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Center for Integrated Nanotechnologies (CINT) Chemical Release Modeling Evaluation

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Center for Integrated Nanotechnologies (CINT)
Chemical Release Modeling Evaluation

Purpose

This evaluation documents the methodology and results of chemical release modeling for operations at Building 518, Center for Integrated Nanotechnologies (CINT) Core Facility. This evaluation is intended to supplement an update to the CINT [Standalone] Hazards Analysis (SHA). This evaluation also updates the original [Design] Hazards Analysis (DHA) completed in 2003 during the design and construction of the facility; since the original DHA, additional toxic materials have been evaluated and modeled to confirm the continued low hazard classification of the CINT facility and operations. This evaluation addresses the potential catastrophic release of the current inventory of toxic chemicals at Building 518 based on a standard query in the Chemical Information System (CIS).

Background

The CINT Building 518 is located on Department of Energy (DOE) property immediately adjacent to Kirtland Air Force Base (AFB) on the West Side of Eubank Boulevard. CINT is Sandia-Controlled and considered an "onsite" facility and operation, per the Sandia National Laboratories *10 CFR 851 Worker Safety and Health Program* (WSHP, PG470246) and the Sandia National Laboratories *Environmental, Safety, and Health Safety Basis Manual* (MN471017). There is no fence surrounding the facility reflecting the open and collaborative operations of the CINT facility.

Internal access to the facility is controlled through a Sandia National Laboratories badge reading system. External access to the facility can be controlled (if/when necessary) with normally open access gates into the parking lot and controlled with normally closed access gates into the receiving/dock area located in the rear, west of the building.

From the dock or receiving area of the facility, the Kirtland AFB fence line is located approximately 50 meters (m) to the west – with the Kirtland AFB family housing located approximately 160 m to the west, inside the Kirtland AFB fence line. Eubank Boulevard is located approximately 210 m to the east from the receiving area. On either side of the CINT facility, two lots of open land owned by the Department of Energy (DOE) are located approximately 225 m to the south and 190 m north of the receiving area. The adjacent property to the west is owned and controlled by Kirtland AFB whereas the property to the north and south are owned and controlled by DOE. The Kirtland fence provides the west boundary of these properties. Because these properties are owned/controlled by either DOE or Kirtland AFB, the nearest property boundary where there could be an offsite impact is to the east along Eubank Boulevard at approximately 210 m.

Release Scenario

To evaluate hazard classification and for site wide comparability, the release scenario modeled is a full container/cylinder release over a fifteen (15) minute period using the IFSB standard modeling protocol. As postulated for gases, an accidental release of toxic materials could result from a cylinder rupture because of mishandling or cylinder failure. An external release is hypothesized with the two general initiating events – (a) the cylinder is accidentally dropped impacting the valve or (b) the cylinder wall, throat, or plug fails.

Historical Modeling

From the 2003 DHA that was completed to support design and construction, a one-pound cylinder of chlorine (Cl_2) gas was determined to be the worst-case chemical release for the facility because chlorine

had the greatest toxic endpoint distance based upon the quantity and toxic endpoint concentration. For the original DHA, DOE approved the adoption of the American Industrial Hygiene Association (AIHA) emergency response planning guidelines (ERPG) for assessing hazard classification, hazard categorization, and risk. Through the Energy Facility Contractors Group (EFCOG), DOE provided guidance to evaluate both onsite and offsite impacts as a result of accidental releases against the ERPG values. The releases were compared with ERPG-2 and ERPG-3 values.

The toxic endpoint determined in the original DHA was at 196 m. This is less than the nearest uncontrolled offsite receptor currently at the CINT boundary to the east; however, this distance is greater than the approximately 50 m distance to the CINT facility boundary to the west. The Kirtland AFB family housing was not present when the facility was originally constructed. Other chemicals evaluated in the 2003 analysis included Ammonia, Boron Trichloride, Fluorine, and Silane.

Current Modeling Methodology

The current evaluation addresses potential catastrophic releases of single containers/cylinder in the current inventory of toxic chemicals at Building 518. A standard query of Sandia's Chemical Inventory System (CIS) was completed in November 2016, and a list of chemicals currently stored at the CINT facility was obtained from this query. Since this review consists of the worst-case scenario of single container failure, the starting quantities assumed for this study are based on the sizes of individual containers of each of the chemicals reviewed. The starting list of chemicals and quantities is included in **Table 1** below.

Table 1. CINT Chemicals and Starting Quantities

Chemical Name	Quantity (lb) [1]
Sulfur Hexafluoride (SF_6)	100
Boron Trichloride (BCl_3)	0.00037
Nitrous Oxide (N_2O)	60
Hydrogen Bromide (HBr)	0.0006
Ethylene Oxide EtO (C_2H_4O)	0.500
Thionyl Chloride ($SOCl_2$)	0.3609
Carbon Monoxide (CO)	2.0270
Ammonia (NH_3)	8
Chlorine (Cl_2)	1
Dichlorosilane DCS (H_2SiCl_2)	8
Phosphorus Oxychloride ($POCl_3$)	0.5456
Iron Carbonyl ($Fe(CO)_5$)	0.2203

1. Modeled quantity based on CIS data obtained November, 2016; quantity represents the size of an individual container of the chemical under review.

Following the current modeling methodology to evaluate consequences to potential onsite and offsite receptors, the release of toxic chemicals are modeled to a toxic endpoint based on Protective Action Criteria (PAC) concentration values. As recommended by DOE and EFCOG, the recommend toxic

endpoint concentration is currently based on PAC values which reflect values based on the following hierarchy of existing chemical exposure limit values:

- Acute Exposure Guideline Level (AEGL) values, provided by EPA and co-developed by the National Academy of Sciences and the National Research Council Committee (NRCC),
- Emergency Response Planning Guideline (ERPG) values, developed by the American Industrial Hygiene Association (AIHA), and
- Temporary Emergency Exposure Limit (TEEL) values, provided by the Subcommittee on Consequence Assessment and Protective Actions (SCAPA), developed by the Department of Energy (DOE) Office of Energy Management (OEM).

PAC values are routinely updated and revised based on changes and updates from these development organizations.

Exposure guidelines for PAC include 3 sets of exposure values: PAC-1, PAC-2, and PAC-3. PAC-3 values consider life-threatening health effects, PAC-2 values consider irreversible and/or long-term health effects, and PAC-1 values consider transient health effects. The standard modeling protocol is to model potential catastrophic releases against the PAC-3 values (the highest tier of the PAC exposure values) in order to determine facility hazard classification. Additional modeling was also completed to review the exposures against PAC-2 values, for informational purposes, and for comparability with the original DHA report.

This analysis used the Areal Locations of Hazardous Atmospheres (ALOHA) computer model (NOAA, 1996) to assess the impacts. ALOHA is jointly produced by the National Oceanographic and Atmospheric Administration (NOAA) and the US Environmental Protection Agency (EPA) Office of Emergency Management. ALOHA is designed to model releases from various sources in order to estimate a resultant hazardous gas cloud concentration at a user-selected location. ALOHA is one of the more commonly used dispersion models for analyzing chemical releases. The model has been used by SNL personnel for emergency planning and facility safety assessments.

To evaluate the consequences against the stated facility classification (i.e., low-hazard) the methodology provided in Toxic Chemical Hazard Classification and Risk Acceptance Guidelines for Use in DOE Facilities, WRSC-MS-92-206 Rev 2 (WRSC, 1995) was used. The WRSC methodology provides guidance for using the ERPG values to determine the facility classification. The methodology looks at impacts to onsite receptors within 100 meters of the release point because hazard classification for a facility is based on impacts within 100 meters of the facility.

Using ALOHA, each chemical found in the CIS database at the CINT facility was modeled to determine the PAC-3 toxic endpoint radius. In the event of a release, local, onsite, and offsite people within the toxic endpoint distance could experience life-threatening effects. The standard modeling protocol methodology for an offsite release assumes 95% worst-case meteorology. **Table 2** below presents the IFSB standard modeling protocol inputs into the ALOHA model for this study.

Table 2. IFSB Standard Modeling Protocol – General Parameters

Variable	Model Input
Wind Speed	1.5 m/s
Wind Input Height	10 meters (m)
Ground Roughness	Open Country
Cloud Cover	0%
Humidity	25%
Air Temperature	20 C
Inversion Height	300 m
Release Quantity	Single Container/Cylinder (lb)
Release Period	15 minutes
Atmospheric Stability Class	F

The ALOHA model provides a distance to the selected (PAC-3) toxic endpoint, which is used to assume an impact zone. The modeled impact zone corresponds to the area within the radius of the calculated toxic endpoint distance from the release point, as modeled with the assumption of a single wind direction. The modeled impact zone encompasses an area much larger than would be impacted by the gas plume or cloud during an actual release. During an actual release, the plume would follow the wind direction to produce a smaller footprint of impact because the plume is generally oriented along an axis in one direction.

Table 3 presents the modeled release rates and toxic endpoints for the starting quantities of the chemicals found in the CIS database for the CINT facility.

Table 3. CINT Chemicals – Toxic Endpoint Distances for PAC-3 Values

Chemical Name	Quantity (lb) [1]	PAC-3 (ppm)	Toxic Endpoint (m)
Sulfur Hexafluoride (SF_6)	100	200000	10
Boron Trichloride (BCl_3)	0.00037	71	11
Nitrous Oxide (N_2O)	60	20000	11
Hydrogen Bromide (HBr)	0.0006	120	11
Ethylene Oxide EtO (C_2H_4O)	0.500	200	13
Thionyl Chloride ($SOCl_2$)	0.3609	14	27
Carbon Monoxide (CO)	2.0270	330	38
Ammonia (NH_3)	8	1100	53
Chlorine (Cl_2)	1	20	54
Dichlorosilane DCS (H_2SiCl_2)	8	50	61[i]
Phosphorus Oxychloride ($POCl_3$)	0.5456	0.85	145[ii]
Iron Carbonyl ($Fe(CO)_5$)	0.2203	0.18	185[iii]

Chemical Name	Quantity (lb) [1]	PAC-3 (ppm)	Toxic Endpoint (m)
Hydrochloric Acid (Byproduct of DCS)	2.89	100	58
Hydrochloric Acid (Byproduct of $POCl_3$)	0.6469	100	30
Carbon Monoxide (Byproduct of $Fe(CO)_5$)	0.2357	330	13

1. Byproducts of DCS, $POCl_3$ and $Fe(CO)_5$ are based on stoichiometric quantities released as byproducts

Results

This model assumes that the Building 518 receiving area is where a potential catastrophic release is considered most likely to occur. The following endpoint distances are considered in this evaluation: the nearest CINT boundary (approximately 50m to the west), the nearest offsite boundary [iv](210m east of the receiving area) and the 100m distance for potential hazard classification.

Note that model results presented here are based on a catastrophic release of hazardous material against acute exposure criteria; estimation of actual releases with corresponding ambient air quality modeling against an 8-hr time weighted average (TWA) was not completed because actual release quantities of hazardous materials released from CINT operations is relatively low in comparison with a catastrophic release.

Offsite Boundary The nearest offsite boundary is approximately 210 meters east of the receiving area. The modeling results demonstrate that a single cylinder release for any of the listed chemicals will not have an offsite release that exceeds the PAC-3 values at the east boundary or at the Kirtland housing to the west. Because the facility is located near a housing area, modeling was also completed for the PAC-2 toxic endpoints. The modeling against the PAC-2 toxic endpoint shows an increase in the distance/impact area greater than shown for the modeling against a PAC-3 toxic endpoint; however, the PAC-2 modeling reflects lower concentrations and consequently lower potential health effects. The PAC-2 model results are included in the results for informational purposes (see attachment) and comparison with the historical modeling completed against the ERPG-2 toxic endpoint.

Hazard Classification Boundary Toxic endpoint distances for two chemicals exceed the 100 m threshold for potential hazard classification: Iron Pentacarbonyl ($Fe(CO)_5$) and Phosphorus Oxychloride ($POCl_3$). Both chemicals spontaneously ignite when exposed to air and therefore releases of these chemicals would not be expected to impact an offsite receptor. Refined modeling of the $Fe(CO)_5$ and $POCl_3$ byproducts (Hydrogen Chloride (HCl) and Carbon Monoxide (CO) respectively) shows that the toxic endpoints for the byproducts of these chemicals do not exceed the PAC-3 values at the east boundary.

CINT Boundary From the list of remaining chemicals, the largest potential toxic endpoint distance potentially occurs from a release of DCS. DCS breaks down to produce Hydrochloric Acid and Silicon Hydrochloride. Because the breakdown of DCS may not occur spontaneously or completely, two potential release scenarios are considered: a release of DCS without breakdown, and a release of DCS as breakdown products.

Figure 1 presents the largest potential impact zone based on a release of DCS to a PAC-3 toxic endpoint at 61m, crossing the Kirtland AFB boundary to the west. Additional refined modeling of HCl determined that the toxic endpoint for this byproduct does not exceed the PAC-3 values at the western boundary.

Modeling demonstrates that a potential catastrophic release of Ammonia, Chlorine, or the HCl byproduct from a DCS release may occur beyond the CINT boundary but within the controlled Kirtland AFB boundary/fenceline.

Attachment 1 provides the modeling analysis and refined calculations from this review. **Attachment 2** provides the printouts from the ALOHA modeling runs completed for this study.

Figure 1. CINT Modeling Results at Approximately 60 m

[i] Modeled byproduct from Dichlorosilane (DCS) reaction as Hydrogen Chloride based on stoichiometric chemistry – DCS can react with (atmospheric water)
[ii] Modeled byproduct from Phosphorus Oxychloride ($POCl_3$) reaction as hydrogen chloride based on stoichiometric chemistry – $POCl_3$ can spontaneously ignite when exposed to air
[iii] Modeled byproduct from Iron Pentacarbonyl ($Fe(CO)_5$) reaction as Carbon Monoxide – $Fe(CO)_5$ can spontaneously ignite when exposed to air
[iv] Offsite boundary in this context means outside of the Kirtland AFB boundary

CINT Toxics Modeling - Chemicals In Inventory

	CAS No	Starting Qty	Release Time	Release Rate	PAC-3	Endpoint	PAC-2	Endpoint
		lb	*min*	*lb/min*	*ppm*	*m*	*ppm*	*m*
Sulfur Hexafluoride	2551-62-4	100	15	6.666666667	200000	10	33000	12
Boron Trichloride	10294-34-5	0.00037	15	2.46667E-05	71	11	2.1	11
Nitrous Oxide	10024-97-2	60	15	4	20000	11	10000	12
Hydrogen Bromide	10035-10-6	0.00055	15	3.66667E-05	120	11	40	11
Ethylene Oxide	75-21-8	0.50044	15	0.033362667	200	13	45	34
Thionyl Chloride	7719-09-7	0.36092	15	0.024061333	14	27	2.4	74
Carbon Monoxide	630-08-0	2.02703	15	0.135135333	330	38	83	77
Ammonia	7664-41-7	8	15	0.533333333	1100	53	160	142
Chlorine	7782-50-5	1	15	0.066666667	20	54	2	194
Dichlorosilane (DCS)	4109-96-0	8	15	0.533333333	50	61	11	161
Phosphorus (v) Oxychloride (POCl3)	10025-87-3	0.5464	15	0.036426667	0.85	145	0.48	198
Iron Pentacarbonyl	13463-40-6	0.22034	15	0.014689333	0.18	185	0.06	333
Hydrochloric Acid (DCS Byproduct)		2.89	15	0.192666667	100	58	22	135
Hydrochloric Acid (POCl Byproduct)		0.6469	15	0.043126667	100	30	22	63
Carbon Monoxide (Iron Pentacarbonyl Byproduct)		0.23571	15	0.015714	330	13	83	26

CINT Toxics Modeling - Chemicals In Inventory

	Evaluation: Toxic Endpoint PAC-3 Exceeds CINT Boundary					Evaluation: Toxic Endpoint PAC-2 Exceeds CINT Boundary				
	KAFB Housing West (m)	Distance West (m)	Distance North (m)	Distance East (m)	Distance South (m)	KAFB Housing West (m)	Distance West (m)	Distance North (m)	Distance East (m)	Distance South (m)
	160	*50*	*190*	*210*	*225*	*160*	*50*	*190*	*210*	*225*
Sulfur Hexafluoride	under	under	under	under	under	under	under	under	under	under
Boron Trichloride	under	under	under	under	under	under	under	under	under	under
Nitrous Oxide	under	under	under	under	under	under	under	under	under	under
Hydrogen Bromide	under	under	under	under	under	under	under	under	under	under
Ethylene Oxide	under	under	under	under	under	under	under	under	under	under
Thionyl Chloride	under	under	under	under	under	under	over	under	under	under
Carbon Monoxide	under	under	under	under	under	under	over	under	under	under
Ammonia	under	over	under	under	under	under	over	under	under	under
Chlorine	under	over	under	under	under	over	over	over	under	under
Dichlorosilane (DCS)	under	over	under	under	under	over	over	under	under	under
Phosphorus (v) Oxychloride (POCl3)	under	over	under	under	under	over	over	over	under	under
Iron Pentacarbonyl	over	over	under	under	under	over	over	over	over	over
Hydrochloric Acid (DCS Byproduct)	under	over	under	under	under	under	over	under	under	under
Hydrochloric Acid (POCl Byproduct)	under	under	under	under	under	under	over	under	under	under
Carbon Monoxide (Iron Pentacarbonyl Byproduct)	under	under	under	under	under	under	under	under	under	under

Attachment 1
CINT Modeling Results

Fe(CO)5	195	g/mol	13463-40-6
Fe	55.85	g/mol	
CO	28.01	g/mol	
Assumed Stoichiometry		(CO)5 + Fe --> Fe(CO)5	

0.08	lbs	x	454	g/lb	=	36.32 g	
36.32	g	/	195	g/mol	=	0.186256 mol	
0.186256	mol Fe(CO)5	x	5	mol CO	/	1 mol Fe(CO)5	= 0.931282 mol CO
0.931282	mol CO	x	28.0101	g/mol CO	=	26.0853 g CO	0.0575 lb CO

Compound Name	**Mol Wt**		**CAS Number**
$POCl_3$	153.3	g/mol	10025-87-3
HCl	36.5	g/mol	
H3PO4	98	g/mol	
Assumed Stoichiometry:		$POCl_3 + 3H_2O$ --> $H_3PO_4 + 3HCl$	

0.55	lbs	x	454	g/lb	=	249.7 g	
249.7	g	/	153.33	g/mol	=	1.628514 mol	
1.628514	mol POCl3	x	3	mol HCl	/	1 mol POCl3	= 4.885541 mol HCl
4.885541	mol CO	x	36.5	g/mol HCl	=	178.3222 g HCl	0.3928 lb HCl

0.55	lbs	x	454	g/lb	=	249.7 g	
249.7	g	/	153.33	g/mol	=	1.628514 mol	
1.628514	POCl3	x	1	mol H3PO4	/	1 POCl3	= 1.628514 mol H3PO4
1.628514	mol H3PO4	x	98	g/mol CO	=	159.5943 g H3PO4	0.3515 lb H3PO4

Compound Name	**Mol Wt**		**CAS Number**
SiH_2Cl_2 (DCS)	101	g/mol	4109-96-0
HCl	36.5	g/mol	
SiHCl	64.5	g/mol	
Assumed Stoichiometry		SiH_2Cl_2 --> SiHCl + HCl	

8	lbs	x	454	g/lb	=	3632 g	
3632	g	/	101	g/mol	=	35.9604 mol	
35.9604	mol DCS	x	1	mol HCl	/	1 mol DCS	= 35.9604 mol HCl
35.9604	mol CO	x	36.5	g/mol HCl	=	1312.554 g HCl	2.89 lb HCl

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Chemical Name: SULFUR HEXAFLUORIDE
  CAS Number: 2551-62-4                    Molecular Weight: 146.06 g/mol
  PAC-1: 3000 ppm    PAC-2: 33000 ppm      PAC-3: 200000 ppm
  Normal Boiling Point: -unavail-
  Vapor Pressure at Ambient Temperature: greater than 1 atm
  Ambient Saturation Concentration: 1,000,000 ppm or 100.0%
  Note: Not enough chemical data to use Heavy Gas option

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country           Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet               Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: 6.66667 pounds/min        Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 3.02 kilograms/min
  Total Amount Released: 45.4 kilograms

THREAT ZONE:
  Model Run: Gaussian
  Red    : less than 10 meters(10.9 yards) --- (200000 ppm = PAC-3)
  Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
  Orange: 12 meters --- (33000 ppm = PAC-2)
  Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
  Yellow: 39 meters --- (3000 ppm = PAC-1)
  Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Warning: BORON TRICHLORIDE can react with water and/or water vapor to
  produce hydrochloric acid and heat.  ALOHA cannot accurately predict the
  air hazard if a reaction occurs.
  Chemical Name: BORON TRICHLORIDE
  CAS Number: 10294-34-5                  Molecular Weight: 117.17 g/mol
  PAC-1: 0.19 ppm    PAC-2: 2.1 ppm       PAC-3: 71 ppm
  Ambient Boiling Point: 7.3° C
  Vapor Pressure at Ambient Temperature: greater than 1 atm
  Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country          Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet              Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: 2.47e-5 pounds/min       Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 0.0112 grams/min
  Total Amount Released: 0.17 grams
  Note: This chemical may flash boil and/or result in two phase flow.

THREAT ZONE:
  Model Run: Heavy Gas
  Red    : 11 meters --- (71 ppm = PAC-3)
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Orange: 11 meters --- (2.1 ppm = PAC-2)
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Yellow: 11 meters --- (0.19 ppm = PAC-1)
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Chemical Name: NITROUS OXIDE
  CAS Number: 10024-97-2                  Molecular Weight: 44.01 g/mol
  PAC-1: 910 ppm     PAC-2: 10000 ppm     PAC-3: 20000 ppm
  Ambient Boiling Point: -91.5° C
  Vapor Pressure at Ambient Temperature: greater than 1 atm
  Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country          Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet              Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: 4 pounds/min             Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 1.81 kilograms/min
  Total Amount Released: 27.2 kilograms
  Note: This chemical may flash boil and/or result in two phase flow.

THREAT ZONE:
  Model Run: Heavy Gas
  Red    : 11 meters --- (20000 ppm = PAC-3)
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Orange: 12 meters --- (10000 ppm = PAC-2)
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Yellow: 52 meters --- (910 ppm = PAC-1)
```

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Chemical Name: HYDROGEN BROMIDE
   CAS Number: 10035-10-6                    Molecular Weight: 80.91 g/mol
   AEGL-1 (60 min): 1 ppm   AEGL-2 (60 min): 40 ppm   AEGL-3 (60 min): 120
ppm
   IDLH: 30 ppm
   Ambient Boiling Point: -70.1° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: 3.67e-5 pounds/min       Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 0.0166 grams/min
   Total Amount Released: 0.25 grams
   Note: This chemical may flash boil and/or result in two phase flow.

 THREAT ZONE:
   Model Run: Heavy Gas
   Red    : 11 meters --- (120 ppm = AEGL-3 [60 min])
   Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
   Orange: 11 meters --- (40 ppm = AEGL-2 [60 min])
   Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
   Yellow: 11 meters --- (1 ppm = AEGL-1 [60 min])
   Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Chemical Name: ETHYLENE OXIDE
  CAS Number: 75-21-8                    Molecular Weight: 44.05 g/mol
  AEGL-1 (60 min): N/A   AEGL-2 (60 min): 45 ppm   AEGL-3 (60 min): 200 ppm
  IDLH: 800 ppm      LEL: 30000 ppm      UEL: 1000000 ppm
  Carcinogenic risk - see CAMEO Chemicals
  Ambient Boiling Point: 5.8° C
  Vapor Pressure at Ambient Temperature: greater than 1 atm
  Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country         Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet             Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: .033363 pounds/min      Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 15.1 grams/min
  Total Amount Released: 227 grams
  Note: This chemical may flash boil and/or result in two phase flow.

THREAT ZONE:
  Model Run: Heavy Gas
  Red    : 13 meters --- (200 ppm = AEGL-3 [60 min])
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Orange: 34 meters --- (45 ppm = AEGL-2 [60 min])
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Yellow: no recommended LOC value --- (N/A = AEGL-1 [60 min])
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Warning: THIONYL CHLORIDE can react with water and/or water vapor to
  produce hydrochloric acid, sulfur dioxide and heat.  ALOHA cannot
  accurately predict the air hazard if a reaction occurs.
  Chemical Name: THIONYL CHLORIDE
  CAS Number: 7719-9-7                    Molecular Weight: 118.97 g/mol
  AEGL-1 (60 min): N/A   AEGL-2 (60 min): 2.4 ppm   AEGL-3 (60 min): 14 ppm
  Ambient Boiling Point: 69.8° C
  Vapor Pressure at Ambient Temperature: 0.13 atm
  Ambient Saturation Concentration: 151,475 ppm or 15.1%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country          Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet              Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: .024061 pounds/min       Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 10.9 grams/min
  Total Amount Released: 164 grams

THREAT ZONE:
  Model Run: Heavy Gas
  Red    : 27 meters --- (14 ppm = AEGL-3 [60 min])
  Note: Threat zone was not drawn because effects of near-field patchiness
    make dispersion predictions less reliable for short distances.
  Orange: 74 meters --- (2.4 ppm = AEGL-2 [60 min])
  Yellow: no recommended LOC value --- (N/A = AEGL-1 [60 min])
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Chemical Name: CARBON MONOXIDE
  CAS Number: 630-8-0                    Molecular Weight: 28.01 g/mol
  AEGL-1 (60 min): N/A   AEGL-2 (60 min): 83 ppm   AEGL-3 (60 min): 330 ppm
  IDLH: 1200 ppm     LEL: 125000 ppm     UEL: 742000 ppm
  Ambient Boiling Point: -193.1° C
  Vapor Pressure at Ambient Temperature: greater than 1 atm
  Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country         Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet             Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: .135135 pounds/min      Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 61.3 grams/min
  Total Amount Released: 919 grams
  Note: This chemical may flash boil and/or result in two phase flow.
     Use both dispersion modules to investigate its potential behavior.

THREAT ZONE:
  Model Run: Gaussian
  Red    : 38 meters --- (330 ppm = AEGL-3 [60 min])
  Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
  Orange: 77 meters --- (83 ppm = AEGL-2 [60 min])
  Yellow: no recommended LOC value --- (N/A = AEGL-1 [60 min])
```

Text Summary

ALOHA® 5.4.7

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Chemical Name: AMMONIA
   CAS Number: 7664-41-7                    Molecular Weight: 17.03 g/mol
   AEGL-1 (60 min): 30 ppm   AEGL-2 (60 min): 160 ppm   AEGL-3 (60 min):
1100 ppm
   IDLH: 300 ppm      LEL: 150000 ppm      UEL: 280000 ppm
   Ambient Boiling Point: -37.0° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: .5333333 pounds/min      Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 242 grams/min
   Total Amount Released: 3.63 kilograms
   Note: This chemical may flash boil and/or result in two phase flow.
      Use both dispersion modules to investigate its potential behavior.

 THREAT ZONE:
   Model Run: Gaussian
   Red    : 53 meters --- (1100 ppm = AEGL-3 [60 min])
   Orange: 142 meters --- (160 ppm = AEGL-2 [60 min])
   Yellow: 338 meters --- (30 ppm = AEGL-1 [60 min])
```

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Chemical Name: CHLORINE
   CAS Number: 7782-50-5                    Molecular Weight: 70.91 g/mol
   AEGL-1 (60 min): 0.5 ppm   AEGL-2 (60 min): 2 ppm   AEGL-3 (60 min): 20
ppm
   IDLH: 10 ppm
   Ambient Boiling Point: -38.1° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: .066667 pounds/min       Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 30.2 grams/min
   Total Amount Released: 454 grams
   Note: This chemical may flash boil and/or result in two phase flow.

 THREAT ZONE:
   Model Run: Heavy Gas
   Red    : 54 meters --- (20 ppm = AEGL-3 [60 min])
   Orange: 194 meters --- (2 ppm = AEGL-2 [60 min])
   Yellow: 410 meters --- (0.5 ppm = AEGL-1 [60 min])
```

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Warning: DICHLOROSILANE can react with water and/or water vapor to
   produce hydrogen chloride and heat.  ALOHA cannot accurately predict the
   air hazard if a reaction occurs.
   Chemical Name: DICHLOROSILANE
   CAS Number: 4109-96-0                    Molecular Weight: 101.01 g/mol
   AEGL-1 (60 min): 0.9 ppm   AEGL-2 (60 min): 11 ppm   AEGL-3 (60 min): 50
ppm
   LEL: 47000 ppm     UEL: 960000 ppm
   Ambient Boiling Point: 3.5° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: .533333 pounds/min       Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 242 grams/min
   Total Amount Released: 3.63 kilograms
   Note: This chemical may flash boil and/or result in two phase flow.

 THREAT ZONE:
   Model Run: Heavy Gas
   Red    : 61 meters --- (50 ppm = AEGL-3 [60 min])
   Orange: 161 meters --- (11 ppm = AEGL-2 [60 min])
   Yellow: 724 meters --- (0.9 ppm = AEGL-1 [60 min])
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Warning: PHOSPHORUS OXYCHLORIDE can react with water and/or water vapor
  to produce hydrogen chloride, phosphine, phosphoric acid and heat.  ALOHA
  cannot accurately predict the air hazard if a reaction occurs.
  Chemical Name: PHOSPHORUS OXYCHLORIDE
  CAS Number: 10025-87-3                  Molecular Weight: 153.33 g/mol
  AEGL-1 (60 min): N/A   AEGL-2 (60 min): N/A   AEGL-3 (60 min): 0.85 ppm
  Ambient Boiling Point: 98.8° C
  Vapor Pressure at Ambient Temperature: 0.032 atm
  Ambient Saturation Concentration: 38,823 ppm or 3.88%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country          Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet              Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: .036427 pounds/min       Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 16.5 grams/min
  Total Amount Released: 248 grams

THREAT ZONE:
  Model Run: Heavy Gas
  Red    : 145 meters --- (0.85 ppm = PAC-3)
  Orange: 198 meters --- (0.48 ppm = PAC-2)
  Yellow: no recommended LOC value --- (N/A = AEGL-1 [60 min])
```

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Warning: IRON PENTACARBONYL can spontaneously ignite when exposed to air.

   ALOHA cannot accurately predict the air hazard if a reaction occurs.
   Chemical Name: IRON PENTACARBONYL
   CAS Number: 13463-40-6                  Molecular Weight: 195.90 g/mol
   AEGL-1 (60 min): N/A   AEGL-2 (60 min): 0.06 ppm   AEGL-3 (60 min): 0.18
ppm
   LEL: 2880 ppm      UEL: 206000 ppm
   Ambient Boiling Point: 96.9° C
   Vapor Pressure at Ambient Temperature: 0.030 atm
   Ambient Saturation Concentration: 35,524 ppm or 3.55%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: .014689 pounds/min       Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 6.66 grams/min
   Total Amount Released: 99.9 grams

 THREAT ZONE:
   Model Run: Heavy Gas
   Red    : 185 meters --- (0.18 ppm = PAC-3)
   Orange: 333 meters --- (0.06 ppm = PAC-2)
   Yellow: no recommended LOC value --- (N/A = AEGL-1 [60 min])
```

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Warning: HYDROGEN CHLORIDE can react with water and/or water vapor.  This
   can affect the evaporation rate and downwind dispersion.  ALOHA cannot
   accurately predict the air hazard if this substance comes in contact with
   water.
   Chemical Name: HYDROGEN CHLORIDE
   CAS Number: 7647-1-0                    Molecular Weight: 36.46 g/mol
   AEGL-1 (60 min): 1.8 ppm   AEGL-2 (60 min): 22 ppm   AEGL-3 (60 min): 100
ppm
   IDLH: 50 ppm
   Ambient Boiling Point: -88.3° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: .192667 pounds/min       Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 87.4 grams/min
   Total Amount Released: 1.31 kilograms
   Note: This chemical may flash boil and/or result in two phase flow.

 THREAT ZONE:
   Model Run: Heavy Gas
   Red    : 58 meters --- (100 ppm = PAC-3)
   Orange: 135 meters --- (22 ppm = PAC-2)
   Yellow: 521 meters --- (1.8 ppm = AEGL-1 [60 min])
```

```
 SITE DATA:
   Location: KIRTLAND AFB, NEW MEXICO
   Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
   Time: December 14, 2016  1334 hours MST (using computer's clock)

 CHEMICAL DATA:
   Warning: HYDROGEN CHLORIDE can react with water and/or water vapor.  This
   can affect the evaporation rate and downwind dispersion.  ALOHA cannot
   accurately predict the air hazard if this substance comes in contact with
   water.
   Chemical Name: HYDROGEN CHLORIDE
   CAS Number: 7647-1-0                    Molecular Weight: 36.46 g/mol
   AEGL-1 (60 min): 1.8 ppm   AEGL-2 (60 min): 22 ppm   AEGL-3 (60 min): 100
ppm
   IDLH: 50 ppm
   Ambient Boiling Point: -88.3° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1.5 meters/second from 0° true at 10 meters
   Ground Roughness: open country          Cloud Cover: 0 tenths
   Air Temperature: 20° C
   Stability Class: F (user override)
   Inversion Height: 300 feet              Relative Humidity: 25%

 SOURCE STRENGTH:
   Direct Source: .043127 pounds/min       Source Height: 0
   Release Duration: 15 minutes
   Release Rate: 19.6 grams/min
   Total Amount Released: 293 grams
   Note: This chemical may flash boil and/or result in two phase flow.

 THREAT ZONE:
   Model Run: Heavy Gas
   Red    : 30 meters --- (100 ppm = PAC-3)
   Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
   Orange: 63 meters --- (22 ppm = PAC-2)
   Yellow: 238 meters --- (1.8 ppm = AEGL-1 [60 min])
```

```
SITE DATA:
  Location: KIRTLAND AFB, NEW MEXICO
  Building Air Exchanges Per Hour: 0.19 (unsheltered single storied)
  Time: December 14, 2016  1334 hours MST (using computer's clock)

CHEMICAL DATA:
  Chemical Name: CARBON MONOXIDE
  CAS Number: 630-8-0                    Molecular Weight: 28.01 g/mol
  AEGL-1 (60 min): N/A   AEGL-2 (60 min): 83 ppm   AEGL-3 (60 min): 330 ppm
  IDLH: 1200 ppm     LEL: 125000 ppm     UEL: 742000 ppm
  Ambient Boiling Point: -193.1° C
  Vapor Pressure at Ambient Temperature: greater than 1 atm
  Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 1.5 meters/second from 0° true at 10 meters
  Ground Roughness: open country         Cloud Cover: 0 tenths
  Air Temperature: 20° C
  Stability Class: F (user override)
  Inversion Height: 300 feet             Relative Humidity: 25%

SOURCE STRENGTH:
  Direct Source: .015714 pounds/min      Source Height: 0
  Release Duration: 15 minutes
  Release Rate: 7.13 grams/min
  Total Amount Released: 107 grams
  Note: This chemical may flash boil and/or result in two phase flow.
     Use both dispersion modules to investigate its potential behavior.

THREAT ZONE:
  Model Run: Gaussian
  Red    : 13 meters --- (330 ppm = PAC-3)
  Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
  Orange: 26 meters --- (83 ppm = PAC-2)
  Note: Threat zone was not drawn because effects of near-field patchiness
     make dispersion predictions less reliable for short distances.
  Yellow: no recommended LOC value --- (N/A = AEGL-1 [60 min])
```