APPENDIX F
ALOHA SIMULATION OF AQUEOUS AMMONIA SPILLS

The Areal Locations of Hazardous Atmospheres (ALOHA), version 5.4, model was used to simulate the volatilization and air dispersion of 19 percent aqueous ammonia (NH_3) spills. ALOHA was jointly developed by the National Oceanic and Atmospheric Administration (NOAA) and the U.S. Environmental Protection Agency. The U.S. Department of Energy's Office of Environmental, Safety, and Health have designated ALOHA as one of six toolbox codes for safety analysis (DOE, 2004). The ALOHA model provides all of the thermodynamic parameter values needed to simulate spills of both anhydrous NH_3 and aqueous NH_3 solutions up to 30 percent. The user enters site specific information concerning the spill volume, the type of spill, and meteorological information.

Three types of 19 percent aqueous NH_3 spills were simulated: a 400-pound (181-kilograms) leak from a valve, an uncontained 23.1-ton (21-metric ton) (6,000-gallon [22,712-liters]) spill from a delivery truck, and a 52-ton (47-metric ton) spill from a storage tank that is surrounded by a 3-foot (0.9-meter) high berm. Each spill is simulated in the ALOHA model as a puddle-evaporation scenario in which the area and mass of aqueous NH_3 are specified. The leaking valve scenario assumes a puddle thickness of 0.4 inch (1 centimeter); the uncontained truck spill assumes a puddle thickness of 4 inches (10 centimeters); and the contained tank spill assumes a puddle thickness of a 3-foot (0.9-meter) berm. A summary of the parameter values used to model the NH_3 spills is given in Table F-1.

Table F-1. Summary of ALOHA Information Used With the 19 Percent Aqueous NH_3 Spill Simulations

	Leaking Valve Scenario	Truck Spill Scenario	Containment Spill Scenario
Description	400-pound (181-kilogram) spill	23-ton (21-metric ton) spill	52-ton (47-metric tons spill
Source type	Evaporating puddle	Evaporating puddle	Evaporating puddle
Source dimensions (length x width)	14.5 feet x 14.5feet (4.43meter x 4.43meter)	49.5 feet x 49.5 feet (15.1 meter x 15.1 meter)	24.5 feet x 24.5 feet (7.47 meter x 7.47 meter)
Source area (square feet [square meters])	211 (19.6)	2,454 (228)	601 (55.8)
Puddle Depth (inch [centimeter])	0.4 (1)	4 (10)	36 (92)
Terrain option	Simple terrain	Simple terrain	Simple terrain
Urban/rural option	Open country	Open country	Open country
Cloud cover	0	0	0
Humidity	50 percent	50 percent	50 percent
Highest daily maximum temperatures	97, 101,104, and 106°F (36, 38, 40 and 41°C)	97, 101,104, and 106°F (36, 38, 40 and 41°C)	97, 101,104, and 106°F (36, 38, 40 and 41°C)
Stability class	Pasquill F	Pasquill F	Pasquill F
Wind speed (feet/second [meter/second])	5 (1.5)	5 (1.5)	5 (1.5)

°F = degree Fahrenheit; ^{0}C = degree Celsius

F.1 WORST-CASE METEOROLOGICAL CONDITIONS

As specified in 40 CFR Part 68.22 for off-site consequence-analysis parameter values (EPA, 1999), the worst-case release analyses are to be based on a wind speed of 5 feet/second (1.5 meters/second), an F atmospheric stability class, and the highest daily maximum temperature in the previous three years. The maximum temperatures are: Tuscola-97°F (36°C), Mattoon-101°F (38°C), Jewett-104°F (40°C), and Odessa-106°F (41°C). The maximum radii to nine different predicted NH_3 concentration levels, down wind of the spills, are predicted for each of the three spill scenarios and for each of the four sites. The nine NH_3 concentration levels are: 30; 110; 160; 220; 390; 550; 1,100; 1,600; and 2,700 parts per million volume (ppmv). These concentrations represent various health-effects criteria levels used in the risk assessment for NH_3 spills (EPA, 2007) (see Section 4.17 for explanation of AEGLs). ALOHA predicts the maximum radius at which each of these concentrations can travel down wind of the spill within the first hour after the spill occurs. Table F-2 presents the predicted maximum radii for the worst-case analysis of the Jewett Site; Table F-3 presents the results for the worst-case analysis at the Tuscola Site; Table F-4 presents the results for the worst-case analysis at the Odessa Site; and, Table F-5 presents the results for the worst-case analysis at the Mattoon Site.

Table F-2. Predicted Maximum Radii for Jewett Site Worst-Case Analysis[1]

Maximum NH_3 (ppmv)	400-pound (181-kilogram) Release[2] (feet [meters])	23-ton (21-metric ton) Release[3] (feet [meters])	52-ton (47-metric ton) Release[4] (feet [meters])
30	2,858 (871)	15,092 (4,600)	8,530 (2,600)
110	1,545 (471)	6,890 (2,100)	3,937 (1,200)
160	1,296 (395)	5,577 (1,700)	3,140 (957)
220	1,122 (342)	4,921 (1,500)	2,618 (798)
390	879 (268)	3,608 (1,100)	1,900 (579)
550	755 (230)	2,907 (886)	1,572 (479)
1,100	548 (167)	1,969 (600)	1,079 (329)
1,600	456 (139)	1,591 (485)	879 (268)
2,700	344 (105)	1,178 (359)	659 (201)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from an evaporating puddle (evaporating puddle, ground, and air at 104°F (40°C) at Jewett, TX, for the worst-case meteorological conditions of 4.9 feet/second (1.5 meters/second) wind speed and Pasquill stability class F.
[2] Initial emission rate of 3.84 kg/min.
[3] Initial emission rate of 41.0 kg/min.
[4] Initial emission rate of 13.3 kg/min.
ppmv = parts per million volume.

Table F-3. Predicted Maximum Radii for Tuscola Site Worst-Case Analysis[1]

Maximum NH_3 (ppmv)	400-pound (181-kilogram) Release[2] (feet [meters])	23-ton (21-metric ton) Release[3] (feet [meters])	52-ton (47-metric ton) Release[4] (feet [meters])
30	2,687 (819)	14,108 (4,300)	7,546 (2,300)
110	1,447 (441)	6,234 (1,900)	3,281 (1,000)
160	1,211 (369)	5,249 (1,600)	2,740 (835)
220	1,050 (320)	4,265 (1,300)	2,287 (697)
390	817 (249)	3,159 (963)	1,667 (508)
550	702 (214)	2,602 (793)	1,381 (421)
1,100	505 (154)	1,752 (534)	948 (289)
1,600	417 (127)	1,414 (431)	771 (235)
2,700	315 (96)	1,043 (318)	577 (176)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from an evaporating puddle (evaporating puddle, ground, and air at 97°F (36°C) at Tuscola, IL, for the worst-case meteorological conditions of 4.9 feet/second (1.5 meters/second) wind speed and Pasquill stability class F.
[2] Initial emission rate of 3.24 kg/min.
[3] Initial emission rate of 33.4 kg/min.
[4] Initial emission rate of 10.5 kg/min.
ppmv = parts per million volume.

Table F-4. Predicted Maximum Radii for Odessa Site Worst-Case Analysis[1]

Maximum NH_3 (ppmv)	400-pound (181-kilogram) Release[2] (feet [meters])	23-ton (21-metric ton) Release[3] (feet [meters])	52-ton (47-metric ton) Release[4] (feet [meters])
30	2,950 (899)	15,584 (4,750)	9,186 (2,800)
110	1,595 (486)	7,874 (2,400)	4,265 (1,300)
160	1,339 (408)	6,562 (2,000)	3,281 (1,000)
220	1,155 (352)	5,577 (1,700)	2,756 (840)
390	906 (276)	3,937 (1,200)	1,998 (609)
550	778 (237)	3,281 (1,000)	1,654 (504)
1,100	568 (173)	2,277 (694)	1,132 (345)
1,600	472 (144)	1,841 (561)	925 (282)
2,700	361 (110)	1,362 (415)	692 (211)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from an evaporating puddle (evaporating puddle, ground, and air at 106°F (41°C) at Odessa, TX, for the worst-case meteorological conditions of 4.9 feet/second (1.5 meters/second) wind speed and Pasquill stability class F.
[2] Initial emission rate of 4.05 kg/min.
[3] Initial emission rate of 52.6 kg/min.
[4] Initial emission rate of 14.3 kg/min.
ppmv = parts per million volume.

Table F-5. Predicted Maximum Radii for Mattoon Site Worst-Case Analysis[1]

Maximum NH_3 (ppmv)	400-pound (181-kilograms) Release[2] (feet [meters])	23-tons (21-metric tons) Release[3] (feet [meters])	52-tons (47-metric tons) Release[4] (feet [meters])
30	2,805 (855)	14,764 (4,500)	8,202 (2,500)
110	1,513 (461)	6,890 (2,100)	3,609 (1,100)
160	1,266 (386)	5,577 (1,700)	2,969 (905)
220	1,096 (334)	4,593 (1,400)	2,477 (755)
390	856 (261)	3,281 (1,000)	1,798 (548)
550	735 (224)	2,785 (849)	1,490 (454)
1,100	532 (162)	1,880 (573)	1,024 (312)
1,600	443 (135)	1,519 (463)	833 (254)
2,700	335 (102)	1,125 (343)	627 (191)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from an evaporating puddle (evaporating puddle, ground, and air at 101°F (38°C) at Mattoon, IL, for the worst-case meteorological conditions of 4.9 feet/second (1.5 meters/second) wind speed and Pasquill stability class F.
[2] Initial emission rate of 3.58 kg/min.
[3] Initial emission rate of 37.5 kg/min.
[4] Initial emission rate of 11.9 kg/min.
ppmv = parts per million volume.

The highest predicted NH_3 concentrations are associated with the 23.1-ton (21-metric ton) truck spill scenario. The 52-ton (47-metric ton) tank spill scenario involves a much larger volume of aqueous NH_3, but the truck spill has the largest spill area (2,454 square feet (228 square meters) versus 601 square feet (55.8 square meters) for the tank spill). The larger the spill area, the greater the mass of NH_3 that is available to evaporate per unit time.

When comparing the same spill scenario for all sites, the only difference used in the simulations was the maximum ambient temperature. The Tuscola site was simulated with a maximum daily temperature of 97°F (36°C) (see Table F-3) and the Odessa site was simulated with a maximum daily temperature of 106°F (41°C) (see Table F-4). There is approximately a 5 percent difference in the travel distance for the NH_3 plume between sites for the same spill scenario. There is little difference among the four sites when comparing the worst-case meteorological conditions. The biggest factor is the type of spill scenario, and the uncontained truck-spill scenario results in the highest potential NH_3 exposures.

F.2 ALOHA SENSITIVITY ANALYSIS FOR 7 DIFFERENT WIND/STABILITY CONDITIONS FOR THE TRUCK SPILL SCENARIO

The effect of different meteorological conditions on the predicted air concentrations of NH_3 resulting from the 23.1-ton (21-metric ton) truck spill was examined. The results presented in Tables F-2 to F-5 were based on the conservative assumption of calm wind conditions at the four sites, defined as a wind speed of 4.9 feet/second (1.5 meters/second) and a Pasquill stability class F. Class F stability corresponds to very stable atmospheric conditions and limited vertical mixing of the NH_3 plume. Hence, the NH_3 plume can travel down wind much further at higher concentrations compared to NH_3 plumes that are subject to greater vertical mixing.

The effect of meteorological conditions on predicted NH_3 concentrations is presented for the 23.1-ton (21-metric ton) truck spill scenario in Table F-6. The Jewett site was selected as a representative site, but the simulation results apply to all four sites. Data for the seven wind speed/stability classes were obtained from the Jewett wind-rose data set in the EIS. The model results in Table F-6 show that for the F/1.5 stability class/wind-condition, elevated NH_3 concentrations extend at least three times further from the source than for the D/8 stability class. The A/2 stability class simulation shows the greatest mixing and the shortest travel distance for elevated NH_3 concentrations. The A stability-class category indicates very unstable air and substantial vertical mixing of the NH_3 plume within the upper air stream. The more unstable the air, the more quickly the NH_3 plume becomes diluted.

Table F-6. Effect of Meteorological Conditions on Predicted NH_3 Concentrations for the 23.1-Ton (21-metric ton) Truck Spill Scenario[1]

Maximum NH_3 (ppmv)	F	A	A	B	B	C	D
	1.5 (20.8 percent)[2]	1 (6.5 percent)	2 (8.7 percent)	3 (27.9 percent)	4 (14.3 percent)	6 (13.4 percent)	8 (8.4 percent)
30	15,092 feet (4,600 meters)	1,289 feet (393 meters)	1,240 feet (378 meters)	1,834 feet (559 meters)	2,024 feet (617 meters)	3,068 feet (935 meters)	5,249 feet (1,600 meters)
110	6,890 (2,100)	669 (204)	643 (196)	948 (289)	1,053 (321)	1,568 (478)	2,493 (760)
160	5,577 (1,700)	554 (169)	528 (161)	784 (239)	873 (266)	1,289 (393)	2,001 (610)
220	4,921 (1,500)	469 (143)	453 (138)	666 (203)	741 (226)	1,096 (334)	1,667 (508)
390	3,608 (1,100)	351 (107)	335 (102)	499 (152)	551 (168)	810 (247)	1,201 (366)
550	2,907 (886)	292 (89)	279 (85)	417 (127)	463 (141)	679 (207)	988 (301)
1,100	1,969 (600)	200 (61)	194 (59)	289 (88)	322 (98)	469 (143)	666 (203)
1,600	1,591 (485)	164 (50)	154 (47)	230 (70)	262 (80)	381 (116)	535 (163)
2,700	1,178 (359)	-	-	171 (52)	194 (59)	282 (86)	390 (119)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from ground puddles (Puddle, ground, and air at 104°F [40°C]) for the 23.1 ton (21 metric ton) release at Jewett, TX. Wind speed/stability-class are obtained from Jewett wind rose data.
[2] Percent of time in stability class.

Table F-7 shows how the truck spill scenario varies between the four sites under the worse-case F/1.5 wind condition. As discussed, there is approximately a 5 percent difference in the predicted characteristics of the NH_3 plume between sites. These differences are only due to the different maximum daily temperatures at each site. Table F-8 compares the predicted NH_3-concentration radii under the second most conservative set of meteorological conditions at each site. At each site, the lengths of the ammonia-concentration radii are almost one-third the lengths of the radii for the worst-case, F stability class condition. There is little different among sites, but large variations at each site for different meteorological conditions and different spill scenarios.

Table F-7. Truck Spill Scenario Across Four Sites[1]

Site	Tuscola	Mattoon	Jewett	Odessa
Stability Class Wind speed (feet/second [meters/second])	F 4.9 (1.5)	F 4.9 (1.5)	F 4.9 (1.5)	F 4.9 (1.5)
Highest daily maximum temperature (°F [°C])	97 (36)	101 (38)	104 (40)	106 (41)
Percent of time for calm wind	4.14 percent	8.14 percent	20.8 percent	4.8 percent
Maximum NH_3 (ppmv)				
30	14,108 feet (4,300 meters)	14,764 feet (4,500 meters)	15,092 feet (4,600 meters)	15,584 feet (4,750 meters)
110	6,234 (1,900)	6,890 (2,100)	6,890 (2,100)	7,874 (2,400)
160	5,249 (1,600)	5,577(1,700)	5,577 (1,700)	6,562 (2,000)
220	4,265 (1,300)	4,593 (1,400)	4,921 (1,500)	5,577 (1,700)
390	3,159 (963)	3,281 (1,000)	3,609 (1,100)	3,937 (1,200)
550	2,602 (793)	2,785 (849)	2,907 (886)	3,281 (1,000)
1,100	1,752 (534)	1,879 (573)	1,969 (600)	2,277 (694)
1,600	1,414 (431)	1,519 (463)	1,591 (485)	1,841 (561)
2,700	1,043 (318)	1,125 (343)	1,178 (359)	1,362 (415)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from an evaporating puddle at Tuscola, Mattoon, and Odessa for the 23.1-ton (21-metric ton) truck release scenario using the worst-case meteorological conditions of 4.9 feet/second (1.5 meters/second) wind speed and Pasquill stability class F. The percent of time for the worst-case condition, which is called calm wind, is obtained from each site's wind rose data.
°F = degree Fahrenheit; °C = degree Celsius

Table F-8. Predicted NH_3-Concentration Radii Under the Second Most Conservative Set of Meteorological Conditions at Each Site[1]

Site	Tuscola	Mattoon	Jewett	Odessa
Stability Class Wind speed (feet/second [meters/second])	D 39.4 (12)	D 39.4 (12)	D 26.2 (8)	D 26.2 (8)
Highest daily maximum temperature (°F [°C])	97 (36)	101 (38)	104 (40)	106 (41)
Percent of time for each combination	2.15 percent	0.27 percent	8.43 percent	20.89 percent
Maximum NH_3 (ppmv)				
30	4,593 feet (1,400 meters)	4,921 feet (1,500 meters)	5,249 feet (1,600 meters)	5,249 feet (1,600 meters)
110	2,126 (648)	2,270 (692)	2,493 (760)	2,589 (789)

Table F-8. Predicted NH_3-Concentration Radii Under the Second Most Conservative Set of Meteorological Conditions at Each Site[1]

160	1,709 (521)	1,824 (556)	2,001 (610)	2,080 (634)
220	1,424 (434)	1,522 (464)	1,667 (508)	1,729 (527)
390	1,027 (313)	1,099 (335)	1,201 (366)	1,247 (380)
550	846 (258)	906 (276)	988 (301)	1,027 (313)
1,100	571 (174)	607 (185)	666 (203)	692 (211)
1,600	456 (139)	489 (149)	535 (163)	558 (170)
2,700	325 (99)	351 (107)	390 (119)	407 (124)

[1] ALOHA predicted maximum radii to specific NH_3 concentrations due to releases from an evaporating puddle at Tuscola, Mattoon, and Odessa for the 23.1-ton (21-metric ton) release scenario using the second worst wind speed/stability class combinations. Meteorological data were obtained from each site's wind rose data.
°F = degree Fahrenheit; °C = degree Celsius

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