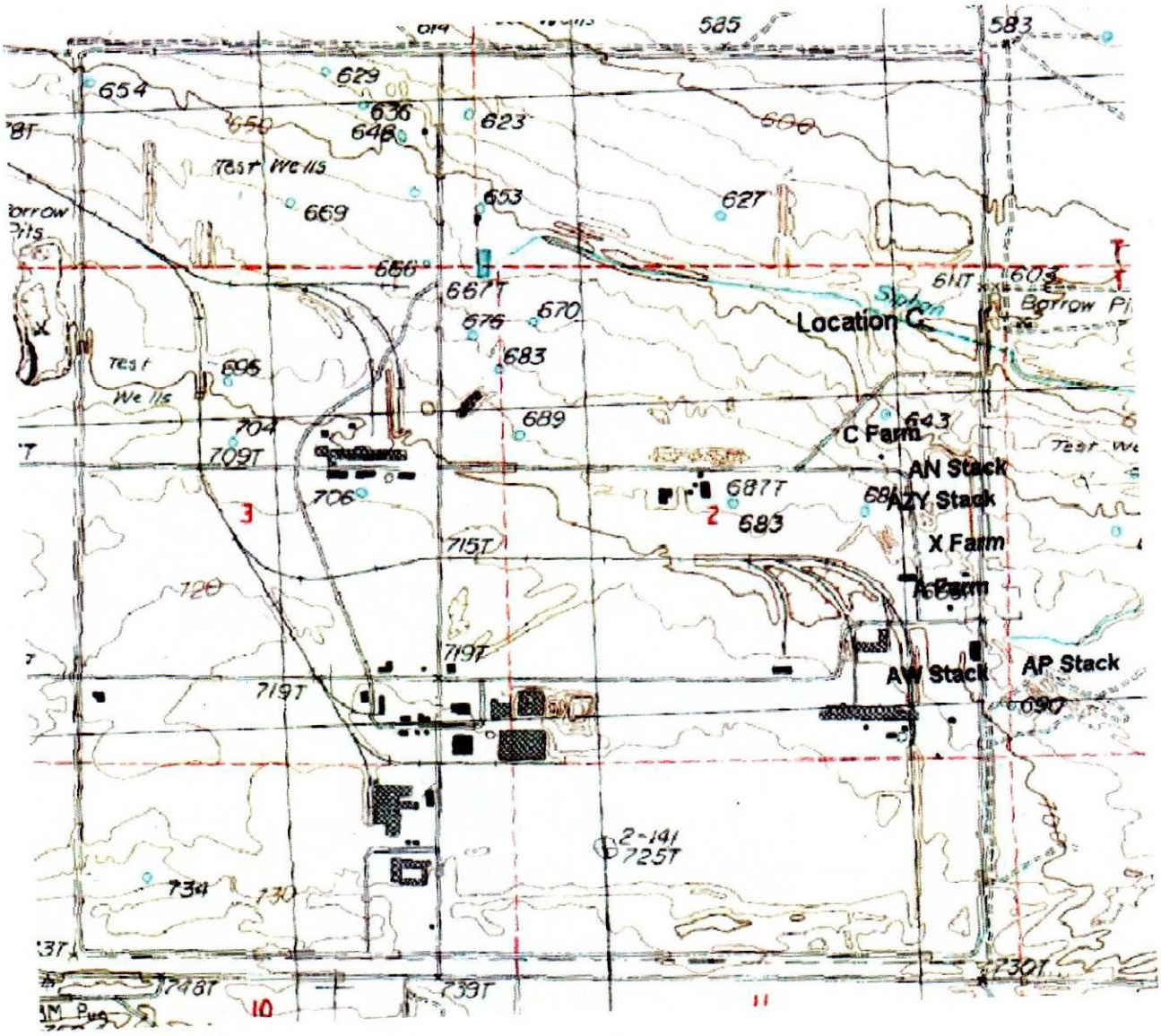


Figure D-2. Location of Meteorological Monitoring Stations at the Hanford Site

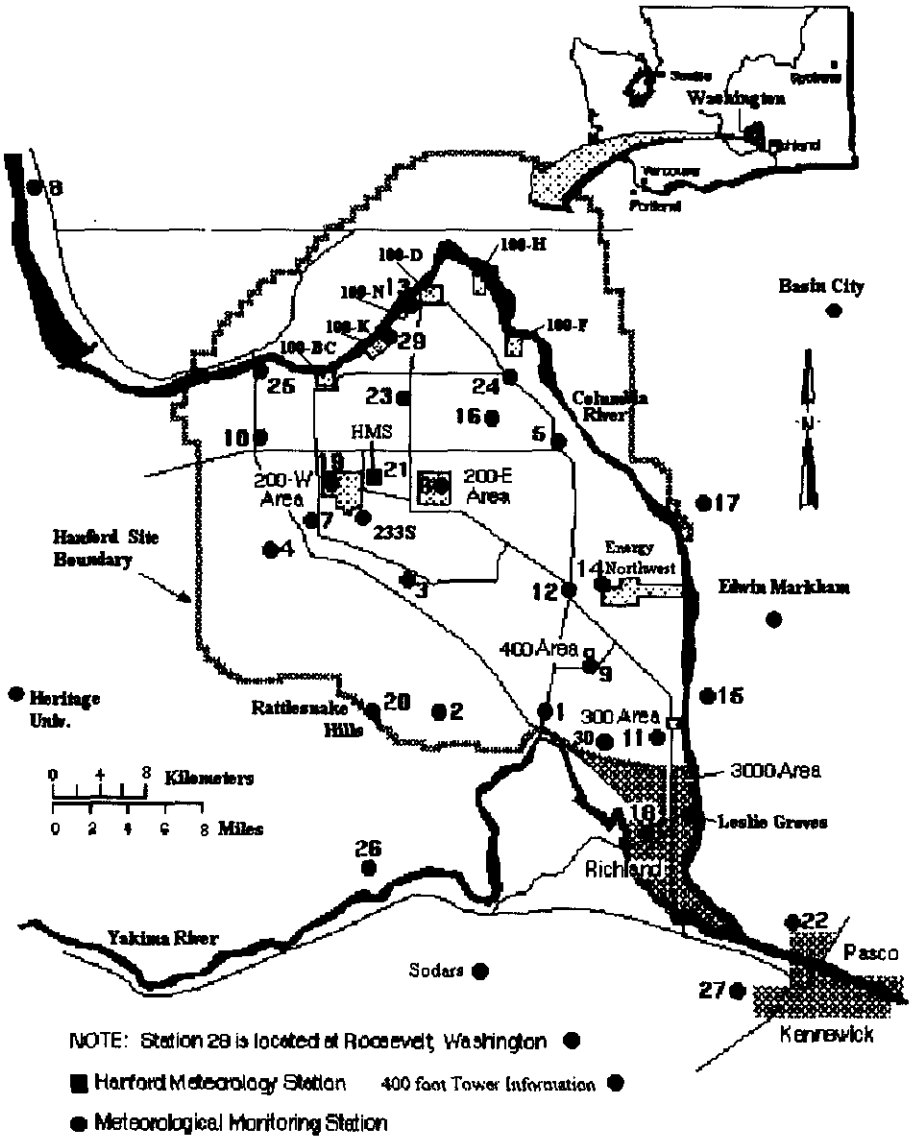
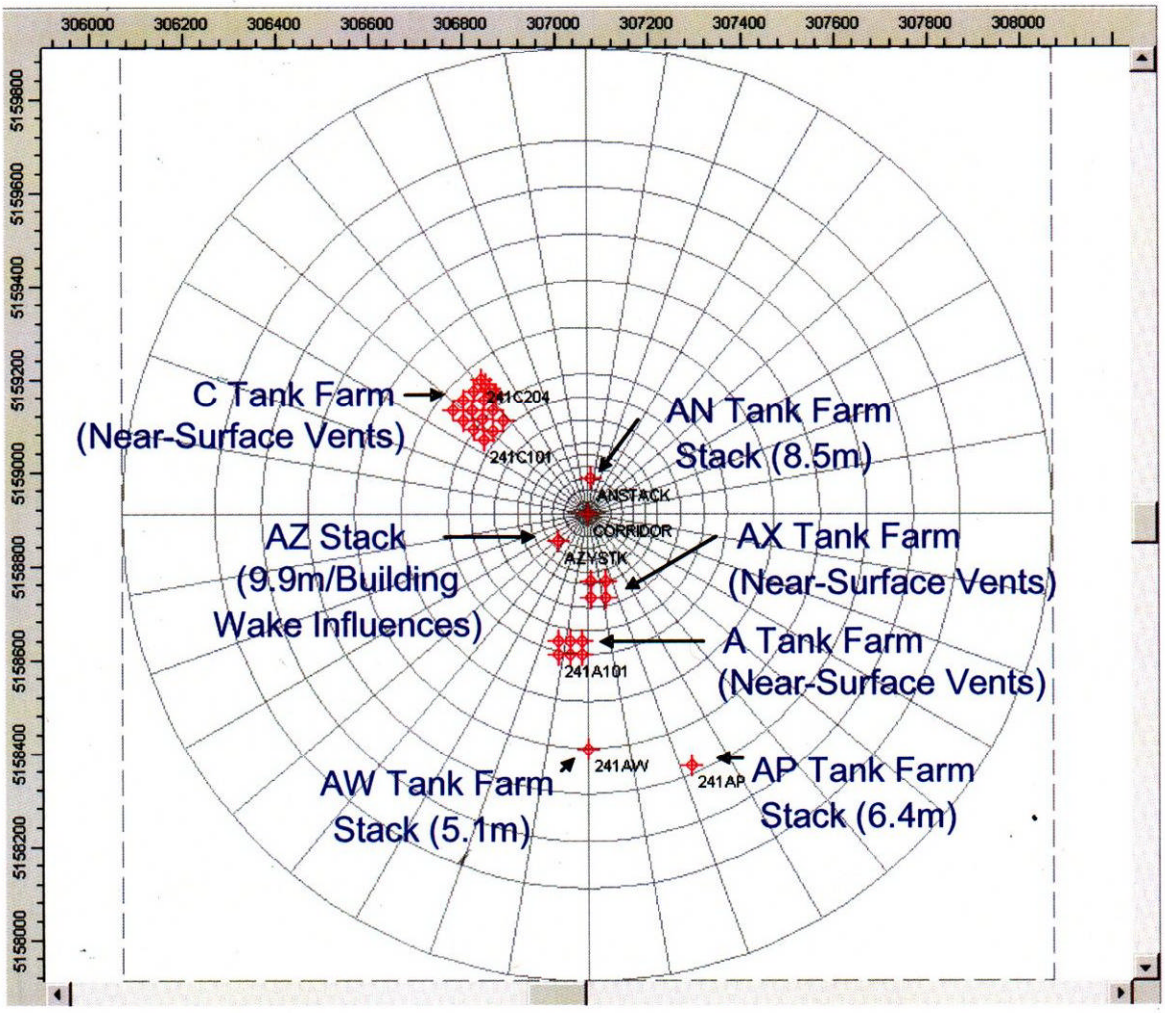


Figure D-3. Vapor Source Release Locations



D3.0 RESULTS

Meteorological and topographical data were combined with the highest measured headspace/stack nitrous oxide and ammonia concentrations to produce the results shown in Figures D-4 and D-5. Figure D-4 plots the estimated 15-minute peak nitrous oxide concentrations over a one-year period. Highest concentrations (0.5 ppmv) are found within the 241-A Tank Farm and southwest of the AN Stack (where the AN stack exhaust plume contacts the ground). There are also areas within C Farm and southwest of AP Stack that have notable (0.2 ppmv) peak concentrations. Strongest influences are from 241-A Farm and the AN Stack, which will become apparent when parametric plots shown in Figures D-6 through D-13 are examined. Peak concentrations are well below the 25 ppmv nitrous oxide Occupational Exposure Limit (OEL).

Figure D-5 plots the highest estimated 15-minute peak ammonia concentrations over a one-year period. Concentration patterns are similar to the nitrous oxide patterns shown in Figure D-5, with some interesting differences. The plots show significant concentrations near the single-shell tank (SST) farms, with the highest concentrations found within the 241-A Farm (1 ppmv). Areas near and within C and AX Farms also have notable peak concentrations (0.2 ppmv). Ammonia from the double-shell tank (DST) stacks appears to be well dispersed with only the AN and AP stack plumes reaching a peak concentration of about 0.1 ppmv. All 15-minute peak ammonia concentrations fall well below the 25 ppmv OEL.

Figures D-6 through D-13 show how SST vents and DST stacks might influence worker breathing zones within the area modeled. A 1 mg/m^3 concentration was assumed to exit each SST vent and DST stack. The plots show the 15-minute peak concentrations over a one-year period. Figure D-6 shows the dispersion pattern from the 242-A Evaporator stack. Even though the 242-A Evaporator stack can influence a large area, 15-minute peak concentrations are three to five orders of magnitude lower than the stack concentration.

Figure D-7 is a plot of the 15-minute average maximum annual concentration given a 1 mg/m^3 release from each of the 16 tanks in 241-C Farm. As indicated in Figure D-7, higher concentrations would be found near the 241-C Farm vents, but 241-C Farm releases could hypothetically influence a large area. Modeling results are consistent with anecdotal evidence that C Farm odors can be smelled quite far away under certain weather conditions.

The analogous model results for 241-A Farm (Figure D-8) are interesting in that 241-A Farm potentially influences a larger area than 241-C Farm. This is a direct result of the higher ventilation rates found in 241-A Farm (see passive ventilation discussion in Section 4.2). Figure D-9 shows that AN Stack can have significant influence over a broad area, particularly locations directly south and southwest. This is consistent with the ammonia results for all sources (Figure D-5) that indicate ammonia concentrations in the worker breathing zones can be heavily influenced by the AN Stack.

Figures D-10 and D-11 show the predicted dispersion from AP and AW Stacks given normalized emissions and no other sources. Comparison of Figures D-10 and D-11 indicates that the AP Stack might influence the workers breathing zone around the AW Stack more than the

AW Stack itself. A similar analysis of AX Farm suggests emission from this farm have only a local influence (Figure D-12). Exhaust from the AZ Stack (Figure D-13) can influence a broad area; however, peak breathing zone concentrations would be two to three orders of magnitude below initial concentrations.

Figure D-4. Predicted Annual Peak Nitrous Oxide Concentration

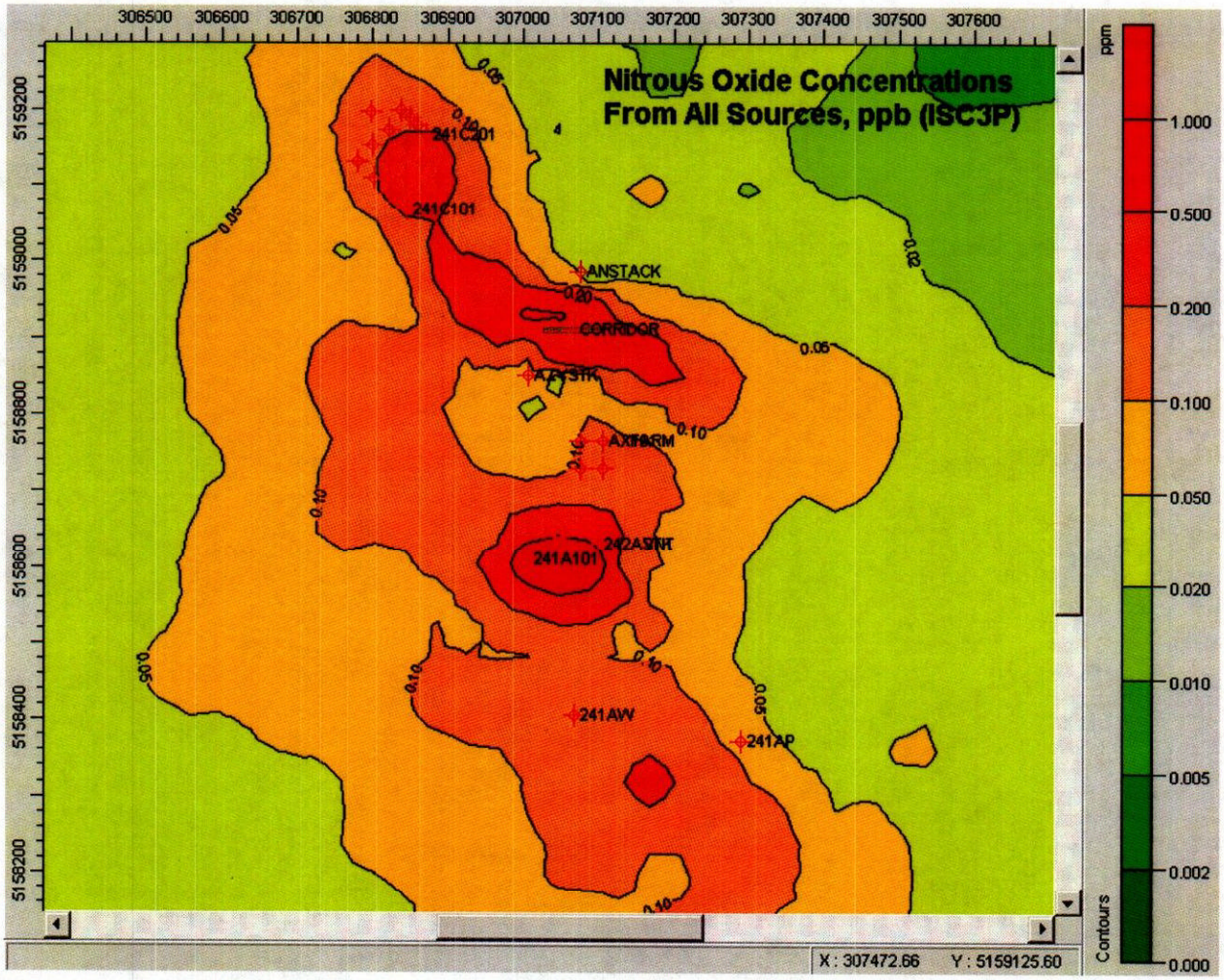


Figure D-5. Predicted Annual Peak Ammonia Concentrations

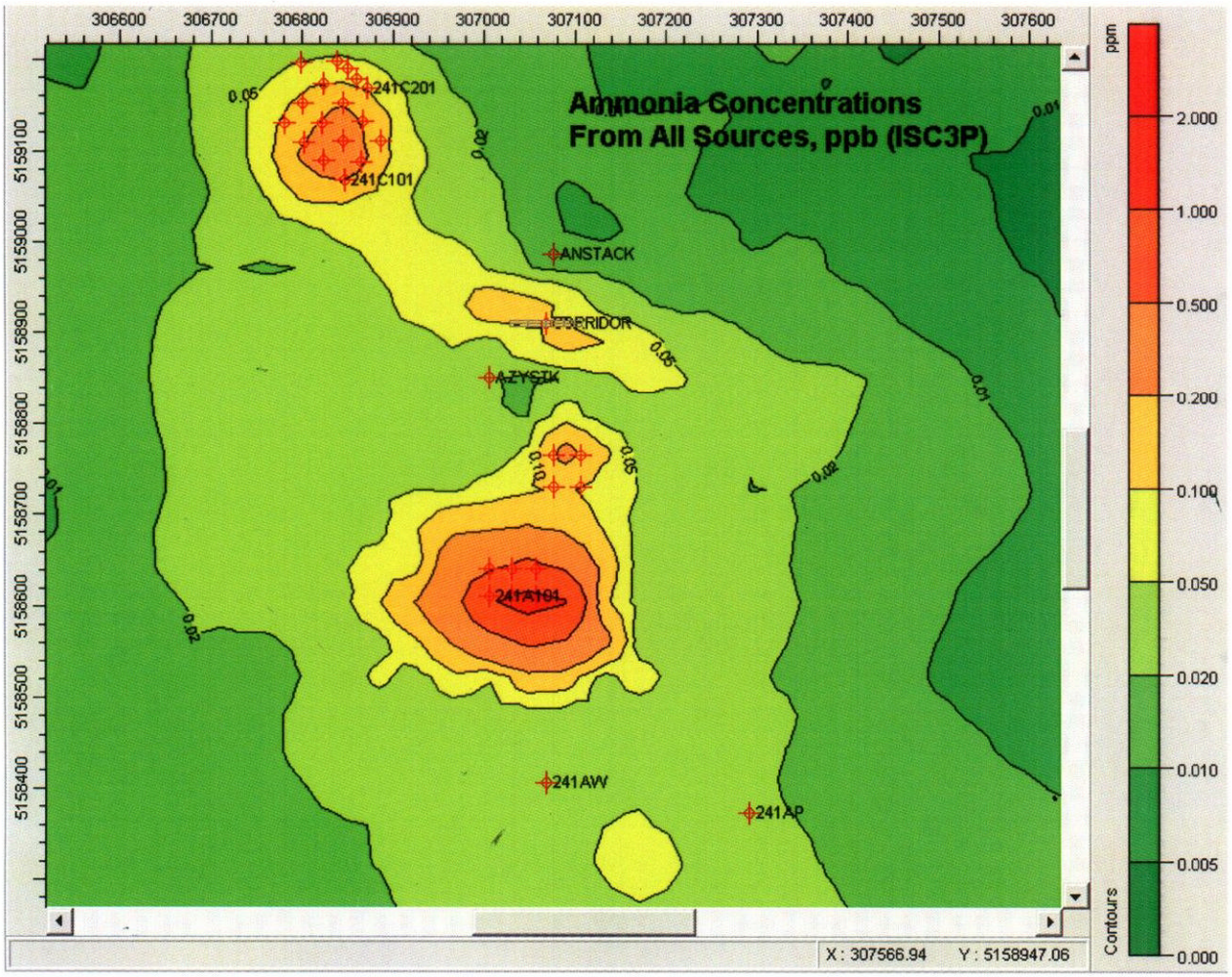


Figure D-6. Predicted 242-A Evaporator Vapor Dispersion

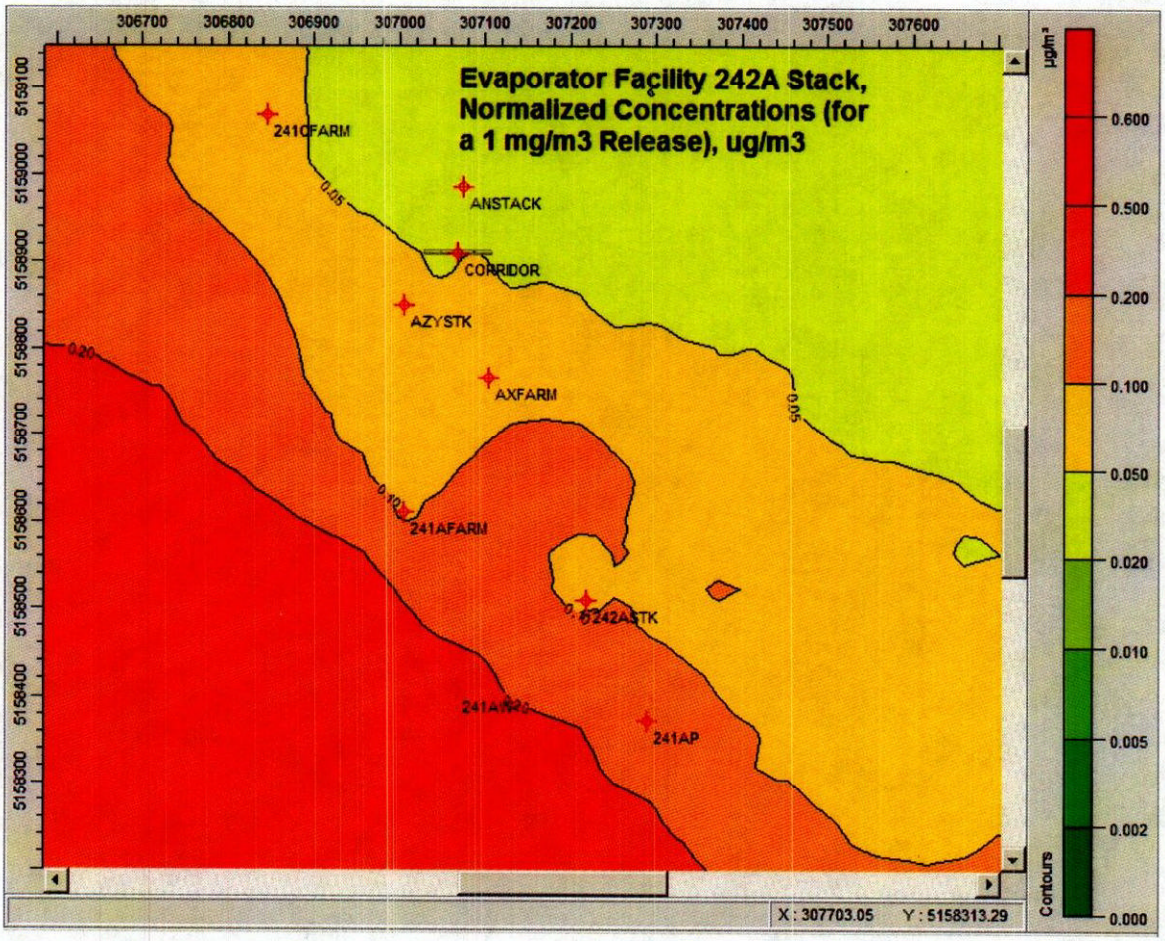


Figure D-7. Predicted C Farm Vapor Dispersion

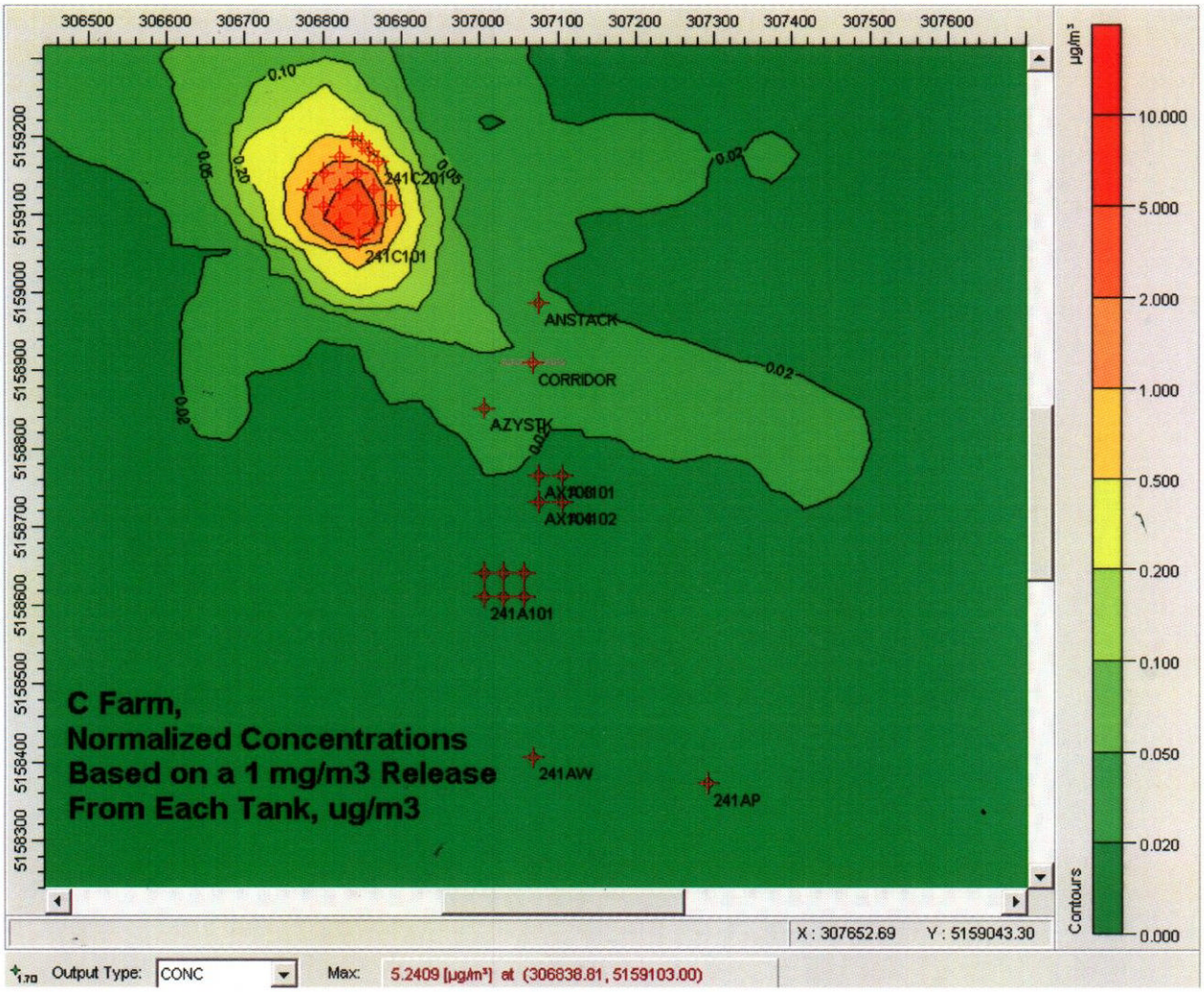


Figure D-8. Predicted A Farm Vapor Dispersion

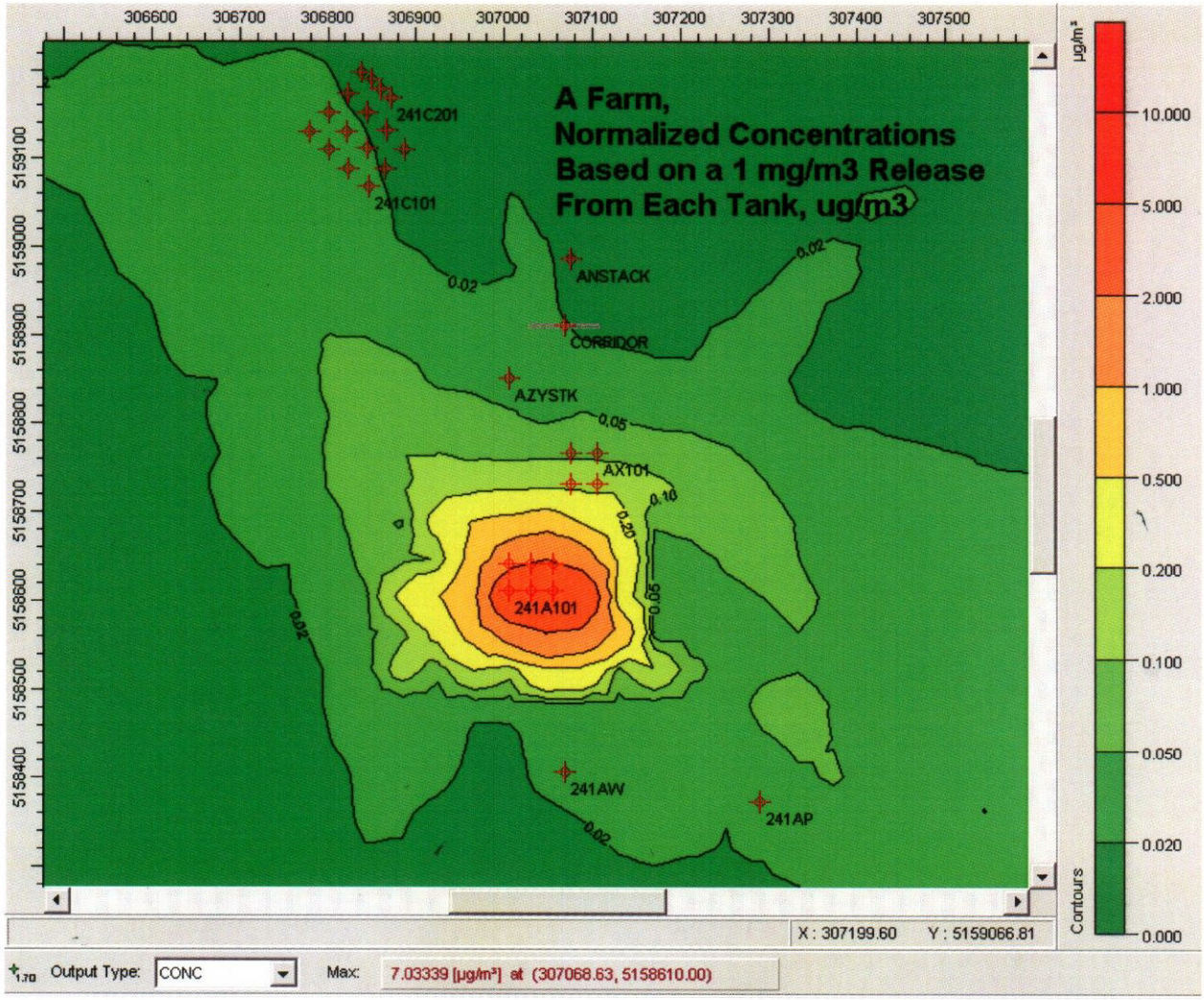


Figure D-9. Predicted AN Stack Dispersion

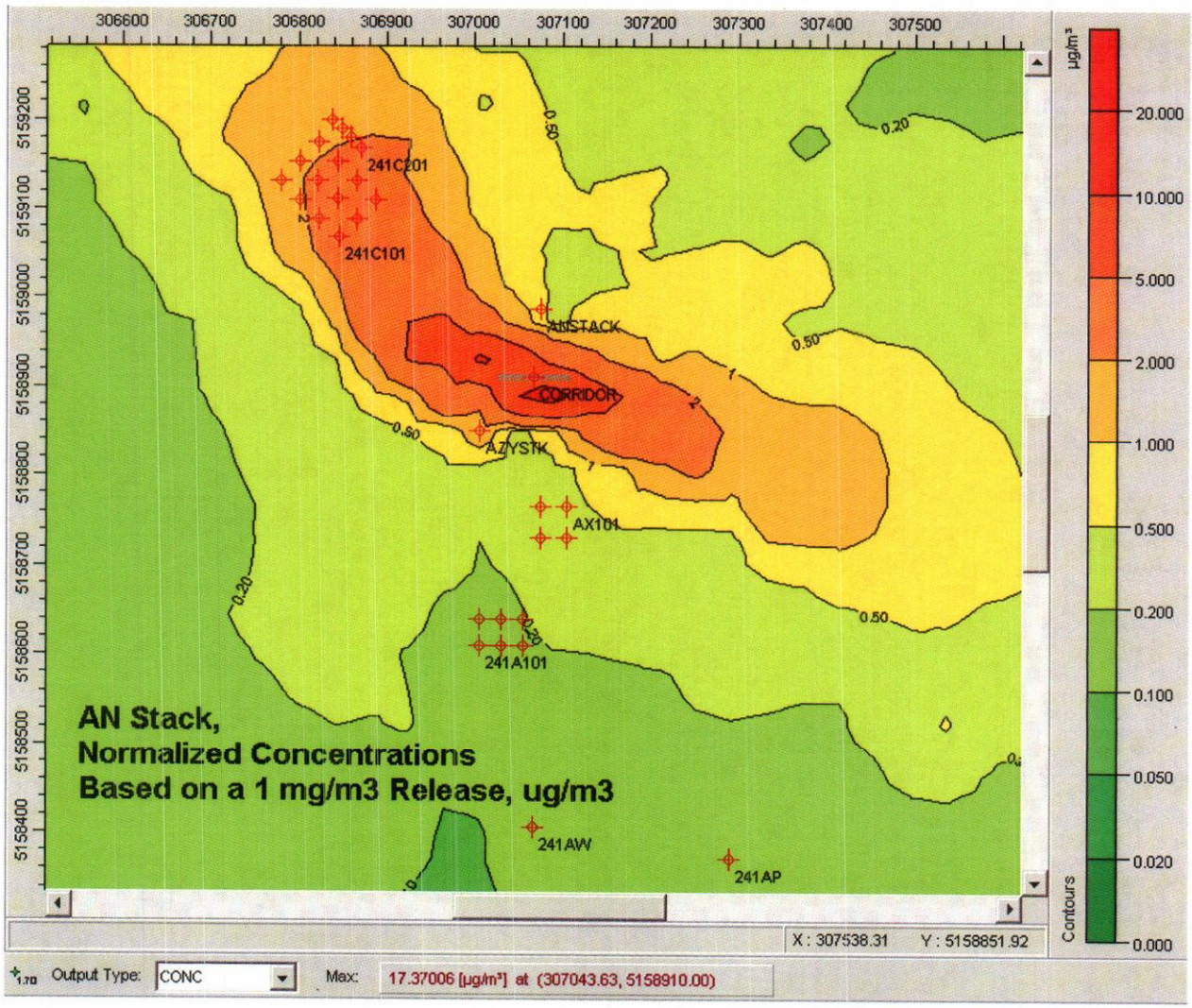


Figure D-10. Predicted AP Stack Vapor Dispersion

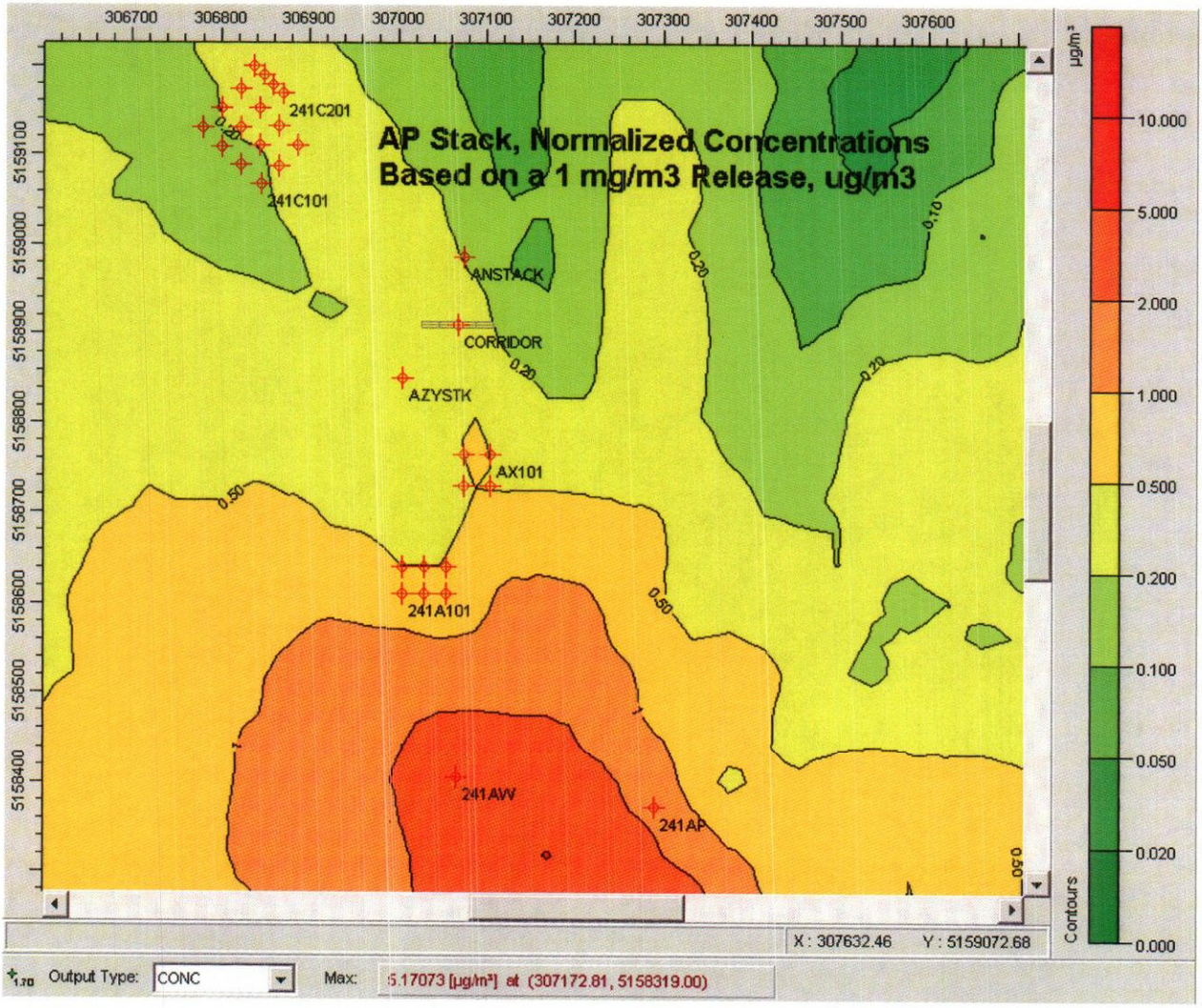


Figure D-11. Predicted AW Stack Vapor Dispersion.

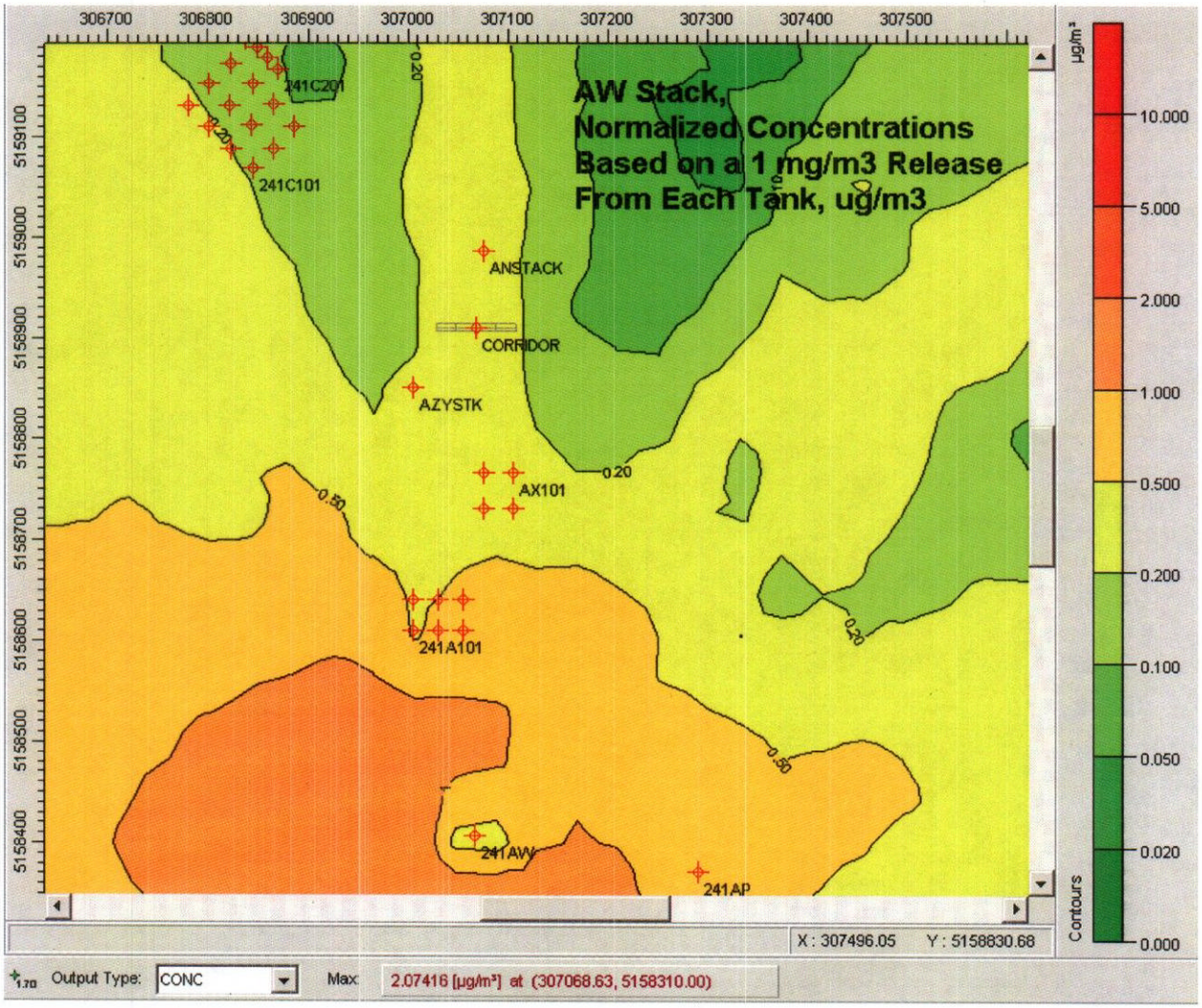


Figure D-12. Predicted AX Farm Vapor Dispersion

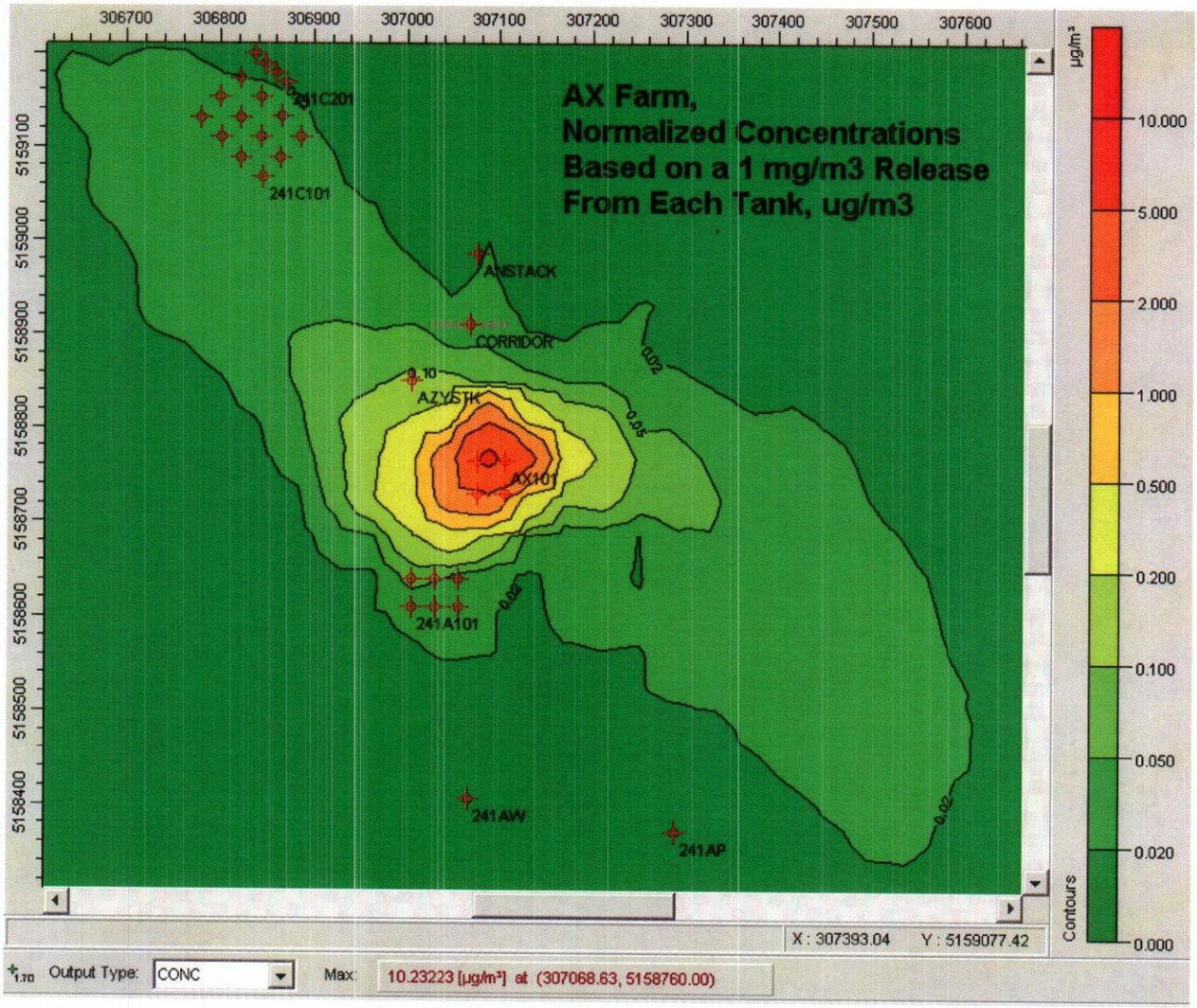
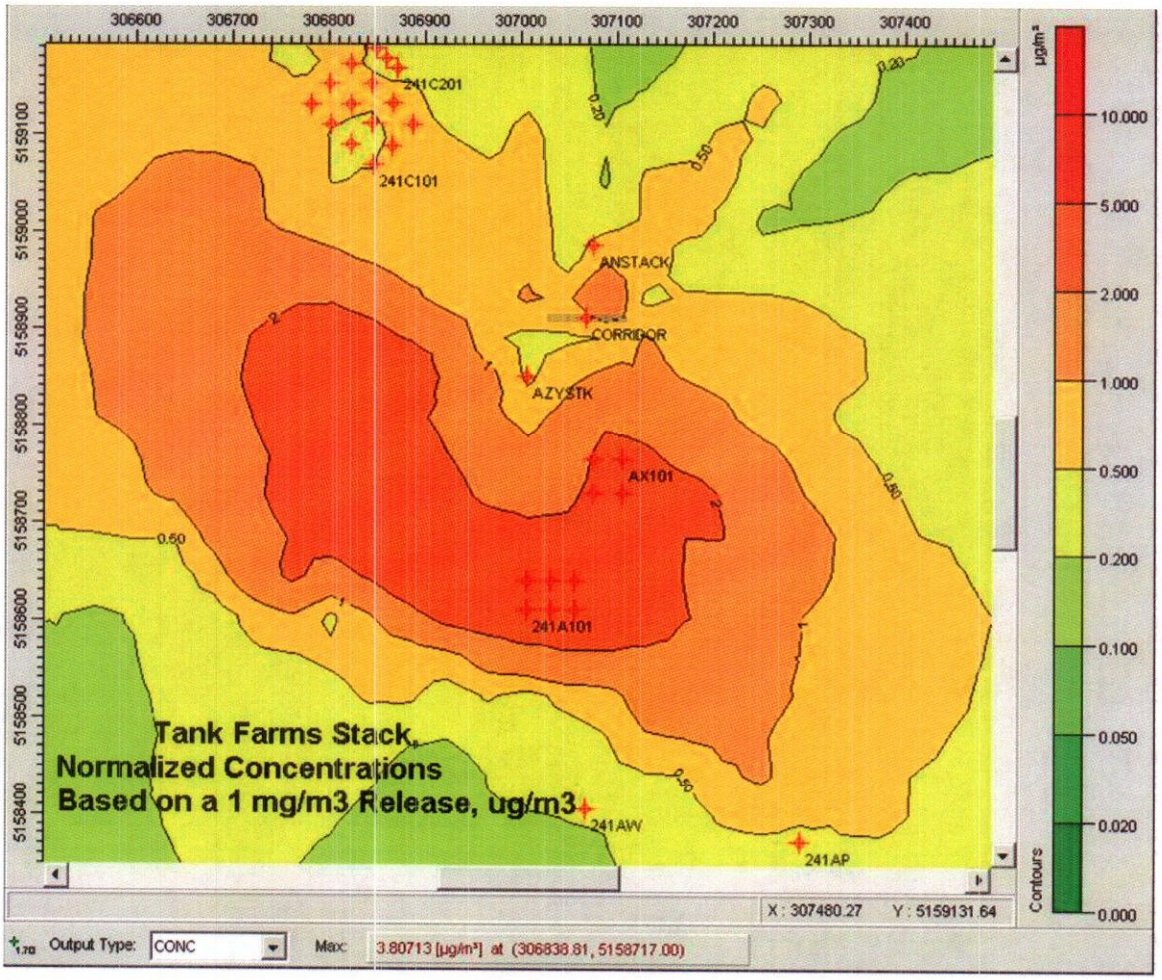


Figure D-13. Predicted AZ Stack Vapor Dispersion



D4.0 CONCLUSIONS

The ISC3P model was used to estimate normalized 15-minute average peak vapor concentrations in the immediate area of tank vents and stacks in the eastern portion of the 200 East Area to address potential worker exposures. Source specific ammonia and nitrous oxide data were combined with topographical and meteorological data to estimate annual peak concentrations. Results indicate that peak ammonia and nitrous oxide concentrations within 241-A and 241-C Farms and south/southwest of the AN Stack. Peak concentrations were more than an order of magnitude less than the 25 ppmv ammonia and nitrous oxide OELs.

Parametric modeling showed that the 242-A Evaporator and AN and AP stacks influenced the largest areas within the A Tank Farm Complex, but that peak concentrations within the worker breathing zones were several orders of magnitude lower than source concentrations.

D5.0 REFERENCES

EPA, 2004, "Approved Methods and Guidance for the Modeling and Assessment of Air Pollutants," http://www.epa.nsw.gov.au/air/amgmaap-06.htm, accessed 12/20/04, U.S. Environmental Protection Agency.

EPA 454/B-95-003a, 1995, *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models. Volume I - User Instructions*, U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Emissions, Monitoring, and Analysis Division, Research Triangle Park, North Carolina.

EPA 454/B-95-003b, 1995, *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models. Volume II - Description of Model Algorithms*, U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Emissions, Monitoring, and Analysis Division, Research Triangle Park, North Carolina.

PNNL-14616, 2004, *Hanford Site Climatological Data Summary 2003 with Historical Data*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14767, 2004, *Characterization of the Near-Field Transport and Dispersion of Vapors Released from the Headspaces of Hanford Site Underground Storage Tanks*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

APPENDIX E

EXPOSURE ASSESSMENT STRATEGY REVIEW GROUP MEETING MINUTES

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CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
March 29, 2005 2440 Stevens

N-Nitrosodimethylamine (NDMA) OEL

Issue: *Determine a safe, effective, and feasible Tank Farms working occupational exposure limit (OEL) for n-nitrosodimethylamine (NDMA).*

Attendees:

Dr. Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Jim Honeyman, CH2M HILL
Jim Huckaby, PNNL
Dr. Terryl Mast, PNNL
Dr. Joseph Samuels, AMH
Gretchen Bruce, Intertox
Dr. Gary Pascoe, Intertox

Agenda:

7:30 CH2M HILL, PNNL – Discuss Tank Farms issues: headspace concentrations, sampling and analytical methods, engineering controls (implications for "stack in the sticks")
8:30 Intertox representatives arrive. Introductions.
9:00 Meeting objectives, expected outcomes and process – Tom Anderson
9:15 Review OEL development process – Tom Anderson
9:45 Background on NDMA in the Tank Farms – Jim Huckaby
10:15 NDMA toxicology and initial OEL calculations – Intertox
11:15 List inputs to a working OEL – facilitated by Tom Anderson
12:00-1:30 Lunch
1:30 Address data gaps, confirm assigned values – facilitated by Tom Anderson
2:00 Working OEL discussions

Meeting Notes:

- The meeting began at 7:30 AM with the CH2M HILL, PNNL, and AMH representatives. Since this was the first meeting of the Review Group, the agenda and procedures were reviewed for comment.

- Joseph Samuels noted that AMH has a non-regulated carcinogen program that sets medical surveillance protocols for IARC-listed carcinogens that do not have established OELs.

- Terri Mast noted that ACGIH and OSHA guidance for NDMA defaults at "as low as reasonably achievable."

- Discussed the DOE TEEL (temporary emergency exposure limit). Since the TEELs are intended as short-term limits, similar to OSHA peaks or ACGIH short-term exposure limits (STELs), they do not apply in this discussion of 8-hr time-weighted averages.

- The Intertox representatives arrived at 8:15. Introductions were made. Tom Anderson reviewed the agenda, then described the process that would be used for setting a working OEL (Attachment 1)

- Existing NDMA OELs and reference levels were reviewed:

Agency	OEL in ppbv	OEL in $\mu g/m^3$
Netherlands, Germany	0.3	1.0
DOE TEEL	1,160.0	3,500.0
Approximate detection limit	0.043	0.13
Canada/U.S.	As low as reasonably achievable	

- Jim Huckaby summarized the known Tank Farms chemistry and headspace concentrations for NDMA
  * TWINS data shows that 19 SSTs and 3 DSTs contain NDMA vapors in headspaces
  * The average concentration is 36 ppbv (109 $\mu g/m^3$)
  * The maximum headspace concentration was measured at 215 ppbv (650 $\mu g/m^3$) in AP-102 (measured by triple sorbent tube on 3/28/2001)
  * The typical detection limit for NDMA has been 8.3 ppbv (25 $\mu g/m^3$) from a 2-L sample volume
  * Headspace vapor measurements are accurate within ± a factor of 10
  * OSHA recommends a 75-L sample volume, which should yield a reliable detection limit of 0.043 ppbv (0.13 $\mu g/m^3$)
  * Jim will contact the Wisconsin WOHL laboratory to inquire why the OSHA detection limit was not achieved
  * Jim feels that a detection limit of at least 0.03 ppbv (0.09 $\mu g/m^3$) is achievable

- Gretchen Bruce and Gary Pascoe presented a detailed review of their methodology and background research for recommendations of a working OEL for NDMA.
  * The EPA formula widely used for setting carcinogen exposure limits is:

$$OEL(\mu g/m^3) = \frac{AcceptableRisk \times AT(d) \times BW(kg) \times 1000 \mu g/mg}{IR(m^3/d) \times EF(d/yr) \times ED(yr) \times CSF(mg/kg-d)^{-1}}$$

Where:
AT = Averaging time; equal to an average lifetime in days
BW = Average adult body weight in kilograms
IR = Inhalation rate, in m^3/day

EF = Exposure frequency, in days worked per year
ED = Exposure duration, or working lifetime, in years
CSF = Cancer slope factor

* Various cancer slope factors were discussed, along with the basis for their development and ways they have been applied in exposure limits.
* The variable inputs to the formula were discussed

- After all the data was presented and reviewed, Tom Anderson facilitated a discussion to decide on the best approach for setting an NDMA OEL.
  * Terri Mast expressed concern that the EPA cancer slope factor might be too conservative for an occupational OEL, since EPA standards are set for 24-hour exposures.
  * Gary Pascoe said he would like to investigate the basis for the Netherlands standard, since they used the above method to generate a relatively high OEL. He took the action to contact the Dutch agency.
  * Tom Anderson presented a table of calculations he had done using various inputs to the EPA formula, resulting in a range of potential OELs.
  * The group decided unanimously to use the EPA formula as the basis for setting the NDMA working OEL, as this formula has wide acceptance and is the most defensible position. It remains to decide which inputs to use in the formula.

- The chemical properties of NDMA were discussed. It was noted that the compound is unstable in sunlight, with a half-life in sunlight of about 1 hour.

- Terri Mast read from the 1985 ACGIH TLV documentation for nitrosamines a passage stating that because of the extreme animal toxicity of nitrosamines, they do not recommend a numerical OEL.
  * Gary Pascoe questioned this reasoning, noting that it did not cite the research study by upon which the EPA cancer slope factor was based.

- Risk factors have an order-of-magnitude effect on the OEL determination from the EPA formula.
  * Gary Pascoe noted that although EPA recommends a range of risk factors from 10^{-4} to 10^{-6}, in practice, OSHA has used risk factors of 10^{-2} to 10^{-3} in several of its final PEL rulings.
  * Gretchen Bruce will produce a chart showing several of these OSHA rulings, including the PELs for carbon tetrachloride, chloroform, and vinyl bromide.
  * Gary Pascoe will call California EPA to learn the justification for their cancer slope factor of 16, as compared to the EPA CSF of 51.

- The group decided by unanimous consensus to investigate a range of potential OELs by using the EPA formula and varying the inputs for:
  * Risk level, from 10^{-3} to 10^{-4}
  * Inhalation rate, from 5 m^3/day (half work day) to 10 (full work day)

* Cancer slope factor, using either the U.S. EPA value of 51 or the Cal EPA value of 16.

- The following inputs to the formula will be held constant:
  * Averaging time: 70 years average lifetime, or 25,500 days
  * Average adult body weight of an adult female: 65 kg
  * Exposure frequency: 200 days/yr (accounting for time away from the Tank Farms due to training, holidays, and vacation).
  * Exposure duration (working life in the Tank Farms): 40 years

- Using these constants and variables, the following is the range of potential OELs under consideration:

$$\textbf{OEL (ug/m3)} = \frac{\textbf{Risk x AT x BW x 1000}}{\textbf{IR x EF x ED x CSF}}$$

Risk factor	**Risk**	**1.00E-04**	**1.00E-03**	**1.00E-04**	**1.00E-03**	
Averaging time (70 yrs)	**AT (d)**	25,550	25,550	25,550	25,550	
Adult body wt (female)	**BW (kg)**	65	65	65	65	
Inhalation rate	**IR (m^3/d)**	**8**	**8**	**10**	**10**	
Exposure frequency	**EF (d/yr)**	200	200	200	200	
Exposure duration	**ED (yr)**	40	40	40	40	
Cancer slope factor	**CSF**	**16**	**16**	**16**	**16**	
	OEL	**0.16**	**1.62**	**0.13**	**1.30**	**ug/m^3**
		0.05	**0.54**	**0.04**	**0.43**	**ppbv**

Risk factor	**Risk**	**1.00E-04**	**1.00E-03**	**1.00E-04**	**1.00E-03**	
Averaging time (70 yrs)	**AT (d)**	25,550	25,550	25,550	25,550	
Adult body wt (female)	**BW (kg)**	65	65	65	65	
Inhalation rate	**IR (m^3/d)**	**8**	**8**	**10**	**10**	
Exposure frequency	**EF (d/yr)**	200	200	200	200	
Exposure duration	**ED (yr)**	40	40	40	40	
Cancer slope factor	**CSF**	**51**	**51**	**51**	**51**	
	OEL	**0.05**	**0.51**	**0.04**	**0.41**	**ug/m^3**
		0.02	**0.17**	**0.01**	**0.13**	**ppbv**

- A final recommendation was not made because more information is needed.
  * Jim Huckaby will provide information on NDMA sampling and analytical methods that should be used to achieve the lowest possible detection limits.
  * Intertox will provide more detailed information on:
    - The OSHA precedent for risk factors in occupational OELs.
    - The cancer slope factors used by Cal EPA and the Netherlands government.
    - The best factor to use for inhalation rate (IR), taking into account increased breathing from exertion for strenuous work and self-contained breathing apparatus (SCBA) use.

- After the meeting, it was noted that, through oversight, a HAMTC representative was not included in the team. Tom Anderson contacted Ed Carter, and will brief him on the details of this meeting. Ed Carter and Jill Molnaa will be invited to participate in all subsequent meetings of the review group.

- A follow-on meeting is planned by phone conference for 9-11 AM Tuesday, Apr 5, chaired by Tom Anderson. A meeting notice with phone number to call will be provided.

- The agenda for the follow-on meeting will be:
  * Briefly review these minutes, note comments or changes (Tom Anderson).
  * Address any questions from HAMTC representatives (Ed Carter/Jill Molnaa).
  * Presentation by Jim Huckaby on sampling and analytical methods.
  * Presentation by Intertox on risk factors, cancer slope factors, and inhalation rates.
  * Use of the above table, or variations as needed, to narrow the range of OEL candidate values.
  * Decision on a consensus working OEL, unless there is dissent – in which case further research may be necessary.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group
Rules for Evaluating Working OELs

This review is for compounds that do not have an established PEL or TLV.

The working OEL decided upon will have a protection equivalent to a PEL or TLV. That is, as stated in the ACGIH TLV documentation: it will set an airborne concentration for chemical gases, vapors, or particulates for which nearly all workers may be exposed repeatedly, day after day, over their working lifetime, without adverse health effects.

The Tank Farms Exposure Assessment Strategy (TFC-PLN-034) sets further levels of protection beyond the OEL, as provided by action limits (50%) of the OEL and administrative control levels (10% of the OEL). Therefore, the working OEL does not need to incorporate these extra protection factors.

In general, the working OEL will be an 8-hr time-weighted average. For compounds that have acute or short-term exposure concerns, a working OEL equivalent to an OSHA ceiling or ACGIH STEL should be considered.

Information sources that will be used for setting the working OEL, in order of priority:

1. Other U.S. federal standards (NIOSH, DOE, EPA)
2. U.S. State standards
3. Acceptable foreign government standards. These standards will be evaluated for equivalency to the U.S. level of protection by comparing OELs set by these governments for related compounds to U.S. PEL/TLV.
4. U.S. toxicology documentation, such as submittals to the PEL or TLV committees for compounds pending standard development.
5. Peer-reviewed published research.

Process for setting the OEL:

1. Consider all standards and sources of information listed above.
2. Use standard risk assessment methodology where applicable (such as for carcinogens).
3. Recommend control strategies, such as engineering or administrative controls, if there are limitations factored into the working OEL.
4. Select a safety factor where necessary – consider amount of information available, reliability of information, toxicity of this and related compounds.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
Phone Conference, April 5, 2005

N-Nitrosodimethylamine (NDMA) OEL

Issue: Determine a safe, effective, and feasible Tank Farms working occupational exposure limit (OEL) for n-nitrosodimethylamine (NDMA).

Attendees (by phone):

Dr. Tom Anderson, CH2M HILL, Chair
Dr. Susan Eberlein, CH2M HILL
Mike Zabel, CH2M HILL
Bob Cash, CH2M HILL
Dr. Joseph Samuels, AMH
Gretchen Bruce, Intertox
Dr. Gary Pascoe, Intertox

Agenda:

- Review minutes of the March 29th meeting.
- Address any questions from HAMTC representatives.
- Presentation by Jim Huckaby on sampling and analytical methods.
- Presentation by Intertox on risk factors, cancer slope factors, and inhalation rates.
- Discuss use of the OEL table from the previous meeting to narrow the range of OEL candidate values.
- Decision on a consensus working OEL.

Meeting Notes:

- Existing NDMA OELs and reference levels were reviewed:

Agency	OEL in ppbv	OEL in $\mu g/m^3$
Netherlands, Germany	0.3	1.0
DOE TEEL	1,160.0	3,500.0
Approximate detection limit	0.043	0.13
Canada/U.S.	As low as reasonably achievable	

- Gretchen Bruce and Gary Pascoe presented a detailed review of their methodology and background research for recommendations of a working OEL for NDMA.
  * The EPA formula widely used for setting carcinogen exposure limits is:

$$OEL(\mu g/m^3) = \frac{AcceptableRisk \times AT(d) \times BW(kg) \times 1000 \mu g/mg}{IR(m^3/d) \times EF(d/yr) \times ED(yr) \times CSF(mg/kg-d)^{-1}}$$

Where:
AT = Averaging time; equal to an average lifetime in days
BW = Average adult body weight in kilograms

IR = Inhalation rate, in m^3/day
EF = Exposure frequency, in days worked per year
ED = Exposure duration, or working lifetime, in years
CSF = Cancer slope factor

* Various cancer slope factors were discussed, along with the basis for their development and ways they have been applied in exposure limits.
* The variable inputs to the formula were discussed

- Risk factors have an order-of-magnitude effect on the OEL determination from the EPA formula.
  * Gary Pascoe noted that although EPA recommends a range of risk factors from 10^{-4} to 10^{-6}, in practice, OSHA has used risk factors of 10^{-2} to 10^{-3} in several of its final PEL rulings.
  * Gretchen Bruce will produce a chart showing several of these OSHA rulings, including the PELs for carbon tetrachloride, chloroform, and vinyl bromide.
  * Gary Pascoe will call California EPA to learn the justification for their cancer slope factor of 16, as compared to the EPA CSF of 51.

- The group decided by unanimous consensus to investigate a range of potential OELs by using the EPA formula and varying the inputs for:
  * Risk level, from 10^{-3} to 10^{-4}
  * Inhalation rate, from 5 m^3/day (half work day) to 10 (full work day)
  * Cancer slope factor, using either the U.S. EPA value of 51 or the Cal EPA value of 16.

- The following inputs to the formula will be held constant:
  * Averaging time: 70 years average lifetime, or 25,500 days
  * Average adult body weight of an adult female: 65 kg
  * Exposure frequency: 200 days/yr (accounting for time away from the Tank Farms due to training, holidays, and vacation).
  * Exposure duration (working life in the Tank Farms): 40 years

- Using these constants and variables, the following is the range of potential OELs under consideration:

Risk factor	Risk	**1.00E-04**	**1.00E-03**	**1.00E-02**	*
Averaging time (70 yrs)	AT (d)	25,550	**25,550**	25,550	
Adult body wt (female)	BW (kg)	65	**65**	65	
Inhalation rate	IR (m^3/d)	10	**10**	10	
Exposure frequency	EF (d/yr)	250	**250**	250	
Exposure duration	ED (yr)	40	**40**	40	
Cancer slope factor	CSF	16	**16**	16	
Derived OEL		0.10	**1.04**	10.38	**µg/m^3**
		0.03	**0.34**	3.43	**ppbv**

* The highlighted box shows inputs to the formula that result in a value nearly identical to the Netherlands OEL

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
June 8, 2005 2440 Stevens

Carcinogen OELs

Issue: Continue discussions on setting an acceptable occupational exposure level (AOEL) for n-nitrosodimethylamine (NDMA), and set a course of action for AOELs for the remainder of the COPC carcinogens.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Jim Honeyman, CH2M HILL
Jim Huckaby, PNNL
Susan Eberlein, CH2M HILL
Gretchen Bruce, Intertox
Gary Pascoe, Intertox
Sandy Rock, AMH
Jill Molnaa, HAMTC Safety
Ed Carter, HAMTC Safety

Agenda:

9:00 Organization and introductions – Tom Anderson
9:15 Review outcome of recent EAS Review Group meetings – Tom Anderson
9:30 Environmental sources of nitrosamines, and how they compare to Tank Farms headspace concentrations
- Gretchen Bruce
- Mike Zabel
- Mark Marcus

10:30 Options for NDMA AOEL; consensus AOEL
11:15 Progress on AOELs for the remainder of the COPC carcinogens – Gretchen Bruce

Meeting Notes:

- After introduction of Sandy Rock to the group, Tom Anderson reviewed activities to date on setting an AOEL for NDMA.

- Jim Huckaby gave an update on NDMA detection limits.
  * Current technology allows detection limits of 3 pptv. To achieve this level requires a rigorous sampling methodology (1,000 L of air over an 8 hr sampling time), plus state-of-the-art analytical methods.
  * A more realistic detection limit is 30 pptv (0.03 ppbv), which requires a 100-L sample.
  * Our current sampling methods take a 100-L sample, and are more in line with the 30 pptv detection limit.

- Gretchen Bruce and Mike Zabel presented their research into background levels and sources of nitrosamines.
  * Jim Huckaby answered a question on the source of nitrosamines in the tanks. They are continually formed and degraded from complexant sources. Formation is enhanced at lower pH, as would occur when water is added to the tanks.
  * Gretchen showed data on nitrosamines in industrial sources, drinking water, soil, air, food, and other media.
    - A representative background NDMA level for the Tank Farms is most likely in the vicinity of 0.01 ppbv – the same as in average suburban air.
    - This background concentration at the Tank Farms would be equivalent to an OEL calculated with the EPA formula using 10^{-4} risk factor and the U.S. EPA cancer slope factor: 0.01 ppbv.
  * Intertox suggested that we consider conducting air sampling outside the Hanford Site, such as in a Tri-Cities park and urban area, for comparison to levels we might detect at the Tank Farms.

- Gretchen presented tables comparing OELs for the 52 COPC between 29 different countries and agencies.
  * In the process it was noted that the NDMA OELs we have been referencing are those of Netherlands and Switzerland (not Germany).
  * The tables show that Netherlands and Swiss OELs are well in line with other countries, and are often more conservative than U.S. OSHA.

- The two most reasonable options for a Tank Farms NDMA AOEL were discussed:
  * Use the OEL established by the Netherlands and Switzerland
    - These are industrialized countries with a judicial and regulatory framework similar to U.S. If the U.S. set an OEL, it likely would be similar, or possibly higher.
    - This standard falls within the range considered by the EAS Review Group
  * Use the EPA formula to generate an AOEL
    - The Independent Toxicology Panel (ITP) recommends a risk factor not higher than 10^{-4}
    - We would have to decide on a cancer slope factor: either the Cal EPA value of 16 or the U.S. EPA value of 51
    - Derive an AOEL by applying these factors to the EPA formula

These options for NDMA are compared in the table below, along with the range of AOELs considered by the EAS Review Group.

Prospective NDMA AOELs

Source	ppbv	$\mu g/m^3$
EAS Review Group range considered*	0.01 – 3.43	0.04 – 10.38
Netherlands, Switzerland OEL	0.3	1.0
EPA formula, CA EPA CSF, 10^{-4} risk	0.04	0.13
EPA formula, U.S. EPA CSF, 10^{-4} risk	0.01	0.04

* Not including the DOE TEEL, which is for short-term emergency exposure and is much higher

Conclusions

- It is reasonable to use foreign government standards, as long as care is taken to ensure that the country employs a methodology comparable to U.S. rulemaking, and the basis for the standard is fully traceable.

- We have to carefully screen OELs to identify any which may have been developed before carcinogenicity was discovered for that agent. If these exist, an OEL that incorporates carcinogenicity data must be used or developed.
  * For PCBs, it is reasonable to use the NIOSH standard rather than the OSHA PEL, because NIOSH accounts for carcinogenicity.

- **The EAS Review Group recommends that AOEL for NDMA will be the Netherlands/Switzerland value: 0.3 ppbv, or 1.0 $\mu g/m^3$**

- Actions for Intertox:
  * Develop an AOEL recommendation for nitrosodipropylamine (NDPA)
  * Develop an AOEL recommendation for all congeners of PCBs as a group
  * Produce a summary table, combining the major elements of Tables A, B, and C presented today

- Actions for Tom Anderson:
  * Expand the rules for AOEL development into a more detailed procedure, as recommended by the ITP
  * Develop a flowchart of the AOEL development process for inclusion in the procedure.

Future Actions

- Review the non-carcinogen AOELs being developed by PNNL.

- Review procedures that are in development by Jim Honeyman, PNNL, and Environmental Health.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
December 6, 2005, 2440 Stevens, Rm 1305C

Purpose: Determine safe, effective, and scientifically justified Tank Farms acceptable occupational exposure levels (AOEL) for butanal, alkyl nitrates, 1-nitrate 1,2,3-propanetriol, dinitrates, and alkyl nitrites.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Jim Honeyman, CH2M HILL
Susan Eberlein, CH2M HILL
Joe Meacham, CH2M HILL
Jim Huckaby, PNNL
Torka Poet, PNNL
Chuck Timchalk, PNNL
Sandy Rock, AMH
Gretchen Bruce, Intertox

The meeting was called to order at 1400 by T. Anderson. Anderson made introductions of all members. He then explained the purpose and schedule for the meetings, which are intended to evaluate a series of AOELs over the course of several days.

Anderson reviewed the overall process for setting AOELs, using the flowcharts for overall OEL process (Attachment 1), non-carcinogen AOELs (Attachment 2), and carcinogen AOELs (Attachment 3).

Discussion:

- How will health effects of vapor mixtures be evaluated? Anderson explained that mixtures will be evaluated as part of the exposure assessment process, using methods such as the OSHA mixture rule. These processes use OELs and AOELS, as inputs. Therefore, the development of AOELs does not have to consider mixture effects.
- Permissible Exposure Limits (PELs) or Threshold Limit Values (TLVs) may have been established for some compounds before carcinogenicity was documented for that compound. How will these be addressed? Anderson stated that carcinogens would be discussed later in the week, and this aspect would be added to the week's agenda.

The main topic of discussion was then started. For each proposed AOEL, the originator gave a presentation on the background for the AOEL. After discussion, a vote was taken on whether to accept the proposed AOEL.

Butanal (123-72-8) – Presented by J. Huckaby and T. Poet

- See Attachment 4.
    - Butanal has been positively identified in the tank headspaces.
    - Its likely source is as a degradation product, via butanol, of tributyl phosphate, an extractant used at PUREX.
    - AIHA has assigned a Workplace Environmental Exposure Level (WEEL) of 25 ppmv.
    - The primary toxicological endpoint is skin and eye irritation.
- Poet recommended that the AIHA WEEL of 25 ppmv be adopted as the AOEL, based on irritation effects, and the fact that it is non-carcinogenic.
- Discussion:
    - Were the nauseating properties of butanal considered? It was mentioned that these effects are seen at levels above 200 ppmv, and so were not relevant.
    - Are there developmental effects? None were detected up to 1,500 ppmv from a similar compound, propanaldehyde.
    - No compelling contrary toxicology was noted.

Action: M. Zabel was asked to research the anticipated odor threshold, and olfactory fatigue level for butanal. This information is not relevant to the AOEL, but is needed evaluating controls and for worker communication.

- Proposal: Adopt the AIHA WEEL of 25 ppmv as the AOEL for butanal. This proposal was unanimously approved.

Short-Chain Alkyl Nitrates – Presented by J. Huckaby and T. Poet

- See Attachment 5.
    - Compounds considered for AOELs were methyl nitrate (598-58-3), ethyl nitrate (625-58-1), and butyl nitrate (928-45-0).
    - These compounds have been seen in headspace sampling as tentatively identified compounds (TICs), and there is reasonable assurance that they are actual headspace constituents.
    - The organic nitrates are used in chemical synthesis of other compounds, including room deodorizers, and rocket propellants.
    - Propyl nitrate has OELs established by OSHA, ACGIH, and NIOSH of 25 ppmv 8-hr TWA. This was used as the surrogate for the other nitrates.
    - Human exposure to propyl nitrate can lead to irritation, headache, and nausea.
- Discussion:
    - The compounds in question all have short-chain R-groups with similar metabolism.

- There was some discussion about whether to adopt the propyl nitrate OEL as the AOEL. An uncertainty factor was recommended because a surrogate is proposed as the point of departure – propyl nitrate – and because little is known about the three compounds in question. Uncertainty factors of three and ten were considered; three was considered appropriate because of the similarity to the surrogate.
- A question was raised about potential carcinogenicity. Three long-term studies were cited on nitrates in food from fertilizers. No cancer potential has been found for these nitrates.
- High levels of nitrates in drinking water from farming have been associated with type I diabetes.
- The potential for both carcinogenicity and diabetes were known and considered when the OEL for propyl nitrate was established.
- Some research has shown that nitrates can affect the thyroid by inhibiting iodide uptake.

- Proposal: Apply an uncertainty factor of 3 to the propyl nitrate OEL of 25 ppmv: 25/3 = 8.33. Round down to an AOEL of 8 ppmv.
  - Further questions were raised about the potential for *in vivo* conversion of nitrates to the more dangerous nitrites. As a result, no vote was taken until more information could be presented.

Action: Poet and Bruce will do further research on the metabolism of nitrates. Voting was deferred until more information could be presented later in the week.

1-Nitrate 1,2,3-propanetriol (624-43-1) – Presented by J. Huckaby and T. Poet

- See Attachment 6.
  - Found as a TIC in one headspace (C-204).
  - It could be formed as a reaction product of nitrate and glycerol, but is unlikely to form at significant concentrations.
  - Chemistry and toxicology should be similar to other nitrates.
  - Propyl nitrate has OELs established by OSHA, ACGIH, and NIOSH of 25 ppmv 8-hr TWA. This was used as the surrogate.
- 1-Nitrate 1,2,3-propanetriol is used in foods and in low-toxicity, environmentally-friendly antifreeze.
- Because of low volatility, it would be most likely seen in Tank Farms as an aerosol.
- Health concerns are low, and parallel those of the alkyl nitrates.
- Proposal: Apply an uncertainty factor of 3 to the propyl nitrate OEL of 25 ppmv: 25/3 = 8.33. Round down to an AOEL of 8 ppmv. This proposal was unanimously approved; however, final approval was deferred pending approval of the alkyl nitrates.

Dinitrates – Presented by J. Huckaby and T. Poet

- See Attachment 7.
    - Compounds in question are: 1,3-propanediol dinitrate (3457-90-7), 1,4-butanediol dinitrate (3457-91-8), 1,2,3-propanetriol 1,3-dinitrate (623-87-0), and 1,5-pentanediol dinitrate (3457-92-9).
    - All have been reported in 1 to 5 tank headspaces, with reasonable assurance of correct assessment.
    - Little direct toxicology information is available, but they should be analogous to propylene glycol dinitrate (PGDN), and other dinitrates, for which adequate information is available.
    - Mode of action is methemoglobinemia and vasodilation..
    - TLVs for several similar dinitrate compounds are 0.05 ppmv.
- Discussion
    - Discussed route of uptake.
    - There was a question about detectability at 5 ppbv (10% of the proposed AOEL). This detection limit is possible with thermal desorption units (TDUs).
    - OELs for similar compounds are based on vasodilation.
    - It was suggested that information from this analysis be used in evaluating the deferred nitrates (above).
    - Several similar dinitrate compounds serve as surrogates; their OEL is 0.05 ppmv. Because of the similarity of the compounds and their mode of action, no uncertainty factor is necessary.
- Proposal: Set an AOEL of 0.05 ppmv for the dinitrates: 1,3-propanediol dinitrate, 1,4-butanediol dinitrate, 1,2,3-propanetriol 1,3-dinitrate, and 1,5-pentanediol dinitrate. This proposal was unanimously approved.

Alkyl Nitrites – Presented by J. Huckaby and T. Poet

- See Attachment 8.
    - Compounds considered were: methyl nitrite (624-91-7), ethyl nitrite (109-95-5), and butyl nitrite (544-16-1).
    - Methyl nitrite and butyl nitrite have been tentatively identified in tank headspace analyses, with reasonable assurance of accuracy. Ethyl nitrite has not been reported in tank vapors.
    - These compounds are used in vasodilating medication, and as drugs of abuse.
    - OSHA, ACGIH, and NIOSH have set OELs for isobutyl nitrite of 1 ppmv.
- Toxicity of nitrites is higher for shorter-chain compounds, and for unbranched compounds.

- Since the alkyl nitrites are short-chain and unbranched, uncertainty factors of 3 should be applied for each of these: 3 (unbranched) x 3 (short-chain) = 9. Rounding up, an uncertainty factor of 10 is recommended.
- It is reasonable to use the isobutyl nitrite surrogate OEL of 1 ppmv as the point of departure, and apply an uncertainty factor of 10, giving an AOEL for alkyl nitrites of 0.1 ppmv.
- **Proposal: Set an AOEL for methyl nitrite, ethyl nitrite, and butyl nitrite of 0.1 ppmv. This proposal was unanimously approved.**

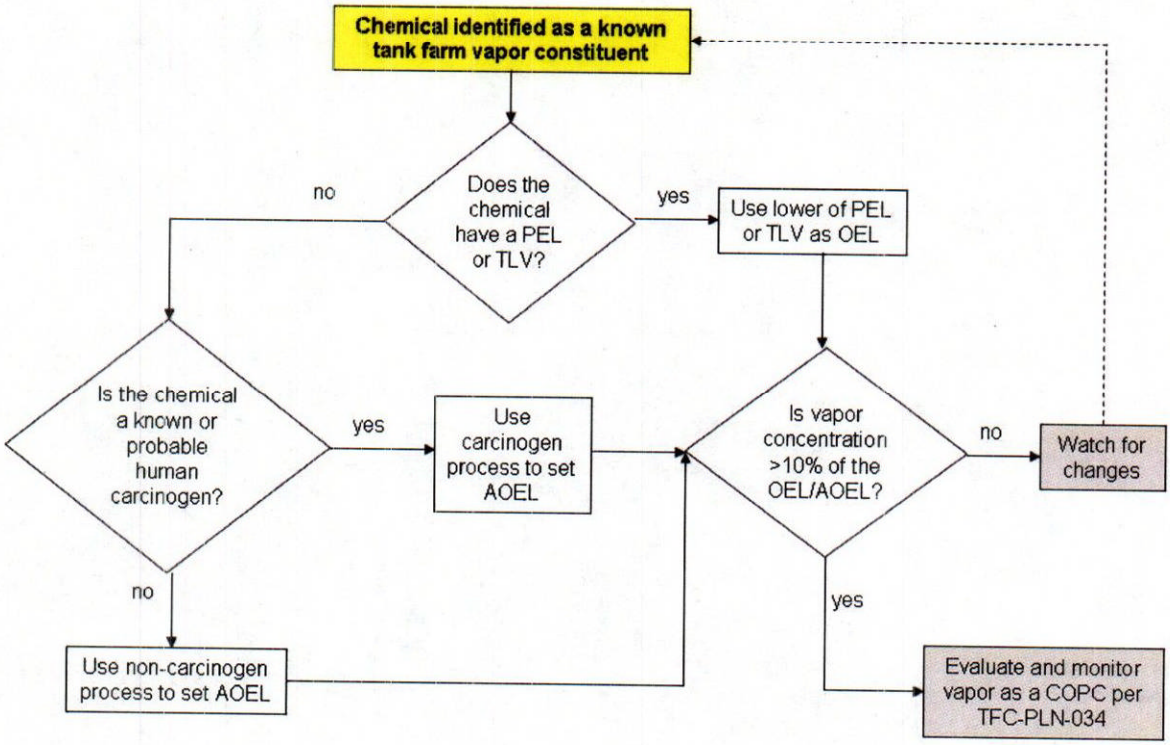
Nitriles – Presented by J. Huckaby and T. Poet

- See Attachment 9.
  - Eleven different saturated and unsaturated nitrile compounds were considered.
  - The mechanism of action proceeds through metabolically-released cyanide, which binds to metalloenzymes, inactivating cytochrome oxidase.
  - Toxic endpoints of concern are fetal development and acute respiratory arrest.
  - A chart is presented showing the LD_{50} of nitriles versus carbon number (from 1 to 9 carbons), for saturated and unsaturated forms. From 2 to 9 carbons the toxicity decreases predictably with higher carbon number (saturated forms).
  - Published OELs for saturated nitriles: 8 ppmv for butanenitrile (NIOSH); 6 ppmv for propanenitrile (ACGIH).
  - Published OELs for unsaturated nitriles: 1 ppmv for methacrylonitrile (ACGIH); 2 ppmv for acrylonitrile (ACGIH).
  - A table is presented showing the 11 nitriles, proposed AOELs, and the basis for the AOEL. Toxicity data are not available for heptanenitrile and decanenitrile.
  - Since the 4- to 8-carbon chain nitriles have a linear relationship between chain length and LD_{50}, their proposed AOEL is based on the NIOSH REL for propanenitrile (6 ppmv). Butanenitrile has a REL of 8 ppmv.
  - There is no toxicity data for heptanenitrile and decanenitrile; therefore, an uncertainty factor of 3 is proposed for these two.
- Discussion
  - Toxicity decreases with chain length after acetonitrile. Unsaturated chains have low LD_{50}s.
  - Is the proposed uncertainty factor for heptanenitrile and decanenitrile too conservative? Since propanenitrile and butanenitrile are more toxic than the higher-chain nitriles, and the proposed AOELs for the 5- to 9-carbon nitriles are based on propanenitrile, is it necessary to apply an uncertainty factor?
- Proposal: Accept the PNNL proposal as shown in the attachment as the AOELs for the 11 nitriles (see list below), but do not apply an uncertainty factor of 3 for heptanenitrile and decanenitrile. This proposal was unanimously approved.

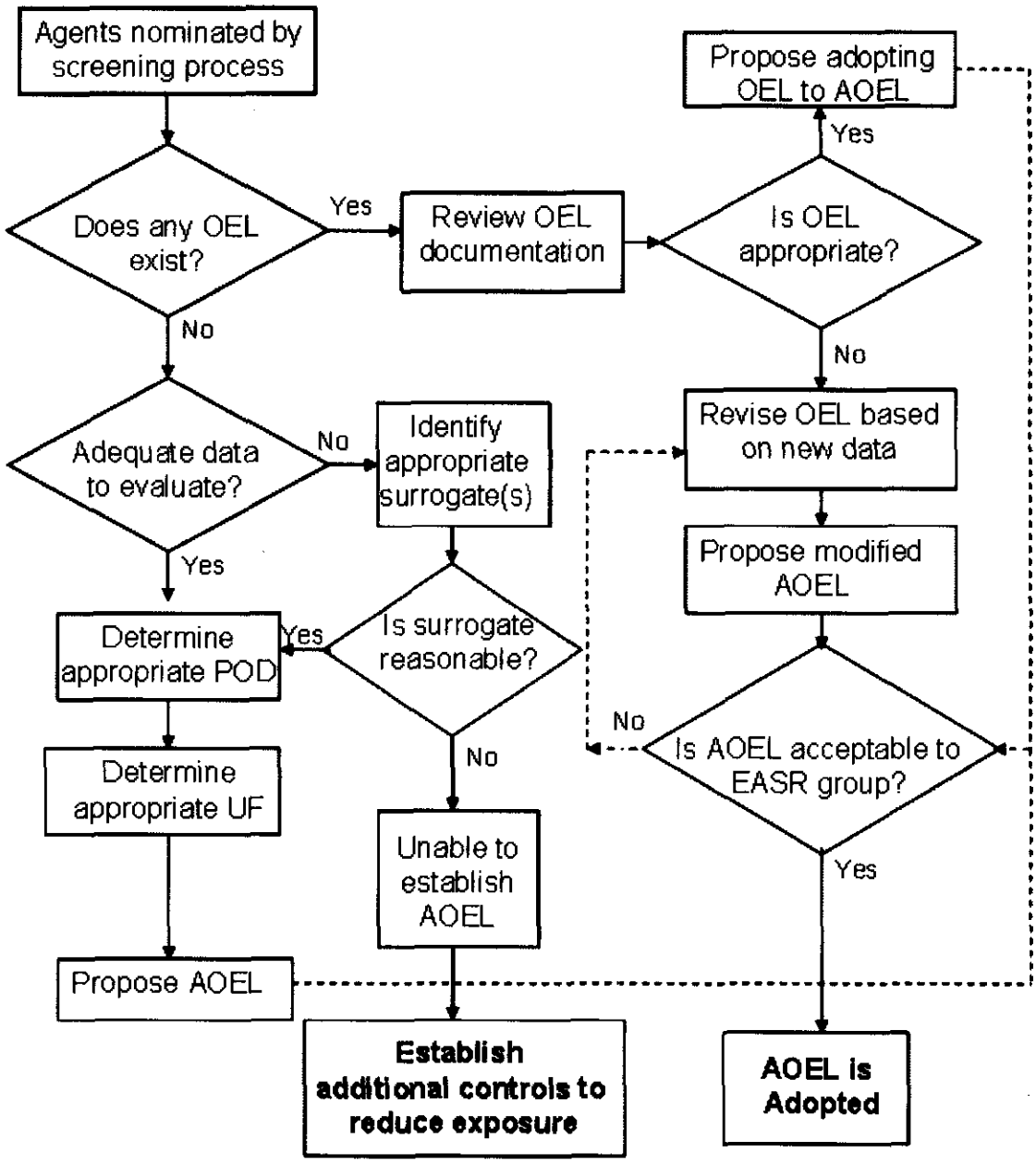
- Approved AOELs for saturated nitriles:
  - Propanenitrile (107-12-0) 6 ppmv
  - Butanenitrile (109-74-0) 8 ppmv
  - Pentanenitrile (110-59-8) 6 ppmv
  - Hexanenitrile (628-73-9) 6 ppmv
  - Heptanenitrile (628-08-3) 6 ppmv
  - Octanenitrile (124-12-9) 6 ppmv
  - Nonanenitrile (2243-27-8) 6 ppmv
  - Decanenitrile (1975-78-6) 6 ppmv
- Approved AOELs for unsaturated nitriles:
  - 3-butenenitrile (109-75-1) 1 ppmv
  - 2-methylene butanenitrile (1647-11-6) 0.3 ppmv
  - 2,4-pentadienenitrile (1615-70-9) 0.3 ppmv

The meeting was adjourned at 1700, to be re-convened the next day with some new members.

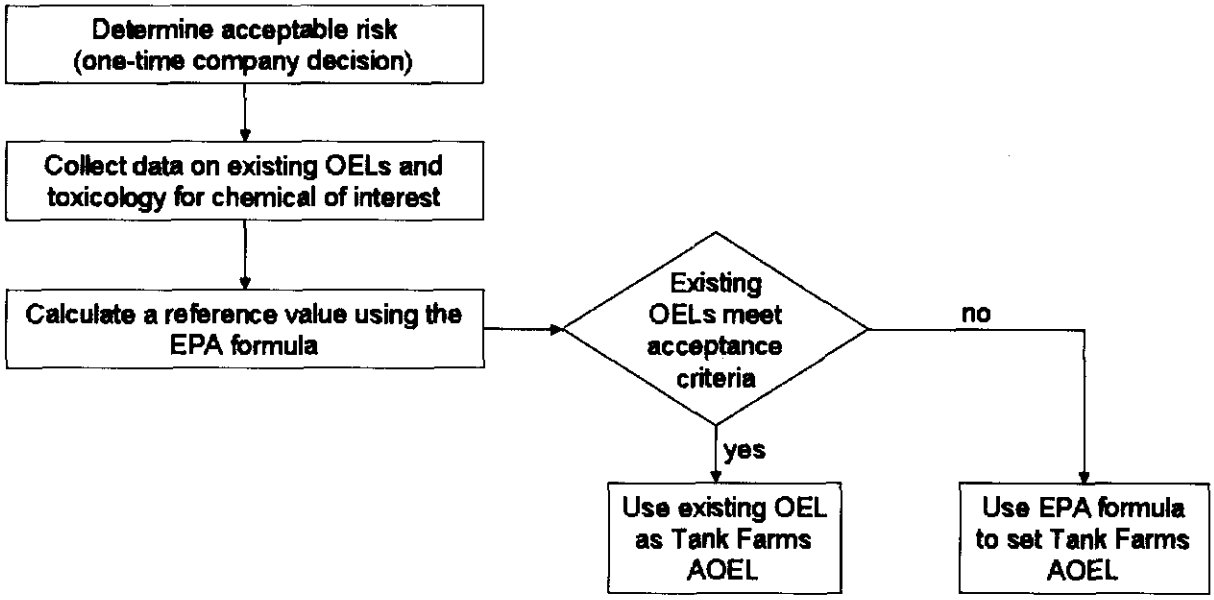
Process for Evaluating the Hazard of Tank Farms Vapors



Non-Carcinogen Process for Establishing AOELs



Carcinogen Process for Establishing AOELs



CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
December 7, 2005, 2440 Stevens, Rm 1305C
Morning Session

Purpose: Review new information on alkyl nitrates and 1-nitrate 1,2,3-propanetriol. Determine safe, effective, and scientifically justified Tank Farms acceptable occupational exposure levels (AOEL) for these, plus polychlorinated biphenyls, acetamide, and decanoates.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Jim Honeyman, CH2M HILL
Susan Eberlein, CH2M HILL
Joe Meacham, CH2M HILL
Jill Molnaa, CH2M HILL
Jim Huckaby, PNNL
Torka Poet, PNNL
Gretchen Bruce, Intertox
Gary Pascoe, representing Intertox

The meeting was called to order at 08:00 by T. Anderson. This is a continuation of a series of meetings started 12/6/2005 to discuss AOELs.

In yesterday's meeting, AOELs were not finalized for short-chain alkyl nitrates and 1-nitrate 1,2,3-propanetriol because there were questions on how these compounds are metabolized in the human body. New information was presented and discussed on these compounds.

Short-Chain Alkyl Nitrates

- Discussion focused on the water solubility of the alkyl nitrates. Due to their water solubility uptake is fairly low and excretion is fairly high, decreasing concerns for toxicity.
- The concerns raised at the previous meeting were adequately addressed, and there were no new concerns.
- Proposal: Apply an uncertainty factor of 3 to the propyl nitrate OEL of 25 ppmv: 25/3 = 8.33. Round down to 8 ppmv as an AOEL for methyl nitrate, ethyl nitrate, and butyl nitrate. This proposal was unanimously approved.

1-Nitrate 1,2,3-propanetriol (624-43-1)

- Chemical properties are similar to the short-chain alkyl nitrates, leading to the same logic as above for solubility and thus toxicity.
- The concerns raised at the previous meeting were adequately addressed, and there were no new concerns.

- Proposal: Apply an uncertainty factor of 3 to the propyl nitrate OEL of 25 ppmv: 25/3 = 8.33. Round down to 8 ppmv as an AOEL for 1-nitrate 1,2,3-propanetriol. This proposal was unanimously approved.

Polychlorinated Biphenyls (PCBs)

- See Attachment 1.
    - This discussion includes any biphenyl molecule containing one or more chlorine atoms. Headspace sampling has identified 14 specific and 3 partially-identified PCBs in 12 tanks.
    - PCBs are present in tank waste from actual PCB material dumped into the tanks.
    - Carcinogenicity has been shown for PCBs with greater than about 50% chlorine content (number of carbons with chlorine attached).
    - Hepatotoxicity is the primary toxicological endpoint of concern.
    - PCBs present in Tank Farms are lower-toxicity congeners.
    - EPA cancer slope factors were presented for low risk and persistence PCB mixtures, such as those present in Tank Farms.
- Discussion
    - The chemical and toxicological characteristics of the various congeners were discussed.
    - The NIOSH REL of 1 $\mu g/m^3$ cites Japanese carcinogenity studies, and is intended for all mixtures of PCBs (low and high chlorine content).
    - The ACGIH TLV of 1 mg/m^3 would not protect against all cases of chloracne.
    - The basis for the EPA cancer slope factors was discussed.
    - The EPA upper-bound slope factor for lowest risk and persistence gives an AOEL of about 26 $\mu g/m^3$. If an uncertainty factor of 30 were applied to the ACGIH TLV, it produces an equivalent value: 1 mg/m^3 / 30 = 33.3 $\mu g/m^3$.
- Proposal: Set an AOEL for Tank Farms PCBs (a mixture of lower-toxicity congeners) of 30 $\mu g/m^3$. This proposal was unanimously approved.

Acetamide (60-35-5)

- See Attachment 2.
    - Acetamide was reported as a tentatively identified compound (TIC) in 2 tanks at very low concentration.
    - High water solubility and low volatility are expected to make headspace concentrations low.
- Current analytical methods will detect acetamide as a TIC if it is present.
- An AOEL for acetamide would be in the ppmv range.

- Acetamide is not likely to be present in tank vapors, and is not likely to reach ppmv levels. It could be screened as a TIC, and if present further action would be taken to set an AOEL.
- Proposal: Screen for acetamide as a TIC at about 1 ppmv, but do not set an AOEL. This proposal was unanimously approved.

Decanoates – J. Huckaby and T. Poet

- See Attachment 3
    - Compounds considered were: 1-methylethyl tetradecanoate (110-27-0) and butyl tetradecanoate (110-36-1).
    - Reported from headspace samples in 7 tanks.
- Decanoates are low-toxicity oils often used as additives in hand lotions and soaps.
- The decanoates seen in headspace sampling are most likely to be contaminants – possibly from hand lotions used by technicians or chemists in the sampling and analytical process. If they were present as a tank waste constituent, other low-carbon-number analogues of the family would also be present – and they are not.
- Proposal: Do not propose an AOEL for 1-methylethyl tetradecanoate and butyl tetradecanoate due to low toxicity and low probability that they are present. This proposal was unanimously approved.

The meeting was adjourned at 1200, to re-convene in the afternoon with some new members.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
December 7, 2005, 2440 Stevens, Rm 1305C
Afternoon Session

Purpose: Determine safe, effective, and scientifically justified Tank Farms acceptable occupational exposure levels (AOEL) for petroleum hydrocarbons, 1-naphthylamine, n-nitrosodipropylamine, furan, and substituted furans. Also to reevaluate the criteria for chemicals of potential concern (COPC).

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Jim Honeyman, CH2M HILL
Dave Farler, CH2M HILL
Joe Meacham, CH2M HILL
Jim Huckaby, PNNL
Torka Poet, PNNL
Chuck Timchalk, PNNL
Gretchen Bruce, Intertox
Gary Pascoe, representing Intertox

The meeting was called to order at 13:20 by T. Anderson.

Petroleum Hydrocarbons – J. Huckaby

- Much of the discussion is based on the report by Carl Mackerer, summarizing work done in the petroleum industry on hydrocarbon streams, such as gasoline, kerosene, and diesel fuel.
- These hydrocarbon streams are grouped by boiling point. Such streams include kerosene, gasoline, and diesel fuel.
- Some hydrocarbons have individual OELs (e.g., benzene). These would continue to be evaluated separately, and would not be included in a stream AOEL.
- Mackerer recommends using the TLV for kerosene as the Tank Farms AOEL because the kerosene encompasses the range of compounds seen in the Tank Farms, and it is conservative.
- The odor threshold for hydrocarbons in much lower than the OELs.
- Proposal: Use the ACGIH TLV of 200 mg/m^3 for kerosene as the AOEL for petroleum hydrocarbons that do not have separate OELs. This proposal was unanimously approved.

1-Naphthylamine (134-32-7)

- See Attachment 1, pp 1-2.
    - No OELs have been established by U.S. agencies or other governments. OSHA and NIOSH list it as an occupational carcinogen (bladder cancers).

- IARC lists 1-naphthylamine as a Group 3 carcinogen (not classifiable as to carcinogenicity).
- No published toxicity criteria are available.
- California EPA published a cancer slope factor for 2-naphthylamine. However, the key step in carcinogen activation for 2-naphthylamine, N-oxidation, occurs only to a limited extent in 1-naphthylamine.
- It would likely be conservative to apply the cancer slope factor (CSF) for 2-naphthylamine in setting an AOEL for 1-naphthylamine.
- Using this approach, the AOEL 1-naphthylamine would be 1 $\mu g/m^3$.

- Discussion
  - The suggested link between 1-naphthylamine and cancer comes from epidemiological studies in the dye manufacturing industry – so there could well be complicating factors from other dye chemicals. No laboratory studies specific for 1-naphthylamine are known.
  - The IARC data is more likely to be based on recent information than OSHA or NIOSH.
  - The detection limit for 1-naphthylamine is likely to be about 0.5 ppbv using a 200-L sample with a semi-volatile thermal desorption unit (TDU).
  - Since N-oxidation is a key question, this discussion will be continued in a future meeting, to allow time for research

Action: Intertox will evaluate the N-oxidation of 1-naphthylamine compared to 2-naphthylamine.

N-nitrosodipropylamine (NDPA) (621-64-7)

- See Attachment 1, p 3.
  - NDPA is on U.S. EPA, IARC, and NTP carcinogenicity lists as a likely or possible human carcinogen.
  - No OELs have been established.
  - Intertox used the U.S. EPA cancer slope factor (CSF) of 7 $(mg/kg/day)^{-1}$ to calculate a proposed AOEL of 0.3 $\mu g/m^3$, or 56 pptv (10^{-4} risk factor).
- Discussion
  - Since nitrosodimethylamine (NDMA) is the most potent of the nitrosamines, it would be conservative to set the AOEL for all nitrosamines at the AOEL that has been approved for NDMA (0.3 ppbv).
- No formal proposal was made, to allow the collection of more information.

Action: Intertox will compile a list of cancer slope factors and OELs for all nitrosamines to rank their relative potency. If this list shows NDMA to be the most potent, a proposal could be made to use the NDMA AOEL for all nitrosamines.

Other Carcinogens

- For some compounds, carcinogenicity was discovered after their PELs or TLVs were established. A question was raised whether new, more conservative AOELs should be considered for these compounds.
- General industries are not taking such actions, but rather are applying the OELs as published. Some government agencies involved in CERCLA activities are reevaluating OELs for environmental contamination on this basis.
- Since there is no compelling regulatory driver for this type of action, undertaking such a major action would go beyond CH2M HILL's current contract scope. Therefore, no action will be taken at this time. This may be considered in future reevaluations of OELs/AOELs.

Furan (110-00-9)

- See Attachment 2.
    - Furan was positively identified in 11 tank headspaces in six different farms.
    - It is a possible carcinogen, causing biliary tract hyperplasia and cholangiocarcinoma in rats, with a very steep dose-response curve.
    - Among the very few standards for comparison are a U.S. EPA reference dose (0.001 mg/kg/day) and a Russian STEL of 0.5 mg/m^3.
    - An empirical study in rats showed 70% carcinogenic response at 4 mg/kg/day. PNNL calculated a dose based on 0.01% response (comparable to 10^{-4} risk) of 0.57 μg/kg/day. This is slightly more conservative than the EPA reference concentration (RfC).
    - This value converts to an AOEL of 3.7 $\mu g/m^3$, or 1.3 ppbv.
- Discussion
    - It would not be reasonable to use the EPA RfC as the basis for the AOEL, because EPA did not include carcinogenicity data in their analysis.
    - Various other models were discussed, but the PNNL method was considered sound.
- Proposal: Use the PNNL calculation as the basis for an AOEL (1.3 ppbv), but round down to a whole number, giving a proposed AOEL for furan of 1 ppbv. This proposal was unanimously approved.

Substituted Furans

- See Attachment 3.
  - This group includes organic compounds with a 4-carbon, 1-oxygen ring, where the ring has at least one double bond.
  - 11 such compounds have been reported in tank headspaces, such as 2-methylfuran, 2,5-dihydrofuran, and 2-propylfuran.
  - Toxicity is likely due to the formation *in vivo* of a reactive epoxide intermediate.
  - The most defensible approach would be to use the furan AOEL.
- Discussion
  - Questions were raised as to whether the substituted furans may be more or less toxic than furan. There is no date or evidence to show that either one is the case.
- Proposal: Use the furan AOEL of 1 ppbv as the AOEL for the substituted furans. This proposal was unanimously approved.

This completed evaluation of AOELs for the current session. Two further agenda items dealt with how carcinogenicity would be addressed in setting AOELs.

Attachment 4 was provided by G. Bruce, giving the basis for OELs set by various agencies. Bruce pointed out the many current OELs were set before carcinogenicity was known for the substance, and the OEL did not take carcinogenicity into account. It was decided that carcinogenicity must be considered when setting AOELs, or when determining whether chemicals should be included on the COPC list. Existing OELs (PELs or TLVs) will not be re-evaluated on this basis.

There was a suggestion that the EASRG review the original technical basis criterion for assigning tank vapors to the chemical of potential concern (COPC) list.

- The original criterion for determining a COPC required that all carcinogens be included on the list, regardless of their headspace concentration. Non-carcinogens are COPC if they are present in headspaces above 10% of their OEL/AOEL.
- These COPC criteria were established early in the technical basis development, when it was not clear whether AOELs would be developed for carcinogens. Now that AOELs are available or under development for all carcinogens, the COPC criteria should be reevaluated.
- Another question was whether COPC should include only chemicals found as vapors in tank headspaces. This proposal requires further evaluation.

Action: Joe Meacham and Jim Huckaby will determine headspace concentrations of chemicals that may have low potential to be present as vapors. These include 1-napthylamine and dichlorodiphenyldichloroethylene (DDE).

- Proposal: Revise the COPC criterion such that a COPC is any chemical present in tank headspaces above 10% of its OEL/AOEL, regardless of whether it is a carcinogen or non-carcinogen. This proposal was unanimously approved.

Action: This change in COPC criteria will not go into effect until Tom Anderson briefs upper management. [Post-note: senior management approved this action on Dec 14.]

The meeting was adjourned at 1600.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
January 16, 2006, 2440 Stevens, Rm 1305B

Purpose: Determine safe, effective, and scientifically justified Tank Farms acceptable occupational exposure levels (AOEL) for various Tank Farms vapors.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Joe Meacham, CH2M HILL
Dave Farler, CH2M HILL
Torka Poet, PNNL
Chuck Timchalk, PNNL
Joseph Samuels, AMH

The meeting was called to order at 0830 by T. Anderson. He explained the purpose for the meetings, which are intended to evaluate a series of AOELs today and tomorrow.

For each proposed AOEL, the originator gave a presentation on the background for the AOEL. After discussion, a vote was taken on whether to accept the proposed AOEL.

2-Fluoropropene (1184-60-7) – Presented by J. Meacham and C. Timchalk

- See Attachment 1.
  - 2-Fluoropropene has been tentatively identified in five tank headspaces.
  - It may be a degradation product of common organic materials used in plutonium processing.
  - It has a relatively high vapor pressure, and due to its volatility it was expected to have dissipated in the past, but it appears to be still present at low levels.
  - Related compounds, the halogenated ethylenes (such as fluoroethylene, or vinyl fluoride), have been classified as known or suspected human carcinogens. There is no available toxicity information for 2-fluoropropene.
  - The most appropriate surrogate is vinyl fluoride, which has been well studied and has an ACGIH TLV of 1 ppmv.
  - The proposed AOEL uses the vinyl fluoride TLV as a point of departure, applying an uncertainty factor of 10 for chemical differences between vinyl fluoride and 2-fluoropropene.
- Discussion:
  - Is there a general pattern of toxicity between the chlorinated, brominated, and fluorinated hydrocarbons? To some extent there is. The fluorinated forms are often less toxic – vinyl bromide is twice as potent as vinyl fluoride.

  - Is the uncertainty factor of 10 consistent with previous applications of uncertainty factors by the EAS Review Group? Yes, because of the potential carcinogenicity an uncertainty factor of 10 is appropriate.

- Proposal: Apply an uncertainty factor of 10 to the ACGIH TLV for vinyl fluoride of 1 ppmv, giving an AOEL for 2-fluoropropene of 0.1 ppmv. This proposal was unanimously approved.

Dibutylbutylphosphonate (78-46-6) – Presented by J. Meacham and C. Timchalk

- See Attachment 2.
  - Dibutylbutylphosphonate has been identified in 7 tank headspaces.
  - It is a known process component of tributyl phosphate, and is difficult to sample properly.
  - It is a phosphoric acid similar to dibutyl phosphate (DBP) and tributyl phosphate (TBP).
  - It has a relatively low vapor pressure.
  - Limited toxicity data is available.
  - Workers exposed to the surrogate TBP have complained of acute effects: nausea and headaches. Based on this, ACGIH set a TLV for TBP of 0.2 ppmv, which is lower than the level that caused the reported symptoms.
  - The proposed AOEL uses the TBP TLV as a point of departure, applying an uncertainty factor of 10 for lack of robust data, and an additional uncertainty factor of 3 for structural differences.
- Discussion
  - A question was asked what the TBP TLV is based upon. It is based on acute effects due to nausea and headache. There has been no association with carcinogenicity.
- Proposal: Apply an uncertainty factor of 30 to the ACGIH TLV for tributyl phosphate of 0.2 ppmv, giving an AOEL for dibutylbutylphosphonate of 0.007 ppmv. This proposal was unanimously approved.

3-Methyl-3-buten-2-one (814-78-8) – Presented by J. Meacham and C. Timchalk

- See Attachment 3.
  - 3-Methyl-3-buten-2-one has been tentatively identified in 2 tank headspaces.
  - It is a potential degradation product of iso-alkanes, and is not expected to be prevalent in tank headspaces.
  - A structurally similar ketone is 3-butene-2-one, which has a TLV of 0.2 ppmv based on skin irritation from direct contact, and respiratory tract irritation from vapors.

  - The surrogate 3-butene-2-one is probably more acutely toxic than 3-methyl-3-buten-2-one.
  - The proposed AOEL uses the 3-butene-2-one TLV of 0.2 ppmv as a point of departure, applying an uncertainty factor of 3 for conversion from the surrogate TLV ceiling to an 8-hour TWA, and an additional uncertainty factor of 10 for differences in toxicological properties and structure.
- Discussion
  - Why is this proposal different than that for dibutylbutylphosphonate? Further discussion arrived at the conclusion that uncertainty factors of 3 for ceiling vs. TLV and 3 for toxicity differences would be applied.
- Proposal: Apply an uncertainty factor of 9 to the ACGIH TLV for 3-butene-2-one of 0.2 ppmv, giving an AOEL for dibutylbutylphosphonate of 0.02 ppmv. This proposal was unanimously approved.

4,7,7-Trimethylbicyclo[4.1.0]heptan-3-one (4176-04-9) – Presented by J. Meacham and C. Timchalk

- See Attachment 4.
  - 4,7,7-Trimethylbicyclo[4.1.0]heptan-3-one has been tentatively identified in 1 tank headspace. It is an unlikely degradation product.
  - It is a natural plant product, similar to camphor.
  - No toxicology studies are available.
  - In humans, prolonged exposure (5 days) to camphor at less than 2 ppmv produced irritation of the eyes and nose.
  - The proposed AOEL uses the camphor TLV of 2 ppmv as a point of departure, applying an uncertainty factor of 3 for differences in toxicological properties and structure.
- Discussion
  - In what types of plants is this found? No information available.
- Proposal: Apply an uncertainty factor of 3 to the ACGIH TLV for camphor of 2 ppmv, giving an AOEL for 4,7,7-trimethylbicyclo[4.1.0]heptan-3-one of 0.7 ppmv. This proposal was unanimously approved.

4-Methyl-2-hexanone (105-42-0) – Presented by J. Meacham and C. Timchalk

- See Attachment 5.
  - 4-Methyl-2-hexanone has been tentatively identified in 4 tank headspaces. It is a degradation product of hydrocarbons.
  - Aliphatic ketones such as this are volatile and can be irritating to eyes, skin, and upper respiratory tract.

  - The most likely surrogate is 2-hexanone, which has a TLV of 5 ppmv, based on animal and human toxicity data. Peripheral neuropathy has been demonstrated for 2-hexanone.
  - The proposed AOEL uses the 2-hexanone TLV of 5 ppmv as a point of departure, applying an uncertainty factor of 10 for differences in toxicological properties and structure.
- Discussion
  - Why is an uncertainty factor of 10 applied here, as opposed to 3 for the previous chemical? This is because the potential neurotoxicity of 2-hexanone is well documented.
- Proposal: Apply an uncertainty factor of 10 to the ACGIH TLV for 2-hexanone of 5 ppmv, giving an AOEL for 4-methyl-2-hexanone of 0.5 ppmv. This proposal was unanimously approved.

6-Methyl-2-heptanone (928-68-7) – Presented by J. Meacham and C. Timchalk

- See Attachment 6.
  - 6-Methyl-2-heptanone has been identified in 115 samples from 30 tank headspaces. It is a degradation product of hydrocarbons.
  - Aliphatic ketones such as this are volatile and can be irritating to eyes, skin, and upper respiratory tract.
  - The most likely surrogates are 2-heptanone (TLV 50 ppmv) and 5-methyl-3-heptanone (TLV 25 ppmv). Limits are based on irritation to eyes, nose, respiratory tract, and mucous membranes. Human results with 5-methyl-3-heptanone are most relevant.
  - The proposed AOEL uses the 5-methyl-3-heptanone TLV of 25 ppmv as a point of departure, applying an uncertainty factor of 3 for minimal differences in chemical structure.
- Discussion
  - Slide 23 (Attachment 6) shows a proposed AOEL of 9 ppmv. Raw arithmetic gives: 25 / 3 = 8.333. Our standard practice has been to truncate the result to the nearest significant figure. This would give a proposed AOEL of 8 ppmv.
- Proposal: Apply an uncertainty factor of 3 to the ACGIH TLV for 5-methyl-3-heptanone of 25 ppmv, giving an AOEL for 6-methyl-2-heptanone of 8 ppmv. This proposal was unanimously approved.

5-Methyl-2-(1-methylethenyl)cyclohexanone (89-82-7) – Presented by J. Meacham and C. Timchalk

- See Attachment 7.
  - 6-Methyl-2-heptanone has been tentatively identified in 2 tank headspaces. Its origin is unknown; it is an unlikely degradation product of hydrocarbons.

- It is also known as pulegone, and is structurally similar to cyclohexanone. Pulegone is a component of pennyroyal, which is used as a flavoring oil in food and drinks.
- In humans, exposure to cyclohexanone at 25 ppmv was not uncomfortable, while at 50 ppmv it was irritating to the throat; at 75 ppmv it was irritating to the eyes, nose, and throat.
- Cyclohexanone has a TLV of 25 ppmv.
- The proposed AOEL uses the cyclohexanone TLV of 25 ppmv as a point of departure, applying an uncertainty factor of 10 for differences in toxicology, metabolism, and chemical structure.

- Discussion
  - Questions were raised on the selection of 10 as an uncertainty factor. It was agreed that this was appropriate based on the differences in metabolism, toxicology, and structure.
- Proposal: Apply an uncertainty factor of 10 to the ACGIH TLV for cyclohexanone of 25 ppmv, giving an AOEL for 5-methyl-2-(1-methylethenyl)cyclohexanone of 2.5 ppmv. This proposal was unanimously approved.

2-nonanone (821-55-6), 3-dodecanone (1524-27-6), 2-tridecanone (593-08-8), and 3-tridecanone (1534-26-5) – Presented by J. Meacham and C. Timchalk

- See Attachment 8.
  - These long-chain ketones have been tentatively identified in up to 21 tank headspaces. They are likely degradation product of hydrocarbons.
  - Long-chain aliphatic ketones have low volatility, but can be irritating to the nose, skin, eyes, and upper respiratory tract.
  - ACGIH has set TLVs for structurally similar ketones 2-heptanone, 3-heptanone, and 4-heptanone (50 ppmv). The TLV was based on irritating effects.
  - Exposure to 2-heptanone at 1,500 ppmv produced irritation, and at 4,800 ppmv produced narcosis.
  - The proposed AOEL uses the 2-heptanone, 3-heptanone, and 4-heptanone TLV of 50 ppmv as a point of departure, applying an uncertainty factor of 3 for slight differences in chemical structure.
- Proposal: Apply an uncertainty factor of 3 to the ACGIH TLV for 2-heptanone, 3-heptanone, and 4-heptanone of 50 ppmv, giving an AOEL for 2-nonanone, 3-dodecanone, 2-tridecanone, and 3-tridecanone of 17 ppmv. This proposal was unanimously approved.

3-Hexanone (589-38-8) – Presented by J. Meacham and C. Timchalk

- See Attachment 9.
    - Long-chain aliphatic ketones have low volatility, but can be irritating to the nose, skin, eyes, and upper respiratory tract.
    - The most likely surrogate, 2-pentanone, has been associated with strong odor, and ocular and upper respiratory tract irritation in humans.
    - The TLV for 2-pentanone is 200 ppmv.
    - The proposed AOEL uses the 2-pentanone TLV of 200 ppmv as a point of departure, applying an uncertainty factor of 3 for slight differences in chemical structure.
- Proposal: Apply an uncertainty factor of 3 to the ACGIH TLV for 2-pentanone of 200 ppmv, giving an AOEL for 3-hexanone of 67 ppmv. This proposal was unanimously approved.

Cyclopentanol (96-41-3) – Presented by J. Meacham and C. Timchalk

- See Attachment 10.
    - This 5-carbon cyclic alcohol has been tentatively identified in 5 tank headspaces. It is a likely degradation product of hydrocarbons.
    - Chronic inhalation exposure (up to 11 weeks) to a likely surrogate, cyclohexanol, at 1000 ppmv resulted in intoxication and 50% mortality.
    - The TLV for the cyclohexanol surrogate is 50 ppmv, based on eye irritation and possible central nervous system effects, such as narcosis and incoordination.
    - The proposed AOEL uses the cyclohexanol TLV of 50 ppmv as a point of departure, applying an uncertainty factor of 10 for differences in toxicology and chemical structure.
- Discussion
    - Although cyclopentanol is likely present in the tanks, the highest measured headspace vapor concentration is suspect. Re-evaluation of the mass spectroscopy showed a probable mis-identification.
- Proposal: Apply an uncertainty factor of 10 to the ACGIH TLV for cyclohexanol of 50 ppmv, giving an AOEL for cyclopentanol of 5 ppmv. This proposal was unanimously approved.

2-Ethyl-1-hexanol (104-76-7) – Presented by J. Meacham and C. Timchalk

- See Attachment 11.
  - This aliphatic, branched alcohol was tentatively identified in 48 tank headspaces. It is an expected hydration product of the extractant bis(2-ethylhexyl)phosphate.
  - Germany set a MAK at 20 ppmv. Documentation was not available to understand the basis for the MAK.
  - Isooctyl alcohol is a likely surrogate, and has the same molecular formula with different structure. The TLV for isooctyl alcohol is 50 ppmv, based on CNS depression. There has been no association with cancer for either of these alcohols.
  - Since the 2-ethyl-1-hexanol MAK is less than half the isooctyl alcohol TLV, the MAK is a conservative AOEL for 2-ethyl-1-hexanol.
- Proposal: Adopt the German MAK of 20 ppmv as the AOEL for 2-ethyl-1-hexanol. This proposal was unanimously approved.

1-Hexadecanol (36653-82-4) and 1-Octadecanol (112-92-5) – Presented by J. Meacham and C. Timchalk

- See Attachment 12.
  - These long-chain aliphatic alcohols were tentatively identified in 15 and 4 tank headspaces, respectively. They are expected oxidation products of trace tank constituents.
  - Both have low toxicity, based on acute toxicity testing. They are common constituents in cosmetics, creams, and lotions.
  - Because of the low toxicity and common use in benign commercial products, an AOEL is not needed.
- Proposal: Do not develop AOELs due to low toxicity and common use in benign commercial products. This proposal was unanimously approved.

1-Methoxybutane (628-28-4) – Presented by J. Meacham and C. Timchalk

- See Attachment 13.
  - Tentatively identified in 3 tank headspaces, as dehydration reaction products of butanal and formaldehyde.
  - Toxicity is expected to be low based on an LC_{50} in mice of about 5 %.
  - A likely surrogate is methyl tert-butyl ether (MTBE). MTBE has low inhalational toxicity, but has been associated with kidney and liver cancer in rats and mice. It has a TLV of 50 ppmv.
  - The proposed AOEL uses the MTBE TLV of 50 ppmv as a point of departure, applying an uncertainty factor of 3 for differences in chemical structure.

- Discussion
    - A question was asked whether there has been any human carcinogenicity associated with 1-methoxybutane. None is known.
- Proposal: Apply an uncertainty factor of 3 to the ACGIH TLV for MTBE of 50 ppmv, giving an AOEL for 1-methoxybutane of 17 ppmv. This proposal was unanimously approved.

Lunch break, 1100-1230. For the afternoon sessions, T. Poet and J. Meacham made the presentations.

2-Methylbut-2-enal (1115-11-3) and 2-Ethylhex-2-enal (645-62-5) – Presented by J. Meacham and T. Poet

- See Attachment 14.
    - Tentatively identified in 1-2 tank headspaces as possible degradation products of diluent and extraction components.
    - In general, the endpoint of concern for aldehydes is irritation.
    - 2-methylbut-2-enal is a rabbit pheromone.
    - Likely surrogates are crotonaldehyde (ceiling 0.3 ppmv) and acrolein (TLV 0.1 ppmv).
    - The proposed AOEL uses the acrolein TLV of 0.1 ppmv as a point of departure
        - For 2-ethylhex-2-enal, apply an uncertainty factor of 3 for conversion from the surrogate TLV ceiling to an 8-hour TWA.
        - For 2-methylbut-2-enal, apply an uncertainty factor of 3 for conversion from the surrogate TLV ceiling to an 8-hour TWA, and an uncertainty factor of 3 for lack of data.
- Discussion
    - What is the detection limit for these compounds? Will they be able to be detected? A detection limit of about 0.003 ppmv is possible, so they would be detected at low levels.
    - Since crotonaldehyde has a more similar structure than acrolein, is it more reasonable to use the crotonaldehyde ceiling as the point of departure? Yes, this is reasonable.
    - The LD_{50} for 2-methylbut-2-enal and 2-ethylhex-2-enal is higher than that for the surrogates acrolein and crotonaldehyde, so 2-methylbut-2-enal and 2-ethylhex-2-enal are less toxic.
    - An alternative AOEL was proposed, using the crotonaldehyde ceiling of 0.3 ppmv as the point of departure.
        - For 2-ethylhex-2-enal, apply an uncertainty factor of 3 for conversion from the surrogate TLV ceiling to an 8-hour TWA.

    - For 2-methylbut-2-enal, apply an uncertainty factor of 3 for conversion from the surrogate TLV ceiling to an 8-hour TWA, and an uncertainty factor of 3 for lack of data.

- Proposal: Use the crotonaldehyde ceiling of 0.3 ppmv as the point of departure. For 2-ethylhex-2-enal, apply an uncertainty factor of 3 for conversion from the ceiling to an 8-hour TWA, giving an AOEL for 2-ethylhex-2-enal of 0.1 ppmv. For 2-methylbut-2-enal, apply an uncertainty factor of 3 for conversion from the ceiling to an 8-hour TWA, and an uncertainty factor of 3 for lack of data, giving an AOEL for 2-methylbut-2-enal of 0.03 ppmv. This proposal was unanimously approved.

1-Nitrobutane (627-05-4) – Presented by J. Meacham and T. Poet

- See Attachment 15.
    - Tentatively identified in 5 tank headspaces, from radical reactions of butyl phosphates or butanol.
    - The primary toxicological effect of the surrogate 1-nitropropane is eye and respiratory tract irritation.
    - The proposed AOEL uses the 1-nitropropane TLV of 25 ppmv as a point of departure, applying an uncertainty factor of 10 for lack of data.
- Proposal: Apply an uncertainty factor of 10 to the ACGIH TLV for 1-nitropropane of 25 ppmv, giving an AOEL for 1-nitrobutane of 2.5 ppmv. This proposal was unanimously approved.

2-Nitro-1-propanol (2902-96-7) – Presented by J. Meacham and T. Poet

- See Attachment 15.
    - Tentatively identified in 1 tank headspace, from radical reactions of various components.
    - No surrogates have been identified containing nitro and alcohol groups.
    - The primary toxicological effect of 2-methyl-2-nitro-1-propanol is eye irritation.
    - The primary toxicological effect of the surrogate 1-nitropropane is eye and respiratory tract irritation.
    - The proposed AOEL uses the 1-nitropropane TLV of 25 ppmv as a point of departure, applying an uncertainty factor of 10 for differences in chemical structure, and 10 for lack of data.
- Discussion
    - A question was asked about the toxicological effects of 1-nitropropane. It is primarily an irritant.

- Questions were asked about the adequacy of toxicological data for 1-nitropropane – is it true there is a "lack of data?" And does this warrant an uncertainty factor of 10? Poet noted that there is some data, and the proper wording should be "limited data." It was decided that the uncertainty factor should be 3 for lack of data.
- There were questions regarding the degree of structural differences between 2-nitro-1-propanol and 1-nitropropane. After considering an uncertainty factor of 3 for structural differences, it was decided to use a factor of 10, as proposed.
- The total uncertainty factor is thus 30.

- Proposal: Apply an uncertainty factor of 30 to the ACGIH TLV for 1-nitropropane of 25 ppmv, giving an AOEL for 2-nitro-1-propanol of 0.8 ppmv. This proposal was unanimously approved.

2-Nitro-2-methylpropane (594-70-7) – Presented by J. Meacham and T. Poet

- See Attachment 15.
  - Tentatively identified in 31 tank headspaces, from radical reactions of various components.
  - The endpoint of concern for the surrogate 2-nitropropane is liver damage. 2-Nitropropane is less lethal than 1-nitropropane.
- Discussion
  - There were questions regarding the degree of structural differences between 2-nitro-2-methylpropane and 2-nitropropane. After considering an uncertainty factor of 10 for structural differences, it was decided to use a factor of 3.
  - Upon further discussion it was decided that there was not adequate toxicity information for the surrogate, 2-nitropropane. It was decided to add an additional uncertainty factor of 10 for lack of data.
  - The total uncertainty factor is thus 30.
- Proposal: Apply an uncertainty factor of 30 to the ACGIH TLV for 2-nitropropane, giving an AOEL for 2-nitro-2-methylpropane of 0.3 ppmv. This proposal was unanimously approved.

N-methylaziridine (1072-44-2) – Presented by J. Meacham and T. Poet

- See Attachment 16.
  - Tentatively identified in 1 tank headspace, from radical reactions of various components.
  - The high bond angle strain of the 3-member ring leads to chemical activity and results in the mutagenic and carcinogenic effects.
  - Aziridine (ethylenimine) has a TLV of 0.5 ppmv. It is irritating to the skin, eyes, and lungs; some kidney damage has also been reported. Exposures at 25 ppmv for more than 4 hours resulted in death in rats and guinea pigs. Embryotoxicity was demonstrated in test animals as low as 0.6 ppmv. Vapor exposures in humans up to 3 hours did not show any health effects.
  - The proposed AOEL uses the aziridine TLV of 0.5 ppmv as a point of departure, applying an uncertainty factor of 10 for lack of data.
- Proposal: Apply an uncertainty factor of 10 to the ACGIH TLV for aziridine, giving an AOEL for n-methylaziridine of 0.05 ppmv. This proposal was unanimously approved.

2,4-Dimethylpyridine (108-47-4) – Presented by J. Meacham and T. Poet

- See Attachment 17.
  - Tentatively identified in 4 tank headspaces. 2,4-Dimethylpyridine is a potential degradation product of polyvinyl resins.
  - Minimal toxicological data is available for 2,4-dimethylpyridine. DOE assigned a TEEL-1 (similar in nature to an OSHA emergency PEL) of 0.5 ppmv.
  - 2,4-Dimethylpyridine is a food additive that is recognized by the World Health Organization as having "no safety concern."
  - A similar compound, pyridine, has a TLV of 1 ppmv. Chronic inhalation exposure to pyridine derivatives in high concentrations produced CNS and GI disturbances, facial paralysis, ataxia (facial tics), and unequal pupils.
  - ACGIH set TLVs for related alkyl pyridines of 2 ppmv.
  - The proposal is to adopt the TEEL-1 as the AOEL.
- Discussion
  - Questions were raised regarding the nature of the TEEL-1. Poet pointed out that this is similar to an OSHA emergency standard. It is equivalent to an 8 hr TWA.
  - The TEEL value is lower (safer) than if we were to apply an uncertainty factor to the TLV for the alkyl pyridines.
- Proposal: Adopt the DOE TEEL-1 of 0.5 ppmv as the AOEL for 2,4-dimethylpyridine. This proposal was unanimously approved.

1,2,3,6-Tetrahydropyridine (694-05-3) – Presented by J. Meacham and T. Poet

- See Attachment 18.
    - Tentatively identified in 2 tank headspaces. 1,2,3,6-Tetrahydropyridine is a potential degradation product of hydrocarbon diluents.
    - No toxicological data is available for 1,2,3,6-tetrahydropyridine. It is similar to pyridine or piperidine.
    - Chronic inhalation exposure to pyridine derivatives in high concentrations produced CNS and GI disturbances, facial paralysis, ataxia (facial tics), and unequal pupils.
    - Piperidines are used as non-sedating antihistamines.
    - 1,2,3,6-Tetrahydropyridine is more structurally similar to piperidine than to pyridine.
    - The TLV for pyridine is 1 ppmv. The AIHA WEEL for piperidine is 1 ppmv.
    - The proposed AOEL uses the piperidine WEEL of 1 ppmv as a point of departure, applying an uncertainty factor of 10 for lack of data and negligible structural differences.
- Proposal: Apply an uncertainty factor of 10 to the AIHA WEEL for piperidine of 1 ppmv, giving an AOEL for 1,2,3,6-tetrahydropyridine of 0.1 ppmv. This proposal was unanimously approved.

The meeting was adjourned at 1415, to reconvene tomorrow.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
January 17, 2006, 2440 Stevens, Rm 1305A

Purpose: Determine safe, effective, and scientifically justified Tank Farms acceptable occupational exposure levels (AOEL) for nitrosamines and 1-naphthylamine.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Joe Meacham, CH2M HILL
Dave Farler, CH2M HILL
Chuck Timchalk, PNNL
Joseph Samuels, AMH
Gretchen Bruce, Intertox – by teleconference
Gary Pascoe, representing Intertox – by teleconference

The meeting was called to order at 0800 by T. Anderson.

For each proposed AOEL, the originator gave a presentation on the background for the AOEL. After discussion, a vote was taken on whether to accept the proposed AOEL.

Nitrosamines – Presented by G. Pascoe

- See Attachment 1.
    - Nitrosamines are formed unintentionally during manufacturing processes, and by reactions with other nitrogen-containing compounds.
    - Potential sources of exposure were discussed.
    - Human and animal epidemiological studies have shown gastric and lung cancers, as well as tumors, from all routes of nitrosamine exposures.
    - A hierarchical approach to assessing toxicity was discussed, scaling the relative toxicity in various ways: by cancer slope factors, inhalation unit risk, and carcinogenic potency (TD_{50}).
    - Germany and the Netherlands have set MAK/MAC values of 0.3 ppbv for both nitrosodimethylamine (NDMA) and nitrosomethyethylamine (NMEA).
    - Reasons were presented for not using toxicity criteria to evaluate toxicity. The essence is that data is inconsistent.
    - A ranking approach was presented.
        - First, determine which of the 2 nitrosamines with OELs is most potent.
        - Identify a metric of carcinogenic potency: the TD_{50} for NMEA was chosen.
        - Derive a potency scale based on the TD_{50} for each nitrosamine, and apply this proportionately to the NMEA OEL.

- The proposed AOEL uses the relative carcinogenic potency ranking scale, based on the NMEA MAK/MAC, as shown in the table on page 7 of Attachment 1.

- Discussion:
  - Who produces the TD_{50} values, are they standard and accepted? See the discussion on page 6 of attachment 1.
  - How were the MAKs/MACs developed, and on what are they based? They use a mix of criteria, similar to the PEL and TLV process: research, toxicity data, feasibility, detection limits, etc.
  - What animal species are the TD_{50} values based upon? Rats, mice, and hamsters.
  - A general discussion of TD_{50} values ensued. They have support by the U.S. EPA, and have been used to develop published standards. How do they compare with our stated acceptable risk of 10^{-4}? They are generally 10^{-3}. This makes them comparable to many of the PELs and TLVs that we have accepted. This is reasonable, based on the fact that they are derived from published OELs – the MAKs/MACs.
  - Can NDEA be detected at 160 pptv? Yes.
  - The values listed in the table are not consistent for significant figures. It was decided to truncate these values to the nearest tenth.

- Proposal: Apply the relative carcinogenic potency ranking scale, based on the NMEA MAK/MAC, resulting in the below-listed AOELS. This proposal was unanimously approved.

- Note that the AOEL for NDMA was set at a previous meeting, adopting the MAK/MAC of 0.3 ppbv.

n-nitrosomethylethylamine (NMEA)	0.3 ppbv
n-nitrosodiethylamine (NDEA)	0.1 ppbv
n-nitrosomorpholine	0.6 ppbv
n-nitrosodipropylamine (NDPA)	1 ppbv
n-nitrosodibutylamine (NDBA)	4 ppbv
n-nitrosopiperidine	8 ppbv
n-nitrosopyrrolidine	4 ppbv

1-Naphthylamine (134-32-7) – Presented by G. Bruce

- See Attachment 2.
  - 1-Naphthylamine is not naturally produced. It is used as chemical intermediates in production of dyes, herbicides, and other chemicals.
  - Studies have shown an association with bladder cancer in humans and dogs, and liver tumors in mice.
  - Little toxicity information is available. No cancer slope factor can be derived for 1-naphthylamine.

  - It is structurally similar to 2-naphthylamine, also a known potent bladder carcinogen.
  - 29 CFR 1910.1003 states that all contact should be avoided.
  - N-oxidation is an important step in carcinogenic activation of 2-naphthylamine. It is uncertain how this may apply to 1-naphthylamine.
  - Based on relative toxicity information for liver cancer in rats, it was suggested that an adjustment factor of 2 (i.e., double) could be applied to the AOEL calculated for 2-naphthylamine using the EPA formula.

- Discussion
  - When OSHA recommends that contact with 1-naphthylamine be avoided, does this include vapors? Yes.
  - It was concluded that there was no convincing evidence to apply an adjustment factor to the AOEL calculated using the cancer slope factor for 2-naphthylamine.

- Proposal: Calculate an AOEL for 1-naphthylamine using the EPA formula for 2-naphthylamine, resulting in an AOEL for 1-naphthylamine of 1 $\mu g/m^3$, or 0.2 ppbv. This proposal was unanimously approved.

The meeting was adjourned at 1000.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
January 26, 2006, 2704HV, G230

Purpose: Review the list of chemicals of potential concern (COPC), determine whether there are chemicals that should be added or removed.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Susan Eberlein, CH2M HILL
Kathleen Hall, CH2M HILL
Jim Honeyman, CH2M HILL
Joe Meacham, CH2M HILL
Dave Farler, CH2M HILL
Jill Molnaa, CH2M HILL
Ed Carter, CH2M HILL
Jim Huckaby, PNNL

The meeting was called to order at 1000 by T. Anderson.

Jim Huckaby led a discussion of proposed COPC list changes (Attachment 1). After discussion, a vote was taken on whether to add or remove individual chemicals or groups.

Huckaby began with a review of the original list of COPC and changes that have been made before today.

- The Industrial Hygiene Technical Basis Document (Tech Basis) Rev. 0 of Oct 2004 published the original list of COPC. This list contained 52 chemicals.
    - A question was asked why the Independent Toxicology Panel (ITP) recommended 4 chemicals on the list. In scanning the 1,837 chemicals listed in the Tech Basis, the ITP thought that these chemicals were particularly dangerous and warranted special review.
- A July 2005 memo from Jim Honeyman made adjustments to the list of 52 COPC.
    - Replaced the two Aroclors with "chlorinated biphenyls."
    - Added pyridine and 3-buten-2-one, which had been erroneously left off the list.
    - Removed carbon monoxide, carbon dioxide, and nitrogen dioxide, since these are common environmental pollutants, not tank waste specific, and they will be evaluated under general industrial hygiene procedures.
    - Removed 7 misidentified chemicals.
    - The result was a list of 42 COPC, plus chlorinated biphenyls.

The 1,837 Tech Basis chemicals were dispositioned as either COPC, non-COPC, or chemicals needing further evaluation. The recent completion of AOELs (see EASRG meeting notes from

16 and 17 January 2006) allowed review and disposition of most of the chemicals requiring evaluation. That review follows.

COPC List Additions #1

- The following are proposed for addition to the COPC list based on the finalized AOEL list.
    - 4-Methyl-2-hexanone (105-42-0)
    - 2,4-Dimethylpyridine (108-47-4)
    - Furan (110-00-9)
    - 2-Methyl-2-butenal (1115-11-3)
    - 2-Fluoro-1-propene (1184-60-7)
    - 1,4-Butandiol dinitrate (3457-91-8)
    - Butyl nitrite (544-16-1)
    - N-Nitrosomorpholine (59-89-2)
    - 1,3-Dinitrate-1,2,3-propanetriol (623-87-0)
    - Methyl nitrite (624-91-9)
    - Heptanenitrile (629-08-3)
    - Dibutylbutylphosphonate (78-46-6)
    - 3-Methyl-3-buten-2-one (814-78-8)
    - Butyl nitrate (928-45-0)
    - 6-Methyl-2-heptanone (928-68-7)
- Discussion
    - Huckaby noted that the origin of 2-fluoro-1-propene in the tanks is unclear.
    - Are there any potential problems with identification of these chemicals? The two nitrites may not have standards available, but they should be able to be seen as TICs (tentatively identified compounds).
    - The 222-S Laboratory will investigate acquiring standards for all COPC, and will plan in advance for analyzing them.
    - Personal monitoring will likely be semi-quantitative.
- Proposal: Add these chemicals to the COPC list. This proposal was unanimously approved.

COPC List Additions #2

- An AOEL was approved by the EASRG for substituted furans. They are proposed for addition to the COPC list.
- The current list of substituted furans detected in tank headspaces is:
    - 2,3-Dihydrofuran (1191-99-7)
    - 2-Methylfuran (534-22-5)
    - 2,5-Dimethylfuran (625-86-5)
    - 2-Ethyl-5-methylfuran (1703-52-2)
    - 4-(1-Methylpropyl)-2,3-dihydrofuran (34379-54-9)

  - 2-Pentylfuran (3777-69-3)
  - 2-(2-Methyl-6-oxoheptyl)furan (51595-87-0)
- Discussion
  - Furan has a separate AOEL and is still listed separately on the COPC list.
  - Discussion was raised on what constitutes a "substituted furan." It was decided that any substitution to the basic unsaturated furan ring is a substitution.
  - Will high-resolution mass spectroscopy be needed for identification? It may be possible to use selected ion monitoring. This will have to be added to the scope of the lab's capabilities.
- Proposal: Add the substituted furans to the COPC list. This proposal was unanimously approved.

COPC List Removals #1 – Carbon Disulfide (75-15-0)

- This is on the COPC list because the Tech Basis required use of the lowest occupational exposure guideline (LOEG). The NIOSH REL of 2 ppmv was used for the Tech Basis initial screening.
- If the LOEG is used as the basis for screening, carbon disulfide becomes a COPC because its maximum headspace concentration was 0.8 ppmv, above 10% of the LOEG.
- The OSHA PEL is 20 ppmv; the ACGIH TLV is 10 ppmv. Thus, carbon disulfide is present in the headspaces below 10% of the TLV.
- Discussion
  - What led NIOSH to set the low REL? This was based on teratogenic potential.
  - Was this ever used as a process chemical? It may have been used as an extractant. It could also be a lab contaminant.
  - The highest headspace concentration was seen in C-103.
  - Is there compelling reason to use the LOEG for screening rather than the TLV? No. To be consistent with DOE O 440.1A and with our current process, it is more reasonable to use the TLV.
  - Carbon disulfide will still be identified as a TIC in sampling, so if it is present it will be detected.
- Proposal: Remove carbon disulfide from the COPC list because it is not present above 10% of the OEL (ACGIH TLV). This proposal was unanimously approved.

COPC List Removals #2 – #8

- These compounds were added to the COPC list under the policy that all probable carcinogens were automatically COPC, regardless of concentration.
- Current policy of the EASRG accepts OELs for carcinogens if the originating agency considered the carcinogenic effects when setting the OEL; it also allows using EPA carcinogen methodology to set AOELs, as has been done for several compounds.

- The following compounds are proposed for removal from the COPC list based on the fact that they were added under the blanket carcinogen policy, their OEL accounts for carcinogenicity, and they are not present above 10% of their OEL:
    - 1,4-Dioxane (123-91-1)
    - Bis(2-ethylhexyl)phthalate (117-81-7)
    - 2-Nitropropane (79-46-9)
    - Chloroform (67-66-3)
    - Carbon tetrachloride (56-23-5)
    - Trichloroethylene (79-01-6)
    - Tetrachloroethylene (127-18-4)
- All of these will still be seen in sampling as TICs.
- Proposal: Remove the above compounds from the COPC list because they are not present above 10% of their OEL. This proposal was unanimously approved.

COPC List Removal #9 – 2-Ethyl-1-Hexanol (104-76-7)

- This compound was added to the COPC list because the Independent Toxicology Panel suggested that it be closely evaluated.
- It is a phosphate degradation product, and is not a carcinogen.
- Its maximum headspace concentration is 0.49 ppmv, 2.5% of the TLV.
- It will still be seen in sampling as a TIC.
- Proposal: Remove 2-ethyl-1-hexanol from the COPC list because it is not present above 10% of the OEL. This proposal was unanimously approved.

COPC List Removal #10 – 3-Hexanone (589-38-8)

- This compound was added to the COPC list because the Independent Toxicology Panel suggested that it be closely evaluated.
- Its maximum headspace concentration is 6.3 ppmv, 9.4% of the TLV.
- It will still be seen in sampling as a TIC.
- Proposal: Remove 3-hexanone from the COPC list because it is not present above 10% of the OEL. This proposal was unanimously approved.

COPC List Removals #11 – 13

- These compounds were determined to be lab contaminants, and are not actually present in the tanks.
    - Chloroethene (75-01-4)
    - 1,2-Dichloroethane (107-06-2)
    - 1,2-Dibromoethane (106-93-4)
- They were seen in blanks at the same levels as in standards.

- Data results were confirmed as suspect by the chemist who reviewed the results. They will be flagged "suspect" when entered into TWINS.
- Proposal: Remove these 3 compounds from the COPC list because they are not actually present in the tanks. This proposal was unanimously approved.

The meeting was adjourned at 11:30.

CH2M HILL Hanford Group Environmental Health
Exposure Assessment Strategy Review Group Meeting
February 15, 2006, 2440 Stevens, Rm 1200

Purpose: Review the list of chemicals of potential concern (COPC), determine whether there are chemicals that should be added or removed.

Attendees:

Tom Anderson, CH2M HILL, Chair
Mike Zabel, CH2M HILL
Susan Eberlein, CH2M HILL
Kathleen Hall, CH2M HILL
Joe Meacham, CH2M HILL
Don Slaugh, CH2M HILL
Jim Huckaby, PNNL

The meeting was called to order at 0700 by T. Anderson.

Jim Huckaby presented the following reviews of proposed changes to the COPC list.

Methylene Chloride (75-09-2)

- This was added to the COPC list under the policy that all probable carcinogens were automatically COPC, regardless of concentration.
- Current policy of the EASRG accepts OELs for carcinogens if the originating agency considered the carcinogenic effects when setting the OEL; it also allows using EPA carcinogen methodology to set AOELs, as has been done for several compounds.
- Methylene chloride has a TLV of 50 ppmv and a PEL of 25 ppmv. Its highest headspace concentration is 1.7 ppmv, or 7% of the PEL.
- The PEL does take into account potential carcinogenicity.
- Proposal: Remove methylene chloride from the COPC list. This proposal was unanimously approved.

Four Proposed New COPCS

- The following are compounds that were on the screening list and have since had acceptable occupational exposure levels (AOELs) established. Their maximum headspace concentrations are above 10% of the AOEL.
    - 2,4-Pentadienenitrile (1615-70-9)
    - 2-Nitro-2-methylpropane (594-70-7)
    - 2-Ethylhex-2-enal (645-62-5)
    - 2-Methylene butanenitrile (1647-11-6)
- Proposal: Add these four compounds to the COPC list. This proposal was unanimously approved.

Four Chemicals from C-204

- The following 4 compounds were detected at concentrations above 10% of the OEL from headspace sampling in C-204 in 1996. Subsequent sampling in C-204 and sampling elsewhere has not detected them at these levels.
    - 1-Nitrobutane (627-05-4)
    - 1,3-Propanediol dinitrate (3457-90-7)
    - 5-Methyl-2-(1-methylethenyl)cyclohexanone (89-82-7)
    - 4,7,7-Trimethylbicyclo[4.1.0]heptan-3-one (4176-04-9)
- The sampling data package from the 1996 sampling has not been found and is presumed lost, so it was not possible to review the data.
- Re-sampling done in 2004 showed much lower levels.
- 1-Nitrobutane was much lower in the triple-sorption tube (TST) sample than in the SUMMA collected at the same time. The last 3 on the list were detected in only 1 of 3 SUMMA samples taken during the 1996 sampling event.
- Discussion
    - Could these chemicals have been released in a "vapor burst" event? Not likely; this kind of event has not been seen elsewhere, and there are other more likely explanations.
    - Are we confident that the 2004 sampling was adequate? Yes, that data was reviewed and no inconsistencies were found.
    - These compounds are not difficult to analyze for.
    - These compounds are easily detected as TICs.
- Proposal: Do not add these four compounds to the COPC list. This proposal was unanimously approved.

2,6-Bis(1,1-dimethylethyl)-4-methylphenol (BHT) (128-37-0)

- This compound was only reported during the first use in 1994 of a new heated manifold sampling system. It is a plasticizer that is very likely to have come from off-gassing of the sampling system itself.
- It is not likely to be a tank vapor.
- Recommend removing from the COPC list.
- Proposal: Remove BHT from the COPC list. This proposal was unanimously approved.

Dichlorodiphenyldichloroethylene (DDE) (72-55-9)

- This is on the COPC list because it is a carcinogen. It was reported in solids samples from C-104; it has never been detected in headspace sampling.
- It is semi-volatile and highly soluble in water.
- Recommend removing from the COPC list.

- Proposal: Remove DDE from the COPC list. This proposal was unanimously approved.

1-Naphthylamine (134-32-7)

- This is on the COPC list because it is a carcinogen. It was reported in solids samples from AW-101 and AN-107; it has never been detected in headspace sampling.
- It is semi-volatile and moderately soluble in water.
- Based on measured non-vapor phase concentrations, dilution with other waste by subsequent retrievals, and the low probability of equilibrium concentrations developing, its vapor concentration could not be above 10% of the AOEL.
- Recommend removing from the COPC list.
- Proposal: Remove 1-naphthylamine from the COPC list. This proposal was unanimously approved.

The only compounds now awaiting determination as to COPC status are methyl isocyanate, sulfur oxides, and ethylamine. Sampling and analysis are underway to make these determinations.

The meeting was adjourned at 0815.

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APPENDIX F

PROCEDURE FOR DEVELOPING NON-CARCINOGEN ACCEPTABLE OCCUPATIONAL EXPOSURE LEVELS

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PROCEDURE FOR DEVELOPING NON CARCINOGEN ACCEPTABLE OCCUPATIONAL EXPOSURE LEVELS

F1.0 PURPOSE

A large number of volatile compounds have been identified in the headspaces of single- and double-shelled tanks used to store mixed chemicals and radioactive waste at the U.S. Department of Energy (DOE) Hanford Site. Concern for the potential exposure of workers to vapors during Tank Farms operations has prompted efforts to evaluate the potential heath risk associated with exposure to these chemicals. Occupational exposure limits (OELs) have not been established for many of these chemicals.

This standard operating procedure (SOP) has been prepared to provide a framework of technical guidance to be used by trained toxicologists or risk assessors. The goal of this SOP is to establish a process for assigning an Acceptable Occupational Exposure Level (AOEL) to non-carcinogenic chemicals or families of chemicals that do not have established OELs identified in the tank waste headspaces at or above preliminary screening values. Hence, there is a need to undertake a more rigorous assessment and establish an AOEL for these chemicals. An AOEL is defined as a level of exposure to a given chemical expected to lead to no adverse health effects that is acceptable to management, professionals, and workers at the Hanford Site.

F2.0 ESTABLISHED EXPOSURE GUIDELINES

OELs are established in this country by the Occupational Health and Safety Administration (OSHA) of the U.S. Department of Labor and are legal obligations for defined industries. The National Institute for Occupational Safety and Health (NIOSH) is an arm of the Centers for Disease Control (CDC) and makes recommendations to OSHA regarding OEL values. The American Conference of Governmental Industrial Hygienists (ACGIH) is a private organization that recommends OEL values to industry for voluntary application. Other human exposure standards have been published, e.g., Emergency Response Planning Guidelines by the American Industrial Hygiene Association (AIHA), Workplace Environmental Exposure Levels by the AIHA, and Acute Exposure Guideline Levels by the U.S. Environmental Protection Agency (EPA). However, their applicability as OEL values for use in Tank Farms must, in each case, be evaluated. The DOE mandates the need to comply with the OSHA and ACGIH standards in its contract with CH2MHILL Hanford Group, Inc.; in cases where both standards exist, the more stringent of the two is applied.

F3.0 APPROACH OVERVIEW

The National Academy of Sciences (NAS 1983; 1994; GAO 2001) has provided overall guidance for chemical risk assessment as further developed and applied by U.S. regulatory agencies. The process for establishing an AOEL for tank waste chemical exposure is modeled upon the generalized scientific approaches used by OSHA and ACGIH to establish OELs for worker exposure. In addition, where appropriate, the scientific approach used by other regulatory agencies such as the EPA to establish reference concentrations (RfC) for airborne pollutants are also considered.

A flow diagram illustrating the key steps in the assessment process is illustrated in Figure F-1. The approach first requires identifying specific chemical agents or classes of chemical agents that are detected in the tank headspace at or above previously established screening values. Chemical agents that exceed the screening values will undergo a more extensive evaluation with the goal of establishing an AOEL for Tank Farms operations. First, a detailed review of relevant OELs will be undertaken. When appropriate exposure guidelines have not been established, available epidemiology and toxicology information on a given chemical or chemical class will be reviewed to identify potential hazards, select critical effects, and estimate dose-response to determine suitable exposure levels (Haber and Maier 2002). Consistent with the technical approaches ACGIH uses for establishing a Threshold Limit Value (TLV), the AOEL will be based on the best scientific information available and will include a critical evaluation of all supporting information (ACGIH 2005).

The goal of the evaluation will be to delineate the most important adverse effects. In evaluating the health effects, human data (e.g., epidemiology studies) are of prime importance, but for chemicals with little or no available human data, a second tier evaluation will be used. The second tier evaluation will focus on the most relevant and sensitive animal toxicity data for the chemical and/or chemical class. In this case, the basis for the AOEL will be the dose-response relationship for the toxic effects of greatest concern, and the point of departure (POD) for calculating the AOEL will be the associated no-observed-effect-level/lowest-observed-effect-levels (NOEL/LOEL). The rationale for the selection of a given toxic effect for the AOEL will be documented.

For setting an AOEL, an appropriate risk assessment approach will be selected based on the critical toxicological effect, the observed dose-response, and the quality of the data used for the assessment (ACGIH 2005). This may include the use of quantitative dose-response models such as the benchmark dose (BMD), and/or the application of added factors to a NOEL/LOEL to address uncertainty.

Before establishing and implementing a formal AOEL for worker protection in the Tank Farms, the proposed exposure level for a given chemical and/or chemical class will be submitted to the Exposure Assessment Strategy Review Group for review. Ideally, the reviewers will include a range of health and science professionals, which could include representatives from occupational medicine, toxicology, risk assessment, industrial hygiene, health physics, and worker groups. The objective of the review will be to critically assess the rationale for establishing the AOEL,

provide the broad base of stakeholders an understanding of the rationale for the AOEL, and provide stakeholders an opportunity to participate in the assessment.

F3.1 DATABASE AND LIGERATURE EVALUATION

F3.1.1. Database Searches

It is imperative that relevant human exposure, epidemiology, and toxicological information be considered in establishing AOELs. A methodical analysis of the available literature as it relates to hazard identification and quantitative dose-response toxicity evaluation is central to the AOEL assessment process. Internet databases such as TOXNET®, TOMES®, PUBMED®, International Agency for Research on Cancer (IARC), and/or STN®, should be utilized as primary sources for initiating searches, and the searches should include both the name and Chemical Abstracts Service registry number of the compound of interest (see Table F-1). These databases contain information applicable to toxicological assessment of chemicals, and the information they provide may overlap. For example, both TOXNET and TOMES contain the RTECS® and HSDB® files. In the event RTECS and/or HSDB files do not exist for a compound or are considered insufficient, the TOXNET literature and/or PUBMED databases should be searched and the original literature evaluated for any relevant information. If relevant information is not located in this manner, PUBMED may be searched directly and/or the chemical abstracts database searched through STN. If information is found in one or more of the above sources but is incomplete, conflicting or considered insufficient, other sources such as NIEHS/NTP, IARC, EPA, and Agency for Toxic Substances and Disease Registry Monographs (ATSDR) may also be searched. Frequently, more in-depth information of the chemical of interest or its surrogate can be located in this way and may be useful in assigning an AOEL.

Table F-1. Abbreviations and Acronyms

Organizations	
ACGIH	American Conference of Governmental Industrial Hygienists
AIHA	American Industrial Hygiene Association
ATSDR	Agency for Toxic Substances and Disease Registry Monographs (ATSDR)
EPA	U.S. Environmental Protection Agency
IARC	International Agency for Research on Cancer
OSHA	Occupational Safety and Health Administration

Databases	
TOXNET®	The Toxicology Data Network, a set of databases covering toxicology, hazardous chemicals, and related areas; it is maintained by the National Library of Medicine (NLM). (http://toxnet.nlm.nih.gov/)
HSDB®	Hazardous Substances Data Bank. Accessible through TOXNET. Provided by the NLM.
PUBMED®	PubMed, provided by the NLM, contains citations for biomedical articles back to the 1950s; sources include MEDLINE and additional life science journals. (http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=PubMed).
RTECS®	Registry of Toxic Effects of Chemical Substances, provided by Thomson Micromedex, Inc. Accessed through TOMES®, which has the same provider.
STN®	STN is the Scientific & Technical Information Network, provided by FIZ Karlsruhe, the American Chemical Society (ACS), and the Japan Science and Technology Corporation (JST). It links to published research in the world's journal and patent literature back to the beginning of the 20th century.
TOMES®	Registry of Toxic Effects of Chemical Substances, provided by Thomson-Micromedex, Inc.

F3.1.2. Literature Evaluation of Published Exposure Guidelines

Initial efforts should focus on a comprehensive evaluation of the available literature that will identify any published exposure guidelines for the chemical of interest or for a reasonable surrogate. The summary documentation used to support the establishment of the OEL should be reviewed to ascertain its relevance, and any AOEL that is adopted based on these published OELs should include appropriate documentation justifying the scientific rationale for its use.

F3.1.3. Use OEL Surrogates

If there are no appropriate exposure guidelines for the chemical of interest, it may be reasonable to identify and assign an OEL based on a structurally related chemical (surrogate). In addition to being structurally related, ideal surrogates should also have a similar toxicological profile (i.e., similar target organs and response); although they may display greater or lesser potency than the chemical of concern. The basis for the choice of the surrogate should be explained and include a brief discussion of the rationale for the assigned OEL for the surrogate.

F4.0 TOXICOLOGY REVIEW

F4.1 TOXICITY REVIEW CRITERIA

In evaluating the toxicity profile for a chemical or chemical class, the assessment should be prioritized based on identification of toxic effects that are particularly relevant for occupational exposure. This would include:

- Identifying chemical agents that have a high acute toxicity potential such as Category 1 chemicals as defined by the Organization for Economic Co-operation and Development (OECD 2004). Chemicals in Category 1 which are considered by OECD to have high acute toxicity potential have LD_{50} and LC_{50} values of $\leq$ 5 mg/kg oral and $\leq$ 100 ppmv inhalation, respectively. These would be of particular concern if the LD_{50}/LC_{50} values do not have large safety margins (<100) between observed toxicity and potential exposure levels.
- Giving priority to the evaluation of studies that utilize the most relevant occupational exposure routes [Inhalation > Oral > Dermal > Others (intravenous/ intraperitoneal)].
- Giving priority to well-characterized dose-response toxicity studies, particularly those that include a more comprehensive evaluation of the toxicity, which includes quantitative in vivo (acute $\rightarrow$ sub-chronic $\rightarrow$ chronic) experiments.

The toxicity testing paradigm suggests that with increasing length of chemical exposures (i.e., acute $\rightarrow$ chronic) the effective dose levels generally decrease such that the lowest NOEL/LOEL will be determined from long-term studies. In addition, long-term chronic studies can identify chemicals that have the potential to produce a broad range of chronic health effects. An important strength of this testing paradigm is that it provides a fairly comprehensive in vivo toxicological evaluation that can be used to link dose-response results across a very broad range of exposure routes (oral vs. inhalation), doses (low vs. high), durations (sub-chronic vs. chronic), and species (rat vs. dog). The use of this type of testing data will provide greater confidence (i.e., less uncertainty) in the AOEL that is established.

F4.2 MINIMAL DATA SETS

As discussed by Haber and Maier (2002), a number of regulatory authorities including the Health Council of the Netherlands (HCN 2000) and the U.S. EPA (EPA 1994) have established minimum data requirements based on the rationale that any value derived from a data set that is less than the minimum prescribed would have too much uncertainty. An alternative approach is to identify the types of data that are particularly useful and utilize a weight-of-evidence approach in the evaluation that looks at the sum total of all available information (SCOEL 1999; Haber and Maier 2002). In this regard, a weight-of-evidence review for the development of an AOEL would focus on evaluating the types of studies that have greater relevance to occupational exposure and are amendable to establishing a dose-response relationship.

F5.0 PROCEDURE FOR CALCULATING AN ACCEPTABLE OCCUPATIONAL EXPOSURE LEVEL

F5.1 POINT OF DEPARTURE (POD)

The overarching goal in evaluating the toxicity databases is to determine a POD for developing an AOEL. Haber and Maier (2002) defined the POD as the concentration to which uncertainty factors are applied to derive an AOEL. The POD is most likely the NOEL/LOEL that was determined from the most appropriate toxicity study. In practice, this is usually the lowest determined NOEL that was experimentally derived. It is also possible to utilize a benchmark dose (BMD) approach, as described below, to determine a POD, particularly when the experimental studies did not identify a NOEL (Fillipsson et al. 2003; Haber and Maier 2002; Crump 1984; Dourson et al. 1985).

F5.2 APPROACH FOR DEVELOPING EXPOSURE LEVELS FOR NON-CANCER EFFECTS

As suggested by Bailey (2002) and others, there are numerous sources of uncertainty in the establishment of an acceptable exposure level. The approach used for identifying an acceptable exposure level for the general population or for occupational-related exposures is to adjust the NOEL or LOEL downward. The magnitude of the downward adjustment reflects the degree of uncertainty concerning the acceptable exposure limits. To address these uncertainties, empirical factors may be used to account for inadequate experimental data, interspecies variability, human variability, or extrapolation for short-term to long-term studies (EPA 2002; Dorne and Renwick 2005). In addition to uncertainty factors, additional modifying factors (MF) have also been occasionally used by some regulatory agencies such as EPA to reflect uncertainties not addressed by other factors. The following will be used to calculate the AOEL.

$$AOEL = \frac{NOEL \text{ or } LOEL}{UFxMF} \qquad \text{(F-1)}$$

The application of empirical uncertainty factors to determine the AOEL is based on the methods utilized by EPA for deriving an RfC (EPA 2002). The default uncertainty factor (UF) generally covers a single order of magnitude (i.e., 10^1), or a value of three is used in place of one-half powers (i.e., $10^{0.5}$). Additional factors could also be considered for inadequate data and for extrapolation from less than lifetime to lifetime exposures. As suggested by the EPA, supporting documentation should include the justification used for the individual factors selected. In addition, as recommended by the EPA (2002), it is advisable to limit the total UF applied to any particular chemical to no more than 3,000 and avoid deriving an exposure guideline that involves the full ten-fold UF in four or more areas of extrapolation. The following uncertainty and modifying factors could be applied:

- ***Extrapolation from animal data to humans (interspecies UF).*** This factor is intended to account for the uncertainty in extrapolating animal data to the case of average healthy human. It assumes that humans are more susceptible to the toxicity than the animal species evaluated.
- ***Variability in the human population (intraspecies UF).*** This factor is intended to account for the variation in sensitivity among humans.
- ***LOEL to NOEL UF.*** This factor is intended to address the uncertainty associated with extrapolation from LOELs to NOELs.
- ***Sub-chronic to chronic duration UF.*** This factor is intended to account for the uncertainty in extrapolating from less than chronic NOELs to chronic NOELs.
- ***Inadequate database UF.*** This factor is intended to account for the inability of any single animal study to adequately address all possible adverse outcomes in humans.
- ***Modifying factors MF.*** This factor is intended to account for any other scientific uncertainties in the study or databases that are not explicitly treated by other UFs. The magnitude of the MF principally depends on professional judgment.

F5.3 ESTABLISHING A NOEL USING BENCHMARK DOSE (BMD)

As noted by Dorne and Renwick (2005), the utilization of a BMD as proposed by Crump (1984) defines a lower statistical confidence for the dose, corresponding to a predefined low level of increase in adverse effects over background. The BMD approach provides a more quantitative alternative to the first step in the dose-response assessment than the NOEL/LOEL process (EPA 2000). This is particularly useful when a NOEL has not been adequately defined from the experimental data.

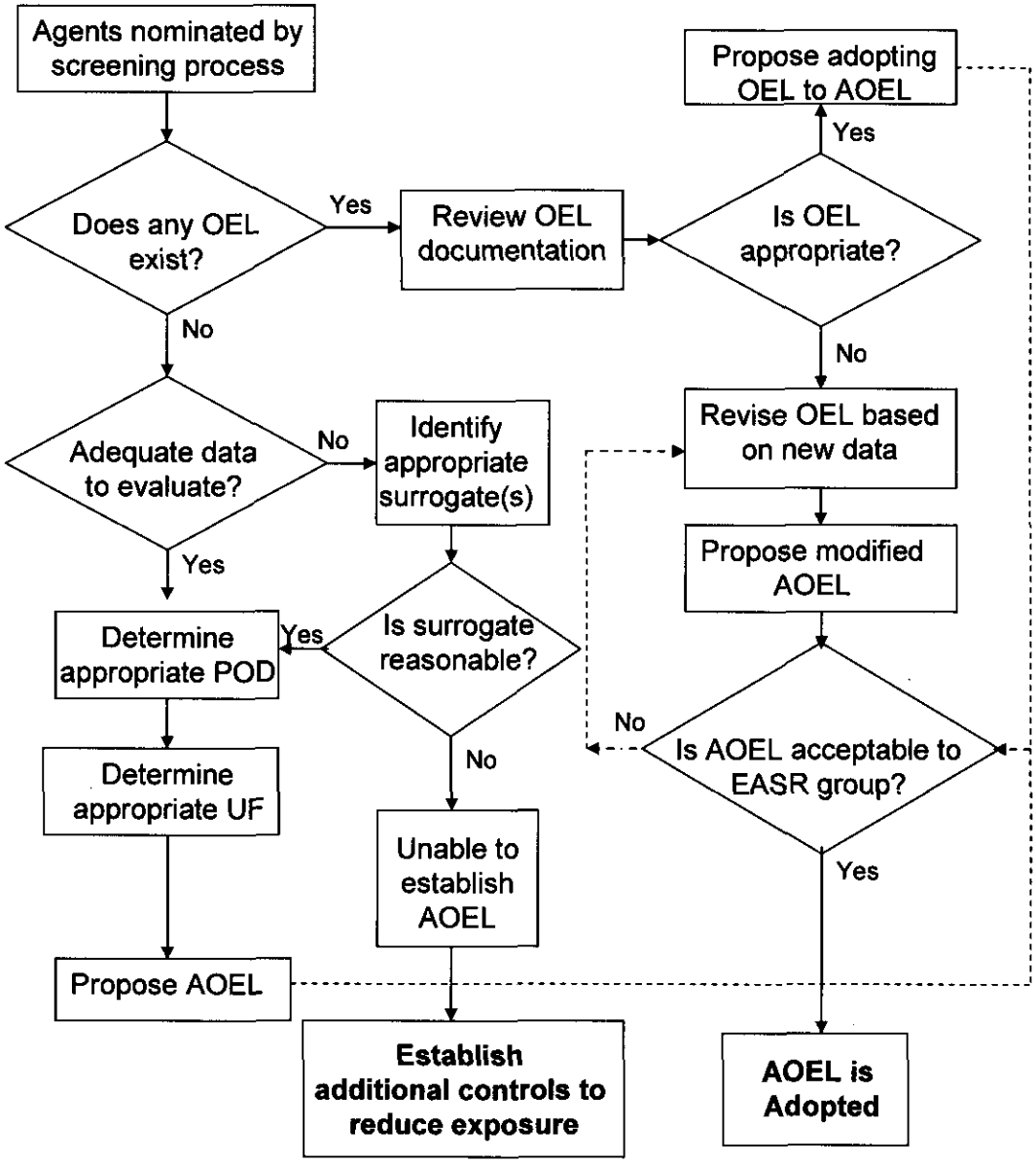
The approach will utilize the EPA's BMD software that is available on the internet (http://www.epa.gov/ncea/bmds.htm). The EPA guidance document (EPA 2000) provides a detailed discussion on a number of important considerations including the types of studies that are appropriate for BMD, selection of the benchmark response values, choice of models for computing BMD, and details concerning the computation of confidence limits for the BMD. Based on the EPA criteria, a 10% response is at or near the limit of sensitivity in most cancer and non-cancer bioassays and will be used as an appropriate Effective Dose (ED10) for the BMD.

As indicated in the EPA guidance (EPA 2000), the primary goal of the mathematical modeling is to fit a model to dose-response data, particularly at the low end of the observable dose-response range. The recommended criteria for selection of an appropriate model for BMDL computation is the Akaike's Information Criterion (AIC). The AIC values are computed for each of the models used in the BMD calculation and compared to select the most appropriate model. Once a BMD value is selected, a lower confidence is placed on the BMD to obtain a dose (BMDL) that ensures with high confidence (95%) the Benchmark Response is not exceeded. The BMDL can then be used in the numerator of Equation F-1 to calculate an AOEL, as described above.

F5.4 FORMAT FOR AOEL DOCUMENT

The AOEL documentation for a given chemical or chemical class will include the following sections. The Executive Summary will be in an abstract format that reasonably communicates the overall process and conclusions of the analysis. A Methodology section will briefly describe the approach used for developing the AOEL, and this will be followed by a section that describes the Available Guidelines that are particularly relevant in developing the AOEL. The Toxicology Summary section will review pertinent human epidemiology and animal toxicology results that are directly relevant to the setting of the AOEL. This will not entail a detailed description of all the available data but will focus on the key studies and results pertinent to the evaluation. The Data Analysis section will describe the process used for setting the AOEL

Figure F-1. Flow Diagram for Establishing an AOEL



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APPENDIX G

PROCEDURE FOR DEVLOPING CARCINOGEN ACCEPTABLE OCCUPATIONAL EXPOSURE LEVELS

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PROCEDURE FOR DEVLOPING CARCINOGEN ACCEPTABLE OCCUPATIONAL EXPOSURE LEVELS

G1.0 PURPOSE

The Hanford Industrial Hygiene Technical Basis has identified more than 1,500 chemicals present in the Tank Farms, including more than 20 known or probable carcinogens. The process described in this procedure will be used to set acceptable occupational exposure levels (AOELs) for carcinogenic chemical compounds that do not have existing U.S. Occupational Safety and Health Administration permissible exposure limits (PEL) or American Conference of Governmental Industrial Hygienists threshold limit values (TLV). If a PEL or TLV exists for a compound under review, the lower of those two standards will be used as the Tank Farms occupational exposure limit (OEL), and this procedure will not be applied.

The end result of this process will be an AOEL that is scientifically justified and consistent with the intent and nature of PELs or TLVs. The AOEL will incorporate a level of protection equivalent to a PEL or TLV. That is, as stated in the ACGIH TLV documentation: it will set an airborne concentration for chemical vapors for which nearly all workers may be exposed repeatedly, day after day, over their working lifetime, without adverse health effects (in this case, incidence of cancer above background rates).

This procedure is intended to be used by occupational health professionals with training and experience in toxicology. The AOELs developed using this procedure will be internally peer reviewed, and then proposed for adoption as Hanford Site Tank Farms AOELs. The Industrial Hygiene Exposure Assessment Strategy (TFC-PLN-034) establishes a committee of professionals known as the Exposure Assessment Strategy Review Group (EASRG). One function of the EASRG is to review the documentation for proposed AOELs and make a technical recommendation to senior management. The final decision on adoption of AOELs is a management decision based on the recommendations of the EASRG. The AOEL values adopted will serve as a basis for future risk management strategies.

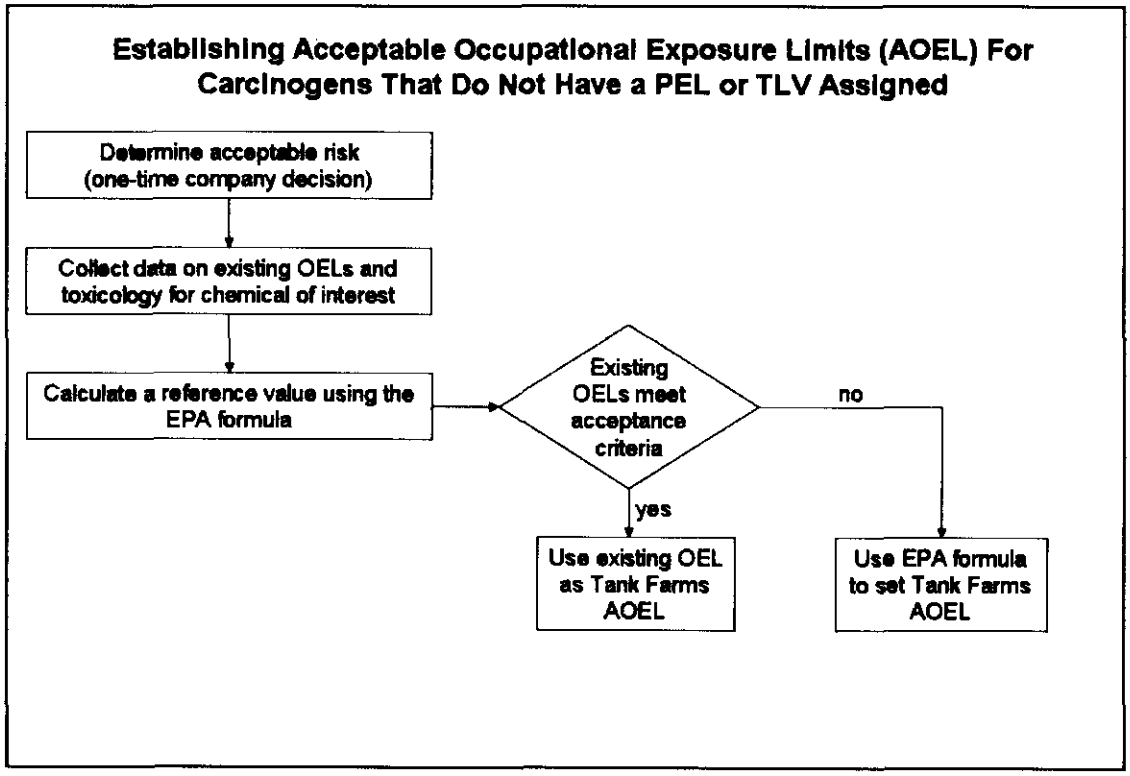
G2.0 PROCESS FOR DETERMINING A CARCINOGEN AOEL

The AOEL established by this process will be an eight-hr time-weighted average for inhalation exposure. For compounds that have acute or short-term exposure concerns in addition to carcinogenic effects, additional safety factors may be considered to account for the acute effects. Non-carcinogenic effects are dealt with in a separate procedure (see Appendix F). There may be cases where Tank Farms exposure scenarios require weighing the relative protection of applying a carcinogen versus non-carcinogen AOEL. In these cases the EASRG will weigh all relevant toxicological and industrial hygiene evidence to determine which AOEL development process is most protective to the worker.

The carcinogen AOEL process, as outlined in Figure G-1, begins with the determination of an acceptable risk factor, a one-time decision that establishes policy on acceptable occupational carcinogen risk. Following this:

1. All relevant toxicology data are compiled;
2. Information is obtained on existing (non-U.S. government) OELs;
3. A reference value is calculated using the EPA carcinogen formula (EPA/630/R-00/004);
4. Existing OELs are evaluated for suitability; and
5. Existing OELs are compared to the standard EPA carcinogen formula value, and a determination is made whether to use existing OELs or the EPA formula value.

Figure G-1. Process for Establishing Carcinogen AOELs



G3.0 ACCEPTABLE RISK LEVEL

In the U.S. EPA Superfund process, a 10^{-6} value (one excess cancer case above background per one million people) is considered a *de minimis* risk, and is the target value for Superfund remediation. The U.S. EPA risk assessment approach to calculating exposure levels typically yields lower values than those calculated by OSHA. This is because EPA limits are designed for 24-hour per day, 7 days per week lifetime exposures, and include extra protection for children and other sensitive individuals. In practice, risk values between 10^{-4} and 10^{-6} are used to make environmental risk management decisions.

In contrast, occupational exposures limits are developed for a "healthy worker" population who are expected to be exposed for a typical work week for not more than 40 years. OSHA has not set an acceptable risk level with regard to cancer risks in occupational settings. Risks considered acceptable by OSHA in establishment of PELs for carcinogens have in practice ranged from 1×10^{-4} to 4.8×10^{-2} (see Table G-1). If the U.S. EPA formula is applied with a 10^{-3} risk level, it yields an occupational exposure limit comparable to many OSHA PELs. For the Hanford Site Tank Farms, a safety factor of ten will be applied above this level: a risk factor of 1×10^{-4} will be used to calculate exposure limits if there are no existing OELs. This is consistent with the EPA process for human health risk assessment, and is more conservative than some OSHA PELs for carcinogens.

G4.0 EVALUATING EXISTING DATA

G4.1 INFORMATION SOURCES

In order to evaluate potential AOELs for a particular carcinogen, existing chemical, toxicological, and regulatory information must be reviewed. Goals of this information review include the following:

- Understand the chemical and physical properties of the compound;
- Understand the health effects (carcinogenic and non-carcinogenic) of the compound in its various forms and species, and routes of exposure;
- Determine whether, when, and where it has been regulated, and the circumstances of this regulation;
- Obtain specific details, such as cancer slope factors;
- Catalogue all exposure limits that have been set for the compound by the various regulatory agencies: governmental and non-governmental; U.S. and foreign; occupational, environmental, emergency, and others;
- Understand the laboratory analytical and field measurement capabilities for the compound of interest; and
- Understand the Tank Farms occupational exposure scenario.

Some information sources are preferable to others. The following order of priority will be considered for setting Tank Farms AOELs:

1. U.S. federal standards (NIOSH, DOE, EPA).
2. U.S. state standards.
3. Acceptable foreign government standards. These standards will be evaluated for equivalency to the U.S. level of protection by comparing OELs set by these governments for related compounds to U.S. PELs/TLVs (see below).
4. U.S. toxicology documentation, such as submittals to the PEL or TLV committees for compounds pending standard development.

G4.2 EVALUATING EXISTING OELS

When considering OELs set by agencies other than OSHA or ACGIH, or by other countries, an evaluation must be made as to whether the OEL establishes a similar degree of protection as that afforded by a PEL or TLV. OELS set by agencies other than OSHA and ACGIH may be acceptable for consideration if they meet these basic criteria:

- Documentation has been made public showing an exhaustive and thorough consideration of all available scientific research and technical information.
- The originating agency has a record of making conservative and protective worker safety decisions.
- There is no evidence that economic or political considerations outweighed health concerns in setting the standard.
- The standard is consistent with toxicological information for the chemical.
- Field measurement or sampling and analytical methods exist (or be developed at reasonable cost) to support the standard.

G4.3 ANALYTICAL METHODS

AOELs used in the Tank Farms must be verifiable using existing sampling and analytical methods. In some cases the toxicological assessment may suggest an AOEL that is lower than the lowest achievable sampling and analytical detection limits. In that case the lowest detection limit achievable will be selected as the AOEL. Therefore, the process of data collection must include an evaluation of sampling and analytical capabilities. This information will then be considered in establishing an AOEL. Depending on the conditions in the field, appropriate risk management techniques will be applied.

G4.4 EPA HUMAN HEALTH RISK ASSESSMENT MODEL

The U.S. EPA human health risk assessment program recommends a quantitative method for establishing threshold exposure levels. The method uses the formula:

$$OEL(\mu g/m^3) = \frac{AcceptableRisk \times AT(d) \times BW(kg) \times 1000 \mu g/mg}{IR(m^3/d) \times EF(d/yr) \times ED(yr) \times CSF(mg/kg-d)^{-1}} \quad \text{(G-1)}$$

For Tank Farms AOEL consideration, the following inputs to the formula will be used:

AT Averaging time; equal to an average human lifetime in days: 25,550 days (70 years).

BW Average adult body weight in kilograms. The OSHA default for adult female weight (65 kg) will be used because it provides a conservative result in the OEL calculation.

IR Inhalation rate: 10 m^3/day,

EF Exposure frequency, in days worked per year: 250 days/yr. Since 250 days/yr represents a maximum work year without deduction for vacation or training time, this is a conservative measure.

ED Exposure duration, or working lifetime, in years: the OSHA default value of 40 years will be used.

CSF Cancer slope factor: specific for each chemical.

CSF is usually calculated as the upper 95th confidence limit of the slope of the dose-response curve. Different CSFs may be calculated for the same chemical compound, depending on which dose-response data set is used, and on varying assumptions about exposure. Toxicologists preparing AOEL recommendations under this procedure are encouraged to calculate different CSFs, and present them to the EASRG with documentation of their underlying assumptions. This will give the EASRG flexibility to select an AOEL with a reasonable set of parameters.

G4.5 SETTING THE AOEL

The Tank Farms AOEL for carcinogens that do not have a PEL or TLV will be set by the following process (see Figure G-1).

1. Use a risk factor of 10^{-4} for all applications of the EPA formula.
2. Conduct a thorough search of scientific research, technical documentation, legislative actions, and other pertinent information. Identify any OELs that have been established by other agencies, states, or foreign governments. In particular, obtain or calculate cancer slope factors (CSFs). Note that different agencies and researchers may assign different CSFs based on varying interpretations of the data. Ensure that

field and laboratory analytical measurement capabilities are taken into account. If necessary, data from studies of chemical surrogates may be used to obtain the needed information, with the application of appropriate uncertainty factors.

3. Use the EPA formula to calculate a reference value for comparison. The value of this exercise is that it yields a number with known parameters that can be used as a basis for evaluating existing OELs.
4. Evaluate existing non-U.S. OELs for acceptance using the criteria in Section G4.0. Document whether any existing OELs meet the acceptance criteria. If existing OELs meet acceptance criteria, they should be proposed as the Tank Farms AOEL.
5. If there are no acceptable existing OELs, the EPA formula will be used to set the proposed AOEL, using the parameters in Section G4.4.
6. The EASRG will evaluate all documentation, and the range of AOELs proposed, and will make a decision consistent with appropriate worker protection.

G5.0 REFERENCES

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Table G-1. OSHA Multistage Model Estimates of Cancer Risks for PELs and Excess Cancer Risks per 1,000 Workers

Chemical	Current Value	Year Set	Former Value	Reference	Current PEL MLE	Current PEL UCL	Former PEL	Risk/1,000 Workers	Concentration at 10^{-4} Risk
Acrylamide	0.03 mg/m^3	1989	0.3 mg/m^3	Preamble [c]	1	5	10-45	6.4	0.00047 mg/m^3
Acrylonitrile	2 ppmv	1993	None	1910.1045	NA	NA	NA	48	0.0041 ppmv
Amitrole	0.2 mg/m^3	1989	None	Preamble	2.7	3.5	NA	NA	NA
Benzene	1 ppmv	1996	None	1910.1028	NA	NA	NA	4	0.024 ppmv
1,3-Butadiene	1 ppmv	1996	1,000 ppmv	1910.1051	<0.1 – 8.1	0.5 – 12.2	NA	11	0.0092 ppmv
Carbon Tetrachloride	2 ppmv	1989	10 ppmv	Preamble	3.7	5.2	17.9 - 26.0	31	0.0064 ppmv
Chloroform	2 ppmv	1989	50 ppmv	Preamble	0.27	1.8	22.4 - 46.1	37	0.0054 ppmv
1,2-Dibromo-3-chloropropane (DBCP)	1 ppbv	1993	None	1910.1044	NA	NA	NA	NA	NA
Ethylene oxide	1 ppmv	1996	None	1910.1047	NA	NA	NA	30	0.0034 ppmv
Formaldehyde	0.75 ppmv	1992	1 ppmv	1910.1048	NA	NA	NA	2	0.038 ppmv
Methylene Dianiline	10 ppbv	1996	None	1910.1050	NA	NA	NA	NA	NA
Methylene Chloride	25 ppmv	1997	500 ppmv	1910.1052	3.6 [e]	NA	126	3.4	0.37 ppmv

Note: NA = not applicable

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