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Modeling Downwind Hazards After An Accidental Release of Chlorine Trifluoride

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INTRODUCTION

Chlorine trifluoride (ClF_3) 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 (U_3O_8). ClF_3 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 m^3 of compressed ClF_3 liquid. An accidental breach of a ClF_3 storage cylinder or tank would result in a release of ClF_3 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, ClF_3 is highly reactive with water vapor in the atmosphere, and therefore, these models would not accurately predict atmospheric concentrations of ClF_3 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 (ClO_2)]. Therefore, a more robust method of predicting downwind atmospheric concentrations of ClF_3 and its reactions 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 ClF_3 AND PRIMARY REACTION PRODUCTS

ClF_3 is a colorless gas, pale yellow liquid, and white solid. It has a slightly sweet, pungent, and irritating odor. At 20°C, ClF_3 has a specific gravity about three times denser than air, and is volatile at normal atmospheric pressure. ClF_3 is classified as a dense gas and if released into the atmosphere will tend to "hug" the ground as it moves downwind. ClF_3 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 ClF_3, as well as its primary atmospheric reaction products, HF and ClO_2.

Due to its high reactivity, ClF_3 is irritating and corrosive to all living tissues. Exposure to skin tissue causes burns and lesions due to formation of hydrofluoric acid. ClF_3 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 ClF_3 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 ClF_3 (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 $(HF)_1$, trimer $(HF)_3$, hexamer $(HF)_6$, octamer $(HF)_8$, and $HF{\cdot}H_2O$.[2] ClO_2 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 CO_2 are highly toxic with strict limits imposed on permissible air concentrations specified by OSHA to protect workers.

CHEMICAL AND THERMODYNAMIC PROCESSES OF ClF_3

The first attempt in combining the atmospheric reactions of ClF_3 with an atmospheric dispersion model was conducted by Bloom *et al.*[4] In the development of their model, Bloom *et al.* combined together a series of hydration reactions into a single equation:

$$16ClF_3 + 27H_2O(g) \rightarrow 10ClO_2(g) + 48HF(g) + HCl(g) + O_2(g) + 5HOCl(g) \quad (1)$$

This overall stoichiometric reaction equation indicates that 16 moles of ClF_3 would "consume" 27 moles of water vapor if the ClF_3 molecule comes into contact with the water molecule (i.e., one mole of water consumes approximately 0.6 moles of ClF_3). This overall reaction is a simplification and does not account for the molar ratio of ClF_3 to water vapor. The availability of water vapor should be considered to determine reaction of ClF_3 and formation of reaction products.

Experiments performed by Bougon *et al.*[5] showed the reaction mechanisms of ClF_3 with water are complicated and vary with the relative proportions of these two reactants. They reported that with an initial molar ratio of ClF_3 to water vapor less than two-thirds (i.e., excess water) the reactions would lead to the formation of HF, Cl_2, and O_2, while a ratio larger that two-thirds (i.e., excess ClF_3) the reactions would yield HF, Cl_2, O_2, ClO_2F, and ClF. A small quantity of ClO_3F also would be generated by the reaction between O_2 and ClO_2F which is formed through the ClF_3–H_2O reaction process. Cooper *et al.*[6] confirmed the findings of Bougon *et al.* that in an excess ClF_3 reaction, H_2O preferentially reacts with ClF_3 rather than other chlorine fluorides such as ClOF. On the other hand, when water is in slight excess, ClO_2 formation is detected but not ClO_2F. More interestingly, if the molar concentration of water vapor is twice that of ClF_3, the probable product is a mixture of HF, HClO, $HClO_2$, and some ClO_2.

When ClF_3 is released to the atmosphere, one of two hydration reactions may occur: (1) initial condition of excess ClF_3 or (2) initial condition of excess water.[4] 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 ClF_3 is described by the following reactions:

$$ClF_3 + H_2O \rightarrow ClOF + 2HF \quad (2a)$$
$$2ClOF \rightarrow ClO_2F + ClF \quad (2b)$$
$$ClO_2F + \tfrac{1}{2}H_2O \rightarrow ClO_2 + \tfrac{1}{4}O_2 + HF \quad (2c)$$
$$ClF + \tfrac{1}{2}H_2O \rightarrow \tfrac{1}{2}Cl_2 + \tfrac{1}{4}O_2 + HF \quad (2d)$$

Adding these reactions together yields the overall reaction under conditions of excess ClF_3:

$$2ClF_3 + 3H_2O \rightarrow ClO_2 + \tfrac{1}{2}Cl_2 + \tfrac{1}{2}O_2 + 6HF \quad (2e)$$

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:

$$4ClF_3 + 6H_2O \rightarrow 2ClO_2 + 2Cl_2O + \tfrac{1}{2}O_2 + 12HF \quad (3a)$$
$$Cl_2O + H_2O \rightarrow 2HOCl \quad (3b)$$

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

$$4ClF_3 + 7H_2O \rightarrow 2ClO_2 + 2\,HOCl + \tfrac{1}{2}O_2 + 12HF \quad (3c)$$

The reaction products for Equation 3c exhibit slow kinetics and are considered stable. The heat of reaction for excess H_2O 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 *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_2O. 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 *et al.*[8] documented thermal decomposition of ClF_3 and ClF_5 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_5, 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 *et al.*[10] and Varma:[11]

$$\alpha + S\beta \rightarrow \text{products} \quad (4)$$

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

$$\dot{R} = \frac{3.6 v_e}{\Lambda}\left[\frac{\bar{\alpha}\bar{\beta}}{\left(\bar{\alpha}\frac{MW_\beta}{MW_a}S\right)+\bar{\beta}}\right] \quad (5)$$

where

v_e is the entrainment velocity (m/s),
Λ is the ratio of the plume cross-sectional area to plume circumference (m),
$\bar{\alpha}$ and $\bar{\beta}$ are the mass fractions of the reaction species, respectively, and
MW_α and MW_β are the molecular weights of the reaction species, respectively.

The entrainment velocity, v_e, 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 Λ is half the plume radius for a circular cross-section.

MODELING ATMOSPHERIC RELEASES OF ClF_3

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 ClF_3 is highly reactive with water vapor, the Gaussian methodology does not adequately describe the behavior of a ClF_3 plume.

Figure 1 (from Bloom, *et al.*[4]) shows a schematic of the potential behavior of a ClF_3 plume. It is likely that ClF_3 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 ClF_3 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, ClF_3 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 ClF_3 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 ClF_3 Chemistry and Thermodynamic Processes into HGSYSTEM

A computerized module has been developed that accounts for the ClF_3 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 (UF_6) 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 UF_6 are similar in many respects to the ClF_3 processes described above.

The ClF_3 module was specifically linked to the HGSYSTEM submodels; AEROPLUME, HEGADAS-S, and PGLUME, and renamed, HGSYSTEM/ClF_3. The following discussion provides some general information on

those submodels; additional details are available in the *HGSYSTEM Version 3.0 Technical Manual*[2] and the *HGSYSTEM Version 3.0 User's Guide*.[15]

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,[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[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 1×10^{-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_3 transitioned to HEGADAS/ClF_3 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^3 at 2000 m). The IDLH for ClO_2 would be exceeded to a downwind distance of about 1500 m. At 2000 m, the ClO_2 concentration would be about 18 mg/m^3. The IDLH for ClF_3 would be exceeded to a downwind distance of about 12 m. At 2000 m, the ClF_3 concentration would be about 6.8×10^{-8} mg/m^3.

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^3. The IDLH for ClO_2 would be exceeded to a downwind distance of about 1400 m. At 2000 m, the ClO_2 concentration would be about 16 mg/m^3. The IDLH for ClF_3 would be exceeded to a downwind distance of about 460 m. At 2000 m, the ClF_3 concentration would be about 5.0×10^{-3} mg/m^3.

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 temperture was lowered to −10°C. HF concentrations exceeded the IDLH to a downwind distance of about 2000 m. The IDLH for ClO_2 would be exceeded to a downwind distance of about 1600 m. At 2000 m, the ClO_2 concentration would be about 19 mg/m^3. The IDLH for ClF_3, would be exceeded to a downwind distance of about 320 m. At 2000 m, the ClF_3 concentration would be 5.5×10^{-3} mg/m^3.

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^3 at 2000 m). The IDLH for ClO_2 would be exceeded to a downwind distance of about 1200 m. At 2000 m, the ClO_2 concentration would be about 20 mg/m^3. The IDLH for ClF_3 would be exceeded to a downwind distance of about 19 m. At 2000 m, the ClF_3 concentration would be about 1.9×10^{-9} mg/m^3.

SUMMARY AND CONCLUSIONS

A module simulating ClF_3 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/ClF_3. Initial model runs simulate the rapid formation of HF and ClO_2 after an atmospheric release of ClF_3. At distances beyond the first several meters from the release point, HF and ClO_2 concentrations pose a greater threat to human health than do ClF_3 concentrations. For most of the simulations, ClF_3 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, ClF_3 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.

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Table 1. Physical characteristics and toxicity information for ClF_3, HF, and ClO_2

Property	ClF_3	HF	ClO_2
Molecular weight, g/g-mol	92.5	20.0	67.5
Vapor pressure at 20°C, atm	1.46	>1 atm	>1 atm
Boiling point at 1 atm, °C	11.8	19.4	9.9
Specific gravity at 20°C (where Air = 1)	3.14		
Liquid density at 0°C, g/ml	1.89	1.00	1.60
IDLH at STP, mg/m^3	67	25	28

Abbreviations: ClF_3 = chlorine trifluoride; HF = hydrogen fluoride; ClO_2 = 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_3

Parameter	Baseline scenario	Sensitivity scenario 1	2	3	4
Release duration, s[a]	30	30	30	30	30
Plume temperature at release, °C[a]	52	52	52	52	52
Plume density at release, kg/m^3[a]	15	15	15	15	15
Release orifice diameter, m[a]	0.13	0.13	0.13	0.13	0.13
Exit velocity from orifice, m/s[a]	31	31	31	31	31
Release angle, where 0° = parallel to ground in the direction of the wind	0	-10	0	0	0
Atmospheric stability class	D	D	D	D	F
Windspeed, m/s	4	4	4	4	2
Relative humidity	70%	70%	10%	70%	70%
Ambient temperature, °C	25	25	25	-10	25

[a]*Source:* R. O. Johnson, Oak Ridge National Laboratory, transmittal to M. D. Cheng, Oak Ridge National Laboratory, October 4, 1994.

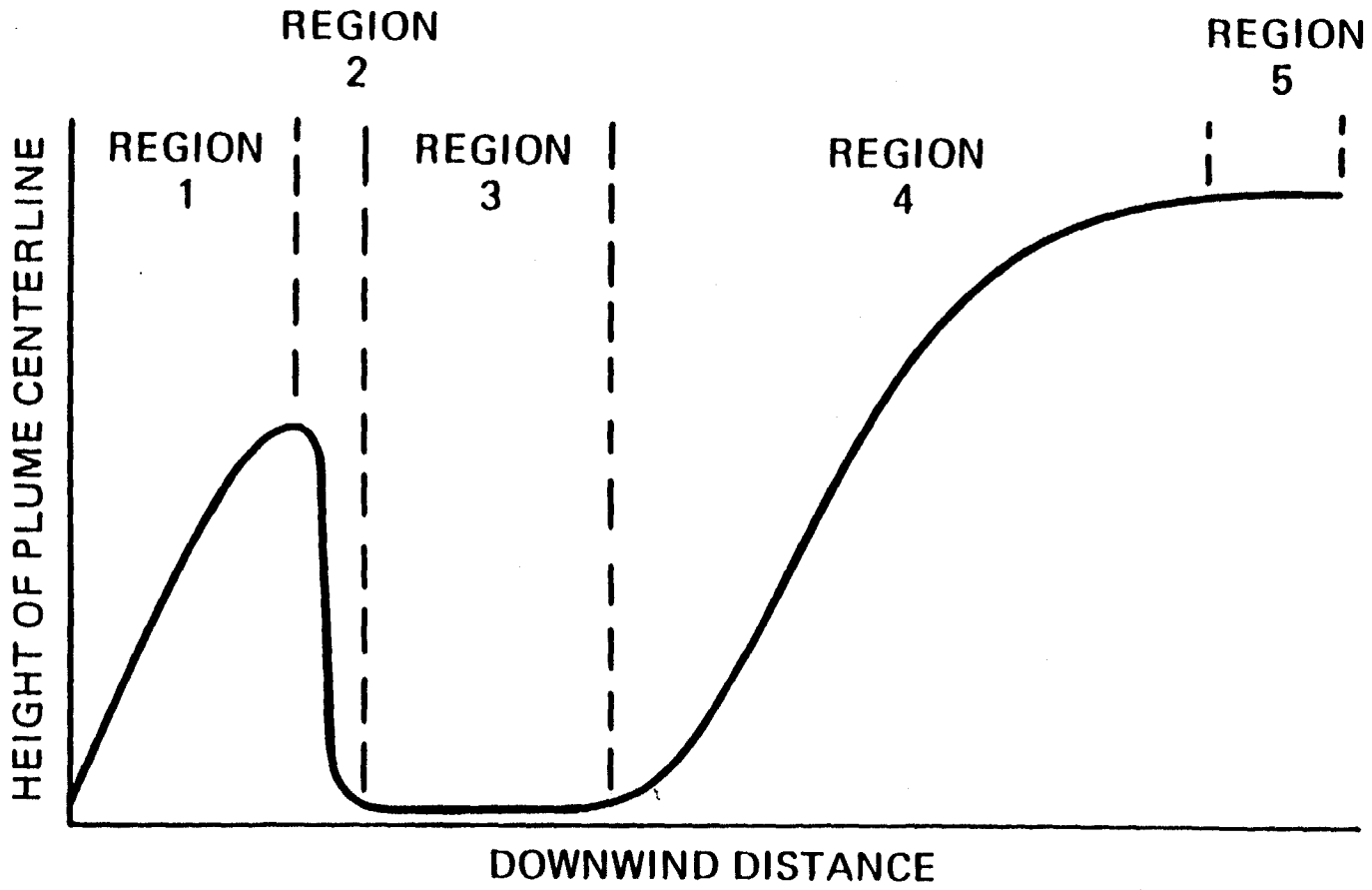

Figure 1. Example of a possible plume trajectory from a moderate velocity, vertical release of ClF_3.
Source: S. G. Bloom, R. A. Just, and W. R. Williams 1989. *A Computer Program for Simulating the Atmospheric Dispersion of UF_6 and Other Reactive Gases Having Positive, Neutral, or Negative Buoyancy*, Report No. K/D-5694, Oak Ridge Gaseous Diffusion Plant, Martin Marietta Energy Systems, Oak Ridge, Tennessee.

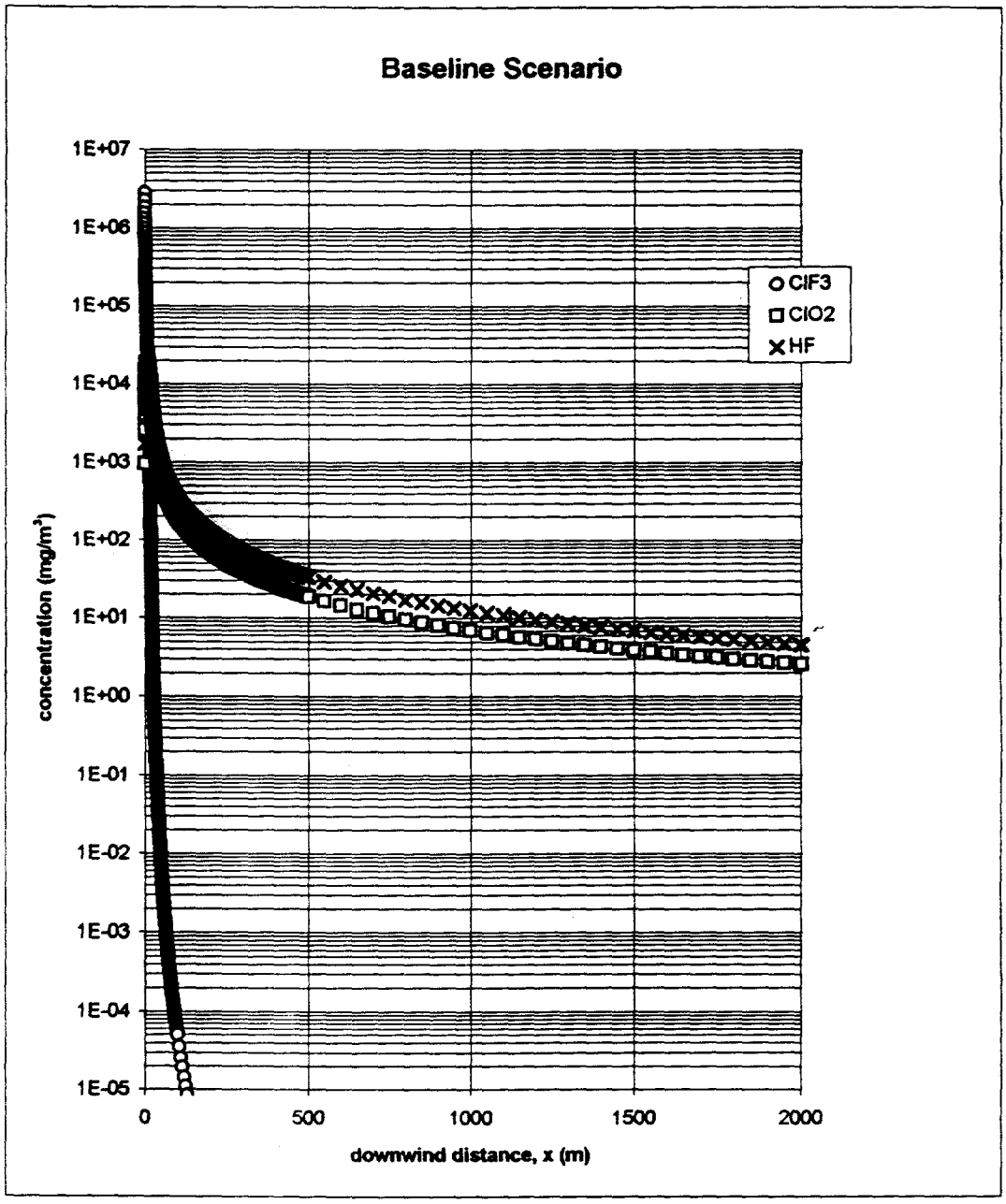

Figure 2. Results of the baseline scenario run. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and relative humidity are 70% and 25°C, respectively, atmospheric stability class is D, and wind speed is 4 m/s.

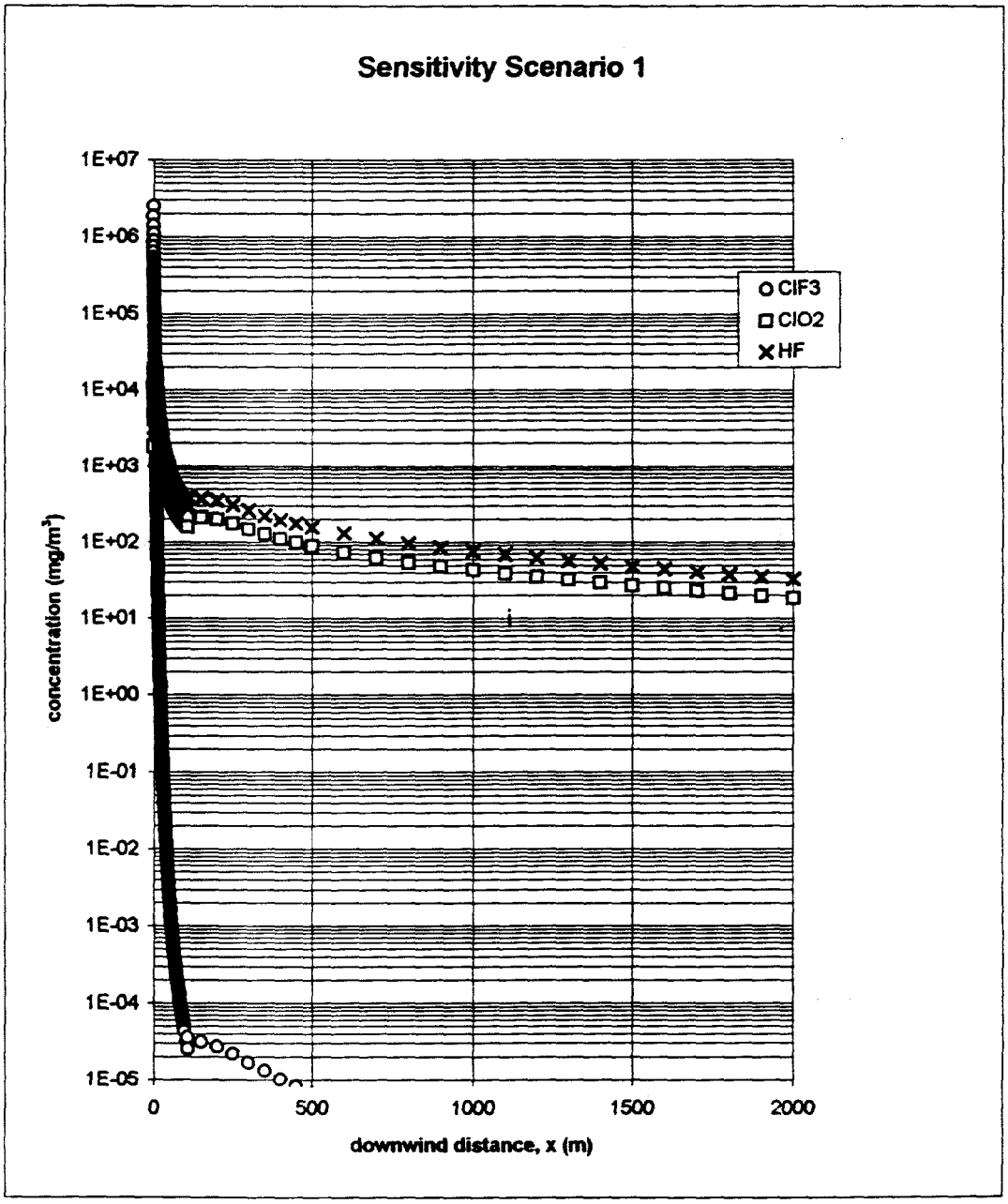

Figure 3. Results of sensitivity scenario 1. Release angle is −45° (where 0° is parallel to the ground in the direction of the wind), ambient relative humidity and temperature are 70% and 25°C, respectively, atmospheric stability class is D, and windspeed is 4 m/s.

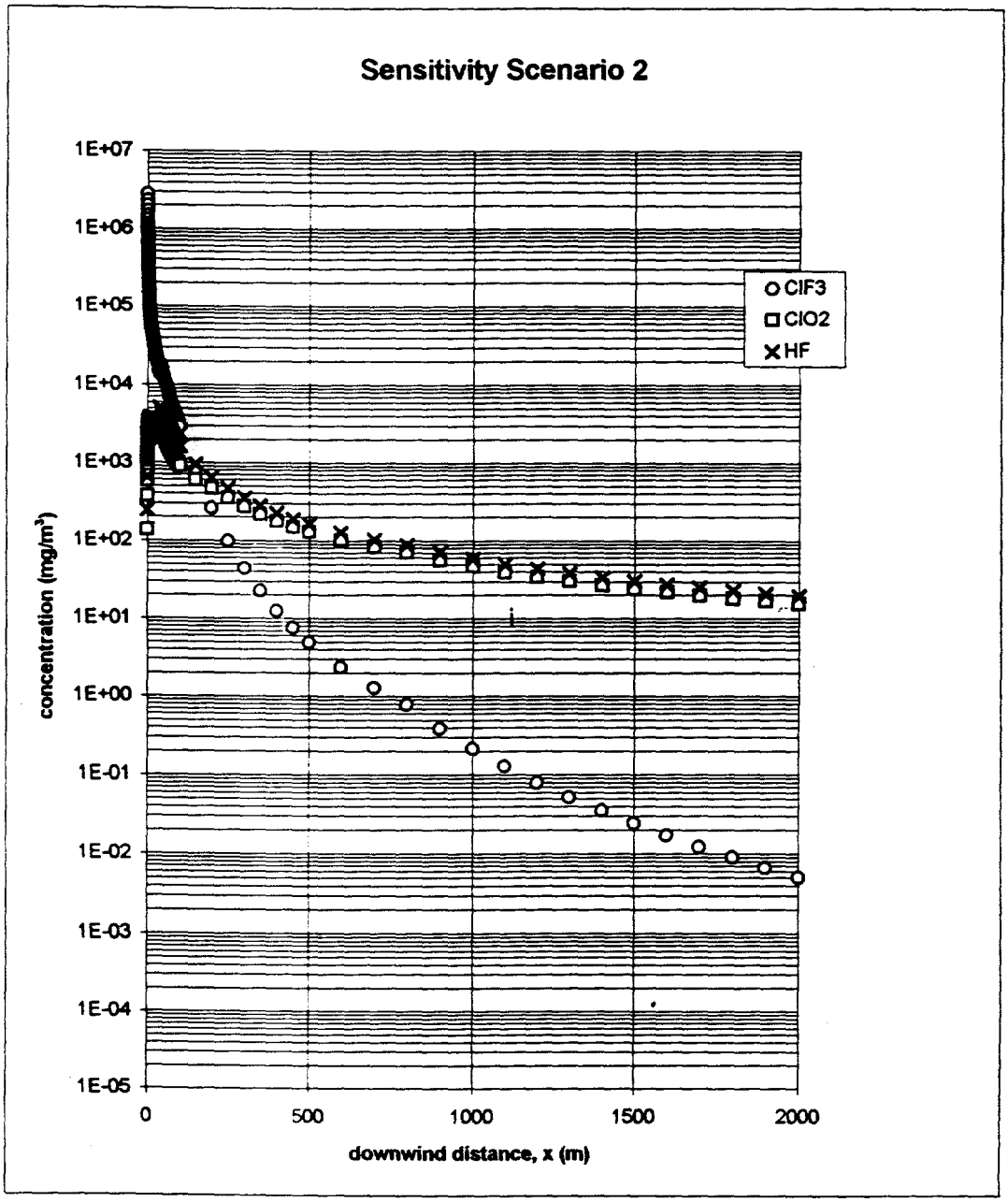

Figure 4. Results of sensitivity scenario 2. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and temperature are 10% and 25°C, respectively, atmospheric stability class is D, and windspeed is 4 m/s.

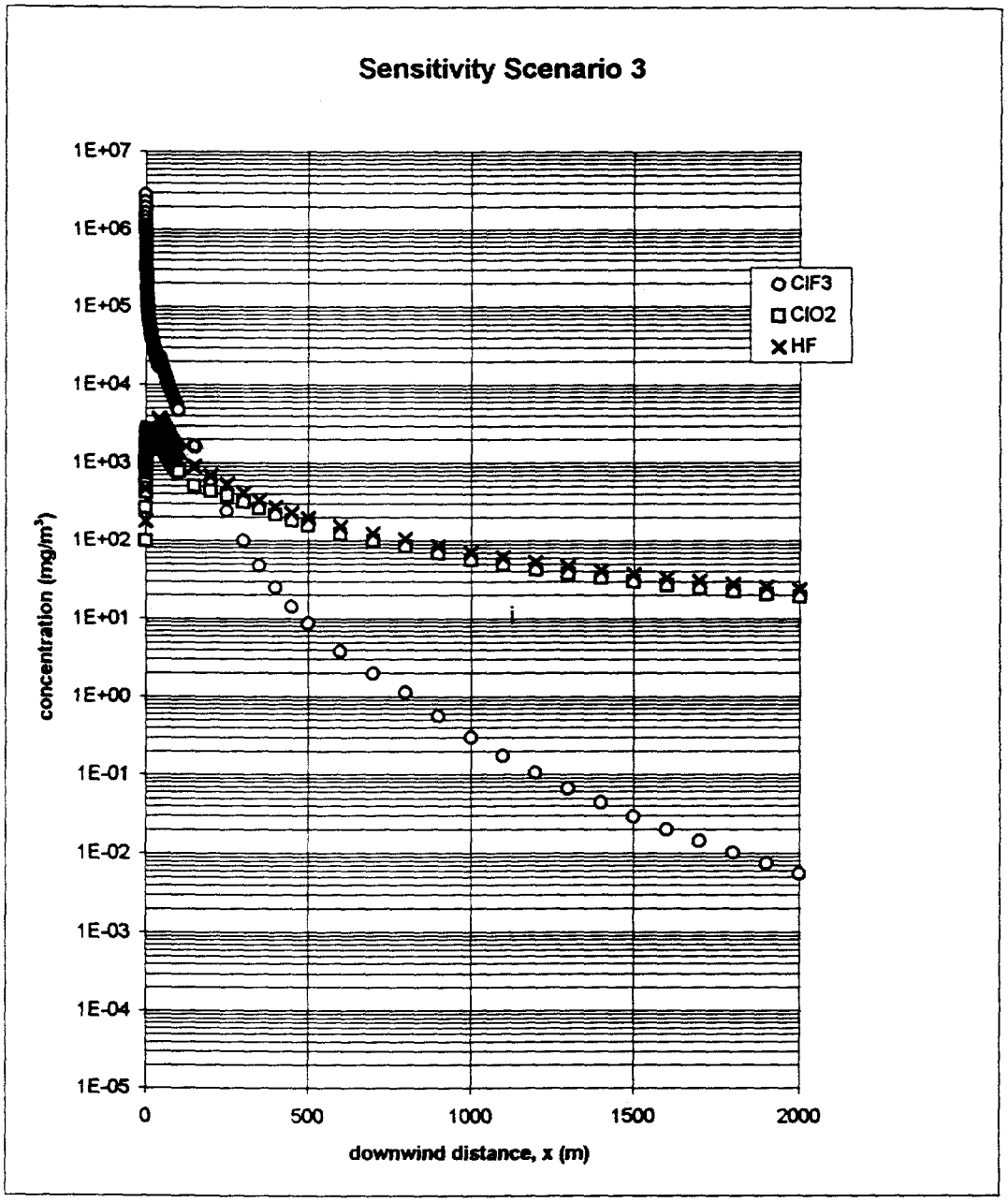

Figure 5. Results of sensitivity scenario 3. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and temperature are 70% and −10°C, respectively, atmospheric stability class is D, and windspeed is 4 m/s.

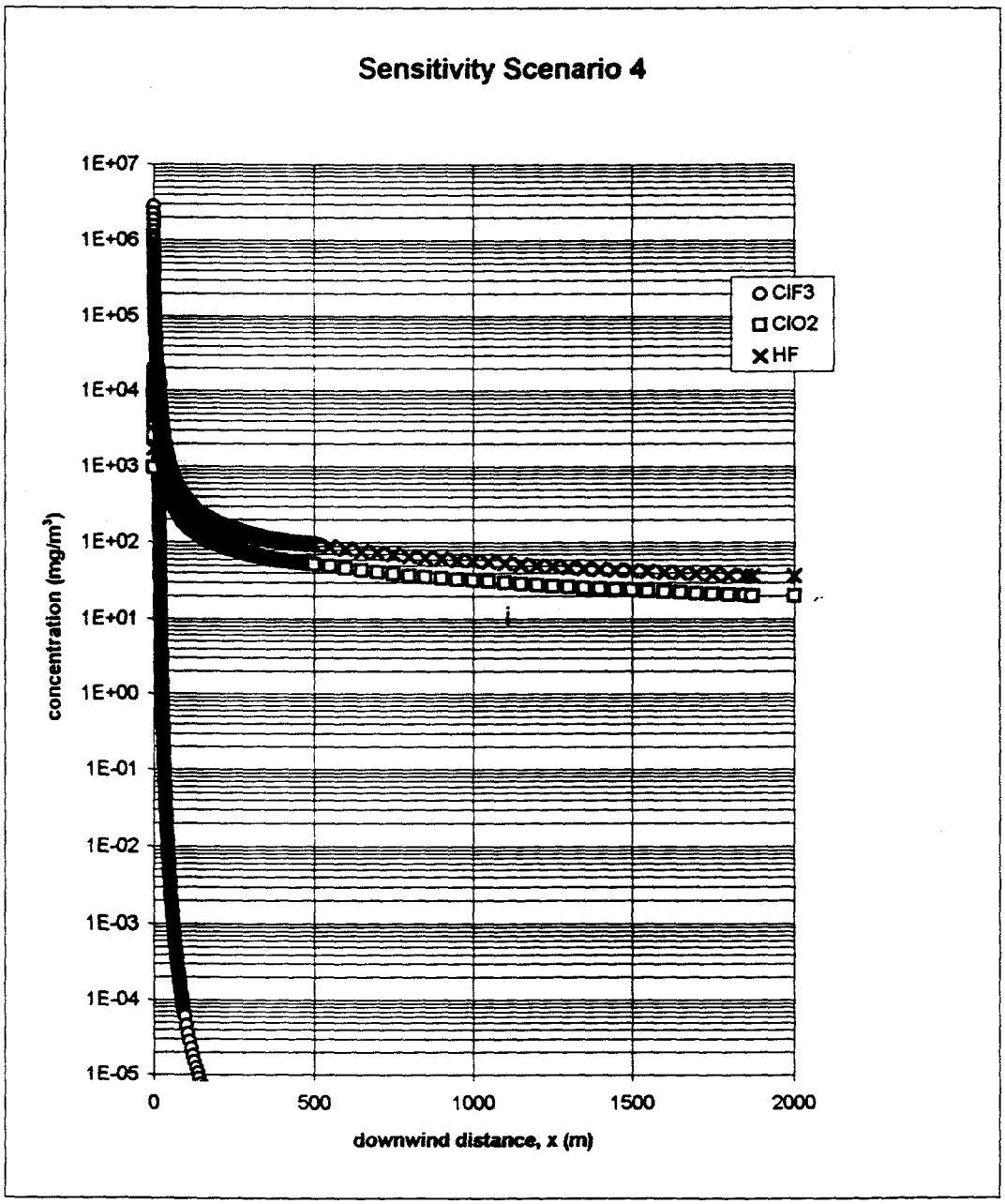

Figure 6. Results of sensitivity scenario 4. Release angle is 0° (parallel to ground in the direction of the wind), ambient relative humidity and temperature are 70% and 25°C, respectively, atmospheric stability class is F, and windspeed is 2 m/s.