An Innovative Approach for Determining Downwind Normalized Concentrations from an Accidental Release

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ABSTRACT

An analysis was performed to evaluate the consequences of a hypothetical release of mercury resulting from a fire at the Spallation Neutron Source (SNS) in Oak Ridge, Tennessee, during facility operation. The potential effects of mercury's chemical toxicity to the public were estimated by using air dispersion modeling to calculate downwind normalized concentrations (χ/Q's). The analysis determined a single 95th percentile χ/Q value (i.e., 5% of the χ/Q's have a value greater than the determined value and 95% of the χ/Q's have a value less than the determined value) representing all wind directions, which was obtained from the dataset of highest calculated 1-hour χ/Q values for all hours of data. For each hour, the highest χ/Q value was selected from values calculated for all receptors under the plume centerline. The 95th percentile χ/Q value was determined using a sorted, aggregated list of these 1-hour maxima. The sensitivity of the results to varying several input parameters was evaluated.

INTRODUCTION

The SNS, which is currently under construction in Oak Ridge, Tennessee, will be a state-of-the-art facility for the production of neutrons for use in scientific research. The facility will consist of 4 main components: (1) a proton source; (2) a linear accelerator; (3) a beam transport and ring system; and (4) an experiment building that will house the mercury target facility. The facility is being built on a previously undeveloped site within the 14,000-hectare Department of Energy reservation that currently houses Oak Ridge National Laboratory (ORNL) and 2 other major industrial complexes (Figure 4).

The site is located on top of Chestnut Ridge, which is one of a series of parallel ridges separated by 1- to 3-km wide valley bottoms oriented along a southwest - northeast axis. Surface elevations range from about 225 m (above mean sea level) along the nearby Clinch River to 415 m at Melton Hill about 5 km south of the site. At a regional scale, the site lies within the Great Valley of Eastern Tennessee between the Cumberland and southern Appalachian mountain ranges. The population center of the city of Oak Ridge is located about 6 km to the northeast and the center of the Knoxville metropolitan area is about 35 km to the east.

The closest reservation boundary to the SNS site is about 2 km to the northwest. In addition, Bethel Valley Road and State Highway 95 traverse the reservation. Unrestricted public access to State Highway 95 is permitted. Although unlimited public access is no longer allowed on Bethel Valley Road, both roads were considered to be available to the public in order to incorporate that possibility in the future.

An accidental release of mercury from the target facility is the primary safety concern of the SNS. Postulated significant adverse impacts to the public would result from events where the mercury is heated and then released through failure of multiple levels of confinement. Because a major fire would likely be required to heat the mercury and breach confinement, this analysis evaluates the effects of mercury's chemical toxicity to the public resulting from such a hypothetical release using air dispersion modeling to calculate downwind normalized concentrations (χ/Q's).

METHODOLOGY

Historically, data used for determining χ/Q values have been stratified with respect to wind direction into 16 or 36 sectors, and separate calculations have been performed for each sector using data with wind directions within each sector. Compliance with regulatory requirements generally has resulted in calculations based on 95th percentile χ/Q values for each sector. Consequently, 16 or 36 (respectively) 95th percentile χ/Q values have been calculated. Frequently, all wind directions within a sector have been adjusted to align with the centerline of the sector. This technique simplifies the calculations and is conservative (forms an upper bound of expected results) because all receptors (along the sector centerline) are also along the downwind plume centerline rather than being offset from the centerline. However, this sector-averaged approach may produce inconsistent results in the Oak Ridge area because of the variability of the terrain within each sector.

Consequently, this analysis determined a single 95th percentile χ/Q value representing all wind directions, which was obtained from a 5-year dataset of highest calculated 1-hour χ/Q values for all hours of data. The 1-hour χ/Q values were calculated using the Industrial Source Complex Short-Term (ISCST3) air dispersion model,[1] which uses a steady-state Gaussian plume algorithm to calculate concentrations. The model was executed with the Complex I switch invoked to treat complex terrain. The base-case runs prior to the sensitivity analyses incorporated stack-tip downwash but not building wake effects.

Given the capabilities of modern computing hardware, a single 95th percentile χ/Q value can be calculated easily using the actual wind directions rather than using the simplifying adjustment that orients the wind directions along the sector centerline. The meteorological data and the receptors were divided into 360 sets, one for each of the 360 integer directions; 360 ISCST3 runs were performed, one for each direction including all hours for which winds blew toward that integer direction. For each run, χ/Q values were calculated for each hour at 100-300 ground-level receptors under the plume centerline for that direction only. For each hour, the highest χ/Q value was selected among all receptors along that direction. The 95th percentile χ/Q value was determined using a sorted, aggregated list of these 1-hour maxima.

Specifically, the calculated χ/Q values were output to "post-processing" files (with one file per direction). For each hour from each file, the highest 1-hour χ/Q value was selected and stored into a single summary file. Thus, the summary file contained the highest 1-hour χ/Q values for all directions and all hours of valid data. The summary file was sorted and ranked according to the magnitude of the χ/Q value. The 95^{th} percentile χ/Q value was determined from the file (i.e., 5% of the 1-hour maximum χ/Q's have a value greater than the determined value and 95% of the 1-hour maximum χ/Q's have a value less than the determined value).

Because the ISCST3 air dispersion model used in the analysis is a straight-line Gaussian model, the highest χ/Q value for any given hour is expected to be located directly downwind from the wind direction during that hour. Maximum χ/Q values were calculated for each hour by establishing the plume centerline at exactly 180° from the wind direction for each hour (e.g., if the wind direction is from 3°, then the downwind plume centerline is at 183°). Receptors from which the maximum χ/Q values were determined are located on the plume centerline (183° in this example).

For an elevated plume, downwind concentrations calculated along slightly off-centerline directions in higher terrain may potentially be greater than concentrations calculated along the plume centerline in lower terrain. Therefore, a test case was run to verify that the off-centerline concentrations would not be sufficiently high to affect the calculations. The inclusion of receptors from 5 adjacent integer directions on either side of the plume centerline (for a total of 11 directions) resulted in no change in the 95^{th} percentile χ/Q value for 5 years of meteorological data (for scenario 2a discussed in the results section). Consequently, no further calculations were made at receptors not on the plume centerline during any given hour. For a nonbuoyant ground-level release in flat terrain, the highest χ/Q value should occur at the nearest downwind receptor, but this assumption cannot be made for this analysis, which included elevated releases, buoyant plumes, and complex terrain.

While selecting the highest χ/Q value for each hour, the distance from the source to that receptor was determined. If the receptor producing the highest χ/Q value was one of the four farthest from the source, then it was considered to be possible that χ/Q values at more distant receptors along that direction could be found. In such cases, additional receptors extending 1 km further were added to that direction and calculations were repeated.

For multi-hour accidents, the methodology was modified to account for cases in which the highest multi-hour concentrations would not be along any of the directions toward which the wind is blowing during an individual hour that contributes to the period of concern. Instead, highest concentrations may be located at neighboring directions for which substantial concentrations are predicted during the period. For this reason, the meteorological data could not be "binned" by direction. Rather, each year's data were processed sequentially. This process made use of the entire receptor grid impractical. When ISCST3 was run with all receptors in one such run, it failed when the post-processing file exceeded 2 gigabytes. In order to reduce the number of receptors used, while ensuring that the maximum values would be captured, the analysis initially used the methodology described above (i.e., a 1-hour fire). Then only those receptors with a χ/Q value greater than zero (more precisely, greater than 1E-8 s/m^3) were selected. Using those receptors, the ISCST3 model was run for each of 5 years of meteorological data. Receptors in each direction had to be processed separately because ISCST3 has a limit on the size of the post-processing file it can produce. Maximum χ/Q values for each hour of each year were determined separately. Maximum value files were then concatenated and sorted to find the overall 95^{th}-percentile χ/Q value.

INPUT DATA

Meteorological Data

Because of the complex terrain in the SNS environs and because some of the accident scenarios involve an elevated release of mercury, there is no obvious way to select a single “worst case” set of meteorological conditions. Instead, modeling was performed using meteorological data recorded for each hour over a 5-year period from ORNL Tower C, located in the valley immediately southeast of Chestnut Ridge. Six years of data (1996–2001) were analyzed initially. Because the year 2000 contained the largest number of missing or invalid hours, that year was eliminated from the analysis. The resulting dataset included a total of 40,939 hours of valid data.

ORNL Tower C is the closest site with meteorological data at a height approximating the SNS facility’s elevation (i.e., elevation above mean sea level). Tower C is located about 50 m south of Bethel Valley Road, approximately 1.3 km east of the State Highway 95/Bethel Valley Road intersection. It measures temperature, wind speed, and wind direction, and calculates sigma-theta (the standard deviation of the wind direction) at 10, 30, and 100 m above ground level. Except for the mixing height calculation discussed below, the 100-m data were used for this analysis. Because the base elevation of the SNS facility on the ridge is approximately 85 m above the base elevation of Tower C in the adjacent valley, an anemometer height of 15 m above ground level was used for input to the ISCST3 model, even though the 100-m data were actually used (i.e., the release height of 15 m above ground level at the SNS site is the same elevation above mean sea level as the data platform height of 100 m above ground level at Tower C).

Stability class was estimated based on sigma-theta data.[2] Hourly mixing height (m) was calculated using the formula in SCREEN3 of 320 times the hourly wind speed (m/s) at 10 m above ground level.[3] Calculated mixing heights of less than 100 m were set equal to 100 m. For stable conditions, however, the ISCST3 model assumes unlimited vertical mixing[1] because it is unlikely that there would be an overlying layer with conditions more stable than the ground-level layer that would confine mixing more than the ground-level layer. Figure 1 displays the number of hours of data in each of the 360 directions toward which the wind blew (directions are in units of degrees, rounded to the nearest integer). The prevailing winds are toward (and also from) the southwest and northeast, which corresponds to the orientation of the valley in which the tower is located.

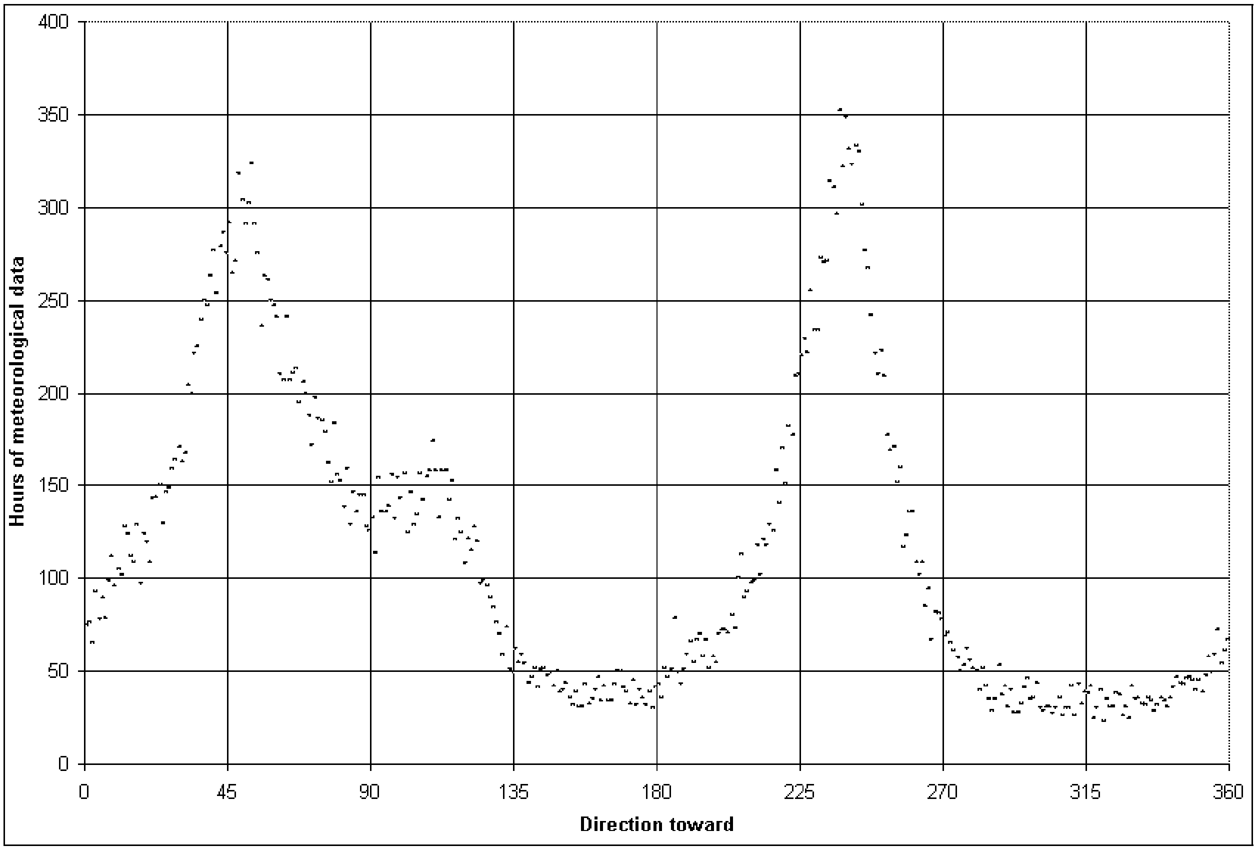

Figure 1. Number of hours of meteorological data in each direction toward which the wind blew (in units of degrees)

Source Data

The release rate used in the ISCST3 model runs was set at 1 g/s so that predicted results would be normalized concentrations (χ/Q's). Because a hypothetical release would be expected from a single source under all scenarios, these χ/Q's can subsequently be multiplied by expected release rates to obtain actual downwind concentrations, if desired. Depending upon the scenario, the release height varied between ground level and 15 m above ground level. Terrain elevations, obtained from the U.S. Geological Survey DEM (digital elevation model) 10-m database, were included for source and receptor locations. However, the ISCST3 model cannot incorporate effects of intervening terrain between the source and receptors.

Two types of scenarios were developed to evaluate the consequences resulting from potential accidental releases of fire-driven mercury. Case 1 is a hypothetical case that does not correspond to any feasible case associated with the facility. It represents an open fire (i.e., not inside a building) that is surrounded by a large pool of mercury. The fire is assumed to continue until the entire amount of mercury (the SNS inventory of 18,000 kg) is vaporized by radiant heat transfer from the fire. For all scenarios associated with Case

1, the release height is set at 15 m for consistency with earlier calculations. Because the entire inventory is assumed to vaporize within the specified durations (1, 2, 3, 4, and 8 hours), the scenarios associated with Case 1 represent fairly large fires with significant upward velocities.

The scenarios associated with Case 2 represent smaller fires with less lofting. These accidental releases are more credible, although still highly unlikely and not "mitigated" in the sense of giving credit for mandatory facility mitigation features. Release heights for these scenarios were obtained as follows:

(a) for scenarios 2a through 2e, half the average building height (7.5 m) was used, based on a hot cell fire within the SNS target facility with varying opening sizes in the structure that surrounds the hot cell;

(b) for scenario 2f, the average building height (15 m) was used, based on an open fire in which the structure surrounding the hot cell has completely collapsed;

(c) for scenario 2g, ground level (0 m) was used, based on no damage to the structural integrity of the building above ground level, and smoke that vents through a roll-top truck door assumed to be open at the time of the fire; and

(d) for scenario 2h, the height of a row of broken windows near the roof of the building (15 m) was used, based on a coincidental, simultaneous fire in the instrument hall of the building resulting from an earthquake.

Table 1 lists the source data used as input in Case 1 and Case 2.[4] For all scenarios, the indicated bulk flow was used. Because bulk flow is not an ISCST3 input parameter, the stack diameter was calculated so that the product of the exit velocity and the area of the stack opening was set equal to the desired bulk flow.

Table 1. Source data used in analysis

Parameter	1a	1b	1c	1d	1e	1f	2a	2b	2c	2d	2e	2f	2g	2h
Fire Size (MW)	25	25	12	7.3	5.2	2.4	1.	1.	1.	1.	1.	1.	1.	1.
Temperature (K)	392	358	332	322	316	307	366	355	341	324	317	301	293	417
Flow Velocity (m/s)	6.5	2.6	2.0	1.7	1.6	1.2	0.42	0.34	0.31	0.24	0.21	0.90	0.001	0.25
Bulk Flow (m^3/s)	169	269	478	142	121	143	0.42	3.4	9.2	19.4	25.6	64.0	25.6	25.9
Stack Diameter (m)	5.75	11.5	10.6	10.2	10.0	9.8	1.13	3.57	6.18	10.1	12.4	9.2	180.5	11.5
Release Height (m)	15	15	15	15	15	15	7.5	7.5	7.5	7.5	7.5	15	0	15
Duration (hour)	1	1	2	3	4	8	1	1	1	1	1	1	1	1

Receptors

A radial receptor grid was created centered on the SNS facility with 360 radials at 1° intervals. For each hour, calculations were performed for receptor(s) along a single radial corresponding with the direction toward which the wind was blowing during that hour. The receptors extend outward from the Oak Ridge reservation boundary at 50-m intervals for at least 2 km in each direction. In addition, locations inside the reservation on Bethel Valley Road and Highway 95 were included as receptors in the appropriate radials. Altogether, 77,691 receptors were used. The number of receptors used in each of the 360 directions is shown in Figure 2. A plot of the receptor grid is shown in Figure 3.

Elevation data were obtained from the U.S. Geological Survey DEM 10-m database. For each receptor point, the elevations of the four closest points in the DEM data were found, from which the elevation of the receptor was interpolated.

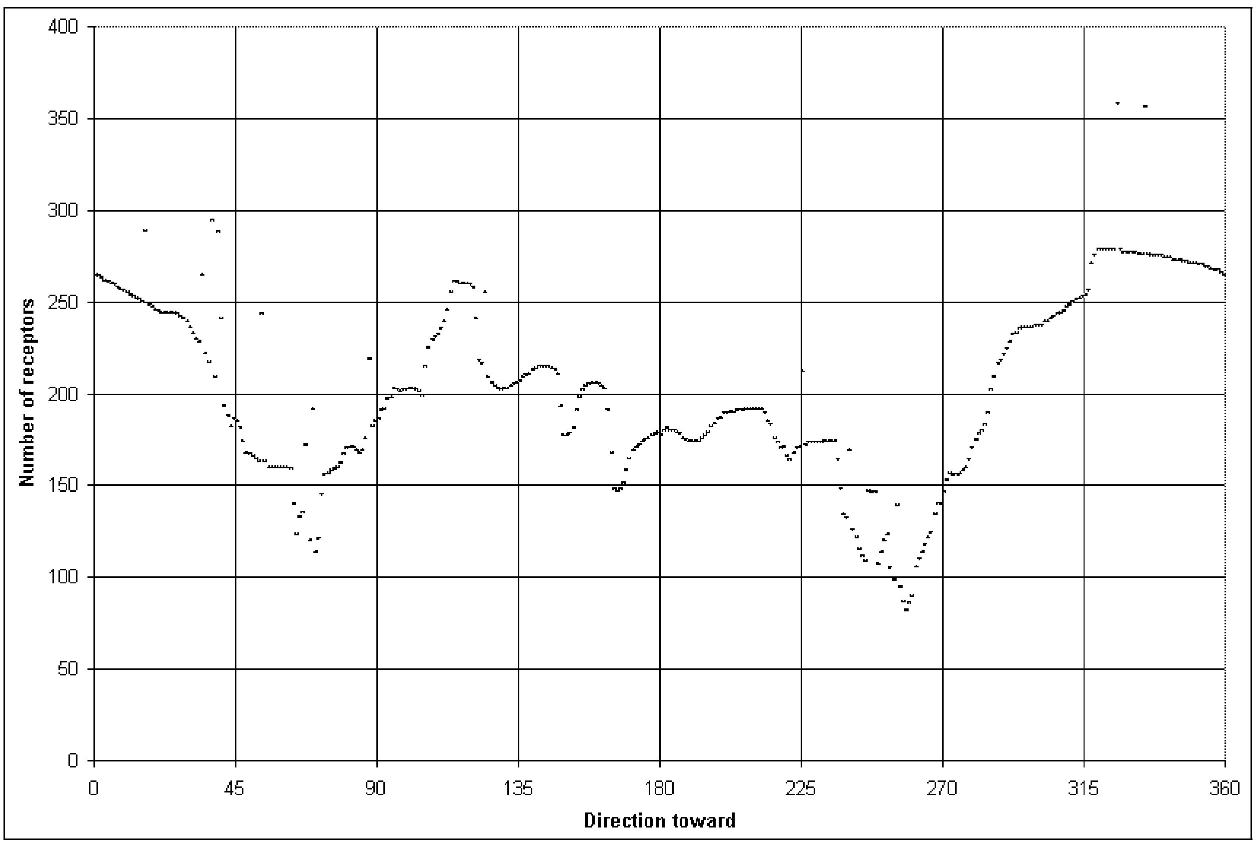

Figure 2. Number of receptors in each direction (degrees)

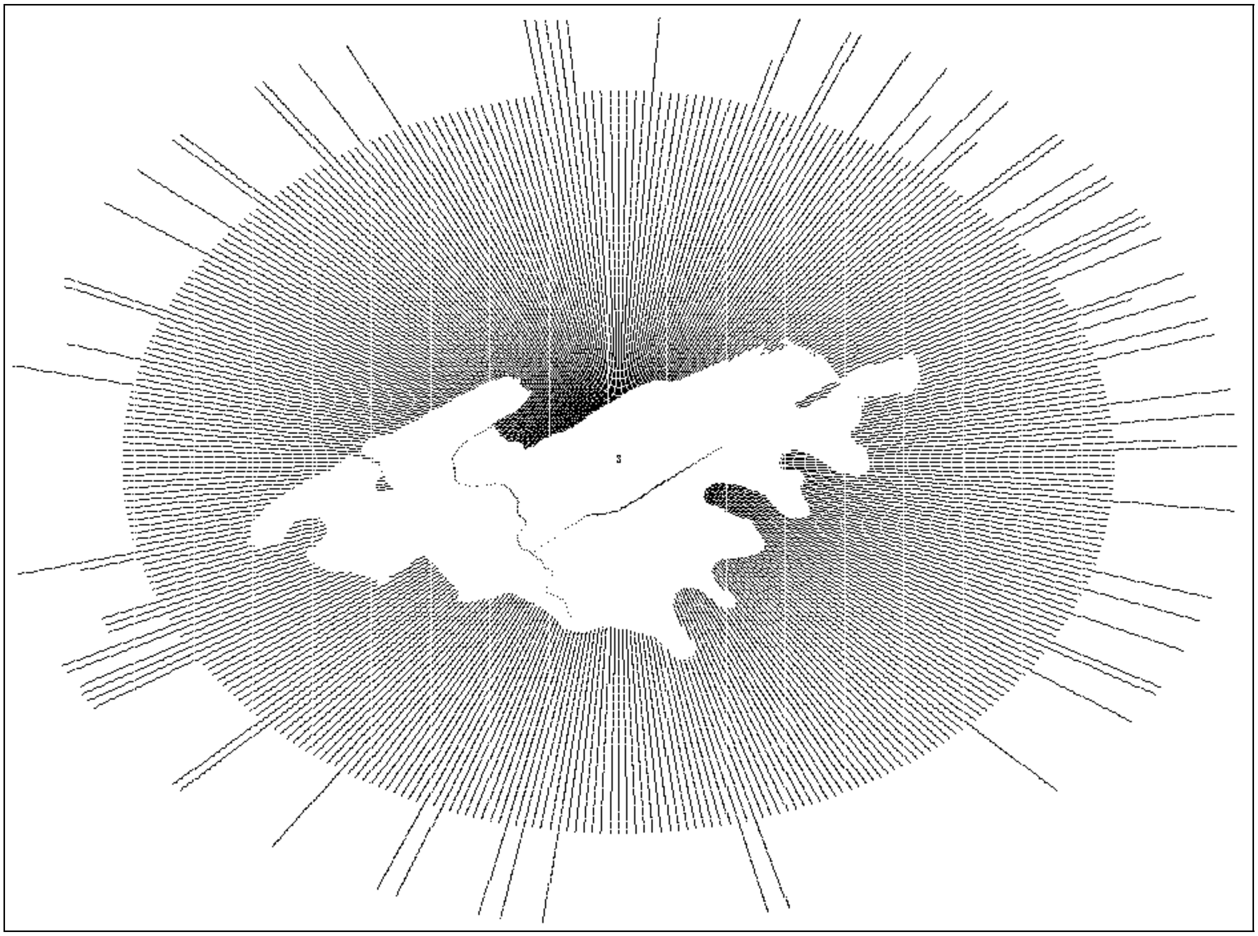

Figure 3. A map of the receptors used in the analysis. The SNS facility is marked with an "S."

RESULTS

Table 2 displays the predicted 95th-percentile χ/Q values resulting from hypothetical mercury releases from the SNS facility without considering the effects of building wake. For all scenarios, the 95th-percentile χ/Q values occur at multiple locations during 3 or more hours. The distance from the SNS facility to the predicted locations varies from 2.6 km to nearly 20 km. The directions from the SNS facility to the predicted locations are distributed fairly evenly rather than being clustered in only a few directions. The number of hours and the closest and furthest locations, as well as the directions to the locations, are included in Table 2.

Table 2. Predicted 95th-percentile mercury χ/Q values (10^{-6} s/m^3) resulting from postulated accidental releases from the SNS facility

Scenario	1a	1b	1c	1d	1e	1f	2a	2b	2c	2d	2e	2f	2g	2h
χ/Q	2.02	2.21	2.31	3.37	3.70	3.99	38.1	32.5	27.2	24.2	23.6	23.4	36.2	14.2
Occurrences (hrs)	183	47	26	4	6	3	8	6	9	9	15	16	8	24
Minimum Distance (km)	3.3	5.1	2.7	3.8	2.7	3.5	4.2	4.5	4.8	2.6	3.3	2.8	3.2	3.0
Direction toward min	343	14	335	5	335	7	25	226	21	314	353	299	302	322
Maximum Distance (km)	16.1	13.9	19.2	8.3	9.6	5.0	6.9	7.3	7.5	7.0	7.7	10.2	6.7	8.5
Direction toward max	255	9	243	155	205	18	114, 46	99	100	46	97	162	160	217

The highest 95th-percentile χ/Q value predicted for any of the scenarios is 3.8 x 10^{-5} s/m^3 for scenario 2a. The 95th-percentile χ/Q values for the other scenarios associated with Case 2 are within a factor of 3 of this highest value. Because of the higher initial upward velocity that drives the plume height above the elevation of the receptors, the 95th-percentile χ/Q values for the scenarios associated with Case 1 are about an order of magnitude less than those for the scenarios associated with Case 2, varying between 2 x 10^{-6} s/m^3 and 4 x 10^{-6} s/m^3.

The locations of the 95th percentile χ/Q values for scenarios 2a and 2g are shown as examples in Figures 4 and 5, respectively. Most of these locations are northwest of the SNS on Blackoak Ridge and Pine Ridge or southeast of the SNS on Stubbs Bluff. The location of these values in elevated terrain implies that the plume height is frequently at or above the elevation of most receptors, even for the smaller fires associated with Case 2. Plots of all χ/Q values calculated for cases 2a and 2g are provided as examples in Figures 6 and 7, respectively.

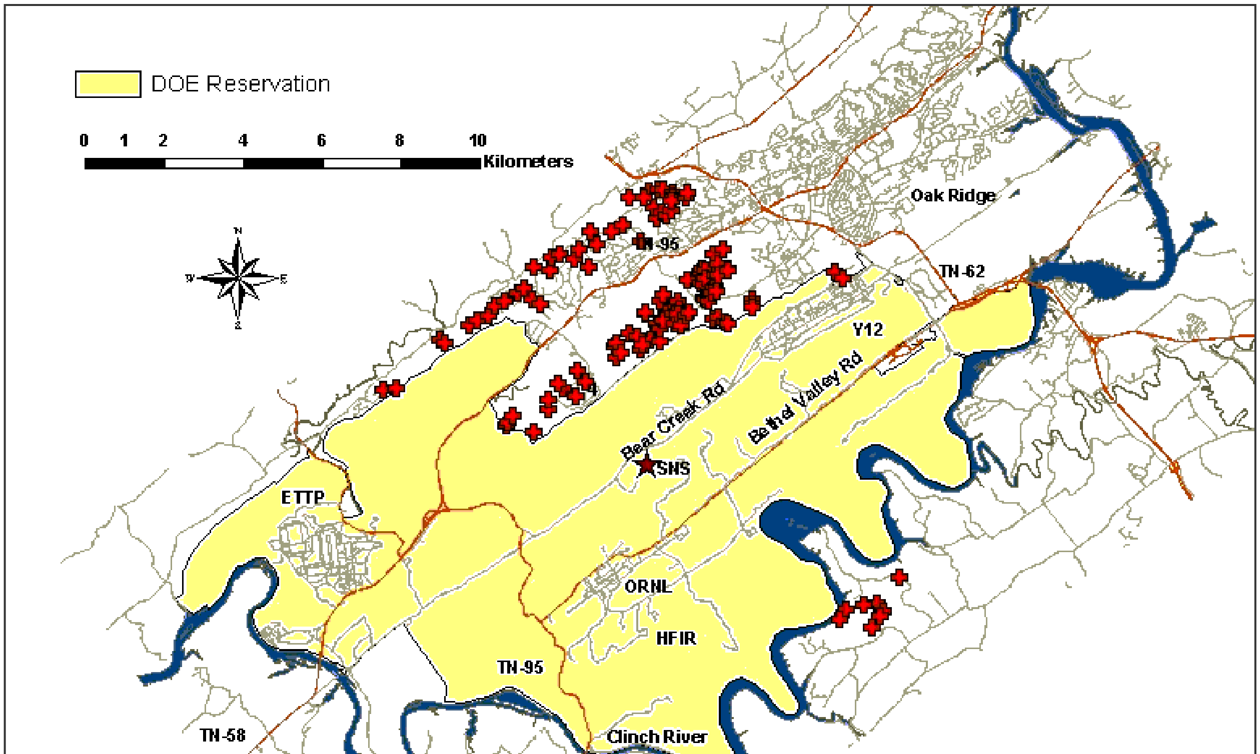

Figure 4. Locations of 95th percentile χ/Q values (indicated by crosses) for case 2a.

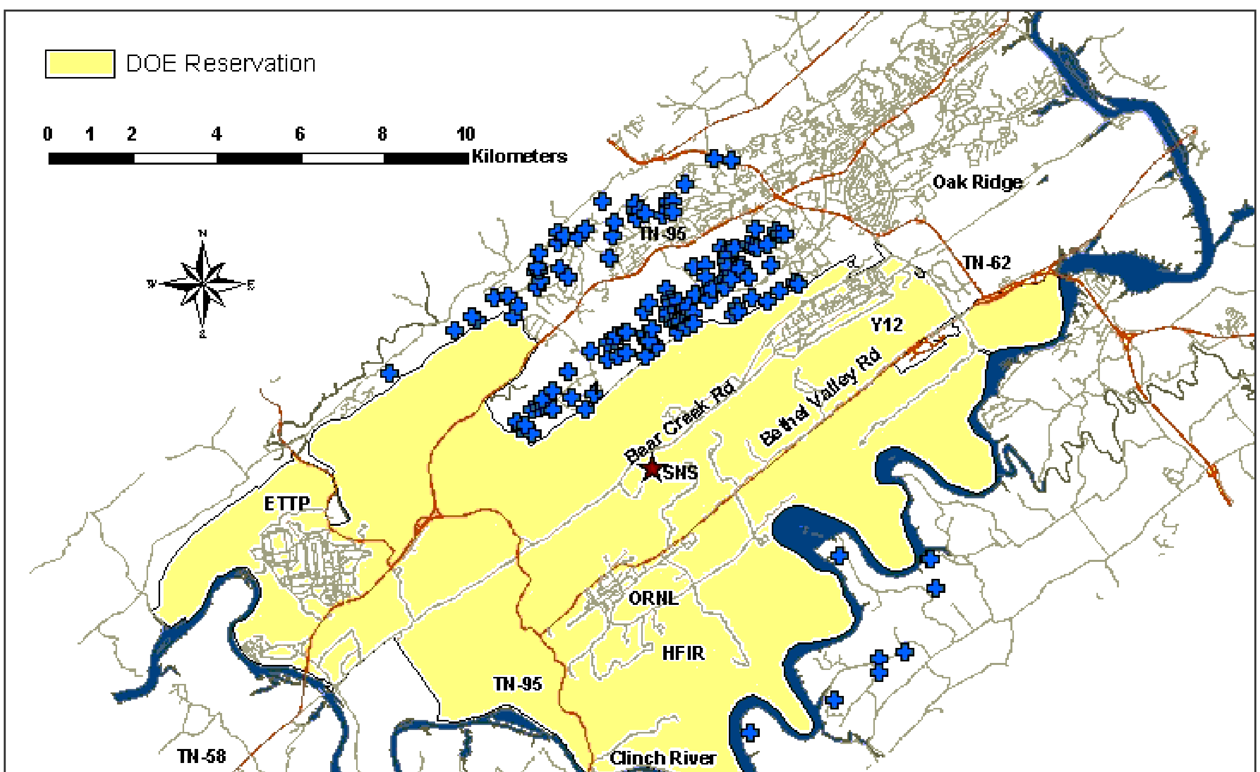

Figure 5. Locations of 95th percentile χ/Q values (indicated by crosses) for case 2g.

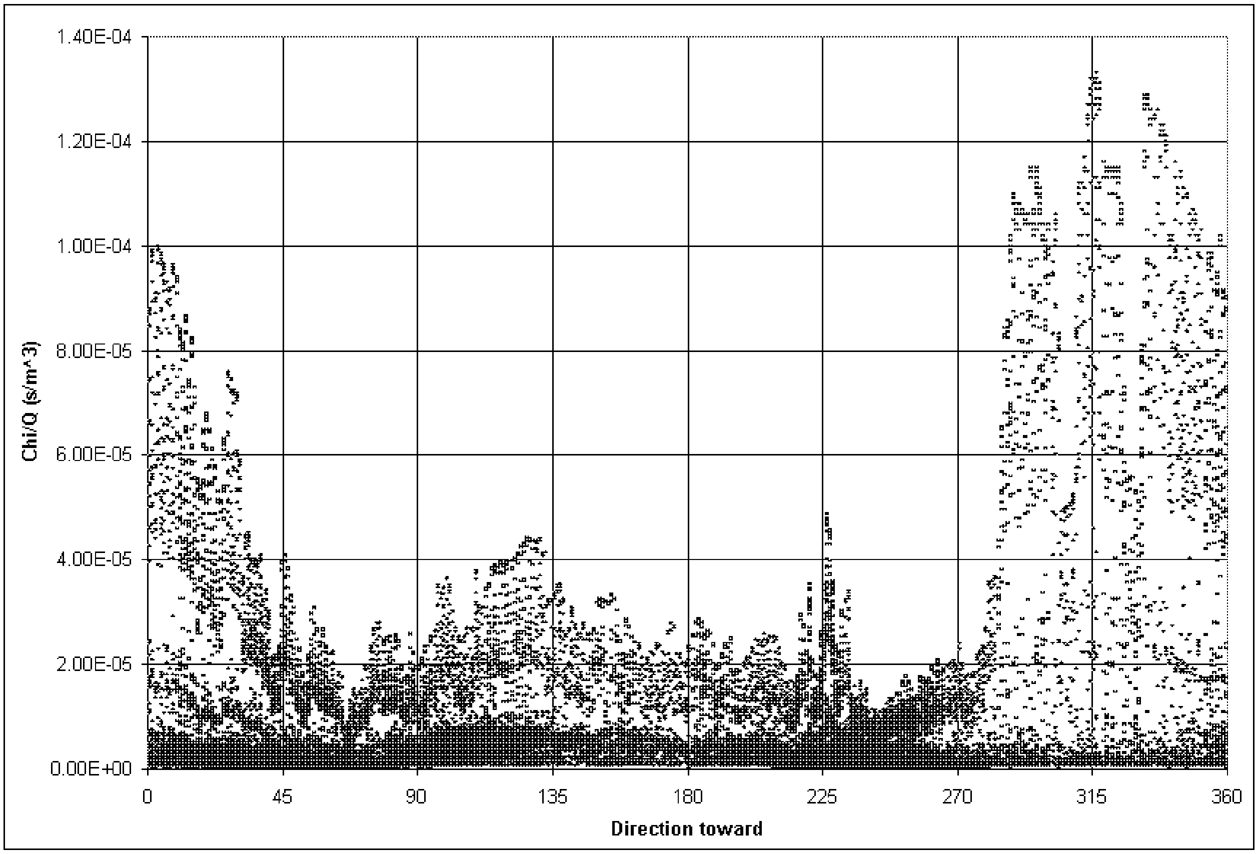

Figure 6. All χ/Q values by direction (in degrees) for case 2a.

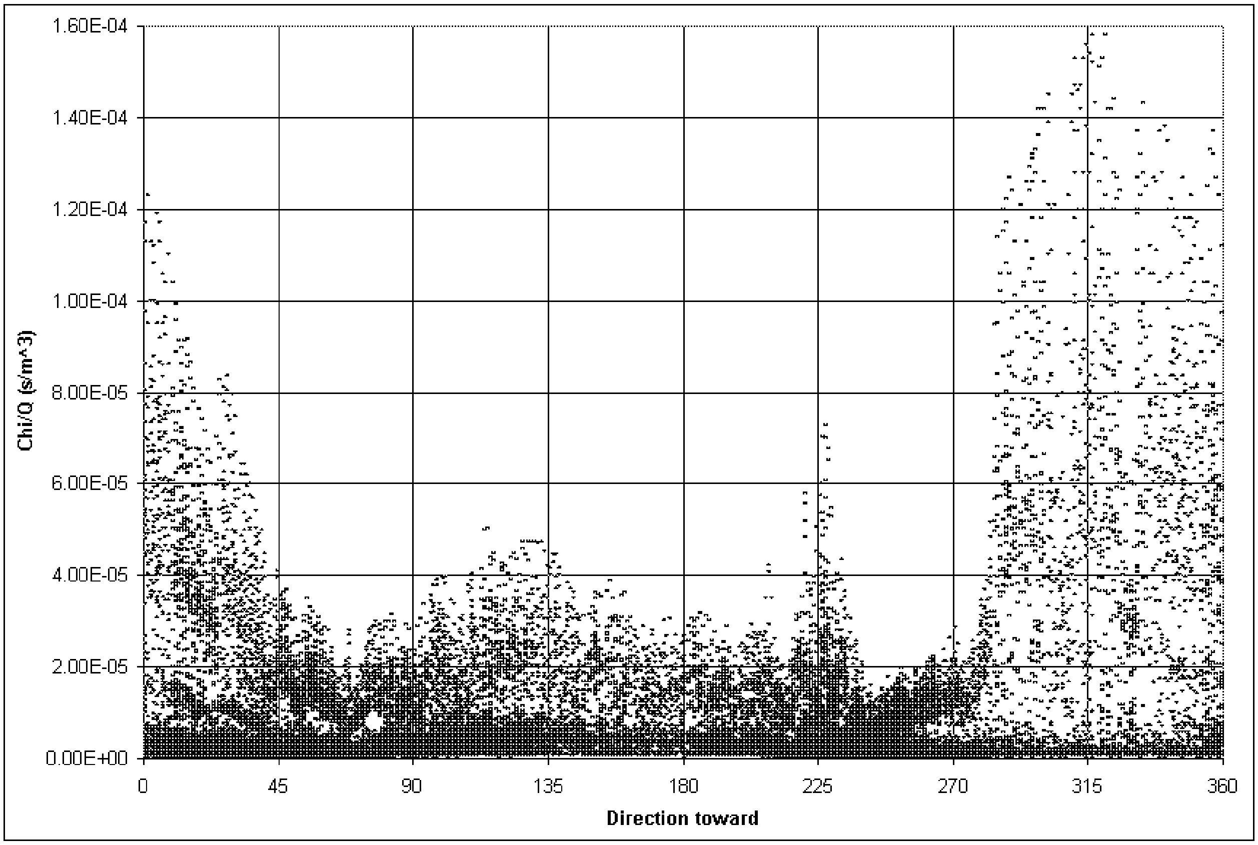

Figure 7. All χ/Q values by direction (in degrees) for case 2g

SENSITIVITY ANALYSES

Four sensitivity analyses were performed using the ISCST3 model. First, the effects of incorporating building wake from the SNS facility were assessed. For all scenarios except 2g, the hypothetical releases were from an elevated height of 7.5 m or 15 m. Scenario 2a, which has the highest 95^{th}-percentile χ/Q value, was selected to illustrate the effects of building wake from an elevated release. The 95^{th}-percentile χ/Q value with building wake was 33.2 x 10^{-6} s/m^3 compared to 38.1 x 10^{-6} s/m^3 without building wake (Table 2). For the lone ground-level release (2g), the 95^{th}-percentile χ/Q value with building wake was 34.2 x 10^{-6} s/m^3 compared to 36.2 x 10^{-6} s/m^3 without building wake (Table 2). Therefore, model runs for the elevated releases and the ground-level release provided conservative (upper-bound) results by excluding building wake effects.

The building wake algorithms in ISCST3 perform two or more of the following adjustments, depending on the magnitude of the building dimensions in relation to the release height: (1) reduce plume rise, (2) enhance vertical mixing of the plume, and (3) enhance lateral mixing of the plume. For elevated releases, a typical net result of these adjustments is to increase ground-level concentrations near the building because the reduced plume rise and enhanced vertical mixing bring the plume to the ground more quickly. However, at the greater distances evaluated in this study, increased vertical and lateral mixing of the plume more than offset the reduction in plume rise caused by building wake. Furthermore, for receptors in elevated terrain near or above plume height, concentrations using building wake algorithms would decrease as a consequence of both reduced plume rise and enhanced mixing. For the single ground-level release (2g), the plume was nearly non-buoyant due to a negligible exit velocity and an exit temperature that was approximately room temperature (293 K). Consequently, building wake effects did not reduce the plume height, which was already at or near ground level, but did enhance the vertical and lateral mixing of the plume. Therefore, maximum concentrations, which occurred along the plume centerline, were reduced by building wake effects.

The second sensitivity analysis evaluated the effects of stack-tip downwash, as calculated by the algorithm in the ISCST3 model. Cases 2f and 2h were used because their release heights were the maximum of 15 m and their 1-hour release duration was easier to evaluate than other cases with longer durations. By turning off stack-tip downwash in the ISCST3 model, the resulting 95th percentile χ/Q values were 16.8 x 10^{-6} s/m^3 and 8.83 x 10^{-6} s/m^3 for cases 2f and 2h, respectively. By comparison, the 95th percentile χ/Q values were 23.4 x 10^{-6} s/m^3 and 14.2 x 10^{-6} s/m^3 for cases 2f and 2h, respectively, using stack-tip downwash (Table 2). Because of the low exit velocities and large stack diameters for these two cases, stack-tip downwash lowers the physical release height to at or near ground level. Because the plume height from the SNS ridge-top release is usually above the receptor elevation, lowering the plume height increases the χ/Q values.

The third sensitivity analysis evaluated the geometry associated with an accidental release through a long line of broken windows at the SNS facility. For a point source, the ISCST3 model requires the inside diameter of the source as an input parameter. ISCST3 was run using both a single source with a large diameter and a line of multiple sources with smaller diameter, in which the cumulative area was equivalent to the area of the single source. This change in source geometry resulted in little difference in χ/Q values, although the single source appeared to be slightly more conservative than the line of multiple sources due to the initial geographical spread of emissions in the latter case.

The final sensitivity analysis evaluated the effects of an accidental release from broken windows on the side of the SNS facility, in which the initial velocity may be in more of a horizontal direction than a vertical direction. Cases 2a and 2f were used to determine the sensitivity of the ISCST3 model to an initial release that is nearly horizontal rather than vertical. For these runs, the data in Table 1 were used, except that the (vertical) exit velocity was set to 0.001 m/s and the diameter, D, was modified by the equation:

D’ = D * (V/0.001)**0.5

where V is the original exit velocity and D’ is the new diameter. This approach is recommended by EPA[5] for hot stack plumes that are interrupted by a rain cap or which are released horizontally. Using this equation, D’ was 23.2 m for case 2a and 276.0 m for case 2f. The resulting 95th percentile χ/Q values were 38.1 x 10^{-6} s/m^3 and 24.1 x 10^{-6} s/m^3 for cases 2a and 2f, respectively. By comparison, the 95th percentile χ/Q values were

38.1×10^{-6} s/m^3 and 23.4×10^{-6} s/m^3 for cases 2a and 2f, respectively, using an initial vertical velocity (Table 2).

The results for the horizontal release are probably affected by one or both of the following mechanisms: (1) increased stack-tip downwash (and thus lowered physical release height) and (2) reduced momentum flux (and thus decreased plume rise when momentum dominates), either of which would lower the plume height. Because the plume height from the SNS ridge-top release is usually above receptor elevations, lowering the plume height would increase the χ/Q values.

However, (1) the above equation to modify the diameter and (2) the equation for the buoyancy flux parameter used in ISCST3 are formulated so that the buoyancy flux would not change for a horizontal vs. vertical release. The results indicate that the χ/Q values from case 2a did not change, while the χ/Q values from case 2f increased slightly for the horizontal release, probably because the release temperature was much warmer for case 2a than case 2f (366 K vs. 301 K, respectively). The plume from case 2a would tend to be more buoyancy dominated, while the plume from case 2f would tend to be more momentum dominated. Thus, the plume height and χ/Q values for case 2f would tend to be more affected by the horizontal release.

ASSUMPTIONS

Several assumptions were incorporated to ensure that the results form an upper bound of actual expected results. Previous evaluations have found that results from the ISCST3 model are biased toward over-predicting concentrations.[6] The 95th-percentile criterion is inherently conservative in that there is a 95% probability that actual concentrations in the event of an accident would be less than predicted values. The probability of a given individual being exposed to predicted concentrations is considerably less than 5% due to the very low probability of the individual's location coinciding with the predicted location. Moreover, some of the receptors are remotely located (e.g., on top of a heavily wooded hill) where it is very unlikely that the duration of personal exposure would extend for the period of time assumed by the release durations in the accident scenarios.

No credit was taken for deposition of material from the plume. Accurate deposition calculations were not possible because the particulate size distribution of the simulated mercury releases was not known. Depending on receptor elevation, the inclusion of deposition algorithms would tend to increase χ/Q values near the SNS facility and reduce values at greater distances (at the receptors of primary interest). Additionally, no credit was taken for consequence mitigation (e.g., sheltering in place or evacuation).

SUMMARY AND CONCLUSIONS

This analysis determined a single 95th percentile χ/Q value representing all wind directions, which was obtained from a dataset of highest calculated 1-hour χ/Q values for all hours of data. Meteorological data and receptors were divided into 360 sets, one for each integer direction; 360 ISCST3 runs were performed, one for each direction including all hours for which winds blew toward that integer direction. For each run, χ/Q values were calculated for each hour at 100-300 ground-level receptors under the plume centerline for that direction only, taking into consideration the release and receptor heights. For each hour, the highest χ/Q value was selected among all receptors along that direction. The 95th percentile χ/Q value was determined using a sorted, aggregated list of these 1-hour maxima.

For all scenarios, the 95th-percentile χ/Q values occurred at multiple locations during 3 or more hours. Distance from the source to the predicted locations varied considerably. The directions to the predicted locations were distributed fairly evenly rather than being clustered in only a few directions. Results of sensitivity analyses indicated that conservative (upper-bound) results were obtained by excluding building wake effects and including stack-tip downwash. A change in source geometry associated with a release through a long line of broken windows had little effect on the results, although the single source appeared to provide slightly higher results than the line of multiple sources. A sensitivity analysis evaluating the effects of a release in which the initial velocity is nearly horizontal yielded the same or slightly higher values than those obtained using a vertical release.

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