Validation of the CHARM® Software Module Including Near-Field Dispersion With Varying Roughness

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Presented
June 24, 2005
Air & Waste Management Association's
98th Annual Conference & Exhibition
Minneapolis, Minnesota

ABSTRACT

As personal computers get faster and more powerful air dispersion models can increase in complexity. This paper briefly discusses modifications made to the CHARM® software package for air dispersion from a Lagrangian puff model to an Eulerian grid model and presents comparisons of the modified model with new wind tunnel (160 points presented here) and existing field data. The wind tunnel data includes near-field data from 3 to 50 meters downwind distance at three surface roughness values. The field data is from previously published reports. The wind tunnel data is presented in tabular form. The comparison of maximum concentration predictions from the modified model gives a Fractional Bias of -0.04 and a Factor of 2 fraction of 0.81. The comparison of off-centerline points gives a Fractional Bias of 0.23 and a Factor of 2 fraction of 0.43.

BACKGROUND

Personal computers have evolved into being capable of much more than just word processing and spreadsheet applications. The PC of today is capable of carrying out calculations so complex that 20 years ago they would have been left to super computers. This paper describes modifications that have been made to a computer model that is designed to predict movement and concentrations of airborne plumes from released chemicals as well as to determine thermal radiation, and explosion overpressures impacts. Comparisons of the modified model's predictions with field data are presented to give an indication of the realism of the estimates.

These comparisons with measured data were done after the model modifications were done. These comparisons act as the initial test of the code. The model was not tuned to the measured value. Coding errors were corrected as they appeared during the simulations and previous simulations re-run. For example, when the surface roughness was greater than 1 meter a variable was not being set and the diffusion coefficient was calculated incorrectly.

There is special treatment for hydrogen fluoride to account for the oligomerization of hydrogen fluoride. This effect is simulated by changing the apparent molecular weight of the chemical in calculations. The degree of the effect is a function of the concentration and temperature of the hydrogen fluoride.

Because of the length of the output and input tables, they are presented in an Appendix to this paper.

THE MODEL

The CHARM® software package[1,2] (Complex Hazardous Air Release Model) began development in 1981 when personal computers began to become popular. Since then, it has gone through continuous development in both functionality and implementation.

Description

Initially, the model was written to simulate the advection and diffusion of a gaseous release. A puff model was used as the core of the calculation. Over time, source-term calculations were added to aid in determining emission rates and release-state parameters. Calculations for simulating jet fires, pool fires, BLEVEs, container explosions, and vapor cloud explosions were also added.

The initial implementation of the program was written in FORTRAN. Graphics were added using the Basic language and Intel Assembler. It was rewritten in C to reduce the maintenance required for a number of languages. Currently, the code is entirely written in C++ and designed for use in Microsoft Windows.

The software is a highly interactive program designed to give output as tables, 2D, and 3D displays.

Modifications

The major modification to the latest version of the model is the replacement of the advection/diffusion Lagrangian approach with a Eulerian grid approach. Moving to a grid model allowed for the addition of many other mechanisms to be considered in a release and its subsequent impacts. Because of the implementation of a grid framework for the calculation, the following considerations have been added:

- Varying terrain altitude in each grid column
- Varying surface roughness in each grid column
- Wind field calculation interacts with terrain to minimize divergence
- Liquid releases can flow over the terrain to become polymorphous sources

Other additions were made to the model at the same time. These changes include:

- Multiple releases in one simulation
- Calculation of coagulation, evaporation, and deposition of particles/droplets

The model has the capability to set up nested grids automatically around a source to ensure a more detailed calculation in the volume where things are changing the quickest. This option was not turned on for these results.

Most data sets for dispersion of releases in the atmosphere are for releases in flat terrain. In model comparisons, the advection and diffusion terms are the largest determiners in the goodness of agreement.

The model software was modified to use the West Wind Field[3]. The West Wind Field considers the effects of vertical temperature stratifications on the wind and diffusion fields and shear flows caused by the atmospheric boundary layer or by terrain effects.

The wind field calculation uses an iterative procedure to minimize the divergence in the field.

The advection/diffusion portion of the model uses a flux-corrected version of Crowely's[4] second-order advection scheme, as implemented by Sklarew and Wilson[5]. The flux corrector method prohibits the calculation of negative concentrations.

The form of the calculation for the advection/diffusion for the n^{th} time step of the concentration (C) of the i^{th} species in the x direction is:

$$C_i^{n+1} = C_i^n + \left(F^n_{i-\frac{1}{2}} - F^n_{i+\frac{1}{2}} \right) \frac{\Delta t}{\Delta x} \quad (\mathbf{1})$$

where

$$F^n_{i+\frac{1}{2}} = \frac{\Delta x}{2\Delta t} \left\{ \left(C_i^n + C_{i+1}^n\right) \alpha_{i+\frac{1}{2}} + \left(C_i^n - C_{i+1}^n\right) \alpha^2_{i+\frac{1}{2}} \right\} + K_{x\,i+\frac{1}{2}} \left(\frac{C_i^n - C_{i+1}^n}{\Delta x} \right) \quad (\mathbf{2})$$

and

$$\alpha_{i+\frac{1}{2}} = u_{i+\frac{1}{2}} \frac{\Delta t}{\Delta x} \quad (\mathbf{3})$$

The air parameters used in the advection/diffusion calculation are those from the West Wind Field with modifications from effects of mass, momentum, and energy from the releases. The first modification is due to the emitted momentum in each direction:

$$u' = \frac{m_a u + p_e}{m_t} \quad (\mathbf{4})$$

where

u' is the new wind speed

u is the atmospheric wind speed

m_a is the mass of air in a cell

m_t is the total mass in a cell

p_e is the momentum in a cell from an emission

The mass from an emission is tracked for each cell as well as the fraction that might be in droplet form. The volume occupied by the mass from an emission can then be calculated. Whatever volume remains in a cell is assumed to be air.

The next modification is only to the vertical component of the velocity and is due to buoyancy. If the difference of the cell's density (ρ) with the ambient density (ρ_a) is greater than one percent of ρ_a, then the vertical velocity may be modified. If the cell's bottom is not in contact with terrain, the vertical velocity changing by:

$$\frac{dw}{dt} = g\left(\frac{\rho_a}{\rho} - 1\right) \qquad \textbf{(5)}$$

where

g = gravitational acceleration = 9.8 m/sec^2

If the bottom of the cell is in contact with the ground and the density difference is less than –0.01, the vertical motion caused by slump is assumed to be transferred to horizontal motion. The horizontal velocity caused by the downward motion is given by:

$$u' = \sqrt{-2g\left(\frac{\rho_a}{\rho} - 1\right)\Delta z} \qquad \textbf{(6)}$$

where

Δz = vertical grid spacing (m)

The emitted momentum and energy are allowed to advect and disperse using the same formulation as used for concentration.

EXPERIMENTAL DATA

There have been a number of controlled releases over the years. These were done to provide a database for evaluating models. The model results have been compared with the measurements from some of those controlled releases. Normally, the results from a field release are given as a number of maximum concentrations measured at various distances downwind from the release site.

In addition to the field releases, a new data set of a number of releases in a wind tunnel has been developed. The importance of this data set is that not only are the maximum concentrations at various downwind distances provided but also concentrations at off centerline locations.

Wind Tunnel Database

Wind tunnel testing was carried out at the facilities of CPP, Inc. in Fort Collins, Colorado. The purpose of the wind tunnel testing was to collect a set of ground-level concentration measurements for full-scale distances out to 50 m for various roughness configurations for use in validating the model. Wind tunnel operating conditions were set using similarity requirements described in the EPA fluid modeling guideline[6].

To meet the wind tunnel modeling objectives, a 1:100 scale model of the various roughness configurations and 1 m surface release were constructed and placed in CPP's wind tunnel. Three different roughness configurations were evaluated during this study as summarized below:

- Configuration A -- This configuration consisted of a pattern of 1 inch high roughness designed to give a full-scale surface roughness length of 5.2 cm.
- Configuration B -- This configuration consisted of a pattern of 2 inch high roughness designed to give a full-scale surface roughness length of 21 cm.
- Configuration C -- This configuration consisted of a pattern of 2 and 8-inch high roughness designed to give a full-scale surface roughness length of 123 cm.

For all tests, a 1 m circular release at ground level was simulated. The release was constructed of a brass tube with steel wool and a screen installed inside to ensure a uniform flow upon exit. The release was supplied with a tracer gas (methane or ethane and helium) with a density identical to methane. Precision mass flow controllers were used to monitor and regulate the discharge velocities.

Concentration measurements were taken in a horizontal/vertical sampling array at four downwind distances (x = 3, 7.5, 15 and 50 m).

The test procedure consists of: 1) setting the proper tunnel wind speed; 2) releasing a metered mixture of source gas of the required density from the release point; 3) withdrawing samples of air from the wind tunnel at designated locations; and 4) analyzing the samples with a flame ionization gas chromatograph (FIGC). The samples are collected simultaneously over a 200 second (approximate) time using CPP's sampling system and consecutively injected into the FIGC.

Results

Table 1 through Table 3 present the results of the wind tunnel experiments for different surface roughness values. Included in the tables is a column labeled "Adjusted Wind Tunnel". Given a continuous-constant release with a constant wind speed, the model predicted an axially symmetric concentration field. The wind tunnel data does not exhibit the same symmetry, although the data indicates that such symmetry exists but somewhat off from the centerline of the tunnel.

The wind tunnel results at each downwind distance were fitted to a Gaussian distribution to estimate what the concentration distribution would be if it were symmetric. These estimates are in the "Adjusted Wind Tunnel" column. The fit was performed to minimize the amount of error in the fit to actual results. The solution is iterative and somewhat dependent upon the initial guess of what the parameters should be. A few of the fits resulted in lower maximum concentrations than those actually measured.

Field Data

To provide range for the comparison readily available data sets were selected. The wind tunnel data is newly available and only covers the near-field region. Other data sets were selected that had releases other than methane, had measurement values further downwind, or were from elevated sources.

The field data used is for the Burro, Desert Tortoise, Goldfish, and Lillestrom releases. The Burro LNG releases occurred at the Naval Weapons Center at China Lake, California, in the summer and fall of 1981. The Desert Tortoise and Goldfish experiments releases were at Liquefied Gaseous Spill Test Facility in Nevada. Ammonia was released in the Desert Tortoise experiments in 1983. Hydrogen fluoride was released in the Goldfish experiments in 1986. The Lillestrom releases were of SF_6 in Lillestrom near Oslo, Norway in 1987.

The release descriptions and results were found on the Transoft International (www.fluidyn.com) and The Albany County Research Corporation (www.ac-research.org) web sites. The Transoft papers compared their models Fluidyn-PANACHE-PANEPR[7] (Burro, Desert Tortoise, Goldfish) and Fluidyn-PANACHE[8] (Lillestrom) to the experimental data, as well as other models, including an earlier version of the CHARM model. The ACRC paper[9] provided descriptions and some of the release information of the experiments.

Results

The results of the model calculations for the various releases are given in Table 4.

MODEL INPUT

The model requires three types of input. The first type is the release description (e.g., emission rate, temperature, location, source size, etc.). The second type is the meteorological conditions. The third type is the grid over which the calculation will take place.

The inputs to the model are given in Table 5 through Table 10.

Wind Tunnel

The emission rates, meteorology, and grid input to the software for the wind tunnel experiments are given in Table 5 and Table 6. Table 5 contains the input that was varied for each experimental run. Table 6 contains the input that was assumed for every simulation.

The grid used for the wind tunnel simulations had a zero elevation at all grid cells. Its largest extent was in the x direction (east-west) with the source near the west end of the grid and the wind from the west.

Field Data

The emission rates, meteorology, and grid input to the software for the field experiments are given in Table 7 through Table 10.

For the Desert Tortoise and Goldfish releases, the elevations of the grid cells were set using USGS DEM data for each area. An editor comes with the model software for processing the DEM data, as well as other information (e.g., maps and chemical data) for use in the main program.

Two grids were used for the Goldfish experiments. One was used for the near field (300 m downwind) with a fine mesh and the other for estimating concentrations beyond 300 m downwind with a coarser mesh. This was done to increase the likelihood that the effects of the oligomerization of hydrogen fluoride would be taken into account at least in the near field. The amount of oligomerization is dependent on concentration. Smaller grid cells results in higher concentrations for a given amount of mass. The Eulerian grid is a three-dimensional collection of grid cells. Since the Goldfish releases were point sources, whichever grid cell received the initial release would determine the initial air concentration.

For the Burro and Lillestrom releases, the grid was assumed to be of a uniform elevation. The terrain for the Burro release was assumed flat because there was some uncertainty of the exact location and nature of the surrounding terrain in the descriptions provided.

MODEL-DATA COMPARISON

To give an objective set of criteria to determine the validity of the model, a number of statistical parameters are given for the maximum concentration and off-center concentration results. The table below shows each statistic and its optimal value. If a model comparison results in an optimal value, it is in perfect agreement with the data.

Fractional Bias (FB)	Normalized Mean Square Error (NMSE)	Geometric Mean (MG)	Geometric Variance (VG)	Fraction of Data with Factor of 2 (FAC2)	Correlation (R^2)
0	0.0	1.0	1.0	1.0	1.0

A model can be deemed acceptable if the statistical parameters fall within the following ranges[10,11]:

FB	NMSE	MG	VG	FAC2
≤ 0.5 ≥ -0.5	≤0.5	≤ 1.25 ≥ 0.75	≤ 1.25 ≥ 1.00	≥ -0.8

Maximums at Distance

Figure 1 presents a plot of the model estimates versus the measured data for the maximum concentrations (presumably at, or near, the plume centerlines). The statistics of the comparison are:

FB	NMSE	MG	VG	FAC2	R^2
-0.04	0.74	0.86	1.41	0.81	0.75

Model results were also compared to the adjusted centerline wind tunnel data. The statistics of the comparison are:

FB	NMSE	MG	VG	FAC2	R^2
-0.02	0.74	0.87	1.44	0.78	0.75

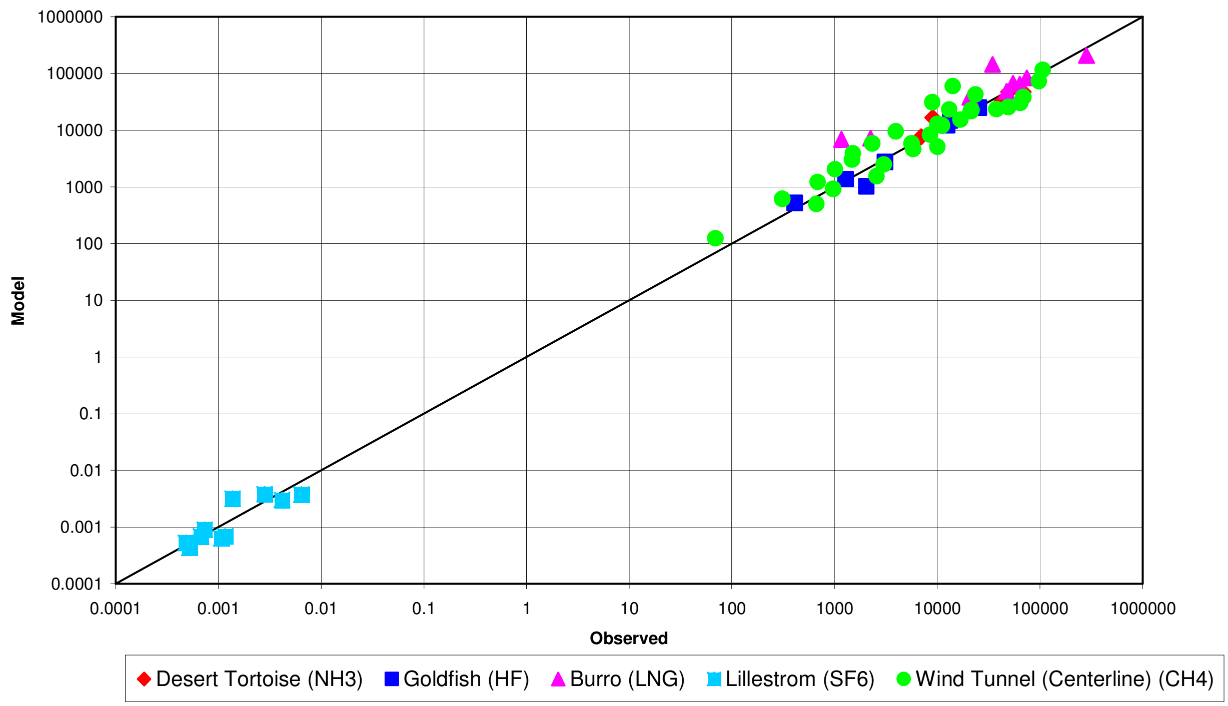

Figure 1. Model vs Observed Maximum Concentrations (ppm)

Off-center Data

Figure 2 presents a plot of the model estimates versus the measured data for the concentrations off-center in the wind tunnel experiments. The statistics of the comparison are:

FB	NMSE	MG	VG	FAC2	R^2
0.23	1.92	2.05	9.93	0.43	0.56

Model results were also compared to the adjusted off-center wind tunnel data. The statistics of the comparison are:

FB	NMSE	MG	VG	FAC2	R^2
0.17	1.06	1.63	5.76	0.39	0.71

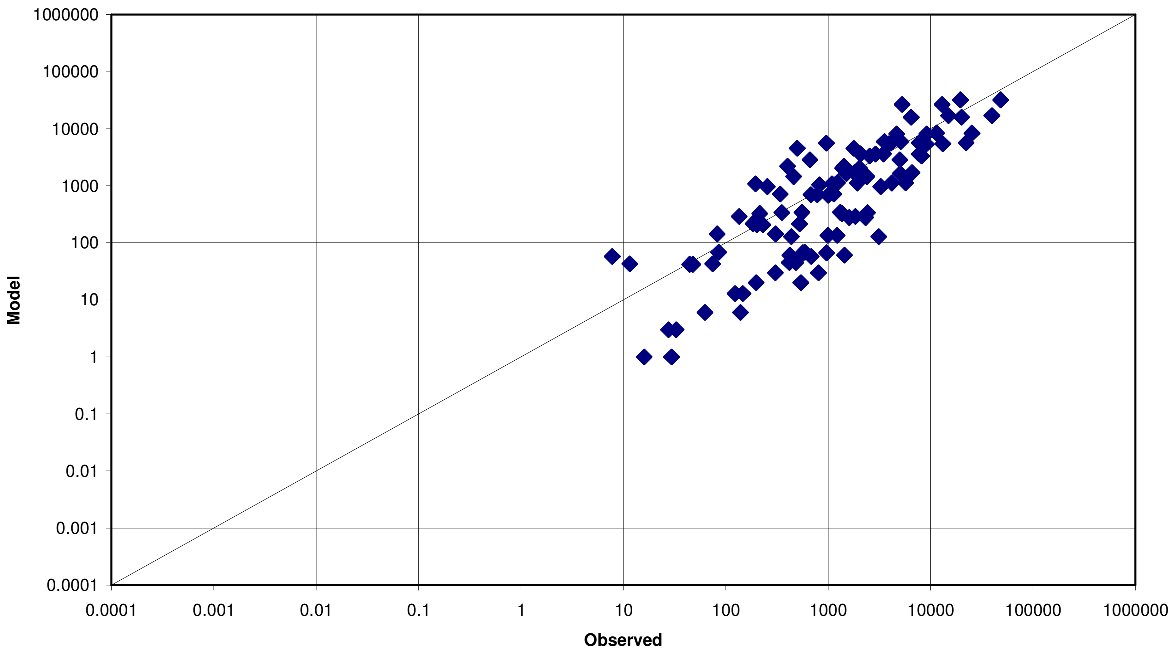

Figure 2. Model vs Observed Off Centerline Concentrations (ppm)

CONCLUSIONS

CHARM is a capable model for estimating concentrations downwind from a release. The model does very well at estimating maximum concentrations downwind of releases. Although not reaching the same level of accuracy as the centerline concentrations, The model does well at predicting off-center concentrations.

Further comparisons of the model with data collected in complex terrain, are planned.

REFERENCES

1. Eltgroth, M.W., (1995): CHARM® Technical Reference Manual, Radian Corporation, Austin, TX.

2. Eltgroth, M.W., (2005): CHARM® Technical Reference Manual (Gridded), URS Corporation, Austin , TX.

3. Fabrick, A.J., R.C. Sklarew, and J. Wilson (1977) ;Point Source Model Evaluation and Development Study. Contract A5-058-87, California Air Resources Board, Science Applications, Inc., 857 Westlake Blvd., Suite 212, Westlake Village, California 91361.

4. Crowley, W. P., (1968): Numerical advection experiments. *Mon. Wea. Rev.*, **96**, 1-12.

5. Sklarew, R. and J. Wilson (1976): Applications of DEPICT to the Farfield, Navajo and Ormond Beach Air Quality Data Base. Science Applications, Inc., 857 Westlake Blvd., Suite 212, Westlake Village, California 91361.

6. EPA, *Guideline for Use of Fluid Modeling of Atmospheric Diffusion*, (1981). U.S. Environmental Protection Agency, Office of Air Quality, Planning and Standards, Research Triangle Park, North Carolina, EPA-600/8-81-009, April 1981.

7. http://www.**fluidyn**.com/validation/Dense_Gas.pdf

8. http://www.**fluidyn**.com/validation/MOLValidationLillestrom.pdf

9. King, S.B., J. Nordin, D. Sheesley, and T. Routh; The Department of Energy HAZMAT Spill Center Data Base. http://www.ac-research.org/stfdb/ DOE%20HSC%20Database%20documentation.PDF

10. Kumar, A., J. Luo, and G. Bennett, "Statistical Evaluation of Lower Flammability Distance (LFD) Using Four Hazardous Release Models", Process Safety Progress, Vol. 12(1), pp. 1-11, 1993.

11. Ahuja, S., and Kumar, A., "Evaluation of MESOPUFF-II SOx Transport and Deposition in the Great Lakes Region", AWMA Specialty Conference on Atmospheric Deposition to the Great Lakes, VIP-72, pp. 283-299, Oct. 28-30, 1996.

APPENDIX

Model vs. Wind Tunnel Measurements

Table 1. Model calculation results for Wind Tunnel releases at 21 cm surface roughness.

Model Run	Ua (m/s)	V (m^3/s)	X (m)	Y (m)	Wind Tunnel (ppm)	Adjusted Wind Tunnel (ppm)	Model (ppm)
1	1.3	0.787	3	-4	497	794	4558
1	1.3	0.787	3	-2	19611	32207	31979
1	1.3	0.787	3	0	106479	110679	116096
1	1.3	0.787	3	2	48323	32207	31979
1	1.3	0.787	3	4	1775	794	4558
1	1.3	0.787	7.5	-5	4111	1988	5601
1	1.3	0.787	7.5	-2.5	12940	9182	26598
1	1.3	0.787	7.5	0	14176	15290	59778
1	1.3	0.787	7.5	2.5	5252	9182	26598
1	1.3	0.787	7.5	5	961	1988	5601
1	1.3	0.787	15	-11	437	682	128
1	1.3	0.787	15	-5.5	5088	4484	5969
1	1.3	0.787	15	0	8954	8399	31199
1	1.3	0.787	15	5.5	3534	4484	5969
1	1.3	0.787	15	11	3116	682	128
1	1.3	0.787	50	-15	1605	1845	279
1	1.3	0.787	50	-7.5	2064	3048	3631
1	1.3	0.787	50	0	3948	3604	9531
1	1.3	0.787	50	7.5	3472	3048	3631
1	1.3	0.787	50	15	2311	1845	279
2	2.7	0.787	3	-4	400	449	2181
2	2.7	0.787	3	-2	14923	26088	16845
2	2.7	0.787	3	0	97754	101027	73496
2	2.7	0.787	3	2	39728	26088	16845
2	2.7	0.787	3	4	1413	449	2181
2	2.7	0.787	7.5	-5	5025	1830	2877
2	2.7	0.787	7.5	-2.5	20056	13275	15897
2	2.7	0.787	7.5	0	23607	25699	43061
2	2.7	0.787	7.5	2.5	6443	13275	15897
2	2.7	0.787	7.5	5	663	1830	2877
2	2.7	0.787	15	-11	421	187	61
2	2.7	0.787	15	-5.5	8184	4823	3333
2	2.7	0.787	15	0	13054	14261	23257
2	2.7	0.787	15	5.5	2547	4823	3333
2	2.7	0.787	15	11	1440	187	61
2	2.7	0.787	50	-15	993	1060	135
2	2.7	0.787	50	-7.5	1378	1814	2034
2	2.7	0.787	50	0	2335	2169	5876
2	2.7	0.787	50	7.5	2026	1814	2034
2	2.7	0.787	50	15	1219	1060	135
3	5.4	0.787	3	-4	195	314	1082

3	5.4	0.787	3	-2	11446	18080	8418
3	5.4	0.787	3	0	68707	69811	38222
3	5.4	0.787	3	2	25327	18080	8418
3	5.4	0.787	3	4	1086	314	1082
3	5.4	0.787	7.5	-5	2390	493	1447
3	5.4	0.787	7.5	-2.5	9185	7886	8096
3	5.4	0.787	7.5	0	21562	19875	22837
3	5.4	0.787	7.5	2.5	4651	7886	8096
3	5.4	0.787	7.5	5	459	493	1447
3	5.4	0.787	15	-11	303	110	30
3	5.4	0.787	15	-5.5	6576	3726	1693
3	5.4	0.787	15	0	10982	12049	12468
3	5.4	0.787	15	5.5	1808	3726	1693
3	5.4	0.787	15	11	805	110	30
3	5.4	0.787	50	-15	565	606	67
3	5.4	0.787	50	-7.5	821	1083	1040
3	5.4	0.787	50	0	1480	1315	3061
3	5.4	0.787	50	7.5	1160	1083	1040
3	5.4	0.787	50	11	962	867	67
4	8.05	0.787	3	-4	338	323	722
4	8.05	0.787	3	-2	7713	14374	5643
4	8.05	0.787	3	0	49147	50924	25691
4	8.05	0.787	3	2	22214	14374	5643
4	8.05	0.787	3	4	1135	323	722
4	8.05	0.787	7.5	-5	3256	982	970
4	8.05	0.787	7.5	-2.5	13136	8685	5455
4	8.05	0.787	7.5	0	16833	17962	15432
4	8.05	0.787	7.5	2.5	3901	8685	5455
4	8.05	0.787	7.5	5	254	982	970
4	8.05	0.787	15	-11	198	66	20
4	8.05	0.787	15	-5.5	5700	2812	1127
4	8.05	0.787	15	0	8486	9841	8335
4	8.05	0.787	15	5.5	1226	2812	1127
4	8.05	0.787	15	11	539	66	20
4	8.05	0.787	50	-15	480	435	45
4	8.05	0.787	50	-7.5	676	770	695
4	8.05	0.787	50	0	1008	932	2050
4	8.05	0.787	50	7.5	783	770	695
4	8.05	0.787	50	15	418	435	45
5	4	0.0787	3	-4	82	90	144
5	4	0.0787	3	-2	1924	3094	1120
5	4	0.0787	3	0	10044	10060	5129
5	4	0.0787	3	2	4164	3094	1120
5	4	0.0787	3	4	306	90	144
6	2.7	0.0787	7.5	-5	1847	581	291
6	2.7	0.0787	7.5	-2.5	5043	3463	1640
6	2.7	0.0787	7.5	0	5822	6280	4647
6	2.7	0.0787	7.5	2.5	1504	3463	1640
6	2.7	0.0787	7.5	5	136	581	291
6	2.7	0.0787	15	-11	63	15	6
6	2.7	0.0787	15	-5.5	2415	968	339
6	2.7	0.0787	15	0	3024	3850	2512

6	2.7	0.0787	15	5.5	351	968	339
6	2.7	0.0787	15	11	140	15	6
6	2.7	0.0787	50	-15	146	129	13
6	2.7	0.0787	50	-7.5	201	231	209
6	2.7	0.0787	50	0	310	280	617
6	2.7	0.0787	50	7.5	230	231	209
6	2.7	0.0787	50	15	123	129	13
7	1.3	0.00787	3	-4	12	32	43
7	1.3	0.00787	3	-2	551	887	340
7	1.3	0.00787	3	0	2571	2686	1551
7	1.3	0.00787	3	2	1316	887	340
7	1.3	0.00787	3	4	74	32	43
7	1.3	0.00787	7.5	-5	683	144	58
7	1.3	0.00787	7.5	-2.5	1358	802	327
7	1.3	0.00787	7.5	0	970	1423	927
7	1.3	0.00787	7.5	2.5	214	802	327
7	1.3	0.00787	7.5	5	8	144	58
7	1.3	0.00787	15	-11	16	4	1
7	1.3	0.00787	15	-5.5	590	226	68
7	1.3	0.00787	15	0	664	878	503
7	1.3	0.00787	15	5.5	85	226	68
7	1.3	0.00787	15	11	29	4	1
7	1.3	0.00787	50	-15	33	29	3
7	1.3	0.00787	50	-7.5	44	50	42
7	1.3	0.00787	50	0	69	61	124
7	1.3	0.00787	50	7.5	47	50	42
7	1.3	0.00787	50	15	28	29	3

Table 2. Model calculation results for Wind Tunnel releases at 5.2 cm surface roughness.

Model Run	Ua (m/s)	V (m^3/s)	X (m)	Y (m)	Wind Tunnel (ppm)	Adjusted Wind Tunnel (ppm)	Model (ppm)
8	8.05	0.787	3	-4	185	2	217
8	8.05	0.787	3	-2	2906	4855	3596
8	8.05	0.787	3	0	64445	65914	30353
8	8.05	0.787	3	2	7713	4855	3596
8	8.05	0.787	3	4	525	2	217
8	8.05	0.787	7.5	-4	1000	2826	679
8	8.05	0.787	7.5	-2	9038	13841	5380
8	8.05	0.787	7.5	0	21300	23506	21740
8	8.05	0.787	7.5	2	19325	13841	5380
8	8.05	0.787	7.5	4	5944	2826	679
9	8.82	0.787	15	-11	56	8	1
9	8.82	0.787	15	-5.5	2437	1723	487
9	8.82	0.787	15	0	10049	10214	12875
9	8.82	0.787	15	5.5	1133	1723	487
9	8.82	0.787	15	11	10	8	1
9	8.82	0.787	50	-15	299	140	4
9	8.82	0.787	50	-7.5	1161	869	463
9	8.82	0.787	50	0	1508	1597	3898
9	8.82	0.787	50	7.5	599	869	463
9	8.82	0.787	50	15	49	140	4

Table 3. Model calculation results for Wind Tunnel releases at 123 cm surface roughness.

Model Run	Ua (m/s)	V (m^3/s)	X (m)	Y (m)	Wind Tunnel (ppm)	Adjusted Wind Tunnel (ppm)	Model (ppm)
10	8.05	0.787	3	-4	920	445	1634
10	8.05	0.787	3	-2	13282	12151	7663
10	8.05	0.787	3	0	37803	36595	23552
10	8.05	0.787	3	2	9502	12151	7663
10	8.05	0.787	3	4	1283	445	1634
10	8.05	0.787	7.5	-4	6278	4809	2689
10	8.05	0.787	7.5	-2	11608	9441	7176
10	8.05	0.787	7.5	0	11133	11821	12115
10	8.05	0.787	7.5	2	7410	9441	7176
10	8.05	0.787	7.5	4	3507	4809	2689
10	8.05	0.787	15	-11	862	486	97
10	8.05	0.787	15	-5.5	4170	3194	1609
10	8.05	0.787	15	0	5643	5985	5870
10	8.05	0.787	15	5.5	2470	3194	1609
10	8.05	0.787	15	11	211	486	97
10	8.05	0.787	50	-15	359	288	114
10	8.05	0.787	50	-7.5	723	550	651
10	8.05	0.787	50	0	685	682	1229
10	8.05	0.787	50	7.5	351	550	651
10	8.05	0.787	50	15	266	288	114

Model vs. Field Data

Table 4. Model calculation results for field releases.

Experiment (Species)	Experiment Number	Distance (m)	Observed Concentration	Model Concentration
Burro (LNG)[1]	3	57	74000	84170
		140	54640	66980
		800	1167	6930
	5	57	63478	64660
		140	47535	48800
		800	2236	7225
	8	57	283390	208900
		140	34507	144400
		800	20810	38350
Desert Tortoise (Ammonia) [1]	1	100	42483	32200
		800	6975	7674
	2	100	68664	47030
		800	8991	16780
	4	100	49307	47420
		800	14562	15810
Goldfish (HF) [1]	1	300	25473	25090
		1000	3098	2741
		3000	411	522
	2	300	13347	14870
		1000	1287	1374
	3	300	12515	12310
		1000	2042	1029
Lillestrom (SF_6)[2]	I-1	160	7.6	4.513
		490	4.8	4.861
		810	3.7	3.071
	I-2	140	8.3	4.912
		440	5.2	6.421
		820	3.4	3.751
	II-1	190	29.6	21.34
		410	9.7	22.59
	II-2	190	45.8	26.62
		430	20	27.14

1. Concentrations are in ppm
2. Concentrations are in $\mu g/m^3$

Model Input

Table 5. Model input that was varied for the Wind Tunnel releases.

Parameter/Run	1	2	3	4	5	6	7	8	9	10
Emission Rate (scfm)	1667	1667	1667	1667	166.7	166.7	16.67	1667	1667	1667
Wind Speed (mph)	3	6	12	18	9	6	3	18	19.7	18
Surface Roughness (cm)	21	21	21	21	21	21	21	5.2	5.2	123

Table 6. Model input used for all Wind Tunnel releases.

Parameter	Value
Species	Methane
Release Height (m)	0
Source Diameter (m)	1
Exit Temperature (ºC)	23
Ambient Temperature (ºC)	23
Relative Humidity (percent)	30
Stability Class	D
Wind Speed Measurement Height (m)	10
Ambient Pressure (atmospheres)	0.85
Grid nx, ny, nz	30, 19, 20
Grid dx, dy, dz (m)	2, 2, 2
Wind Direction (degrees)	270
Source Grid Cell Location (zero-based x, y, z)	1, 9, 0

Table 7. Model input for the Burro releases.

Parameter/Run	3	5	8
Location (Latitude)	35º 45.0406' N	35º 45.0406' N	35º 45.0406' N
Location (Longitude)	117º 36.3480' W	117º 36.3480' W	117º 36.3480' W
Emission Rate (kg/s)	88	81.8	116.9
Duration (sec)	167	190	107
Release Height (m)	0	0	0
Source Diameter (m)	58	58	58
Temperature (ºC)	33.8	40.5	33.1
Relative Humidity (percent)	5.2	5.6	4.5
Ambient Pressure (mb)	948	941	941
Wind Speed (m/s)	5.4	7.4	1.8
Wind Direction (degrees)	269	263	279.8
Wind Measurement Height (m)	2	2	2
Stability Class	B	C	E
Surface Roughness (cm)	0.02	0.02	0.02
Grid nx, ny, nz	41, 9, 5	41, 9, 5	41, 9, 5
Grid dx, dy, dz (m)	25, 25, 4	25, 25, 4	25, 25, 4
Grid SW Corner (Latitude)	35° 44.9941' N	35° 44.9941' N	35° 44.9941' N
Grid SW Corner (Longitude)	117° 36.4374' W	117° 36.4374' W	117° 36.4374' W
Elevation (m)	665	665	665
Averaging Time (sec)	10	10	10

Table 8. Model input for the Desert Tortoise releases.

Parameter/Run	1	2	4
Location (Latitude)	36° 48.1018' N	36° 48.1018' N	36° 48.1018' N
Location (Longitude)	115° 57.3907' W	115° 57.3907' W	115° 57.3907' W
Species	Ammonia	Ammonia	Ammonia
Emission Rate (kg/s)	81	117	107.9
Duration (sec)	126	255	381
Release Height (m)	0.79	0.79	0.79
Source Diameter (m)	0.0945	0.0945	0.0945
Exit Temperature (ºC)	21.5	20.1	24.1
Hole Facing (degrees)	45	45	45
Horizontal Exit Velocity (m/s)	81.2	85.2	92.5
Ambient Temperature (ºC)	29.3	30.5	33
Relative Humidity (percent)	13.2	17.5	21
Ambient Pressure (mb)	909	910	903
Wind Speed (m/s)	7.42	5.76	5.5
Wind Direction (degrees)	267.3	271.2	274.3
Wind Measurement Height (m)	2	2	2
Stability Class	D	D	D
Met Site Location (Latitude)	36° 48.0182' N	36° 48.0182' N	36° 48.0182' N
Met Site Location (Longitude)	115° 57.4453' W	115° 57.4453' W	115° 57.4453' W
Surface Roughness (cm)	0.3	0.3	0.3
Grid nx, ny, nz	21, 21, 15	21, 21, 15	21, 21, 15
Grid dx, dy, dz (m)	50, 50, 5	50, 50, 5	50, 50, 5
Grid SW Corner (Latitude)	36° 47.8018' N	36° 47.8018' N	36° 47.8018' N
Grid SW Corner (Longitude)	115° 57.5163' W	115° 57.5163' W	115° 57.5163' W
Minimum Elevation (m)	969	969	969
Maximum Elevation	972	972	972
Averaging Time (sec)	30	30	30

Table 9. Model input for the Goldfish releases.

Parameter/Run	1	2	3
Location (Latitude)	36° 48.1018' N	36° 48.1018' N	36° 48.1018' N
Location (Longitude)	115° 57.3907' W	115° 57.3907' W	115° 57.3907' W
Species	Hydrogen Fluoride	Hydrogen Fluoride	Hydrogen Fluoride
Emission Rate (kg/s)	30.2	10.4	10.4
Duration (sec)	125	360	360
Release Height (m)	1	1	1
Source Diameter (m)	0.0945	0.0945	0.0945
Exit Temperature (ºC)	40	38	39
Hole Facing (degrees)	With wind	With wind	With wind
Horizontal Exit Velocity (m/s)	3.89	1.34	1.34
Ambient Temperature (ºC)	37	36	26.5
Relative Humidity (percent)	4.9	10.5	27.6
Ambient Pressure (mb)	891	900	900
Wind Speed (m/s)	5.6	4.2	5.4
Wind Direction (degrees)	270	270	270
Wind Measurement Height (m)	2	2	2
Stability Class	D	D	D
Met Site Location (Latitude)	36° 48.0182' N	36° 48.0182' N	36° 48.0182' N
Met Site Location (Longitude)	115° 57.4453' W	115° 57.4453' W	115° 57.4453' W
Surface Roughness (cm)	0.3	0.3	0.3
Grid nx, ny, nz	35, 21, 10	33, 29, 20	33, 29, 20
Grid dx, dy, dz (m)	100, 100, 4	100, 100, 2	100, 100, 2
Grid SW Corner (Latitude)	36° 47.6010' N	36° 47.7801' N	36° 47.7801 N
Grid SW Corner (Longitude)	115° 57.5774' W	115° 58.1525' W	115° 58.1525' W
Near Field (300 m) Grid nx, ny, nz	46, 30, 10	46, 30, 10	46, 30, 10
Near Field (300 m) Grid dx, dy, dz (m)	10, 10, 4	10, 10, 4	10, 10, 4
Near Field (300 m) Grid SW Corner (Latitude)	36° 47.9989' N	36° 47.9989' N	36° 47.9989' N
Near Field (300 m) Grid SW Corner (Longitude)	115° 57.4699' W	115° 57.4699' W	115° 57.4699' W
Minimum Elevation (m)	969	968	968
Maximum Elevation	972	973	973
Averaging Time (sec)	67	67	67

Table 10. Model input for the Lillestrom releases.

Parameter/Run	I-1	I-2	II-1	II-2
Location (Latitude)	59° 53.3400' N	59° 53.3400' N	59° 53.3400' N	59° 53.3400' N
Location (Longitude)	11° 3.0600' E	11° 3.0600' E	11° 3.0600' E	11° 3.0600' E
Species	Sulfur Hexafluoride	Sulfur Hexafluoride	Sulfur Hexafluoride	Sulfur Hexafluoride
Emission Rate (g/s)	0.102	0.102	0.102	0.102
Duration (min)	15	15	15	15
Release Height (m)	36	36	36	36
Source Diameter (cm)	0.15	0.15	0.15	0.15
Exit Temperature (ºC)	87	87	85	85
Hole Facing (degrees)	With wind	With wind	With wind	With wind
Horizontal Exit Velocity (m/s)	6.5	6.5	5.75	5.75
Ambient Temperature (ºC)	-25.65	-25.65	-12.75	-12.75
Relative Humidity (percent)	45	45	45	45
Ambient Pressure (mb)	1000	1000	1000	1000
Wind Speed (m/s)	2.1	1.7	0.5	0.4
Wind Direction (degrees)	270	270	270	270
Wind Measurement Height (m)	10	10	10	10
Stability Class	D	D	D	D
Met Site Location (Latitude)	59° 53.3400' N	59° 53.3400' N	59° 53.3400' N	59° 53.3400' N
Met Site Location (Longitude)	11° 3.0600' E	11° 3.0600' E	11° 3.0600' E	11° 3.0600' E
Surface Roughness (cm)	50	50	50	50
Grid nx, ny, nz	35, 11, 25	35, 11, 25	20, 11, 25	20, 11, 25
Grid dx, dy, dz (m)	40, 40, 4	40, 40, 4	40, 40, 4	40, 40, 4
Grid SW Corner (Latitude)	59° 53.2203' N	59° 53.2203' N	59° 53.2203' N	59° 53.2203' N
Grid SW Corner (Longitude)	11° 2.9469' E	11° 2.9469' E	11° 2.9469' E	11° 2.9469' E
Elevation (m)	110	110	110	110