

For Presentation at the Air & Waste Management Association's 90th Annual Meeting & Exhibition, June 8-13, 1997, Toronto, Ontario, Canada

JUN 17 1997

OSTI

97-MP8.04

## Releases of $UF_6$ to the Atmosphere After a Potential Fire in a Cylinder Storage Yard

**Douglas A. Lombardi**

Oak Ridge National Laboratory, P. O. Box 2008, MS-6200, Bldg. 4500N, Oak Ridge, TN 37831-6200

**W. Reid Williams**

**James C. Anderson**

**Robert A. Just**

**Sanford A. Bloom**

Lockheed Martin Energy Systems, P. O. Box 2008, MS-6332, Bldg. 1000, Oak Ridge, TN 37831-6332

*The submitted manuscript has been authored by a contractor of the U.S. Government under contract no. DE-AC05-96OR22464. Accordingly, the U.S. Government retains a non-exclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.*

### Introduction

Uranium hexafluoride ( $UF_6$ ), a toxic material, is stored in just over 6200 cylinders at the K-25 site in Oak Ridge, Tennessee. The safety analysis report (SAR)<sup>1</sup> for cylinder yard storage operations at the plant required the development of accident scenarios for the potential release of  $UF_6$  to the atmosphere. In accordance with DOE standards and guidance<sup>2</sup>, the general approach taken in this SAR was to examine the functions and contents of the cylinder storage yards to determine whether safety-significant hazards were present for workers in the immediate vicinity, workers on-site, the general public off-site, or the environment, and to evaluate the significance of any hazards that were found. A detailed accident analysis was performed to determine a set of limiting accidents that have potential for off-site consequences. One of the limiting accidents identified in the SAR was the rupture of a cylinder engulfed in a fire.

The fire accident scenario assumes that a vehicle accident near a storage cylinder results in a spill of gasoline or diesel fuel. The fuel would flow under the storage cylinder and ignite a fire of sufficient duration and temperature to cause a rupture, releasing liquid and vapor  $UF_6$ . The fire is assumed to occur for a period of time after the rupture during which  $UF_6$  would sublime to vapor form. After the fire is extinguished,  $UF_6$  would continue to sublime to vapor until the cylinder cools below 56.5°C. Vehicles likely to be involved in a cylinder accident would be traveling in the storage yard or on roads adjacent to

## **DISCLAIMER**

**This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.**

**DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

the storage yard. Also, vehicles transporting cylinders between storage yards may be involved in an accident. The remainder is divided into four topical areas: (1) reactions and dispersion of UF<sub>6</sub> in the atmosphere, (2) chemical toxicity of UF<sub>6</sub> hydrolysis reaction products, (3) development of the atmospheric source term, and (4) results of the downwind consequence assessment.

## Reactions and Dispersion of UF<sub>6</sub> in the Atmosphere

As shown in Figure 1, UF<sub>6</sub> exists only as a solid at normal atmospheric temperatures and pressures. However, if a cylinder were involved in a fire, the solid UF<sub>6</sub> would sublime to vapor at temperatures above 56.5°C. In turn, the UF<sub>6</sub> vapor would pressurize the cylinder forming liquid UF<sub>6</sub> at pressures greater than 0.150 MPa and temperatures greater than 64.1°C. If exposed directly to atmospheric temperatures and pressures (e.g., during a fire-induced breach of a storage cylinder), liquid UF<sub>6</sub> would flash (i.e., immediately partition) to a mixture of vapor and solid particles. The solid UF<sub>6</sub> will sublime to the vapor form within a few minutes after release. As shown in Equation 1, the UF<sub>6</sub> vapor, which is about 12 times as dense as ambient air, would react exothermically with atmospheric water vapor entrained by the plume, forming hydrogen fluoride (HF) vapor and solid uranyl fluoride (UO<sub>2</sub>F<sub>2</sub>).

**Equation 1.** UF<sub>6</sub> hydrolysis reaction.



The UF<sub>6</sub> hydrolysis reaction (Equation 1) releases approximately 58 kJ per g mole of H<sub>2</sub>O, which heats the plume. At the same time, the sublimation of solid UF<sub>6</sub> to the vapor phase cools the plume. At normal atmospheric pressures, HF vapor is assumed to polymerize and depolymerize as an equilibrium mixture of the monomer (HF)<sub>1</sub>, hexamer (HF)<sub>6</sub>, octamer (HF)<sub>8</sub>, and the HE·H<sub>2</sub>O compound (hydrofluoric acid) as described in Schotte<sup>3</sup>.

The UF<sub>6</sub> plume may alternate between negative, neutral, and positive buoyancy caused by varying plume density. Figure 2 shows the special complications in simulating plume behavior caused by the varying plume density. This diagram schematically represents a moderate velocity, vertical release of UF<sub>6</sub> to the atmosphere. Although the plume is initially much denser than the ambient air, the momentum of the vertical release initially causes the plume to rise as it moves downwind, as shown in region 1 of the figure. As the vertical momentum decreases, the plume may sink as shown in region 2 of the figure, because the plume can be much denser than the surrounding air. If it contacts 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, UF<sub>6</sub> reactions with water vapor occur and release more heat than is removed by sublimation of solid UF<sub>6</sub>. The net heat added, combined with the entrainment of relatively light air, can 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 becomes neutrally buoyant because concentrations of uranium and HF are small, the bulk density of the plume is approximately equal to that of the surrounding air, reactions are essentially complete, and the temperature is close to ambient. The Gaussian plume methodology for passive, non-buoyant plumes is appropriate to model plume behavior in region 5.

The schematic plume trajectory shown in Figure 2 is only one of many patterns that can result from various potential combinations of physical factors and chemical states, all of which vary with time. For example, the release rate and release mode (e.g., from a rapidly swinging feed line or a stationary

cylinder) may favor rapid entrainment of ambient air, causing the plume to become neutrally buoyant (region 5) very quickly. Alternatively, the  $UF_6$  mixture may be released downward causing a strong interaction with the ground and a direct transition into region 3. For a pure  $UF_6$  gas release, the plume density may decrease by up to a factor of 12 (the ratio, approximately 350/29, between the molecular weights of  $UF_6$  and dry air) between the release point and a downwind distance of only a few hundred meters.

## **Chemical Toxicity of $UF_6$ Hydrolysis Reaction Products**

The hydrolysis reaction forming  $UO_2F_2$  and HF (Equation 1) occurs relatively quickly. Consequently, the health effects of  $UF_6$  releases are based on the uranium (bound in the  $UO_2F_2$ ) and HF formed in the reaction. Toxicological evaluation guidelines (EGs) for assessing human health effects of air contamination were developed for the SAR to estimate downwind consequences of potential accidental  $UF_6$  releases. For the fire release scenario, the following toxicological EGs were used<sup>1</sup>:

- uranium chemical toxicity: 30 mg uranium inhalation intake/event, and
- HF toxicity concentration: 16.4 mg/m<sup>3</sup> (1-hr average concentration).

The uranium chemical toxicity EG (30 mg intake) corresponds to a level of 3  $\mu$ g uranium per gram of kidney tissue following an acute intake of soluble uranium by inhalation, assuming the metabolism of an average person. The HF toxicity concentration corresponds to the Emergency Response Planning Guideline Level 2 (ERPG-2) established by the American Industrial Hygiene Association as the highest average concentration to which individuals could be exposed for up to one hour without experiencing or developing irreversible health effects<sup>1</sup>.

## **Development of the Atmospheric Source Term**

The first step in estimating consequences for comparison to EGs is the development of an atmospheric source term for the fire release scenario. For this analysis, the fire duration (30 minutes) and temperature (800°C) selected were based on Nuclear Regulatory Commission (NRC) regulations regarding hypothetical transportation accidents (10 CFR 71.73). In these regulations, NRC considered the potential range of thermal environments and package contents for evaluating and licensing containers of radiological materials. In addition to duration and temperature, the following fire and heat transfer properties were used in the analysis based on guidance from 10 CFR 71.73:

- the  $UF_6$  storage cylinder is fully engulfed in the fire,
- the fire emissivity is 0.9,
- the cylinder surface absorptivity is 0.8, and
- the heat transfer to the cylinder is convective.

A lumped parameter heat transfer/stress analysis model (6FIRE)<sup>5</sup> was used to estimate the time of rupture of the  $UF_6$  cylinders engulfed in the 30-minute, 800°C fire. The model also provides information on the amount of each phase (i.e., liquid and vapor) released at the time of rupture. The 6FIRE model permits evaluation of transient effects such as changing cylinder wall temperatures,  $UF_6$  phase

temperatures, and internal pressure. Cylinder rupture is assumed to occur when the internal pressure results in a hoop stress exceeding the ultimate stress of the cylinder wall material. The post-rupture release of  $UF_6$  (i.e., the  $UF_6$  sublimed during the remainder of the fire and post-fire cool-down) was evaluated using the SUBLIME model<sup>6</sup>.

Many types of cylinders are used in the storage yards. Steel thin-walled, 1.2 m diameter (48 in.) cylinders (designated as 48G) containing up to 12,700 kg of  $UF_6$  were used in this analysis. These cylinders comprise the majority (about 68%) of storage yards cylinders that would be at risk to a fire. Also, 48G cylinders contain the most  $UF_6$ , and therefore, would provide an upper-bound estimate of source material released to the atmosphere. Table 1 lists the results of the 6FIRE and SUBLIME simulations for a 30-minute, 800°C fire engulfing a 48G storage cylinder.

There are many uncertainties in the results shown in Table 1, including: (1) fire properties (e.g., fire duration and temperature), (2) cylinder conditions (e.g., mechanical defects or corrosion), (3) portion of cylinder immersed in the fire, (4) fire fighting activity effects, (5) internal conditions of  $UF_6$  inside the cylinder, and (6) amount of  $UF_6$  inside the cylinder. Due to the considerable uncertainty in the source term estimates, three initial release amounts of  $UF_6$  (i.e., amounts of  $UF_6$  released at the time of rupture) were considered in the dispersion calculation to provide a range of consequence estimates. The three initial release amounts were 181 kg, 1814 kg, and 3629 kg.

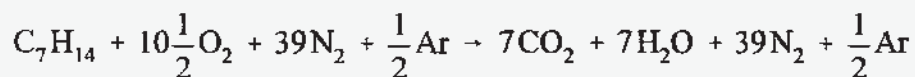
At the time of failure, liquid and vapor  $UF_6$  in the heated cylinder would be released to the atmosphere. The proportions of each phase calculated for the 48G cylinder using 6FIRE (Table 1) were applied to the different release amounts. For this specific case, a total of 1740 kg of  $UF_6$  would be released with 92% (1600 kg) as liquid and 8% (142 kg) as vapor. At the time of rupture, the liquid  $UF_6$  would be at a temperature of 127°C and the vapor  $UF_6$  would be at a temperature of 356°C. The liquid  $UF_6$  is assumed to isentropically flash to vapor and solid when released to the atmosphere, with a flashing temperature of 56.5°C.

The amount of solid and vapor  $UF_6$  created during flashing were calculated by the MIX code, developed by S. G. Bloom, Lockheed Martin Energy Systems, Oak Ridge, Tennessee, based on the subroutines developed by Williams<sup>7</sup>. The code simulates the mixing of up to four streams into a constant volume or constant pressure compartment, and is able to simulate chemical and thermodynamic properties associated with flashing of liquid  $UF_6$ , sublimation of solid  $UF_6$ , and reactions of  $UF_6$  vapor with water vapor.

The initial release amounts were assumed to mix with 10 m<sup>3</sup> of air for every m<sup>3</sup> of  $UF_6$  released (0.823 kg of air for every kg of  $UF_6$  released). The mixing air was divided into two different streams. The first mixing air stream was the combustion stream assumed to be at the temperature of the fire (800°C). The volume of this stream was calculated assuming an upward fire velocity of 5 m/s (based on Zamejc and Chao<sup>8</sup>) and an assumed fire diameter of 5 m. Using these values, the fire flux would be about 100 m<sup>3</sup>/s. For the 181 kg case, the released  $UF_6$  was assumed to reside over the fire for about 3 s, resulting in about 300 m<sup>3</sup> of combustion air entrained into the initial volume. For the 1814 kg and 3629 kg release cases, the residence time was assumed to be slightly longer at 5 s, resulting in about 500 m<sup>3</sup> of combustion air entrained into the initial volume.

The fuel in the fire was assumed to be gasoline ( $C_7H_{14}$ ). Equation 2 shows the reaction of gasoline with dry air in the fire, assuming complete combustion.

**Equation 2.** The complete combustion reaction of gasoline with dry air.



The combustion stream mixing with the released  $UF_6$  is assumed to be defined by the right-hand side of Equation 2. Therefore, the molecular weight of the combustion stream would be about 28.9 kg/kgmol. At 800°C, the density of the combustion stream would be 0.328 kg/m<sup>3</sup>, with the resulting mass of combustion air equal to 98.3 kg for the 181-kg release case and 164 kg for the 1814-kg and 3629-kg release cases. For the 181-kg release case, 8.01 kg of water vapor would be in the combustion stream and for the 1814-kg and 3629-kg release cases, 13.4 kg of water vapor would be in the combustion stream.

The second mixing air stream was the ambient stream and was calculated as the additional air required to assure a 10 to 1 initial mixing (volume basis). The ambient air stream was assumed to be at 26.7°C and 60% relative humidity (typical summertime conditions at the K-25 site).

The MIX code was used to calculate the final composition, volume, and temperature of the plume after initial mixing and before dispersion. The four streams (liquid  $UF_6$ , vapor  $UF_6$ , combustion air, and ambient air) at the conditions specified above were input into the code for each of the three release cases (see Table 2). The composition of the mixed volume (i.e., the initial state of the plume before dispersing downwind) calculated by the MIX code for each case is shown in Table 3.

The initial temperature and volume of the plume after mixing calculated by the MIX code for each release amount is shown in Table 4. The initial shape of the plume is assumed to be a hemisphere. The center of the release is assumed to occur at the centroid of the hemisphere at height,  $h$  (m), above the ground calculated using Equation 3. Assumed release heights for each release case are shown in Table 4.

**Equation 3.** Centroid height of a hemisphere.

$$h = \frac{4r}{3\pi}$$

where:

$r$  is the radius of the hemisphere

The material is assumed to be released from the initial volume as a slow horizontal jet directed downwind of the release. This is a conservative assumption (i.e., results in relatively high consequence estimates) because a vertical jet release would result in more upward momentum of the plume and

slightly lower downwind consequence estimates. Also, a relatively fast jet would result in increased entrainment, higher initial plume dilution, and lower downwind consequences. For each release case, the diameter of the jet was chosen so that the jet velocity would be slightly greater than the ambient wind speed. Keeping the jet speed close to ambient wind speed decreases entrainment of ambient air into the plume, resulting in higher consequence estimates. Another criterion for selecting release diameter was to ensure that the plume angle did not exceed  $-45^\circ$  (with respect to a horizontal surface) before impacting the ground. A sharper jet angle would have necessitated the use of a different model. For most of the scenarios, the diameter had to be decreased (i.e., the release jet velocity was increased) so the plume did not strike the ground at a sharp angle. Because two ambient wind speeds (1 m/s and 4 m/s) were simulated for each release case, two jet diameters were selected for each release case [selection of meteorological parameters (e.g., wind speed and stability class) is discussed in the following section]. Jet diameters for each release case are shown in Table 4.

The release was assumed to occur over 2 minutes (120 s) because the breach resulting from a hydraulic failure of the cylinder would be large allowing much of the mass to escape quickly. Release durations less than 2 minutes would result in only slightly higher consequence estimates near the source (i.e., within a few hundred meters) and virtually no difference in consequence estimates at downwind distances greater than a few hundred meters. Releases lasting more than 2 minutes would result in less injection of pollutant to the air per unit time, which would lead to reduced concentrations and reduced consequences. The total mass flux of the plume from the initial volume is calculated as the total mass of the initial volume ( $\text{UF}_6$  vapor + dry air +  $\text{UO}_2\text{F}_2$  + HF) divided by the release duration (2 minutes). For each release case, the total mass of the plume, calculated using the MIX code, and the mass flux flowing out of the initial volume are shown in Table 4. All of the source parameters listed in Table 4 were used as input for dispersion model simulations.

## Results of the Downwind Consequence Estimate

The AEROPLUME/RK model, part of HGSYSTEM/ $\text{UF}_6$ <sup>9,10</sup>, was used to estimate downwind uranium and HF concentrations. AEROPLUME/RK estimates near-field (i.e., downwind distances ranging from tens to hundreds of meters) dispersion of elevated, two-phase (aerosol and vapor) pressure-driven momentum jets of  $\text{UF}_6$  and its reaction products ( $\text{UO}_2\text{F}_2$  and HF). This model applies to releases from pressurized tanks or cylinders from the point of release until they either (1) strongly interact with the ground and become a dense ground-hovering plume; or (2) become passive (i.e., chemical reactions cease and the density approaches ambient air density). The letters RK signify that a robust Runge-Kutta differential equation solver has been included, which enables the user to model situations where the plume angle changes rapidly with time, such as  $\text{UF}_6$  releases with steep jet angles (between  $-10^\circ$  and  $-45^\circ$  from the horizontal) pointing downward toward the ground. The Runge-Kutta numerical solver replaces the SPRINT solver employed in HGSYSTEM Version 3.0, which could not consistently simulate  $\text{UF}_6$  releases with steep jet angles<sup>9</sup>. AEROPLUME/RK employs sophisticated  $\text{UF}_6$  chemistry and thermodynamics modules necessary to simulate  $\text{UF}_6$  plume dispersion (as described earlier in this paper).

For some of the release cases, the plume would be dense and ground-hovering very close to the release. However, for all release cases, plume buoyancy increases substantially within about 60 m downwind of the release due to (1) dilution by entrainment of ambient air and (2) generation of heat by the  $\text{UF}_6$  hydrolysis reaction. The plume centerline would tend to rise with increasing buoyancy, with the final

effective plume centerline height being several meters above the ground at farther downwind distances. The height of final plume rise is determined by several factors including the magnitude of the fire and the meteorological conditions. Higher wind speeds would tend to push the plume in the horizontal direction, limiting the final plume height. A less stable, more turbulent atmosphere would spread the plume down to ground-level nearer the source. To demonstrate these effects, two common meteorological conditions were examined for each release case: (1) a stable atmosphere (stability class F) with light wind speed (1 m/s), designated F1; and (2) a neutral atmosphere (stability class D) with moderate wind speed (4 m/s), designated D4. A total of six AEROPULME/RK simulations were made for the fire event release (i.e., two meteorological conditions for each of the three release amounts).

Because the releases were assumed to be transient (i.e., 2 minutes), a post-processor (POSTAP) was developed to convert steady-state results from AEROPULME/RK to transient data. The POSTAP code accounts for the finite duration of the release and the spreading of the plume in the direction of the wind. POSTAP was developed from the POSTHEG code, an enhancement to HGSYSTEM/UF<sub>6</sub><sup>9</sup>. The development of POSTAP is reported by Lombardi<sup>11</sup>.

As noted in the preceding section, the ambient air temperature and relative humidity were selected to be 26.7°C and 60%, respectively, for all simulations. These values represent typical summertime values at the K-25 site.

Figures 3 and 4 show downwind consequence estimates for uranium and HF, respectively. Uranium intake was calculated using Equation 4.

**Equation 4.** Uranium inhalation intake.

$$U = C_{U-a} \times T_{exp} \times BR$$

where:

- $U$  is the uranium inhalation intake (mg)
- $C_{U-a}$  is the average uranium concentration (mg/m<sup>3</sup>)
- $T_{exp}$  is the time of exposure
- $BR$  is the breathing rate of the exposed individual

For this analysis,  $BR$  was assumed to be 0.000417 m<sup>3</sup>/s (1.5 m<sup>3</sup>/hr), corresponding to light exercise<sup>12</sup>. Average (over the time of exposure) HF concentrations were calculated using assuming stoichiometric proportions with uranium as shown in Equation 5.

**Equation 5.** Average HF concentration.

$$C_{a-HF} = 0.336 \times C_{a-U}$$

where:

$C_{a-HF}$  is the average uranium concentration ( $\text{mg}/\text{m}^3$ )

The value 0.336 is obtained from the  $\text{UF}_6$  hydrolysis reaction (Equation 1) and is the ratio of 4 times the molecular weight of HF (20) to the molecular weight of uranium (238).

Consequence estimates within 300 m of the release show that estimated uranium intake and HF concentrations are greatest for the highest release case (3629 kg). Concentration estimates are greatest under D4 conditions at downwind distances ranging from 100 to 800 m because the plume centerline height is estimated to be lower for the higher-wind speed cases, and because the plume is allowed to spread and contact the ground more rapidly in the vertical direction with a neutral atmosphere than with a stable atmosphere. At greater downwind distances (i.e., greater than about 800 m), the higher plumes in a stable, lower-wind speed atmosphere have begun to spread sufficiently to contact the ground appreciably; whereas, the neutral case plumes have begun to experience substantial dilution due to atmospheric dispersion. Therefore, for the highest release case (3629 kg), consequence estimates under F1 conditions are higher than D4 conditions at downwind distances beyond 800 m.

The 3629 kg release under D4 conditions exceeds the uranium inhalation intake EG (30 mg) to greater downwind distances (about 350 m) than any other case. The shortest distance to the Oak Ridge Reservation site boundary from the  $\text{UF}_6$  cylinder storage yards is about 610 m. Therefore, the uranium intake EG would not be exceeded at the nearest site boundary. The HF exposure EG ( $16.4 \text{ mg}/\text{m}^3$ ) is exceeded at or beyond the nearest site boundary for all cases except the 181-kg and 1814-kg releases under F1 conditions. However plume exposure times were estimated to be 12 minutes or less; thus a direct comparison with the 1-hour average EG value (i.e., the HF ERPG-2) does not reflect actual health effects. As reported in the SAR<sup>1</sup>, an equivalent EG for 12-minute exposure would be about  $35 \text{ mg}/\text{m}^3$ . Only the 181-kg release under D4 conditions would exceed this equivalent EG value at or beyond the site boundary (i.e., concentrations would exceed  $35 \text{ mg}/\text{m}^3$  to a downwind distance of approximately 700 m). Compared to the other release cases, plume height would be lowest at the site boundary for the 181-kg release under D4 conditions. Although the initial temperature of the released volume is relatively high for this case, the small size of the initial volume released (Table 4) implies that the plume achieves neutral buoyancy quickly and plume rise is limited. Under D4 conditions, the plume centerline height for the 181-kg release is only 20 m at the site boundary compared to 65 m for the 1814-kg release with a much larger initial volume.

## References

1. Lockheed Martin Energy Systems, Inc.(LMES); *K-25 Site Cylinder Storage Yards Final Safety Analysis Report*; Oak Ridge K-25 Site: Oak Ridge, Tennessee 1997; K/D-SAR-29.
2. U. S. Department of Energy (DOE); *Preparation Guide for U. S. Department of Energy Nonreactor Nuclear Safety Analysis Reports*; Washington, D.C. 1994; DOE-STD-3009-94.
3. Schotte. W.; "Fog formation of hydrogen fluoride in air," *Ind. Eng. Chem. Res.* **1987**, *26*, 300-306.

4. U. S. Department of Energy (DOE); "Updated SCAPA ERPG Working List," *Attachment I, to the Subcommittee on Consequence Assessment and Protective Actions April 18-19, 1995 Meeting Minutes*; Savannah, Georgia 1995.
5. Williams, W.R.; *Overview of UF<sub>6</sub> Cylinder-Fire Modeling with Specific Discussion of 6FIRE*; Lockheed Martin Energy Systems, Inc., Engineering Analysis: Oak Ridge, Tennessee 1996; DAC-EA-710660-A001.
6. Anderson, J.C.; *SUBLIME: A Model for Evaluating the Sublimation of UF<sub>6</sub> for a Ruptured/Breached Cylinder During and After a Fire*; Lockheed Martin Energy Systems, Inc., Engineering Analysis: Oak Ridge, Tennessee 1996; DAC-EA-710660-A002.
7. Williams, W.R.; *Calculational Methods for Analysis of Postulated UF<sub>6</sub> Releases, Volume 1*; prepared for the U. S. Nuclear Regulatory Commission by the Oak Ridge National Laboratory: Oak Ridge, Tennessee 1985; ORNL/ENG/TM-31/V1, NUREG/CR-4360.
8. Zamejc, E.R.; Chao C.C.; "Consequence Analysis of PCB-containing liquid Pool Fires;" presented at the *AIChE Meeting*: Orlando, Florida March 18-20, 1990.
9. Hanna, S. R.; Chang, J.C.; *HGSYSTEM/UF<sub>6</sub> Model Enhancements for Plume Rise and Dispersion Around Buildings, Lift-off of Buoyant Plumes, and Robustness of Numerical Solver*; prepared by Earth Tech, Corp.: Concord, Massachusetts for the Gaseous Diffusion Plant Safety Analysis Report Upgrade Program: Oak Ridge, Tennessee 1997; K/SUB/93-XJ947/2R1.
10. Hanna, S. R.; Chang, J.C.; Zhang, J.X.; *Technical Documentation of HGSYSTEM/UF<sub>6</sub> Model*; prepared by Earth Tech, Corp.: Concord, Massachusetts for the Gaseous Diffusion Plant Safety Analysis Report Upgrade Program: Oak Ridge, Tennessee 1997; K/SUB/93-XJ947.
11. Lombardi, D.A.; *Dispersion Analysis for the K-25 Site UF<sub>6</sub> Cylinder Storage Yards Safety Analysis Report*; Oak Ridge National Laboratory: Oak Ridge, Tennessee 1996; DAC-19045-CCA-84.
12. ICRP (International Commission on Radiological Protection); *Human Respiratory Tract Model for Radiation Protection*; Elsevier Science Ltd.: Oxford, England 1994; ICRP Publication 66.

**Table 1.** Results of 6FIRE and SUBLIME simulations for a type-48G UF<sub>6</sub> storage cylinder<sup>a</sup>.

---

<i>6FIRE Results</i>	
Initial UF <sub>6</sub> mass, kg	12,700
Time at which rupture occurs, min	12.2
Mass of solid at rupture, kg (% of total in cylinder)	10,960 (86.3)
Mass of liquid at rupture, kg (% of total in cylinder)	1598 (12.6)
Mass of vapor at rupture, kg (% of total in cylinder)	142 (1.1)
Cylinder pressure at rupture, MPa	23.41
Liquid temperature at rupture, °C	126.7
Vapor temperature at rupture, °C	355.9
Average shell temperature at rupture, °C	607.2
Initial release, kg	1740
<i>SUBLIME Results</i>	
Time from rupture to end of fire, min	17.8
Vapor sublimated during remainder of fire, kg	1349
Vapor temperature at the end of fire, °C	488.9
Vapor sublimated after fire, kg	540.7
Duration of post-fire release, min	91.4
<i>Combine Results</i>	
Total UF <sub>6</sub> released, kg (% of initial UF <sub>6</sub> in cylinder)	3630 (28.6)

---

<sup>a</sup>The estimates provided show the indicated number of significant figures for information. The precision of this calculation is probably one to two significant figures

**Table 2.** Composition and temperature of the four streams input into the MIX code for the cylinder storage yard fire release scenario.

Release case	Mixing streams			Ambient air
	Liquid UF <sub>6</sub>	Vapor UF <sub>6</sub>	Combustion air	
181 kg	UF <sub>6</sub> mass = 166.6 kg Temp. = 126.7°C Pressure = 23.48 MPa	UF <sub>6</sub> mass = 14.85 kg Temp. = 355.9°C Pressure = 23.48 MPa	Dry air mass = 90.28 kg Water mass = 8.010 kg Temp. = 801.7°C Pressure = 0.101 MPa	Dry air mass = 59.01 kg Water mass = <i>a</i> Temp. = 26.67°C Pressure = 0.101 MPa
1814 kg	UF <sub>6</sub> mass = 1666 kg (3673 lb) Temp. = 126.7°C (260.0°F) Pressure = 23.48 MPa	UF <sub>6</sub> mass = 148.5 kg Temp. = 355.9°C Pressure = 23.48 MPa	Dry air mass = 150.5 kg Water mass = 13.35 kg Temp. = 801.7°C Pressure = 0.101 MPa	Dry air mass = 1342 kg Water mass = <i>a</i> Temp. = 26.67°C Pressure = 0.101 MPa
3629 kg	UF <sub>6</sub> mass = 3332 kg (7345 lb) Temp. = 126.7°C (260.0°F) Pressure = 23.48 MPa	UF <sub>6</sub> mass = 297.0 kg (654.7 lb) Temp. = 355.9°C (672.7°F) Pressure = 23.48 MPa	Dry air mass = 150.5 kg Water mass = 13.35 kg Temp. = 801.7°C Pressure = 0.101 MPa	Dry air mass = 2835 kg Water mass = <i>a</i> Temp. = 26.67°C Pressure = 0.101 MPa

<sup>a</sup>For the ambient air stream, the water vapor mass was calculated by the MIX code assuming 60% relative humidity at 26.67°C.

**Table 3. Initial plume composition for the cylinder storage yard fire release scenario.**

Release case	Dry air, kg (% of total)	HF, kg (% of total)	UF <sub>6</sub> vapor, kg (% of total)	UO <sub>2</sub> F <sub>2</sub> , kg (% of total)
181 kg	149.3 (43.97)	19.50 (5.74)	95.67 (28.18)	75.07 (22.11)
1814 kg	1493 (44.72)	68.58 (2.05)	1513 (45.32)	263.9 (7.91)
3629 kg	2986 (44.80)	111.9 (1.68)	3137 (47.06)	430.5 (6.46)

Table 4. Release conditions input to the AEROPLOUME/RK model for the cylinder yard fire release scenario.

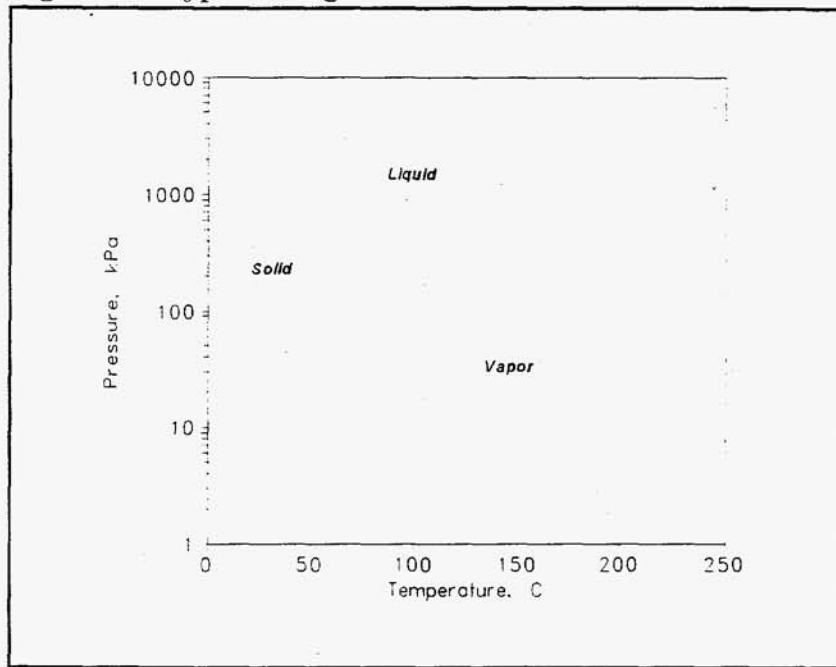
Mass of UF <sub>6</sub> released, kg	Initial plume temperature after mixing, °C <sup>a</sup>	Initial plume volume after mixing, m <sup>3a</sup>	Height of release, m <sup>b</sup>	Diameter of release jet, m (ft)		Mass of the initial volume after mixing, kg <sup>a</sup>	Mass flux out of the initial volume after mixing, kg/s <sup>c</sup>
				u = 1 m/s	u = 4 m/s		
181	464.7	387	2.418	2.0	1.0	339.5	2.829
1814	111.2	1869	4.086	2.0	2.0	3338	27.82
3629	73.2	3341	4.959	2.0	2.0	6664	55.54

<sup>a</sup>Initial plume temperature, volume, and mass after mixing were calculated using the MIX code.

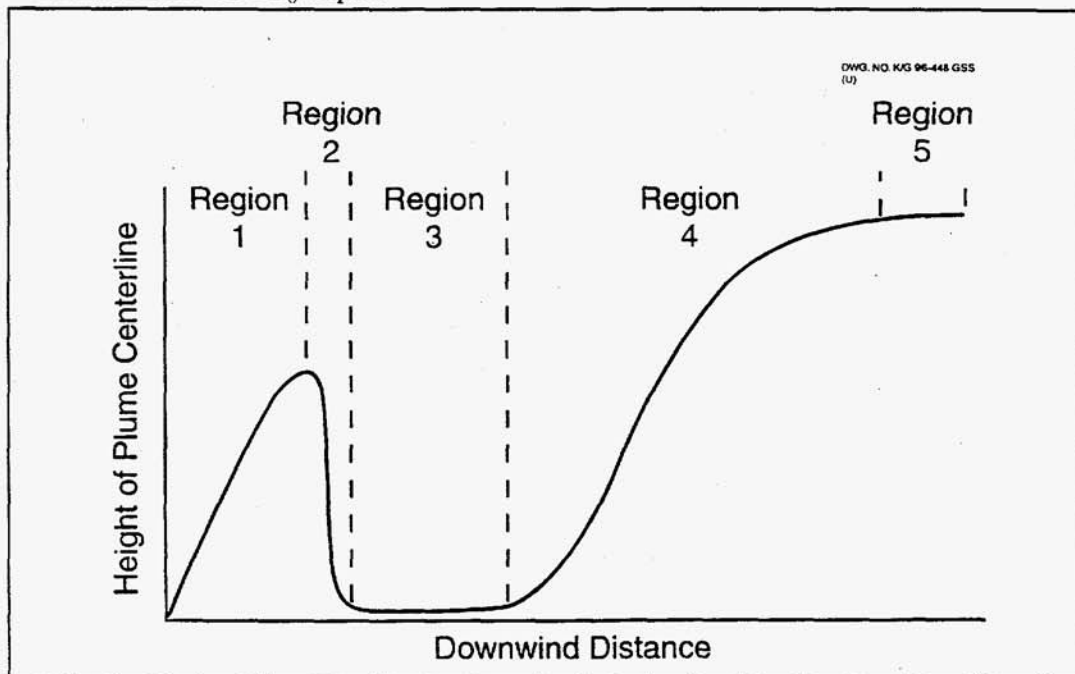
<sup>b</sup>Assuming the initial plume volume is a hemisphere, the release height was selected as the centroid of the hemisphere.

<sup>c</sup>The mass flux was calculated using an assumed release duration of 2 minutes (120 s).

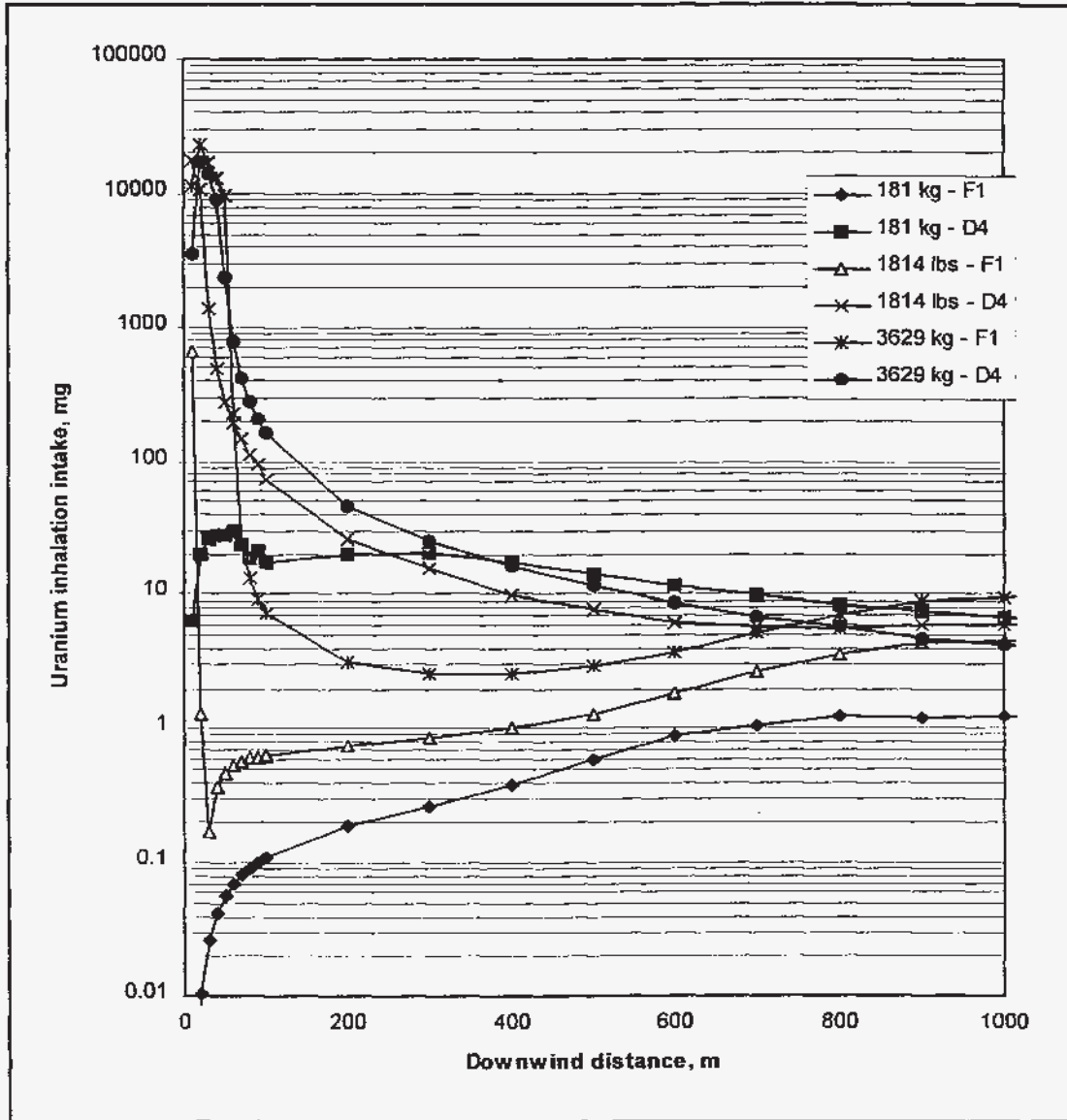
**Figure 1.**  $UF_6$  phase diagram.



**Figure 2.** Example of a possible plume trajectory from a moderate velocity, vertical release of  $UF_6$  vapor.



**Figure 3.** Estimated uranium inhalation intake from the cylinder storage yard fire release scenario.



**Figure 4.** Estimated average (over the time of exposure) hydrogen fluoride (HF) concentrations from the cylinder storage yard fire release scenario.

