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Chemical Inventory Limits for Investigation, Remediation, and Restoration of Material Disposal Area B Nuclear Environmental Site

Prepared by the
Environmental Stewardship–Environmental Remediation and Surveillance Division

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1.0 INTRODUCTION

Los Alamos National Laboratory (LANL, or the Laboratory) document LA-UR-05-XXXX, "Documented Safety Analysis for Investigation, Remediation, and Restoration of Material Disposal Area B Nuclear Environmental Site" (LANL 2006), identified the development of an Above-Ground Material Management Plan as a technical safety requirement (TSR) specific administrative control (SAC). Inventory limits specified by the Above-Ground Material Management Plan will mitigate the consequences in the event of an accidental release of a hazardous material/substance during the investigation, remediation, and restoration (IRR) of Material Disposal Area (MDA) B. This report provides the methodology used to develop chemical inventory limits for MDA B IRR and identifies those limits for a subset of chemicals. Additionally, the methodology described in this report will be used by field personnel to determine inventory limits for those chemicals identified during MDA B IRR that are not evaluated by this report.

Waste inventory information for MDA B is anecdotal. The Laboratory did not maintain waste inventory records during the active disposal life of this area (1945 to 1948). Therefore, while subject matter experts (SMEs) generated a list of contaminants of concern (CoCs) using historical documentation, investigation and characterization activities are necessary before the Laboratory will know the exact contents of MDA B. As such, inventory limits identified by the Above-Ground Material Management Plan will be applicable only to those chemicals (liquids and gases) staged/stored in the Definitive Identification Facility (DIF) and the surrounding storage/staging area (327 m from the maximally-exposed offsite individual [MEOI]) that the Laboratory has fully characterized. Field personnel will rely upon post-excavation containment (e.g., overpacking, cylinder coffins, etc.) and good work practices (as described by the Above-Ground Material Management Plan) to ensure the safety of the public, workers, and the environment during work within the excavation enclosure, during onsite transportation, and during work with unidentified hazardous materials/substances.

The primary consideration in the development of chemical inventory limits is to ensure no irreversible or other serious health effects or symptoms to the public at the nearest site boundary. Therefore, chemical inventories will be limited to the quantity of material that, given a chemical spill or release, will not meet or exceed 60-minute Acute Exposure Guideline Level 2 (AEGL-2), Emergency Response Planning Guideline 2 (ERPG-2), or Temporary Emergency Exposure Level 2 (TEEL-2) airborne concentration limits at the site boundary. In accordance with "AEGLs, ERPGs, or Rev. 21 TEELs for Chemicals of Concern 2005" (Craig 2005), AEGL values (final or interim) will be used to determine inventory limits, when available. In the absence of AEGL values, analysts will reference ERPG values. TEEL values will be used when no AEGL or ERPG values exist for a given chemical. Analysts will use the threshold quantities given by 29 CFR 1910.119 (Appendix A, List of Highly Hazardous Chemicals, Toxics, and Reactives) and 40 CFR 68.130 (Tables 1 and 2, List of Regulated Toxic Substances and Threshold Quantities for Accidental Release Prevention; Tables 3 and 4, List of Regulated Flammable Substances and Threshold Quantities for Accidental Release Prevention) in lieu of the quantities calculated based on AEGL/ERPG/TEEL-2 limits when the threshold quantities are more restrictive. Storage limits for flammable and combustible liquids and hazardous and toxic gases as specified by LIR 402-510-01, "Chemical Management," will take precedence over the limits identified in this report when they are more restrictive.

2.0 METHODOLOGY

An initial list of chemicals was developed using the CoC list provided in the documented safety analysis (DSA) (LANL 2006), the results of the pore gas and surface sampling conducted in 1998 and 2001 (LANL 2004), and a general list of volatile organic compounds (VOCs). Analysts identified a subset of this list for

inventory control. Analysts established inventory limits for those chemicals that the Laboratory may find in a readily dispersible form in MDA B. Liquids and gases were considered if they have a vapor pressure (VP) greater than 0.5 mm Hg and/or a boiling point (BP) less than 100°C. Chemicals normally found in a solid form were not analyzed. Although particles smaller than about 10 µm in diameter are respirable, a liquid or gas is expected to have greater consequences in terms of area of impact and time urgency. This criterion ensures that the analysis included those chemicals that may pose a high vaporization/dispersion hazard and is consistent with the chemical accident screening used in DOE/EIS-0238, "Site-Wide Environmental Impact Statement for Continued Operation of the Los Alamos National Laboratory" (DOE 1999).

Analysts used two separate air dispersion models to determine the inventory limit for a given chemical of concern: Areal Locations of Hazardous Atmospheres (ALOHA) Version 5.3.1 and Emergency Prediction Information Code (EPIcode) Version 7.0.

ALOHA is a public domain code that is part of a system of software known as the Computer-Aided Management of Emergency Operations (CAMEO), which was developed to plan for and respond to chemical emergencies. It is also widely used throughout the Department of Energy (DOE) complex for safety analysis applications. The Environmental Protection Agency (EPA), through its Chemical Emergency Preparedness and Prevention Office (CEPPO), and the National Oceanic and Atmospheric Administration (NOAA) Office of Response and Restoration jointly sponsor ALOHA. EPIcode was developed by Homann Associates, Inc., which maintains and upgrades the code. Homann Associates, Inc. developed EPIcode to automate the implementation of the EPA 'Green Book' guidance regarding dispersion of hazardous chemicals. The DOE Office of Environment, Safety, and Health designated both ALOHA and EPIcode as DOE "toolbox" codes. DOE-EH-4.2.1.3-ALOHA Code Guidance (DOE June 2004a) and DOE-EH-4.2.1.3-EPIcode Code Guidance (DOE June 2004b) provide detailed descriptions of the software and DOE-recommended guidance for use of the software in safety analysis applications.

ALOHA and EPIcode are well-developed computer models that are capable of calculating χ/Q values with the weather conditions provided, such as stability class, temperature, wind speed, and distance from release. These codes use a centerline Gaussian-dispersion plume model to represent chemical releases that are neutrally buoyant. ALOHA will also model heavy gas releases.

ALOHA and EPIcode use the Gaussian model to predict how gases that are about as buoyant as air will disperse in the atmosphere. Such "neutrally-buoyant" gases have about the same density as air. According to this model, wind and atmospheric turbulence are the forces that move the molecules of a released gas through the air, so as an escaped cloud is blown downwind, "turbulent mixing" causes it to spread out in the crosswind and upward directions. According to the Gaussian model, any crosswind slice of a moving pollutant cloud looks like a bell-shaped curve, high in the center and lower on the sides.

"Heavy gases" form vapor clouds that are heavier and denser than air. Heavy gases include not only gases with molecular weights heavier than air (the average molecular weight of air is about 29 kg/kmol), but sometimes also gases such as anhydrous ammonia that are normally lighter than air, but that are stored liquefied under pressure. Liquefied gases typically escape from storage as a cold, heavy cloud containing a mixture of gas and fine aerosol droplets. A release of such a mixture is called a two-phase flow. The aerosols weigh the cloud down and make it more dense, and their evaporation cools the cloud.

Heavy gases behave in a complicated way when they escape from storage. A heavy gas cloud first slumps away from the source in all directions, then flows downwind like water, propelled by the wind, gravitational slumping, and its forward momentum. As it moves downwind, air is stirred into the cloud, and it becomes less and less dense, eventually behaving like a neutrally buoyant gas.

The basis for identifying the potential for heavy gas effects is the Richardson (Ri) number. The Ri number represents a relative measure of the potential energy of the cloud with respect to the mechanical turbulent energy of the atmosphere. The source Ri (Ri_0) number, above which heavy gas transport effects are assumed important, is typically considered about 50 (Hanna, 1996). An absolute threshold value does not actually exist. Heavy gas effects may begin to appear for Ri_0 values as low as one and become more pronounced as Ri_0 is increased. ALOHA uses a critical Ri_0 value of one.

ALOHA's heavy gas model typically (as seen in this analysis) produces results that allow for a much higher inventory limit than those produced by EPIcode. Other analyses have used the results of ALOHA when heavy gas transport and dispersion are characteristic, since EPIcode does not have a heavy gas model. However, due to the lack of an absolute threshold value for the Ri_0 number and the tendency for heavy gas releases to transition to a neutrally buoyant plume, analysts chose the more conservative results of the two models (typically EPIcode) to set the inventory limits for MDA B IRR.

2.1 Input Parameters

Table 2.1-1 provides the basic input parameters used to run ALOHA and EPIcode. All releases are assumed to take place outdoors. No credit is taken for confinement structures or ventilation/filtration. Following sections provide the specific input parameters used to model liquid spills and gaseous releases.

**Table 2.1-1
Input Parameters for EPIcode and ALOHA**

Input Parameter	EPIcode	ALOHA	Justification
Source Location/ Site Data	Lat: 34.00879 N Long: 106.44313 W Source Altitude: 2069 m (6789 ft)	Los Alamos, NM Lat: 35° 31.2 min N Long: 106° 11.4 min W Elevation: 2069 m (6789 ft)	Latitude, longitude, and altitude are input into EPIcode; specific latitude, longitude, and elevation information is provided by ALOHA when Los Alamos, NM is chosen by the user.
Building Type	N/A	Default is sheltered single story	Not applicable to this analysis—receptor is conservatively located outside.
Date and Time	N/A	June 30, 2005; 0600 hours MDT	ALOHA uses a number of parameters, including date and time, to determine the evaporation rate; these parameters must also be consistent with the desired atmospheric stability class. The date and time have been selected to ensure the recommendation of Stability Class F.
Terrain/Ground Roughness	Standard (rural)	Open Country (rural)	Rural terrain is chosen for conservatism. EPIcode's rural model produces concentrations approximately 10 times greater than its urban model; ALOHA's rural model produces concentrations approximately 3 times greater than its urban model.
Atmospheric Stability Class	F	F	Atmospheric Stability Class F is conservatively chosen to represent unfavorable, worst-case

**Table 2.1-1
Input Parameters for EPIcode and ALOHA**

Input Parameter	EPIcode	ALOHA	Justification
			conditions.
Cloud Cover	N/A	Clear (0 tenths)	ALOHA primarily uses the cloud-cover input to estimate the amount of incoming solar radiation that is incident upon the puddle formed by a liquid spill (cloud cover is expected to also have an effect at night on the long wave radiation calculations and therefore a small effect on evaporation). Zero tenths cloud cover is conservative and consistent with the selection of Atmospheric Stability Class F.
Wind Speed/ Measurement Height	1.5 m/s at 10 m	1.5 m/s at 10 m	1.5 m/s at 10 m is the DOE-recommended wind speed and conservative reference height for use with Stability Class F (DOE June 2004a; DOE June 2004b). Thoman, et. al., further demonstrates the conservatism of choosing a reference height of 10 m (as opposed to the 2 m default for EPIcode and 3 m default for ALOHA) (Thoman, et. al. 2005).
Wind Direction	Any direction	Any direction	Downwind concentration results are not sensitive to this input parameter specification.
Inversion Height	200 m	200 m	200 m has been conservatively chosen to ensure the worst-case downwind concentrations are represented—the lower the inversion height, the higher the downwind concentration.
Temperature	32.2°C	32.2°C	95 th percentile value of a five-year record of

**Table 2.1-1
Input Parameters for EPIcode and ALOHA**

Input Parameter	EPIcode	ALOHA	Justification
			daily high temperatures for Los Alamos (measurements obtained from TA-53 monitoring station— 10/31/00 to 10/30/05).
Humidity	N/A	50%	50% is the DOE-recommended value (DOE June 2004a). This value is used to calculate the evaporation rate only. ALOHA does not model chemical reactions resulting from moisture.
Release Height	0 m (ground-level release)	0 m (ground-level release)	All release scenarios assume a ground-level release.
Receptor Height	0 m	0 m (only option)	A receptor height of 0 m is most appropriate and conservative for a ground-level release (DOE June 2004b).
Deposition Velocity	0 cm/s	0 cm/s (only option)	Plume depletion is conservatively not considered given the close proximity of the MEOI.
Airborne Fraction	1.00	N/A	All of the material involved is conservatively assumed to be released to the atmosphere.
Sample/Averaging Time	10 minutes	3 minutes (only option)	Default values; these low sampling/averaging times are conservative as they provide for higher downwind concentrations.
Dispersion Model	Gaussian	Gaussian and Heavy Gas, as applicable	EPIcode uses the Gaussian model only; ALOHA decides the most appropriate of the Gaussian and Heavy Gas model to use for a given chemical.

2.1.1 Puddle Source/Liquid Spill

Analysts chose ALOHA's puddle source model and EPIcode's liquid spill model to model the release of chemicals in a liquid form. These two models assume that the total inventory of a specified chemical has spilled onto the ground and has formed one puddle or pool that has a uniform depth and is not changing in area. Catastrophic failure of a storage vessel is an example of a scenario that could quickly progress to a puddle source or liquid spill configuration. The source term is proportional to the pool surface area, which is defined by the presence of a berm (or similar type barrier) or by assuming that the liquid spreads to some uniform thickness (e.g., 1 cm).

ALOHA (EPA/NOAA 2004)

ALOHA's puddle source model can model evaporation from puddles that are boiling or that are cooler than the boiling point of the liquid that they contain. To model evaporation from a puddle, ALOHA accounts for the effects of wind speed, atmospheric turbulence, air temperature and pressure, viscosity, and other properties of the spilled chemical. It accounts for the effects on puddle temperature of solar heating, evaporative cooling, and several other ways in which heat is exchanged between a puddle and its environment. For example, on a sunny day, ALOHA will expect heat energy from the sun to warm the puddle. It expects puddle temperature to directly influence evaporation rate so that the higher the puddle temperature, the faster the evaporation rate. It accounts for changes in puddle temperature and hence in evaporation rate over time. The types of heat transfer that ALOHA expects to affect puddle temperature fall into the following three categories:

- incoming solar radiation (affected by location, time and date, and cloud cover),
- heat transfer with the air (affected by air temperature, humidity, and initial puddle temperature), and
- heat transfer with the ground (affected by ground temperature, ground type, and initial puddle temperature).

The puddle source model requires the following specific inputs in addition to those given in Table 2.1-1:

- puddle area or diameter;
- volume, mass, or depth of the puddle;
- ground type;
- ground temperature; and
- initial puddle temperature.

The puddle area/diameter and the volume/mass/depth of the puddle characterize the quantity of the chemical spilled and provide the physical dimensions of the puddle or pool that are necessary for the evaporation calculation. Analysts determined the surface area of a spilled chemical using the following equation:

$$A = V/\Delta h \quad \text{(Equation 2.2-1)}$$

where, A is the surface area of the puddle, V is the volume of the puddle (or total amount of material spilled), and Δh is the depth of the puddle. The purpose of this analysis was to determine the maximum

quantity of a specified chemical that will not meet or exceed AEGL/ERPG/TEEL-2 at the site boundary. Therefore, analysts estimated the volume of the puddle until a quantity was identified that yielded a concentration just less than the AEGL/ERPG/TEEL-2 threshold for the chemical modeled. The DOE code guidance for ALOHA (DOE June 2004a) recommends a puddle depth (Δh) of 1 cm, a depth that is commonly used and suggested by EPA guidance. Therefore, analysts used a puddle depth of 1 cm for this analysis.

Ground type influences the amount of heat energy transferred from the ground to an evaporating puddle. As it computes heat transfer from ground to puddle, ALOHA assumes that the ground does not absorb any of the spilled chemical. ALOHA offers four choices for ground type:

- default—unwetted soil not covered by rock or concrete;
- concrete—concrete, cement, asphalt, or otherwise paved surfaces;
- sandy—sandy, dry soil; and
- moist—sandy, moist soil.

ALOHA expects heat to be transferred most readily from a default or concrete ground into a puddle, and least readily from sandy ground. The more heat energy that is transferred into the puddle, the higher the evaporation rate and the downwind concentration. Analysts chose the default ground type (unwetted soil not covered by rock or concrete) as the most representative and conservative choice for this analysis.

ALOHA uses ground temperature to predict the amount of heat transferred from the ground to an evaporating puddle. The warmer the ground relative to the temperature of the puddle, the more heat energy will be transferred into the puddle, and the faster the puddle will evaporate. The DOE code guidance for ALOHA (DOE June 2004a) recommends a specification based on statistical analysis of measurements of ground surface temperature, and when such data is not available, the ground temperature should be set equal to the air temperature. Analysts conservatively set the ground temperature equal to the air temperature (32.2°C) for this analysis.

To predict the rate of evaporation from a puddle of spilled liquid, ALOHA must know the initial temperature of the puddle. It assumes the initial temperature to be the same throughout the depth and width of the puddle. The DOE code guidance for ALOHA (DOE June 2004a) recommends that the initial puddle temperature be consistent with the storage/operating temperature or the ambient temperature. Therefore, analysts assumed that the initial puddle temperature was equal to the air/ground temperature. The initial puddle temperature must be above the liquid's freezing point (ALOHA cannot predict sublimation rate from a frozen puddle) and equal to or less than the liquid's ambient boiling point.

EPIcode (Homann Associates, Inc. 2003)

EPIcode's liquid spill model is not as complex as ALOHA's puddle source model. EPIcode's evaporation methodology is based on an EPA model (EPA 1987) and considers the windspeed, molecular weight of the spilled material, surface area of the spilled material, vapor pressure of the spilled material at a given temperature, and the temperature of the spilled material. For liquid spill scenarios, EPIcode prompts the analyst for inputs of total quantity of liquid that is spilled, surface area of pool that forms from the spill (calculated by EPIcode), the chemical vapor pressure (calculated by EPIcode), and the liquid temperature. From these inputs, EPIcode calculates the evaporative release rate to the atmosphere and the duration of the release.

As with the ALOHA model, analysts estimated the total quantity of liquid spilled until a quantity was identified that yielded a concentration just less than the AEGL/ERPG/TEEL-2 threshold for the chemical modeled. Once the analyst specifies a quantity, EPIcode provides three possible spill areas—one based on a 1 cm pool depth, one based on a 1 mm pool depth, and one based on a 1 in. pool depth. For an unmitigated analysis, as with ALOHA, the DOE code guidance for EPIcode (DOE June 2004b) recommends that a minimum depth of 1 cm be specified.

The evaporation rate is directly proportional to the chemical vapor pressure, and the vapor pressure of the chemical constituent is a strong function of its temperature in the liquid state. EPIcode typically provides the vapor pressure at a given temperature (e.g., 25°C) for each chemical. EPIcode recalculates the vapor pressure based on the specified spill temperature. The DOE code guidance for EPIcode (DOE June 2004b) recommends that the analyst first consider the range of possible liquid temperatures, consistent with the storage/operating temperature or the environment temperature, and then specify the spill temperature. As with the ALOHA model, analysts conservatively set the spill temperature equal to the air/environment temperature (32.2°C) for this analysis.

Very small particles and gases or vapors are deposited on surfaces as a result of turbulent diffusion and Brownian motion. Chemical reactions, impaction, and other biological, chemical, and physical processes combine to keep the released substance at ground level. As this material is deposited on the ground, the plume above becomes depleted, and downwind concentrations are lower than would be the case without plume depletion. EPIcode uses a source-depletion algorithm to adjust the air concentration in the plume to account for this removal of material. The deposition velocity input determines plume depletion. The most conservative results are generally obtained with the deposition velocity set to zero; however, this assumption could lead to unrealistically large concentration predictions for particles, particularly at large distances downwind. The DOE code guidance for EPIcode (DOE June 2004b) recommends the default values of 0 cm/s for gases and vapors and 0.3 cm/s for solids, although other values may be used with justification. Due to the close proximity of the MEOI, analysts conservatively assumed a deposition velocity of 0 cm/s for liquid spills.

Additional input parameters include the airborne fraction and the physical height of the spill. Analysts conservatively assumed the airborne fraction, the fraction of the total quantity of material involved in the spill that is released to the atmosphere, to be 1.00. For MDA B IRR activities, the physical height of a chemical spill will be 0 m.

2.1.2 Gaseous Release

Analysts chose ALOHA's direct source model and EPIcode's term release model to model the release of chemicals in a gaseous form.

ALOHA (EPA/NOAA 2004)

The direct source model is used when the emission rate of a gas is known. The emission rate remains constant throughout the duration of the release. A continuous (lasting more than one minute) or instantaneous release (lasting one minute) may be chosen. For the purposes of this analysis, analysts modeled all gases as a continuous 10-minute release. This is consistent with modeling performed for the LANL site-wide environmental impact statement (DOE 1999). As for the liquid spill, analysts estimated the total quantity of gas released until a quantity was identified that yielded a concentration just less than the AEGL/ERPG/TEEL-2 threshold for the chemical modeled. Analysts assumed a ground-level release, so the source height was set to 0 m.

EPIcode (Homann Associates, Inc. 2003)

EPIcode defines a term release as a release that is of finite duration. As the release duration increases, the results from the term-release model approach that from the continuous release model for equivalent specifications of release rates and other input variables. At the other end of the spectrum for term releases (i.e., releases of very short duration) is the instantaneous release. When the user specifies an instantaneous term release, EPIcode uses the puff model. For other term releases (i.e., non-instantaneous), EPIcode automatically selects the puff or plume equation at each downwind location based on the relative dimension of the cloud width with respect to the cloud length. When the cloud length is less than the cloud width, the puff equation is considered a more accurate model of the dispersion.

As with ALOHA, analysts modeled all gases as a continuous 10-minute release and estimated the total quantity of gas released until a quantity was identified that yielded a concentration just less than the AEGL/ERPG/TEEL-2 threshold for the chemical modeled. The effective release height was set to 0 m. Analysts conservatively assumed the airborne fraction to be 1.00. No plume depletion was credited, and the deposition velocity was set to 0 cm/s.

3.0 CHEMICAL INVENTORY LIMITS

Tables 3.0-1 through 3.0-5 provide the inventory limits at 327 m identified through modeling for each of the chemicals analyzed. The chemicals are presented based on their Department of Transportation (DOT) hazard class. Appendix B provides the results of the modeling for both ALOHA and EPIcode. Modeling was performed at various distances and for both AEGL/ERPG/TEEL-2 and -3 to accommodate changes that may occur during the MDA B IRR planning phase. An activity or facility with greater than 100,000 lbs of a hazardous material/substance is considered to be in a production mode. Therefore, any limits identified at greater than 100,000 lbs were set at 100,000 lbs.

Table 3.0-1
Chemical Inventory Limits for DOT Class 2: Gases (Flammable, Non-Flammable, Toxic)

Chemical	Form	CAS No.	Limit (lbs)—327 m
Bromomethane (also Methyl Bromide)	Gas	74-83-9	30
Chloroethane (also Ethyl chloride)	Gas	75-00-3	410
Chloromethane (also Methyl chloride)	Gas	74-87-3	128
Dichlorodifluoromethane	Gas	75-71-8	7750
Hydrogen bromide, anhydrous (also Hydrobromic acid, anhydrous)	Gas	10035-10-6	1.5
Hydrogen Chloride, anhydrous	Gas	7647-01-0	5
Hydrogen Fluoride, anhydrous	Gas	7664-39-3	3
Hydrogen iodide, anhydrous (also Hydriodic acid 4)	Gas	10034-85-2	0.4
Sulfur dioxide	Gas	7446-09-5	0.3
Vinyl Chloride	Gas	75-01-4	1975 ^a

^a10% LEL ≤ AEGL/ERPG/TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account

Table 3.0-2
Chemical Inventory Limits for DOT Class 3: Flammable and Combustible Liquids

Chemical	Form	CAS No.	Limit (lbs)—327 m
1,1-Dichloroethane	Liquid	75-34-3	13,100
1,1-Dichloroethylene (also Vinylidene Chloride)	Liquid	75-35-4	26
1,2,4-Trimethylbenzene	Liquid	95-63-6	11,500
1,2-Dichloroethane (also Ethylene Dichloride)	Liquid	107-06-2	1975
1,2-Dichloropropane	Liquid	78-87-5	1600
1,3,5-Trimethylbenzene (also Mesitylene)	Liquid	108-67-8	5600
1,3-Dichloropropane	Liquid	142-28-9	4700
2,2-Dichloropropane	Liquid	594-20-7	530
2-Butanone (also Ethyl Methyl Ketone)	Liquid	78-93-3	20,000 ^a
2-Chloroethyl vinyl ether	Liquid	110-75-8	100
2-Chlorotoluene (also O-Chlorotoluene)	Liquid	95-49-8	95,000
2-Hexanone (also Methyl Butyl Ketone)	Liquid	591-78-6	3150
4-Chlorotoluene	Liquid	106-43-4	100,000
4-Methyl-2-pentanone (also Methyl Isobutyl Ketone)	Liquid	108-10-1	7000
Acetone	Liquid	67-64-1	10,000 ^a
Acrylonitrile	Liquid	107-13-1	126
Benzene	Liquid	71-43-2	750
Bromobenzene	Liquid	108-86-1	3750
Carbon disulfide (also Carbon bisulfide)	Liquid	75-15-0	325
Chlorobenzene	Liquid	108-90-7	53,700
cis-1,3-Dichloropropylene (also cis-1,3-Dichloro-1-propene)	Liquid	10061-01-5	84
Ethylbenzene	Liquid	100-41-4	8900
Ethyl ether (also Diethyl ether)	Liquid	60-29-7	395
Isopropylbenzene (also Cumene)	Liquid	98-82-8	7100
m-Xylene	Liquid	108-38-3	17,500
p-Xylene	Liquid	106-42-3	16,500
n-Butylbenzene	Liquid	104-51-8	100,000
n-Propylbenzene	Liquid	103-65-1	100,000
Kerosene	Liquid	8008-20-6	6400
o-Xylene	Liquid	95-47-6	23,500
sec-Butylbenzene	Liquid	135-98-8	16,000
Styrene (also Styrene monomer)	Liquid	100-42-5	31,500
tert-Butylbenzene	Liquid	98-06-6	68,000
Toluene	Liquid	108-88-3	12,500
trans-1,2-Dichloroethylene	Liquid	156-60-5	2700
trans-1,3-Dichloropropylene	Liquid	10061-02-6	93

^a10% LEL ≤ AEGL/ERPG/TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account

Table 3.0-3
Chemical Inventory Limits for DOT Class 6: Toxic Substances and Infectious Substances

Chemical	Form	CAS No.	Limit (lbs)—327 m
1,1,1,2-Tetrachloroethane	Liquid	630-20-6	5300
1,1,1-Trichloroethane	Liquid	71-55-6	5100
1,1,2,2-Tetrachloroethane	Liquid	79-34-5	775
1,2,3-Trichloropropane	Liquid	96-18-4	3100
1,2-Dibromoethane (also Ethylene Dibromide)	Liquid	106-93-4	3200
1,2-Dichlorobenzene (also O-Dichlorobenzene)	Liquid	95-50-1	47,000
1,2-Dichloroethane (also Ethylene Dichloride)	Liquid	107-06-2	1975
1,3-Dichlorobenzene (also M-Dichlorobenzene)	Liquid	541-73-1	6500
2-Chloroethylvinyl ether	Liquid	110-75-8	100
Acrylonitrile	Liquid	107-13-1	126
Bromochloromethane	Liquid	74-97-5	10,800
Bromoform	Liquid	75-25-2	300
Carbon disulfide (also Carbon bisulfide)	Liquid	75-15-0	325
Carbon tetrachloride	Liquid	56-23-5	2030
Chloroform	Liquid	67-66-3	310
Dibromochloromethane (also Chlorodibromomethane)	Liquid	124-48-1	150
Dibromomethane	Liquid	74-95-3	51
Iodomethane (also Methyl iodide)	Liquid	74-88-4	195
Methylene chloride (also Dichloromethane)	Liquid	75-09-2	1470
Tetrachloroethylene (also Perchloroethylene)	Liquid	127-18-4	18,000
Trichloroethylene	Liquid	79-01-6	7100
Trichlorofluoromethane	Gas	75-69-4	1250

Table 3.0-4
Chemical Inventory Limits for DOT Class 8: Corrosives

Chemical	Form	CAS No.	Limit (lbs)—327 m
Ammonium Hydroxide (10-35% ammonia; 21-72% ammonium hydroxide; water is balance)	Liquid	1336-21-6	102
Hydrogen bromide, anhydrous (also Hydrobromic acid, anhydrous)	Gas	10035-10-6	1.5
Hydrogen bromide, solution (48%)	Liquid	10035-10-6	700
Hydrogen Chloride, anhydrous	Gas	7647-01-0	5
Hydrogen chloride, solution (30-40%)	Liquid	7647-01-0	155
Hydrogen Fluoride, anhydrous	Gas	7664-39-3	3
Hydrogen Fluoride, solution (47-52%)	Liquid	7664-39-3	590
Nitric acid, anhydrous	Liquid	7697-37-2	270
Nitric acid, solution (70%)	Liquid	7697-37-2	450
Sulfur dioxide	Gas	7446-09-5	0.3

Table 3.0-5
Chemical Inventory Limits for DOT Class 9: Miscellaneous Hazardous Materials

Chemical	Form	CAS No.	Limit (lbs)—327 m
1,1,2-Trichloroethane	Liquid	79-00-5	600
Bromodichloromethane (also Dichlorobromomethane)	Liquid	75-27-4	90
Trichlorotrifluoroethane (also 1,1,2-Trichloro-1,2,2-trifluoroethane) (Note: This chemical not regulated by DOT)	Liquid	76-13-1	6250

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Appendix A

Acronyms/Abbreviations and Glossary

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A-1.0 ACRONYMS AND ABBREVIATIONS

AEGL	acute exposure guideline level
ALOHA	Areal Locations of Hazardous Atmospheres
BP	boiling point
CAMEO	Computer-Aided Management of Emergency Operations
CEPPO	Chemical Emergency Preparedness and Prevention Office
CoC	contaminant of concern
DIF	Definitive Identification Facility
DOE	Department of Energy
DOT	Department of Transportation
DSA	documented safety analysis
EPA	Environmental Protection Agency
EPIcode	Emergency Prediction Information Code
ERPG	emergency response planning guideline
IRR	investigation, remediation, and restoration
LANL	Los Alamos National Laboratory
MDA	material disposal area
MEOI	maximally-exposed offsite individual
NOAA	National Oceanic and Atmospheric Administration
OSHA	Occupational Safety and Health Administration
SAC	specific administrative control
SME	subject matter expert
TEEL	temporary emergency exposure level
TSR	technical safety requirement
VOC	volatile organic compound
VP	vapor pressure

A-2.0 GLOSSARY

AEGL-2—The airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3—The airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

ERPG-2—The maximum concentration in air below which it is believed nearly all individuals could be exposed for up to one hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action.

ERPG-3—The maximum concentration in air below which it is believed nearly all individuals could be exposed for up to one hour without experiencing or developing life-threatening health effects.

TEEL-2—Same as ERPG-2.

TEEL-3—Same as ERPG-3.

Appendix B

Modeling Results

	Chemical	CAS No.	DOT Hazard Class	Form	VP	BP	AELG/ERPG/TEEL	Distance to MEOI (m)	ALOHA			EPIcode			Inventory Limit (lbs)	
									Quantity (lbs)	Concentration	Model	Quantity (lbs)	Concentration	Model		
1	1,1,1,2-Tetrachloroethane	630-20-6	6	Liquid	14 mm Hg at 25°C	135.1°C	60 ppm (TEEL-2)	127	---	---	---	860	59 ppm	Liquid Spill	860	CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical
								227				2650	59 ppm		2650	
								297				4400	59 ppm		4400	
								327				5300	59 ppm		5300	
								357				6250	59 ppm		6250	
								127				3450	190 ppm		3450	
								227				10,550	190 ppm		10,550	
								297				17,600	190 ppm		17,600	
								327				21,050	190 ppm		21,050	
								357				24,800	190 ppm		24,800	
2	1,1,1-Trichloroethane	71-55-6	6	Liquid	100 mm Hg at 20°C	73.9°C	600 ppm (AELG-2 interim)	127	4,050	593 ppm	Puddle (Heavy Gas)	825	590 ppm	Liquid Spill	825	CERCLA chemical; reportable quantity = 1000 lbs EPCRA Section 313 chemical
								227	11,750	598 ppm		2550	590 ppm		2550	
								297	19,100	595 ppm		4250	590 ppm		4250	
								327	22,750	595 ppm		5100	590 ppm		5100	
								357	26,750	598 ppm		6050	590 ppm		6050	
								127				8800	4100 ppm	Liquid Spill	8800	
								227				26,500	4100 ppm		26,500	
								297				44,500	4100 ppm		44,500	
								327				53,000	4100 ppm		53,000	
								357				62,500	4100 ppm		62,500	
3	1,1,2,2-Tetrachloroethane	79-34-5	6	Liquid	5 mm Hg at 20°C	146.4°C	5 ppm (TEEL-2)	127	170	4.91 ppm	Puddle (Gaussian)	125	4.8 ppm	Liquid Spill	125	CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical
								227	1150	4.97 ppm	(Heavy Gas)	390	4.9 ppm		390	
								297	2050	4.89 ppm		650	4.8 ppm		650	
								327	2550	4.9 ppm		775	4.8 ppm		775	
								357	3100	4.9 ppm		925	4.9 ppm		925	
								127				3650	99 ppm	Liquid Spill	3650	
								227				11,100	99 ppm		11,100	
								297				18,500	99 ppm		18,500	
								327				22,300	99 ppm		22,300	
								357				26,000	99 ppm		26,000	
4	1,1,2-Trichloroethane	79-00-5	9	Liquid	16.7 mm Hg at 20°C	113.9°C	15 ppm (TEEL-2)	127	275	14.8 ppm	Puddle (Heavy Gas)	95	14 ppm	Liquid Spill	95	CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical
								227	1000	14.9 ppm		300	14 ppm		300	
								297	1800	14.9 ppm		500	14 ppm		500	
								327	2200	14.8 ppm		600	14 ppm		600	
								357	2700	14.9 ppm		700	14 ppm		700	
								127				780	99 ppm		780	
								227				2400	99 ppm		2400	
								297				4000	99 ppm		4000	
								327				4800	99 ppm		4800	
								357				5700	99 ppm		5700	
5	1,1-Dichloroethane	75-34-3	3	Liquid	182 mm Hg at 20°C	57.2°C	3000 ppm (TEEL-2 and TEEL-3)	127	7500	2930 ppm	Puddle (Heavy Gas)	2100	2900 ppm	Liquid Spill	2100	CERCLA chemical; reportable quantity = 1000 lbs EPCRA Section 313 chemical
								227	20,500	2920 ppm		6500	2900 ppm		6500	
								297	33,200	2990 ppm		10,950	2900 ppm		10,950	
								327	38,500	2920 ppm		13,100	2900 ppm		13,100	
								357	46,500	2970 ppm		15,450	2900 ppm		15,450	
6	1,1-Dichloroethylene (also Vinylidene Chloride) (Note: ALOHA initial puddle temperature is set at 24.6°C—the ambient boiling point.)	75-35-4	3	Liquid	602 mm Hg at 25°C	37°C	20 ppm (TEEL-2)	127	9	19.7 ppm	Puddle (Heavy Gas)	4	18 ppm	Liquid Spill	4	CAA Section 112(r) chemical; threshold quantity = 10,000 lbs CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical
								227	35	19.3 ppm		13	19 ppm		13	
								297	65	19.7 ppm		22	19 ppm		22	
								327	80	19.6 ppm		26	19 ppm		26	
								357	99	19.8 ppm		31	19 ppm		31	
								127				145	590 ppm	Liquid Spill	145	
								227				450	590 ppm		450	
								297				750	590 ppm		750	
								327				900	590 ppm		900	
								357				1050	590 ppm		1050	

7	1,2,3-Trichloropropane (EPIcode specific gravity incorrect; specific gravity corrected to 1.39 per CAMEO.)	96-18-4	6	Liquid	3 mm Hg at 25°C	156.2°C	10 ppm (TEEL-2)	127	490	9.96 ppm	Puddle (Gaussian)	510	9.9 ppm	Liquid Spill	490	EPCRA Section 313 chemical	
								227	4000	9.89 ppm	(Heavy Gas)	1575	9.9 ppm	1575			
								297	7250	9.94 ppm		2600	9.8 ppm	2600			
								327	9000	9.98 ppm		3100	9.8 ppm	3100			
								357	10,900	9.99 ppm		3700	9.9 ppm	3700			
							100 ppm (TEEL-3)	127				7800	99 ppm	Liquid Spill	7800		
								227				24,000	99 ppm	24,000			
								297				39,500	99 ppm	39,500			
								327				47,500	99 ppm	47,500			
								357				56,000	99 ppm	56,000			
8	1,2,4-Trimethylbenzene	95-63-6	3	Liquid	1 mm Hg at 13.3°C	168.9°C	36.6 ppm (TEEL-2)	127	7750	36.1 ppm	Puddle (Heavy Gas)	1850	36 ppm	Liquid Spill	1850	EPCRA Section 313 chemical	
								227	25,750	36.3 ppm		5750	36 ppm	5750			
								297	44,500	36.4 ppm		9500	36 ppm	9500			
								327	54,000	36.4 ppm		11,500	36 ppm	11,500			
								357	63,500	36 ppm		13,500	36 ppm	13,500			
							(NOTE: LEL = 8000 ppm; 10% LEL ≤ TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)	1500 ppm (TEEL-3)	127						Liquid Spill		100,000
								227				>100,000		>100,000			
								297				>100,000		>100,000			
								327				>100,000		>100,000			
								357				>100,000		>100,000			
9	1,2-Dibromoethane (also Ethylene Dibromide)	106-93-4	6	Liquid	12 mm Hg at 20°C	131.1°C	30 ppm (TEEL-2)	127	2400	29.7 ppm	Puddle (Heavy Gas)	520	29 ppm	Liquid Spill	520	CERCLA chemical; reportable quantity = 1 lb EPCRA Section 313 chemical	
								227	8000	29.7 ppm		1600	29 ppm	1600			
								297	14,000	29.9 ppm		2650	29 ppm	2650			
								327	17,000	29.8 ppm		3200	29 ppm	3200			
								357	20,000	29.4 ppm		3750	29 ppm	3750			
							100 ppm (TEEL-3)	127				2010	99 ppm	Liquid Spill	2010		
								227				6150	99 ppm	6150			
								297				10,250	99 ppm	10,250			
								327				12,350	99 ppm	12,350			
								357				14,550	99 ppm	14,550			
10	1,2-Dichlorobenzene (also O-Dichlorobenzene)	95-50-1	6	Liquid	1 mm Hg at 20°C	180.6°C	50 ppm (TEEL-2)	127	35,000	49.6 ppm	Puddle (Heavy Gas)	7750	49 ppm	Liquid Spill	7750	CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical	
								227	>100,000			23,800	49 ppm	23,800			
								297	>100,000			39,000	49 ppm	39,000			
								327	>100,000			47,000	49 ppm	47,000			
								357	>100,000			55,000	49 ppm	55,000			
							200 ppm (TEEL-3)	127				54,850	190 ppm	Liquid Spill	54,850		
								227				>100,000		>100,000			
								297				>100,000		>100,000			
								327				>100,000		>100,000			
								357				>100,000		>100,000			
11	1,2-Dichloroethane (also Ethylene Dichloride)	107-06-2	3.6	Liquid	64 mm Hg at 20°C	83.3°C	200 ppm (ERPG-2)	127	1700	199 ppm	Puddle (Heavy Gas)	320	190 ppm	Liquid Spill	320	CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical	
								227	5300	198 ppm		990	190 ppm	990			
								297	9000	199 ppm		1650	190 ppm	1650			
								327	11,500	198 ppm		1975	190 ppm	1975			
								357	13,500	196 ppm		2300	190 ppm	2300			
							300 ppm (ERPG-3)	127				500	290 ppm	Liquid Spill	500		
								227				1560	290 ppm	1560			
								297				2600	290 ppm	2600			
								327				3115	290 ppm	3115			
								357				3695	290 ppm	3695			
12	1,2-Dichloropropane	78-87-5	3	Liquid	40 mm Hg at 20°C	96.7°C	110 ppm (TEEL)	127	1250	108 ppm	Puddle (Heavy Gas)	260	100 ppm	Liquid Spill	260	CERCLA chemical; reportable quantity = 1000 lbs EPCRA Section 313 chemical	
								227	4000	107 ppm		800	100 ppm	800			
								297	7000	109 ppm		1325	100 ppm	1325			
								327	8350	108 ppm		1600	100 ppm	1600			
								357	10,000	108 ppm		1875	100 ppm	1875			

						400 ppm (TEEL-3)	127				1140	390 ppm	Liquid Spill	1140		
							227				3510	390 ppm		3510		
							297				5800	390 ppm		5800		
							327				7000	390 ppm		7000		
							357				8200	390 ppm		8200		
13	1,3,5-Trimethylbenzene (also Mesitylene)	108-67-8	3	Liquid	2.73 mm Hg at 25°C	164.7°C	25 ppm (TEEL-2)	127	3500	24.3 ppm	Puddle (Heavy Gas)	900	24 ppm	Liquid Spill	900	
								227	12,000	24.4 ppm		2800	24 ppm		2800	
								297	20,500	24 ppm		4650	24 ppm		4650	
								327	25,500	24.3 ppm		5600	24 ppm		5600	
								357	30,500	24.2 ppm		6600	24 ppm		6600	
							500 ppm (TEEL-3)	127				52,000	490 ppm	Liquid Spill	52,000	
								227				>100,000			100,000	
								297				>100,000			100,000	
								327				>100,000			100,000	
								357				>100,000			100,000	
14	1,3-Dichlorobenzene (also M-Dichlorobenzene)	541-73-1	6	Liquid	2.13 mm Hg at 25°C	172°C	15 ppm (TEEL-2)	127	3500	14.7 ppm	Puddle (Heavy Gas)	1050	14 ppm	Liquid Spill	1050	CERCLA chemical; reportable quantity = 100 lbs
								227	12,000	14.7 ppm		3200	14 ppm		3200	EPCRA Section 313 chemical
								297	20,000	14 ppm		5450	14 ppm		5450	
								327	26,500	14.9 ppm		6500	14 ppm		6500	
								357	31,750	14.9 ppm		7700	14 ppm		7700	
							75 ppm (TEEL-3)	127				7875	74 ppm	Liquid Spill	7875	
								227				23,750	74 ppm		23,750	
								297				39,750	74 ppm		39,750	
								327				47,500	74 ppm		47,500	
								357				56,000	74 ppm		56,000	
15	1,3-Dichloropropane	142-28-9	3	Liquid	18.1 mm Hg at 25°C	120.4°C	100 ppm (TEEL-2)	127	3350	99.4 ppm	Puddle (Heavy Gas)	765	99 ppm	Liquid Spill	765	CERCLA chemical; reportable quantity = 5000 lbs
								227	10,500	97.3 ppm		2350	99 ppm		2350	
								297	18,000	97.5 ppm		3900	99 ppm		3900	
								327	22,000	98.4 ppm		4700	99 ppm		4700	
								357	26,000	97.8 ppm		5500	99 ppm		5500	
							350 ppm (TEEL-3)	127				3300	340 ppm	Liquid Spill	3300	
								227				10,150	340 ppm		10,150	
								297				16,850	340 ppm		16,850	
								327				20,200	340 ppm		20,200	
								357				23,750	340 ppm		23,750	
16	2,2-Dichloropropane	594-20-7	3	Liquid	126 mm Hg at 22°C	70.5°C	110 ppm (TEEL-2)	127				85	100 ppm	Liquid Spill	85	
								227				260	100 ppm		260	
								297				440	100 ppm		440	
								327				530	100 ppm		530	
								357				620	100 ppm		620	
							400 ppm (TEEL-3)	127				350	390 ppm	Liquid Spill	350	
								227				1090	390 ppm		1090	
								297				1800	390 ppm		1800	
								327				2150	390 ppm		2150	
								357				2550	390 ppm		2550	
17	2-Butanone (also Ethyl Methyl Ketone)	78-93-3	3	Liquid	71 mm Hg at 20°C	79.6°C	2700 ppm (AEGL-2 interim)	127	12,000	2620 ppm	Puddle (Heavy Gas)	3300	2600 ppm	Liquid Spill	3300	CERCLA chemical; reportable quantity = 5000 lbs
	(NOTE: LEL = 14,000 ppm; 10% LEL ≤ AEGL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)							227	35,000	2640 ppm		10,250	2600 ppm		10,250	EPCRA Section 313 chemical
								297	57,000	2670 ppm		17,000	2600 ppm		17,000	
								327	67,000	2640 ppm		20,000	2600 ppm		20,000	
								357	78,000	2630 ppm		24,000	2600 ppm		24,000	
	(NOTE: LEL = 14,000 ppm; 10% LEL ≤ AEGL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)						4000 ppm (AEGL-3 interim)	127				5600	3900 ppm	Liquid Spill	5600	
								227				17,250	3900 ppm		17,250	
								297				28,500	3900 ppm		28,500	
								327				34,000	3900 ppm		34,000	
								357				40,000	3900 ppm		40,000	

						2000 ppm (TEEL-3)	357	50,000	995 ppm		12,700	990 ppm		12,700		
							127				3900	1900 ppm	Liquid Spill	3900		
							227				12,000	1900 ppm		12,000		
							297				19,975	1900 ppm		19,975		
							327				23,875	1900 ppm		23,875		
							357				28,100	1900 ppm		28,100		
29	Bromodichloromethane (also Dichlorobromomethane)	75-27-4	9	Liquid	50 mm Hg at 20°C	88.5°C	30 mg/m ³ (TEEL-2)	127	--	--	--	14.5	29 mg/m ³	Liquid Spill	14.5	CERCLA chemical; reportable quantity = 5000 lbs EPCRA Section 313 chemical
								227				45	29 mg/m ³		45	
								297				75	29 mg/m ³		75	
								327				90	29 mg/m ³		90	
								357				105	29 mg/m ³		105	
							150 mg/m ³ (TEEL-3)	127				75	140 mg/m ³		75	
								227				230	140 mg/m ³		230	
								297				385	140 mg/m ³		385	
								327				465	140 mg/m ³		465	
								357				545	140 mg/m ³		545	
30	Bromoform	75-25-2	6	Liquid	5 mm Hg at 20°C	149.4°C	1 ppm (TEEL-2)	127	60	0.9 ppm	Puddle (Gaussian)	48	0.93 ppm	Liquid Spill	48	CERCLA chemical; reportable quantity = 100 lbs EPCRA Section 313 chemical
								227	200	0.918 ppm		150	0.94 ppm		150	
								297	500	0.965 ppm	(Heavy Gas)	250	0.94 ppm		250	
								327	600	0.927 ppm		300	0.94 ppm		300	
								357	750	0.976 ppm		350	0.93 ppm		350	
							850 ppm (TEEL-3)	127				>100,000		Liquid Spill	100,000	
								227				>100,000			100,000	
								297				>100,000			100,000	
								327				>100,000			100,000	
								357				>100,000			100,000	
31	Bromomethane (also Methyl Bromide)	74-83-9	2	Gas	1690 mm Hg at 25°C	3.3°C	50 ppm (ERPG-2)	127	22	49.9 ppm	Direct Continuous (Heavy Gas)	4.75	48 ppm	Term Release	4.75	CERCLA chemical; reportable quantity = 1000 lbs EPCRA EHS chemical; threshold planning quantity = 1000 lbs EPCRA Section 313 chemical OSHA (29 CFR 1910.119) chemical; threshold quantity = 2500 lbs
								227	70	49.1 ppm		15	49 ppm		15	
								297	120	48.7 ppm		25	49 ppm		25	
								327	150	49.7 ppm		30	49 ppm		30	
								357	175	48.9 ppm		35	48 ppm		35	
							200 ppm (ERPG-3)	127				19	190 ppm	Term Release	19	
								227				59	190 ppm		59	
								297				99	190 ppm		99	
								327				119	190 ppm		119	
								357				141	190 ppm		141	
32	Carbon disulfide (also Carbon bisulfide)	75-15-0	3.6	Liquid	297 mm Hg at 20°C	46.7°C	160 ppm (AEGL-2 interim)	127	240	158 ppm	Puddle (Heavy Gas)	50	150 ppm	Liquid Spill	50	CAA Section 112(r) chemical; threshold quantity = 20,000 lbs CERCLA chemical; reportable quantity = 100 lbs EPCRA EHS chemical; threshold planning quantity = 10,000 lbs EPCRA Section 313 chemical
								227	900	158 ppm		160	150 ppm		160	
								297	1575	158 ppm		270	150 ppm		270	
								327	1925	159 ppm		325	150 ppm		325	
								357	2275	158 ppm		375	150 ppm		375	
							480 ppm (AEGL-3 interim)	127				170	470 ppm	Liquid Spill	170	
								227				525	470 ppm		525	
								297				880	470 ppm		880	
								327				1060	470 ppm		1060	
								357				1250	470 ppm		1250	
33	Carbon tetrachloride	56-23-5	6	Liquid	91 mm Hg at 20°C	76.7°C	190 ppm (AEGL-2 interim)	127	1750	188 ppm	Puddle (Heavy Gas)	330	180 ppm	Liquid Spill	330	CERCLA chemical; reportable quantity = 10 lbs EPCRA Section 313 chemical
								227	5350	188 ppm		1015	180 ppm		1015	
								297	9000	189 ppm		1695	180 ppm		1695	
								327	10,750	189 ppm		2030	180 ppm		2030	
								357	12,700	189 ppm		2400	180 ppm		2400	
							520 ppm (AEGL-3 interim)	127				1020	510 ppm	Liquid Spill	1020	
								227				3120	510 ppm		3120	
								297				5150	510 ppm		5150	
								327				6200	510 ppm		6200	
								357				7350	510 ppm		7350	
34	Chlorobenzene	108-90-7	3	Liquid	12 mm Hg at 25°C	167.8°C	500 ppm (TEEL-2)	127	30,000	498 ppm	Puddle (Heavy Gas)	8875	490 ppm	Liquid Spill	8875	CERCLA chemical; reportable quantity = 100 lbs

							227	85,000	490 ppm		27,000	490 ppm		27,000	EPCRA Section 313 chemical	
							297	>100,000			44,900	490 ppm		44,900		
							327	>100,000			53,700	490 ppm		53,700		
							357	>100,000			63,000	490 ppm		63,000		
							1000 ppm (TEEL-3)				23,600	990 ppm	Liquid Spill	23,600		
							127				71,000	990 ppm		71,000		
							227				>100,000			100,000		
							297				>100,000			100,000		
							327				>100,000			100,000		
							357				>100,000			100,000		
35	Chloroethane (also Ethyl chloride)	75-00-3	2	Gas	1310 mm Hg at 25°C	12.2°C	1000 ppm (TEEL-2)	127	390	983 ppm	Direct Continuous (Heavy Gas)	65	970 ppm	Term Release	65	CAA Section 112(r) chemical; threshold quantity = 10,000 lbs
								227	1120	990 ppm		205	990 ppm		205	CERCLA chemical; reportable quantity = 100 lbs
								297	1820	994 ppm		340	980 ppm		340	EPCRA Section 313 chemical
								327	2160	993 ppm		410	980 ppm		410	
								357	2500	982 ppm		480	980 ppm		480	
	(LEL = 36,000 ppm; 10% LEL ≤ TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account)						3800 ppm (TEEL-3)	127				250	3700 ppm	Term Release	250	
								227				775	3700 ppm		775	
								297				1300	3700 ppm		1300	
								327				1550	3700 ppm		1550	
								357				1840	3700 ppm		1840	
36	Chloroform	67-66-3	6	Liquid	160 mm Hg at 20°C	61.7°C	64 ppm (AEGL-2 interim)	127	220	63 ppm	Puddle (Heavy Gas)	50	63 ppm	Liquid Spill	50	CAA Section 112(r) chemical; threshold quantity = 20,000 lbs
								227	750	62.8 ppm		155	63 ppm		155	CERCLA chemical; reportable quantity = 10 lbs
								297	1300	62.6 ppm		260	63 ppm		260	EPCRA EHS chemical; threshold planning quantity = 10,000 lbs
								327	1600	63.2 ppm		310	63 ppm		310	EPCRA Section 313 chemical
								357	1900	62.9 ppm		365	63 ppm		365	
							3200 ppm (AEGL-3 interim)	127				3700	3100 ppm	Liquid Spill	3700	
								227				11,000	3100 ppm		11,000	
								297				19,000	3100 ppm		19,000	
								327				22,700	3100 ppm		20,000	
								357				26,750	3100 ppm		20,000	
37	Chloromethane (also Methyl chloride)	74-87-3	2	Gas	4220 mm Hg at 25°C	-24.4°C	400 ppm (ERPG-2)	127	110	390 ppm	Direct Continuous (Heavy Gas)	20	380 ppm	Term Release	20	CAA Section 112(r) chemical; threshold quantity = 10,000 lbs
								227	340	391 ppm		64	390 ppm		64	CERCLA chemical; reportable quantity = 100 lbs
								297	580	396 ppm		105	390 ppm		105	EPCRA Section 313 chemical
								327	700	398 ppm		128	390 ppm		128	OSHA (29 CFR 1910.119) chemical; threshold quantity = 15,000 lbs
								357	820	395 ppm		151	390 ppm		151	
							1000 ppm (ERPG-3)	127				52	990 ppm	Term Release	52	
								227				160	990 ppm		160	
								297				268	990 ppm		268	
								327				322	990 ppm		322	
								357				380	990 ppm		380	
38	cis-1,3-Dichloropropylene (also cis-1,3-Dichloro-1-propene)	10061-01-5	3	Liquid	43 mm Hg at 25°C	104.3°C	5 ppm (TEEL-2)	127	--	--	--	13.5	4.9 ppm	Liquid Spill	13.5	
								227				42	4.9 ppm		42	
								297				70	4.9 ppm		70	
								327				84	4.9 ppm		84	
								357				98	4.9 ppm		98	
							12.5 ppm (TEEL-3)	127				33	12 ppm	Liquid Spill	33	
								227				100	12 ppm		100	
								297				170	12 ppm		170	
								327				210	12 ppm		210	
								357				250	12 ppm		250	
39	Dibromochloromethane (also Chlorodibromomethane)	124-48-1	6	Liquid	54.9 mm Hg at 23.9°C	116°C	40 mg/m ³ (TEEL-2)	127	--	--	--	24	39 mg/m ³	Liquid Spill	24	CERCLA chemical; reportable quantity = 100 lbs
								227				75	39 mg/m ³		75	
								297				125	39 mg/m ³		125	
								327				150	39 mg/m ³		150	
								357				175	39 mg/m ³		175	

						150 mg/m ³ (TEEL-3)	127				90	140 mg/m ³	Liquid Spill	90		
							227				285	140 mg/m ³		285		
							297				475	140 mg/m ³		475		
							327				570	140 mg/m ³		570		
							357				675	140 mg/m ³		675		
40	Dibromomethane	74-95-3	6	Liquid	44.9 mm Hg at 25°C	95.6°C	10 mg/m ³ (TEEL-2)	127	12	9.81 mg/m ³	Puddle (Heavy Gas)	8	9.5 mg/m ³	Liquid Spill	8	CERCLA chemical; reportable quantity = 1000 lbs EPCRA Section 313 chemical
							227	40	9.5 mg/m ³		25	9.6 mg/m ³		25		
							297	71	9.82 mg/m ³		43	9.9 mg/m ³		43		
							327	86	9.96 mg/m ³		51	9.8 mg/m ³		51		
							357	102	9.95 mg/m ³		60	9.8 mg/m ³		60		
							500 mg/m ³ (TEEL-3)	127				470	490 mg/m ³	Liquid Spill	470	
							227				1460	490 mg/m ³		1460		
							297				2435	490 mg/m ³		2435		
							327				2920	490 mg/m ³		2920		
							357				3445	490 mg/m ³		3445		
41	Dichlorodifluoromethane	75-71-8	2	Gas	4980 mm Hg at 25°C	-30°C	10,000 ppm (TEEL-2)	127	4950	9980 ppm	Direct Continuous (Heavy Gas)	1250	9900 ppm	Term Release	1250	CERCLA chemical; reportable quantity = 5000 lbs EPCRA Section 313 chemical
							227	14,750	9960 ppm		3850	9900 ppm		3850		
							297	25,000	9960 ppm		6450	9900 ppm		6450		
							327	30,000	9870 ppm		7750	9900 ppm		7750		
							357	36,500	9980 ppm		9150	9900 ppm		9150		
							15,000 ppm (TEEL-3)	127				1820	14,000 ppm	Term Release	1820	
							227				5625	14,000 ppm		5625		
							297				9400	14,000 ppm		9400		
							327				11,300	14,000 ppm		11,300		
							357				13,350	14,000 ppm		13,350		
42	Ethylbenzene	100-41-4	3	Liquid	10 mm Hg at 26°C	136.2°C	125 ppm (TEEL-2)	127	6250	124 ppm	Puddle (Heavy Gas)	1450	120 ppm	Liquid Spill	1450	CERCLA chemical; reportable quantity = 1000 lbs EPCRA Section 313 chemical
							227	19,500	124 ppm		4450	120 ppm		4450		
							297	33,000	124 ppm		7450	120 ppm		7450		
							327	39,500	124 ppm		8900	120 ppm		8900		
							357	47,000	124 ppm		10,500	120 ppm		10,500		
	(LEL = 8000 ppm; 10% LEL ≤ TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account)						800 ppm (TEEL-3)	127				16,250	790 ppm	Liquid Spill	16,250	
							227				49,500	790 ppm		49,500		
							297				82,000	790 ppm		82,000		
							327				97,500	790 ppm		97,500		
							357				>100,000			100,000		
43	Ethyl ether (also Diethyl ether)	60-29-7	3	Liquid	442 mm Hg at 20°C	34.6°C	500 ppm (TEEL)	127	295	497 ppm	Puddle (Heavy Gas)	63	490 ppm	Liquid Spill	63	CAA Section 112(r) chemical; threshold quantity = 10,000 lbs
	(Note: ALOHA initial puddle temperature is set at 27.5°C—the ambient boiling point.)						227	975	494 ppm		195	490 ppm		195	CERCLA chemical; reportable quantity = 100 lbs	
							297	1650	490 ppm		330	490 ppm		330		
							327	2050	499 ppm		395	490 ppm		395		
							357	2425	496 ppm		465	490 ppm		465		
	(LEL = 17,000 ppm; 10% LEL ≤ TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account)						1900 ppm (TEEL-3)	127				260	1800 ppm	Liquid Spill	260	
							227				800	1800 ppm		800		
							297				1350	1800 ppm		1350		
							327				1600	1800 ppm		1600		
							357				1900	1800 ppm		1900		
44	Hydrogen bromide, anhydrous (also Hydrobromic acid, anhydrous)	10035-10-6	2.8	Gas	760 mm Hg at 66.5°C	-66.5°C	3 ppm (TEEL-2)	127	0.5	2.92 ppm	Direct Continuous (Heavy Gas)	0.24	2.9 ppm	Term Release	0.24	OSHA (29 CFR 1910.119) chemical; threshold quantity = 5000 lbs
							227	1.6	2.97 ppm		0.75	2.9 ppm		0.75		
							297	2.5	2.92 ppm		1.25	2.9 ppm		1.25		
							327	3.1	2.93 ppm		1.5	2.9 ppm		1.5		

								297											
								327											
								357											
50	Hydrogen iodide, anhydrous (also Hydriodic Acid 4)	10034-85-2	2	Gas	5940 mm Hg at 25°C	-35.38°C	0.5 ppm (TEEL-2)	127	0.1	0.399 ppm	Direct Continuous (Heavy Gas)	0.065	0.49 ppm	Term Release	0.065				
	(Note: Modeling assumes this chemical does not come into contact with water. A reaction with water could affect the downwind dispersion.)																		
								227	0.35	0.448 ppm		0.2	0.49 ppm		0.2				
								297	0.65	0.492 ppm		0.3	0.44 ppm		0.3				
								327	0.75	0.48 ppm		0.4	0.48 ppm		0.4				
								357	0.9	0.493 ppm		0.45	0.46 ppm		0.45				
							5 ppm (TEEL-3)	127	1.5	4.91 ppm	Direct Continuous (Heavy Gas)	0.65	4.9 ppm	Term Release	0.65				
								227	5.1	4.94 ppm		2	4.9 ppm		2				
								297	9	4.91 ppm		3.3	4.8 ppm		3.3				
								327	11	4.89 ppm		4	4.8 ppm		4				
								357	13.5	4.95 ppm		4.75	4.9 ppm		4.75				
51	Iodomethane (also Methyl iodide)	74-88-4	6	Liquid	402 mm Hg at 25°C	42.8°C	50 ppm (ERPG-2)	127	120	49.6 ppm	Puddle (Heavy Gas)	31	48 ppm	Liquid Spill	31				
								227	460	49.5 ppm		97	49 ppm		97				
								297	800	49.5 ppm		163	49 ppm		163				
								327	960	49 ppm		195	49 ppm		195				
								357	1150	49 ppm		230	49 ppm		230				
							125 ppm (ERPG-3)	127				82	120 ppm	Liquid Spill	82				
								227				250	120 ppm		250				
								297				420	120 ppm		420				
								327				505	120 ppm		505				
								357				600	120 ppm		600				
52	Isopropylbenzene (also Cumene)	98-82-8	3	Liquid	10 mm Hg at 38.3°C	152°C	50 ppm (TEEL-2)	127	4700	49.7 ppm	Puddle (Heavy Gas)	1150	49 ppm	Liquid Spill	1150				
								227	15,000	48.7 ppm		3500	49 ppm		3500				
								297	26,000	49 ppm		5900	49 ppm		5900				
								327	32,000	49.7 ppm		7100	49 ppm		7100				
								357	38,000	49.5 ppm		8300	49 ppm		8300				
	(NOTE: LEL = 8000 ppm; 10% LEL ≤ TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)						900 ppm (TEEL-3)	127				60,000	890 ppm	Liquid Spill	60,000				
								227				>100,000			100,000				
								297				>100,000			100,000				
								327				>100,000			100,000				
								357				>100,000			100,000				
53	m-Xylene	108-38-3	3	Liquid	8.35 mm Hg at 25°C	138.8°C	200 ppm (TEEL-2)	127	12,000	190 ppm	Puddle (Heavy Gas)	2900	190 ppm	Liquid Spill	2900				
								227	38,000	198 ppm		8500	190 ppm		8500				
								297	63,000	199 ppm		14,000	190 ppm		14,000				
								327	75,000	197 ppm		17,500	190 ppm		17,500				
								357	87,000	194 ppm		20,500	190 ppm		20,500				
							900 ppm (TEEL-3)	127				23,000	890 ppm	Liquid Spill	23,000				
								227				70,000	890 ppm		70,000				
								297				>100,000			100,000				
								327				>100,000			100,000				
								357				>100,000			100,000				
54	p-Xylene	106-42-3	3	Liquid	10 mm Hg at 27.3°C	138.5°C	200 ppm (TEEL-2)	127	12,000	199 ppm	Puddle (Heavy Gas)	2700	190 ppm	Liquid Spill	2700				
								227	36,000	198 ppm		8350	190 ppm		8350				
								297	60,000	199 ppm		13,750	190 ppm		13,750				
								327	72,000	199 ppm		16,500	190 ppm		16,500				
								357	84,000	197 ppm		19,500	190 ppm		19,500				
							900 ppm (TEEL-3)	127				21,500	890 ppm	Liquid Spill	21,500				
								227				65,000	890 ppm		65,000				
								297				>100,000			100,000				
								327				>100,000			100,000				

CERCLA chemical; reportable quantity = 100 lbs
EPCRA Section 313 chemical
OSHA (29 CFR 1910.119) chemical; threshold quantity = 7500 lbs

CERCLA chemical; reportable quantity = 5000 lbs
EPCRA Section 313 chemical

CERCLA chemical; reportable quantity = 1000 lbs
EPCRA Section 313 chemical

CERCLA chemical; reportable quantity = 100 lbs
EPCRA Section 313 chemical

	(NOTE: LEL = 7000 ppm; 10% LEL ≤ TEEL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)																		
						750 ppm (TEEL-3)	127												
							227												
							297												
							327												
							357												
66	Tetrachloroethylene (also Perchloroethylene)	127-18-4	6	Liquid	14 mm Hg at 20°C	121.1°C	230 ppm (AEGL-2 interim)	127	12,500	224 ppm	Puddle (Heavy Gas)	3000	220 ppm	Liquid Spill	3000				
								227	37,500	224 ppm		9000	220 ppm		9000				
								297	61,000	223 ppm		15,000	220 ppm		15,000				
								327	75,000	229 ppm		18,000	220 ppm		18,000				
								357	88,000	228 ppm		21,000	220 ppm		21,000				
							1200 ppm (AEGL-3 interim)	127											
								227				25,500	1100 ppm	Liquid Spill	25,500				
								297				78,000	1100 ppm		78,000				
								327				>100,000			>100,000				
								357				>100,000			>100,000				
67	Toluene	108-88-3	3	Liquid	20 mm Hg at 18.3°C	111.1°C	510 ppm (AEGL-2 interim)	127	9000	508 ppm	Puddle (Heavy Gas)	2050	500 ppm	Liquid Spill	2050				
								227	26,500	505 ppm		8200	500 ppm		8200				
								297	43,500	503 ppm		10,500	500 ppm		10,500				
								327	52,000	501 ppm		12,500	500 ppm		12,500				
								357	61,500	505 ppm		14,500	500 ppm		14,500				
	(NOTE: LEL = 11,000 ppm; 10% LEL ≤ AEGL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)						2900 ppm (AEGL-3 interim)	127											
								227				20,500	2800 ppm	Liquid Spill	20,500				
								297				60,500	2800 ppm		60,500				
								327				100,000	2800 ppm		100,000				
								357				>100,000			>100,000				
68	trans-1,2-Dichloroethylene (also trans-1,2-Dichloroethene)	156-60-5	3	Liquid	331 mm Hg at 25°C	48°C	1000 ppm (AEGL-2 interim)	127	2050	975 ppm	Puddle (Heavy Gas)	440	990 ppm	Liquid Spill	440				
								227	6400	994 ppm		1360	990 ppm		1360				
								297	10,400	993 ppm		2250	990 ppm		2250				
								327	12,400	993 ppm		2700	990 ppm		2700				
								357	14,500	992 ppm		3200	990 ppm		3200				
	(NOTE: LEL = 56,000 ppm; 10% LEL ≤ AEGL < 50% LEL; safety considerations against the hazard(s) of explosion(s) must be taken into account.)						17,000 ppm (AEGL-3 interim)	127											
								227				13,200	16,000 ppm	Liquid Spill	13,200				
								297				40,300	16,000 ppm		40,300				
								327				66,000	16,000 ppm		66,000				
								357				79,600	16,000 ppm		79,600				
												93,300	16,000 ppm		93,300				
69	trans-1,3-Dichloropropylene	10061-02-6	3	Liquid	30 mm Hg at 20°C	112°C	5 ppm (TEEL-2)	127				15	4.9 ppm	Liquid Spill	15				
								227				47	4.9 ppm		47				
								297				78	4.9 ppm		78				
								327				93	4.9 ppm		93				
								357				112	4.9 ppm		112				
							25 ppm (TEEL-3)	127											
								227											
								297											
								327											
								357											
70	Trichloroethylene	79-01-6	6	Liquid	58 mm Hg at 20°C	87.2°C	450 ppm (AEGL-2 interim)	127	5400	446 ppm	Puddle (Heavy Gas)	1150	440 ppm	Liquid Spill	1150				
								227	17,000	446 ppm		3550	440 ppm		3550				
								297	28,000	446 ppm		5950	440 ppm		5950				
								327	33,100	444 ppm		7100	440 ppm		7100				
								357	39,500	448 ppm		8300	440 ppm		8300				

