Modeling Downwind Hazards After An Accidental Release of Chlorine Trifluoride

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INTRODUCTION

Chlorine trifluoride (CIF₃) is a chemical compound used in the gaseous diffusion process to enrich uranium at two plants, one in Portsmouth, Ohio (PORTS) and the other in Paducah, Kentucky (PGDP). This compound is employed in gaseous diffusion to fluorinate uranium yellow cake (U₃O₈). CIF₃ is shipped to the two gaseous diffusion plants as compressed liquid in cylinders. These cylinders are stored on-site until they are emptied into large storage tanks that hold about 57 m³ of compressed CIF₃ liquid. An accidental breach of a CIF₃ storage cylinder or tank would result in a release of CIF₃ vapor to the atmosphere, which is a concern for plant managers and safety engineers because of its extreme toxicity. Many atmospheric dispersion models are available to model the release of inert airborne contaminants; however, CIF₃ is highly reactive with water vapor in the atmosphere, and therefore, these models would not accurately predict atmospheric concentrations of CIF₃ downwind of a potential release. Additionally, these models do not predict the formation of reaction products that also are toxic [i.e., hydrogen fluoride (HF) and chlorine dioxide (ClO₂)]. Therefore, a more robust method of predicting downwind atmospheric concentrations of CIF₃ and its reaction products is needed to assess potential release hazards. This paper discusses the development of a chemistry and thermodynamics module that has been integrated into the dense gas dispersion model, HGSYSTEM.¹

CHARACTERISTICS AND TOXICITY OF CIF₃ AND PRIMARY REACTION PRODUCTS

CIF₃ is a colorless gas, pale yellow liquid, and white solid. It has a slightly sweet, pungent, and irritating odor. At 20°C, CIF₃ has a specific gravity about three times denser than air, and is volatile at normal atmospheric pressure. CIF₃ is classified as a dense gas and if released into the atmosphere will tend to "hug" the ground as it moves downwind. CIF₃ is the most reactive of the halogen fluorides, reacting with nearly all inorganic and organic compounds, and violently with water. Table 1 shows some physical properties of CIF₃, as well as its primary atmospheric reaction products, HF and ClO₂.

Due to its high reactivity, CIF₃ is irritating and corrosive to all living tissues. Exposure to skin tissue causes burns and lesions due to formation of hydrofluoric acid. CIF₃ exposure to the eye causes damage that may result in blindness. Burn activity continues while residual fluorides remain on the skin and eye tissue. If CIF₃ is inhaled, it can cause inflammation of the respiratory tract and abnormal, potentially fatal, buildup of fluids in the lungs. Due to its high toxicity, the Occupational Safety and Health Administration (OSHA) has established strict regulatory limits on permissible air concentrations of CIF₃ (Table 1).

Anhydrous HF (i.e., HF free from water) is a liquid that readily volatilizes into a colorless gas with a strong, irritating odor. At normal atmospheric pressures, HF vapor is assumed to exist as an equilibrium mixture of the monomer (HF)₂, trimer (HF)₆, hexamer (HF)₉, octamer (HF)₁₂, and HF·H₂O.² ClO₂ is a yellow to red gas or a red-brown liquid (below 11°C) with an unpleasant odor similar to chlorine or nitric acid.³ Both HF and CO₂ are highly toxic with strict limits imposed on permissible air concentrations specified by OSHA to protect workers.
CHEMICAL AND THERMODYNAMIC PROCESSES OF CIF₃

The first attempt in combining the atmospheric reactions of CIF₃ with an atmospheric dispersion model was conducted by Bloom et al. In the development of their model, Bloom et al. combined together a series of hydration reactions into a single equation:

\[
16\text{CIF}_3 + 27\text{H}_2\text{O}(g) \rightarrow 10\text{ClO}_2(g) + 48\text{HF}(g) + \text{HCl}(g) + \text{O}_2(g) + 5\text{HOCl}(g)
\] (1)

This overall stoichiometric reaction equation indicates that 16 moles of CIF₃ would “consume” 27 moles of water vapor if the CIF₃ molecule comes into contact with the water molecule (i.e., one mole of water consumes approximately 0.6 moles of CIF₃). This overall reaction is a simplification and does not account for the molar ratio of CIF₃ to water vapor. The availability of water vapor should be considered to determine reaction of CIF₃ and formation of reaction products.

Experiments performed by Bougon et al. showed the reaction mechanisms of CIF₃ with water are complicated and vary with the relative proportions of these two reactants. They reported that with an initial molar ratio of CIF₃ to water vapor less than two-thirds (i.e., excess water) the reactions would lead to the formation of HF, Cl₂, and O₂, while a ratio larger that two-thirds (i.e., excess CIF₃) the reactions would yield HF, Cl₂, O₂, ClO₂F, and CIF. A small quantity of ClO₂F also would be generated by the reaction between O₂ and ClO₂F which is formed through the CIF₃–H₂O reaction process. Cooper et al. confirmed the findings of Bougon et al. that in an excess CIF₃ reaction, H₂O preferentially reacts with CIF₃ rather than other chlorine fluorides such as ClOF. On the other hand, when water is in slight excess, ClO₂ formation is detected but not ClO₂F. More interestingly, if the molar concentration of water vapor is twice that of CIF₃, the probable product is a mixture of HF, HClO, HClO₂, and some ClO₂.

When CIF₃ is released to the atmosphere, one of two hydration reactions may occur: (1) initial condition of excess CIF₃ or (2) initial condition of excess water. The initial environmental conditions, specifically, the availability of water, are critical in directing the hydration reactions to different pathways and the formation of different reaction products. The first hydration sequence, involving excess CIF₃ is described by the following reactions:

\[
\begin{align*}
\text{ClF}_3 + \text{H}_2\text{O} & \rightarrow \text{ClOF} + 2\text{HF} \quad (2a) \\
2\text{ClOF} & \rightarrow \text{ClO}_2\text{F} + \text{ClF} \quad (2b) \\
\text{ClO}_2\text{F} + \frac{1}{2}\text{H}_2\text{O} & \rightarrow \text{ClO}_2 + \frac{1}{4}\text{O}_2 + \text{HF} \quad (2c) \\
\text{ClIF} + \frac{1}{2}\text{H}_2\text{O} & \rightarrow \frac{1}{2}\text{Cl}_2 + \frac{1}{4}\text{O}_2 + \text{HF} \quad (2d)
\end{align*}
\]

Adding these reactions together yields the overall reaction under conditions of excess CIF₃:

\[
2\text{ClF}_3 + 3\text{H}_2\text{O} \rightarrow \text{ClO}_2 + \frac{1}{2}\text{Cl}_2 + \frac{1}{4}\text{O}_2 + 6\text{HF} \quad (2e)
\]

The reactions products on the right-hand side of Equation 2e have slow reaction kinetics; therefore, compared to downwind plume travel time, these reactants would be stable in the atmosphere. The heat of reaction was determined by subtracting the sum of heats of formation of the products from the sum of heats of formation of the reactants. The heat of reaction was found to be 243.2 kJ/mole.
The second sequence, excess water vapor is described by the following reactions:

\[ 4\text{ClF}_3 + 6\text{H}_2\text{O} \rightarrow 2\text{ClO}_2 + 2\text{Cl}_2\text{O} + \frac{1}{2}\text{O}_2 + 12\text{HF} \]  

\[ \text{Cl}_2\text{O} + \text{H}_2\text{O} \rightarrow 2\text{HOCI} \]

Adding these reactions yields the overall reaction under the conditions of excess water vapor:

\[ 4\text{ClF}_3 + 7\text{H}_2\text{O} \rightarrow 2\text{ClO}_2 + 2\text{HOCI} + \frac{1}{2}\text{O}_2 + 12\text{HF} \]

The reaction products for Equation 3c exhibit slow kinetics and are considered stable. The heat of reaction for excess H\(_2\)O was calculated to be 228.0 kJ/mole.

A review of the open literature (M. D. Cheng, Oak Ridge National Laboratory, Memorandum to Ken Keith, Oak Ridge K-25 Plant, and Don Lee, Oak Ridge National Laboratory, January 10, 1994) found that ClF\(_3\) reactions with species other than water vapor may occur during normal atmospheric conditions. Axworthy \textit{et al.}\(^7\) found that ClF\(_3\) was photochemically decomposed by ultraviolet radiation in the 200–350 nm wavelength range leading to the formation of ClF\(_2\)O. However, protons of these wavelengths are relatively sparse in the lower atmosphere where a release of ClF\(_3\) is likely to occur; therefore, this reaction mechanism would occur much less frequently than hydration reactions. Blauer \textit{et al.}\(^8\) documented thermal decomposition of ClF\(_3\) and ClF\(_2\) in the temperature range of 530 to 1030°C, which is well outside the temperature experienced in the lower atmosphere. Christie\(^9\) described the reaction mechanism between chlorine compounds (including ClF, ClF\(_3\), ClF\(_4\), and ClO\(_2\)) and hydroxyl compounds in the condensed phase. These reactions only would be relevant if ClF\(_3\) releases occurred during rain or fog events. Only then could ClF\(_3\) be incorporated into the aqueous phase. Based on the literature review, the authors concluded that hydration reactions of ClF\(_3\) are clearly the dominant mechanism to be considered for atmospheric releases (i.e., those reactions described by Equations 2e and 3c).

For Equations 2e and 3c, the reaction rate under turbulent conditions follows the single-step reaction formula developed by Varma \textit{et al.}\(^\text{10}\) and Varma.\(^\text{11}\)

\[ \alpha + S\beta \rightarrow \text{products} \]

where \(S\) is the number of moles of species \(\beta\) that reacts with one mole of species \(\alpha\) (i.e., \(S\) is the stoichiometric constant). Based on this single step reaction, the reaction rate \(\dot{R}\) (mole/s\(^2\)), adopted by Bloom \textit{et al.} for use in PLUME89A, is expressed as:

\[ \dot{R} = \frac{3.6\nu}{\Lambda} \left[ \frac{\alpha\beta}{\left( \frac{\alpha}{MW_{\beta}} + \frac{\beta}{MW_{\alpha}} \right)} \right] \]
where
\[ v^* \] is the entrainment velocity (m/s),
\[ \Delta \] is the ratio of the plume cross-sectional area to plume circumference (m),
\[ \alpha \] and \[ \beta \] are the mass fractions of the reaction species, respectively, and
\[ MW_{\alpha} \] and \[ MW_{\beta} \] are the molecular weights of the reaction species, respectively.

The entrainment velocity, \( v^* \), is in the order of 0.6 times the jet speed (m/s) or 0.6 times the ambient friction velocity for a low-momentum, ground-hovering plume. The ratio \( \Delta \) is half the plume radius for a circular cross-section.

### MODELING ATMOSPHERIC RELEASES OF CIF₃

**Plume Behavior After an Atmospheric Release**

Gaussian dispersion models historically have been used to model transport and dispersion of pollutants released to the atmosphere. These models assume that the pollutants are inert and neutrally buoyant (about the same density as the surrounding air). Because CIF₃ is highly reactive with water vapor, the Gaussian methodology does not adequately describe the behavior of a CIF₃ plume.

Figure 1 (from Bloom, et al.⁴) shows a schematic of the potential behavior of a CIF₃ plume. It is likely that CIF₃ and its reaction products would be released from its storage container in a jet due to the reactions occurring inside the breached container (R. O. Johnson, Oak Ridge National Laboratory, transmittal to M. D. Cheng, Oak Ridge National Laboratory, October 4, 1994). If the jet is pointed upward, the momentum of the jet will initially cause the plume to rise as it moves downwind, as shown in region 1 of the figure. As the momentum slows, the plume may sink as shown in region 2 of the figure, because CIF₃ gas can be much denser than the surrounding air. If it sinks all the way to the ground, the plume is designated a ground-hovering plume, as shown in region 3 of the figure. During (and preceding) this ground-hovering plume phase, CIF₃ reactions with water vapor would occur and release heat. The heat released during this reaction and the entrainment of air would cause the plume to become less dense. In turn, the plume may rise as shown in region 4 of the figure. In region 5, the plume would become neutrally buoyant because CIF₃ concentrations would be reduced and reactions would generate less heat. The Gaussian methodology would be sufficient to model plume behavior in region 5.

**Integration of CIF₃ Chemistry and Thermodynamic Processes into HGSYSTEM**

A computerized module has been developed that accounts for the CIF₃ chemistry and thermodynamic processes modeled by Equations 2e, 3c and 5. This module was incorporated into the latest version of HGSYSTEM (Ver. 3.0). HGSYSTEM, approved by the U. S. Environmental Protection Agency as an alternative regulatory model (40 CFR 51, Appendix W), is actually a suite of codes that model dense gas dispersion and HF chemical and thermodynamic processes. HGSYSTEM has been previously selected to simulate the atmospheric dispersion of uranium hexafluoride (UF₆) releases in support of the Gaseous Diffusion Plant (GDP) Safety Analysis Report (SAR) Upgrade Program.¹²,¹³,¹⁴ Chemical and thermodynamic processes of atmospheric releases of UF₆ are similar in many respects to the CIF₃ processes described above.

The CIF₃ module was specifically linked to the HGSYSTEM submodels; AEROPLUME, HEGADAS-S, and PGLUME, and renamed, HGSYSTEM/CIF₃. The following discussion provides some general information on
those submodels; additional details are available in the *HGSYSTEM Version 3.0 Technical Manual* \(^\text{15}\) and the *HGSYSTEM Version 3.0 User's Guide*.

**AEROPLUME.** This submodel estimates near-field (tens to hundreds of meters) dispersion of elevated, two-phase (aerosol and vapor) momentum jets of ClF\(_3\), ClO\(_2\), and HF. This submodel applies to releases from pressurized tanks or cylinders at the point of release to the time when they either (1) strongly interact with the ground and become a dense ground-based plume or (2) become passive (i.e., the density approaches ambient air density and chemical reactions cease).

**HEGADAS-S.** This submodel applies to continuous, steady-state, ground-hovering plumes. The submodel is used for either (1) area source releases (i.e., spills) or (2) at the point where AEROPLUME predicts that the dense plume will be in direct contact with the ground.

**PGPLUME.** This submodel is used in the final passive phase of the elevated plume where the Gaussian plume methodology is applicable. No chemical reactions or thermodynamic processes are modeled in PGPLUME. AEROPLUME will transition to PGPLUME if the plume remains elevated.

**Performance of HGSYSTEM/ClF\(_3\)**

One baseline release scenario and four sensitivity scenarios were simulated to test the performance of HGSYSTEM/ClF\(_3\). Table 2 lists the input parameters into HGSYSTEM/ClF\(_3\) for the baseline and sensitivity scenarios. The baseline scenario simulated an atmospheric release from a ClF\(_3\) storage cylinder breach. According to the PGDP SAR prepared in 1985,\(^\text{16}\) 82 kg of ClF\(_3\) would be released in a cylinder rupture. In the PGDP SAR, the duration of such a release was reported to be less than 60 seconds. For the purpose of this study, the release time was assumed to be 30 seconds. The release parameters were determined from information in the PGDP SAR and Braker and Mossman\(^\text{17}\) (R. O. Johnson, Oak Ridge National Laboratory, transmittal to M. D. Cheng, Oak Ridge National Laboratory, October 4, 1994).

Figure 2 shows the results of the baseline scenario run. AEROPLUME/ClF\(_3\) was used to initially simulate dispersion. ClF\(_3\) concentrations rapidly decrease, while HF and ClO\(_2\) are rapidly created. In the baseline scenario, AEROPLUME/ClF\(_3\) did not transition to HEGADAS-S/ClF\(_3\) or PGPLUME/ClF\(_3\) up to a 2000 m distance downwind from the release point. Concentrations were calculated out to a distance of 2000 m to provide concentration estimates at the farthest GDP facility boundaries.

For the baseline scenario, HF concentrations would exceed the immediately dangerous to life and health (IDLH) threshold value of 25 mg/m\(^3\) [at standard temperature and pressure (STP)] at distances less than 600 m. The IDLH was established by the National Institute of Occupational Safety and Health as the maximum atmospheric concentration from which a person could escape within 30 minutes without a respirator and without experiencing health effects or escape-impairing effects (e.g., severe eye irritation). At 2000 m, the HF concentration would be about 4.5 mg/m\(^3\). The IDLH for ClO\(_2\) (28 mg/m\(^3\) at STP) would be exceeded to a downwind distance of 375 m. At 2000 m, the ClO\(_2\) concentration would be about 2.6 mg/m\(^3\). The IDLH for ClF\(_3\) (67 mg/m\(^3\) at STP) would be exceeded at downwind distances less than 19 m. At 2000 m, the ClF\(_3\) concentration would be about \(1 \times 10^{-13}\) mg/m\(^3\).
Figures 3 through 6 show the results of the scenarios used to test the sensitivity of the model. Figure 3 shows the sensitivity to adjusting the release angle from 0° (i.e., parallel to the ground in the direction of the wind) used in the baseline scenario to -45° (i.e., toward the ground in the direction of the wind). The release simulates a strong interaction of the jet with the ground resulting in a substantial decrease in jet momentum. For this simulation, AEROPLUME/ClF<sub>3</sub> transitioned to HEGADAS/ClF<sub>3</sub> at a downwind distance of 108 m. A slight jump is seen in HF concentrations at 70 m due to the difference in the way that plume concentrations are calculated in AEROPLUME and HEGADAS-S. In AEROPLUME, plume concentrations are assumed to be uniform over the cross-sectional area of the plume. In HEGADAS-S, plume concentrations are assumed to have Gaussian-like profiles. The distribution of concentrations in the plume is such that the greatest concentrations are at the plume centerline and at ground-level. Therefore, HF concentrations increase slightly at the transition point as concentrations change from plume average to maximum centerline value.

For sensitivity scenario 1, HF concentrations exceeded the IDLH to a downwind distance beyond 2000 m (HF concentration would be about 33 mg/m<sup>3</sup> at 2000 m). The IDLH for ClO<sub>2</sub> would be exceeded to a downwind distance of about 1500 m. At 2000 m, the ClO<sub>2</sub> concentration would be about 18 mg/m<sup>3</sup>. The IDLH for ClF<sub>3</sub> would be exceeded to a downwind distance of about 12 m. At 2000 m, the ClF<sub>3</sub> concentration would be about 6.8 × 10<sup>-8</sup> mg/m<sup>3</sup>.

Figure 4 shows the sensitivity of the module to ambient relative humidity. The ambient relative humidity for the baseline scenario was chosen to be 70%. This represents a typical ambient relative humidity at the GDPs. For sensitivity scenario 2, the relative humidity was lowered to 10%. HF concentrations exceeded the IDLH to a downwind distance of about 1700 m. At 2000 m, the HF concentration would be about 19 mg/m<sup>3</sup>. The IDLH for ClO<sub>2</sub> would be exceeded to a downwind distance of about 1400 m. At 2000 m, the ClO<sub>2</sub> concentration would be about 16 mg/m<sup>3</sup>. The IDLH for ClF<sub>3</sub> would be exceeded to a downwind distance of about 460 m. At 2000 m, the ClF<sub>3</sub> concentration would be about 5.0 × 10<sup>-3</sup> mg/m<sup>3</sup>.

Figure 5 shows the sensitivity of the module to ambient temperature. The ambient temperature for the baseline scenario was chosen to be 25°C. For sensitivity scenario 3, the ambient temperature was lowered to -10°C. HF concentrations exceeded the IDLH to a downwind distance of about 2000 m. The IDLH for ClO<sub>2</sub> would be exceeded to a downwind distance of about 1600 m. At 2000 m, the ClO<sub>2</sub> concentration would be about 19 mg/m<sup>3</sup>. The IDLH for ClF<sub>3</sub>, would be exceeded to a downwind distance of about 320 m. At 2000 m, the ClF<sub>3</sub> concentration would be 5.5 × 10<sup>-3</sup> mg/m<sup>3</sup>.

In the baseline scenario, concentrations were calculated using neutral (Pasquill-Gifford stability class D) atmospheric conditions with wind speeds equal to 4 m/s. These parameters represent typical meteorological conditions at the GDPs that result in high concentration estimates compared to other frequently occurring conditions. For the final sensitivity run (sensitivity scenario 4 as shown in Figure 6), concentrations were calculated using stable (Pasquill-Gifford stability class F) atmospheric conditions with wind speeds equal to 2 m/s. HF concentrations exceeded the IDLH to a downwind distance beyond 2000 m (HF concentrations would be about 36 mg/m<sup>3</sup> at 2000 m). The IDLH for ClO<sub>2</sub> would be exceeded to a downwind distance of about 1200 m. At 2000 m, the ClO<sub>2</sub> concentration would be about 20 mg/m<sup>3</sup>. The IDLH for ClF<sub>3</sub> would be exceeded to a downwind distance of about 19 m. At 2000 m, the ClF<sub>3</sub> concentration would be about 1.9 × 10<sup>-9</sup> mg/m<sup>3</sup>. 
SUMMARY AND CONCLUSIONS

A module simulating CIF₃ chemical reactions with water vapor and thermodynamic processes in the atmosphere after an accidental release has been developed. This module was linked to HGSYSTEM and named HGSYSTEM/CIF₃. Initial model runs simulate the rapid formation of HF and ClO₂ after an atmospheric release of CIF₃. At distances beyond the first several meters from the release point, HF and ClO₂ concentrations pose a greater threat to human health than do CIF₃ concentrations. For most of the simulations, CIF₃ concentrations rapidly fall below the IDLH (i.e., within about 20 m). For releases occurring in ambient conditions with low relative humidity and/or ambient temperature, CIF₃ concentrations exceed the IDLH up to almost 500 m.

The performance of this model needs to be determined for potential release scenarios that will be considered in the GDP SAR Upgrades. These release scenarios are currently being developed.

REFERENCES


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**Table 1. Physical characteristics and toxicity information for ClF<sub>3</sub>, HF, and ClO<sub>2</sub>**

<table>
<thead>
<tr>
<th>Property</th>
<th>ClF&lt;sub&gt;3&lt;/sub&gt;</th>
<th>HF</th>
<th>ClO&lt;sub&gt;2&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight, g/g-mol</td>
<td>92.5</td>
<td>20.0</td>
<td>67.5</td>
</tr>
<tr>
<td>Vapor pressure at 20°C, atm</td>
<td>1.46</td>
<td>&gt;1 atm</td>
<td>&gt;1 atm</td>
</tr>
<tr>
<td>Boiling point at 1 atm, °C</td>
<td>11.8</td>
<td>19.4</td>
<td>9.9</td>
</tr>
<tr>
<td>Specific gravity at 20°C (where Air = 1)</td>
<td>3.14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid density at 0°C, g/ml</td>
<td>1.89</td>
<td>1.00</td>
<td>1.60</td>
</tr>
<tr>
<td>IDLH at STP, mg/m³</td>
<td>67</td>
<td>25</td>
<td>28</td>
</tr>
</tbody>
</table>

Abbreviations: ClF<sub>3</sub> = chlorine trifluoride; HF = hydrogen fluoride; ClO<sub>2</sub> = chlorine dioxide; STP = standard temperature and pressure (25°C and 1 atm); IDLH = Immediately Dangerous to Life and Health.

**Table 2. Scenario release parameter input to HGSYSTEM/ClF<sub>3</sub>**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Baseline scenario</th>
<th>Sensitivity scenario 1</th>
<th>Sensitivity scenario 2</th>
<th>Sensitivity scenario 3</th>
<th>Sensitivity scenario 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release duration, s&lt;sup&gt;a&lt;/sup&gt;</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>Plume temperature at release, °C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>52</td>
<td>52</td>
<td>52</td>
<td>52</td>
<td>52</td>
</tr>
<tr>
<td>Plume density at release, kg/m³&lt;sup&gt;a&lt;/sup&gt;</td>
<td>15</td>
<td>15</td>
<td>15</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Release orifice diameter, m&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>Exit velocity from orifice, m/s&lt;sup&gt;a&lt;/sup&gt;</td>
<td>31</td>
<td>31</td>
<td>31</td>
<td>31</td>
<td>31</td>
</tr>
<tr>
<td>Release angle, where 0° = parallel to ground in the direction of the wind</td>
<td>0</td>
<td>-10</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Atmospheric stability class</td>
<td>D</td>
<td>D</td>
<td>D</td>
<td>D</td>
<td>F</td>
</tr>
<tr>
<td>Windspeed, m/s</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>Relative humidity</td>
<td>70%</td>
<td>70%</td>
<td>10%</td>
<td>70%</td>
<td>70%</td>
</tr>
<tr>
<td>Ambient temperature, °C</td>
<td>25</td>
<td>25</td>
<td>25</td>
<td>-10</td>
<td>25</td>
</tr>
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</table>

<sup>a</sup>Source: R. O. Johnson, Oak Ridge National Laboratory, transmittal to M. D. Cheng, Oak Ridge National Laboratory, October 4, 1994.
Example of a possible plume trajectory from a moderate velocity, vertical release of ClF₃.

Figure 2. Results of the baseline scenario run. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and relative humidity are 70% and 25°C, respectively, atmospheric stability class is D, and wind speed is 4 m/s.
Figure 3. Results of sensitivity scenario 1. Release angle is $-45^\circ$ (where $0^\circ$ is parallel to the ground in the direction of the wind), ambient relative humidity and temperature are 70% and 25°C, respectively, atmospheric stability class is D, and windspeed is 4 m/s.
Results of sensitivity scenario 2. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and temperature are 10% and 25°C, respectively, atmospheric stability class is D, and windspeed is 4 m/s.
Figure 5. Results of sensitivity scenario 3. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and temperature are 70% and -10°C, respectively, atmospheric stability class is D, and windspeed is 4 m/s.
Results of sensitivity scenario 4. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and temperature are 70% and 25°C, respectively, atmospheric stability class is F, and windspeed is 2 m/s.