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Chemical Emission Scenarios and Detection Limits for Active Infrared Remote Sensing

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Summary

This report presents results from the calculation of chemical emission rates from various military and human activities: diesel electric generator exhaust, diesel exhaust from a missile transport vehicle, evaporation of light organic compounds from stored diesel fuel, evaporation of spilled SCUD missile fuel, burning ammunition, burning sarin, human breath, cook stove exhaust, septic system and landfill emissions. Also presented are the results of Gaussian puff dispersion calculations of the different chemical compounds in each of the plume scenarios. These calculations allow concentration-pathlengths for the compounds to be determined, and, using this information, estimates are made of the infrared absorption cross sections for the compounds. Calculated infrared absorbance spectra of the compounds are also presented along with the absorbance spectra of compounds found in the atmosphere that may interfere with detection of the target compounds. The methodology used in this study is presented in detail in the Introduction.

The results of this study will be used to determine the feasibility of detecting the target compounds using infrared systems. The results suggest that it may be possible to detect compounds in this manner from activities that produce copious amounts of emissions such as the diesel electric generator exhaust, spilled SCUD missile fuel, burning ammunition, and burning sarin. The results of the study are summarized in the Conclusion section.

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1.0 Introduction

This report presents calculated concentration-pathlengths in plumes of gas phase compounds that may be emitted during various military and industrial situations and activities. The concentration-pathlength, which is the product of the distance through a section of the plume and the average concentration in that section of the plume, is used as a "first cut" in determining the feasibility of using infrared laser, active remote sensing to detect and quantify the chemical compound of interest. For example, diesel engines may produce an exhaust plume with a unique chemical signature.

A detailed discussion of the laser and detection system and the transmission of infrared laser light through the atmosphere will be given in a subsequent report. This report will identify and determine an emission rate for the most abundant compounds in a particular emission scenario, calculate and display the plume dimensions and concentrations for each compound, identify "atmospheric windows" where infrared transitions for the compounds of interest could be observed, and calculate the absorptance for the infrared transitions used for detection. A table in the Conclusion section summarizes the results.

1.1 Emission Scenarios

To give the emission scenarios operational verisimilitude and consistency, a hypothetical military facility was devised. Details of the facility are described below, but briefly, it is assumed to be a hard rock tunnel used as a SCUD storage, maintenance, and launch site, and a command and control facility that is guarded by infantry and an artillery battery. The list of emission scenarios is not exhaustive, but may be considered as representative of three categories of operations: operations, battle damage assessment, and human activities. The scenarios are listed below.

- Operations:
  - diesel electric generator exhaust
  - diesel exhaust from a missile transporter, erector, launcher vehicle
  - evaporation from stored diesel fuel
  - evaporation from spilled SCUD missile fuel

- Battle Damage Assessment:
  - burning ammunition
  - burning sarin

- Human Activities:
  - human breath
  - cook stove exhaust
  - septic system emissions
  - landfill emissions

Other emission scenarios were considered but not modeled for this report. These include emissions from grinding and welding in a machine shop, emission from a fuel fire, and human effluents other than breath. Tables for these scenarios are given in Appendixes A, B, and C.

No specific (actual) military facility was modeled for the scenarios in this report. The details of the hypothetical tunnel facility and the emission scenarios were pieced together from a number of sources in the open literature. Missing details were filled in with what the authors felt were reasonable assumptions. It is important to remember that small details will have a profound affect on the detectability of a specific chemical compound or activity. For example, the sulfur content of diesel fuel will determine the sulfur dioxide content in the engine's exhaust. The age and maintenance of the engine will also affect exhaust output by altering the molar ratios of specific compounds. Is the diesel exhaust vented straight from the engine or is it first mixed with tunnel air? What is the temperature of the exhaust, what are the number and sizes of the vents, what is the ventilation rate, etc.? If diesel exhaust is vented at a temperature significantly above ambient, it may be possible to detect the carbon dioxide using infrared spectroscopy: rovibrational transitions of hot carbon dioxide will appear in atmospheric windows. If the carbon dioxide comes out at ambient temperature, it would not be possible to distinguish exhaust CO_2 from background CO_2. In this case, it would be necessary to employ a chemical-based carbon dioxide detector dropped in the vicinity of a suspected vent.

Another important detail to consider is the specificity of detection; that is, how are chemical signatures to be sorted to determine the type and level of activity? How can one distinguish between carbon dioxide given off by diesel generators, diesel trucks, and cook stoves; or between hydrocarbons given off by the evaporation of diesel fuel and solvents. Here again, other types of information will be important in sorting out the field data. Information regarding the background chemical signature for a suspected military site is imperative. Is the site near an urban area? What kinds of industries are nearby? If the site is in a forested area what kinds of trees are present (terpenes from trees will mask or confuse interpretation of hydrocarbon emissions)? These and many more questions will have to be addressed before a complete picture of a specific activity can be determined using infrared sensing.

1.2 Facility Description

Given below is a detailed description of the underground military facility that was used to establish various parameters used in modeling the effluent scenarios.

The tunnel is a ballistic surface-to-surface missile storage, maintenance, and launch facility. It also contains a command and control center and artillery battery. The total complement in the tunnel is one thousand men. There are twenty-five missiles and six launchers stored within the tunnel and sixty motor vehicles. The artillery battery has one hundred tons of stored artillery shells.

The location is in mountainous terrain where the tunnel entrances are at an elevation of ~270 m; the tunnel exits are at ~ 340 m. The highest elevation in the area is 500 m. The tunnels run perpendicular to two roads and a river path. The nearest railroad is 5 to 6 km away over rough terrain and there are no tracks closer to the tunnel.

The mountain ranges have typical elevations of 400 m or more and the soil types are typically weathered granite rock and low in fertility. Flooding occurs regularly near the river area from the heavy rains and mountain run-off.

The climate in the area consists of long, cold winters and hot, humid summers. The humidity is high and heavy rainfall is the norm for the mountainous region. About 60 percent of the precipitation (monsoon season) occurs from June to September. The average precipitation is ~1000 to 1500 mm (39 to 59 in). The average snowfall averages 37 days during the winter, and the temperature averages between -3°C and -13°C. The summer temperatures average between 20 and 29°C, and there are typhoons at least once every summer. Spring and fall are transitional seasons marked by mild temperatures and variable winds. The average wind velocity is 2 to 4 m/s in the mountain areas, except for the summers, when sustained hard winds over 30m/s have been recorded.

The tunnel has two corridors, one is 1230 m in length and the other is 1430 m in length. The distance between the entrances is 215 m. The distance between the exits is 700 m. The corridor size is estimated to be ~ 10 m high and 10 m wide—enough to drive two trucks side by side in some lengths of the tunnel. The chamber heights are 20 m. There is a joint corridor that connects the main corridors near the middle of both corridors. The tunnel area is estimated to be 141,000 m^2 and its volume is approximately 2×10^6 m^3. There are four large main vents and four main adits to the tunnel. The vents are angled and are not vertical. The vents are circular in cross section and are 2 m in diameter. The ventilation rate is 2×10^3 m^3/min/vent. The typical ventilation device consists of several large fans and there are no scrubbers or filters attached.

There are four 30,000-liter water tanks for storing potable water, and two 250 m^3 vented septic tanks. The living, kitchen, and toilet facilities for the main troops are located in four separate areas in the tunnels.

The tunnel typically houses one-thousand men who manage the command and control center, provide maintenance on the vehicles and equipment, keep the missile systems in a battle-ready condition, and provide tunnel defense. There is also housing for additional troop and military support along the roads outside of the tunnel area. There are twenty-three buildings/structures located along the main canyon roads that contain additional storage, electrical power generation facilities, and dwellings. Gasoline is scarce, coal is abundant and an outside electrical power grid is typically used for power. Diesel is used to fuel backup power generators and for powering vehicles.

The four backup diesel generators (500 kW each) supply electrical power for lights, ventilation and other services in the tunnel when the outside power grid is no longer accessible. The command and

control center contains computers and communication devices, as well as some living quarters and a kitchen/dining area that will house twenty-five men. This section contains separate waste and water tanks. This portion of the tunnel is vented into the larger vents and is hardened from the rest of the facility with blast doors and a separate generator.

The twenty-five missiles stored within the tunnel are Russian SCUD-type missiles. The SCUD-C is 10 m long and 2 m in diameter. The missiles are transported on six launchers (Transporter-Erector-Launchers, or TELs) such as the MAZ-543. The TEL is 9.4 m long, 3.1 m wide, and weighs 42,150 kg fully loaded (Lennox 1991). The other vehicles stored consist of munitions-transport trucks, fuel trucks, and troop-movement trucks. The typical travel routes include the river, the railroad, and some roads. A machine shop for maintaining the missiles and vehicles includes typical unalloyed steel and stainless steel milling, turning, grinding, welding, and degreasing operations.

Figure 1 is a topographic representation of the tunnel complex and the surrounding areas.

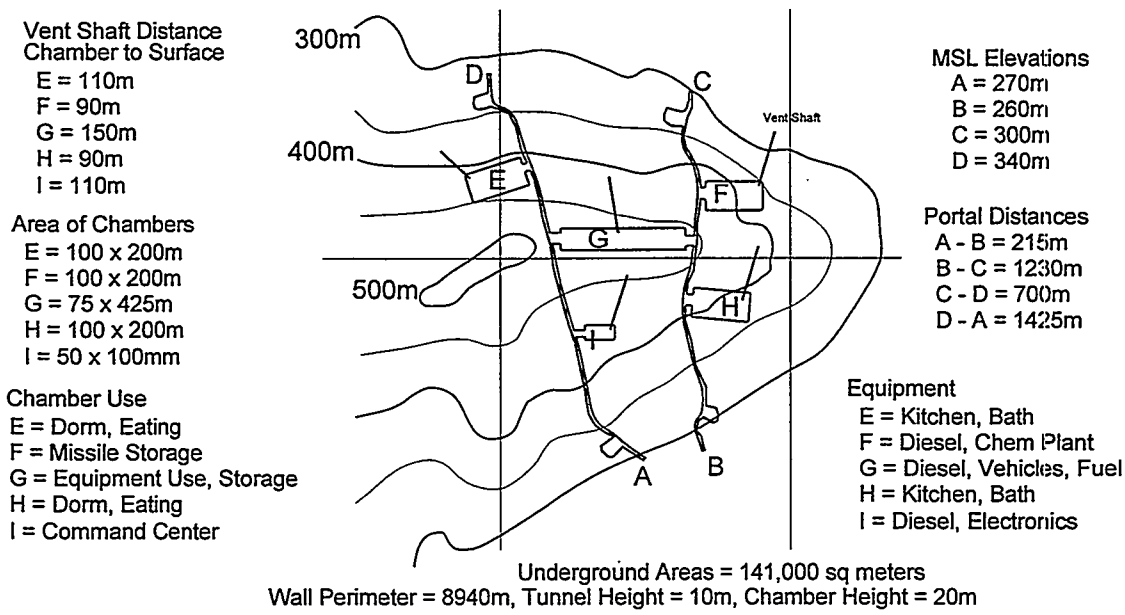

Figure 1. Hypothetical Underground Facility with Surface Topography

1.3 Plume Modeling

Once the physical details of a scenario had been decided upon, the chemicals emitted and their emission rate had to be determined. This was done by searching the open literature looking for similar or relevant information and then scaling the emission rate to match the details of the given scenario. The compounds and their emission rates are given in a table for each scenario. Details as to how the emission rates were determined are given below each table. Though this is given only brief mention here, this was the most time consuming portion of this project. To look for the needed information, standard reference

materials such as encyclopedias, textbooks, and monographs such as *Jane's Defense Series*, were searched. The World Wide Web was also searched. References are given below each table. For specific chemical or physical property data, Chem Abstracts was searched using SciFinder, or the Beilstein and Gmelin databases were searched using Crossfire.

To model the emission plume a commercial software package known as CHARM was used. CHARM, written by Radian Corporation,[a] simulates chemical plumes using a Gaussian puff model and is typically used to determine the level of disaster response to accidental releases of hazardous compounds from factories, rail cars, etc. Details regarding the model are given elsewhere (Radian Corp. 1991; AICE 1996; Zannetti 1990). CHARM takes as input the name of the compound of interest, its emission rate, the size of the puff (that is, the dimension of the vent the compound is coming out of, or the size of the pool it is evaporating from), the release height (for a vent release, this would be the height of vent above the ground), the temperature of the gas in the plume, initial horizontal and vertical puff speed, and air fraction. CHARM has a database of compounds that allows it to look up any needed physical or chemical properties (vapor pressure, molecular weight, etc.). The database is limited to common industrial compounds, but new compounds can be added once the properties for the compound can be found or measured. CHARM also inputs meteorological data such as ambient temperature, relative humidity, and wind speed and direction. Surface roughness and stability class are also input. The surface roughness used in the modeling done here was 10 cm, which corresponds to low-level vegetation. This number is used to calculate the ambient turbulence, and is important in determining at what distance the plume can be expected to be thoroughly mixed with the air. The stability class used throughout is D in the Pasquill-Gifford rating scheme (neutral stability, lapse rate -1.5 to -0.5°C 10^{-2} m^{-1}) and corresponds to a neutral lapse rate. An ambient temperature of 25°C, relative humidity of 50 percent, a constant wind speed of 5 m/sec, and constant wind direction are assumed throughout. For each compound modeled in each scenario, the CHARM input file is included in the report.

CHARM allows for variable wind speed and direction, though, as mentioned above, these have been kept constant. CHARM also allows for a variable release rate, but this too was kept constant in the modeling. Two release types were used for the work done here: a user defined release through a vent or a pool evaporation. For the former, an emission rate is input for the compound coming out of a stack or vent either as a pure compound or mixed with a certain air fraction. For the latter, a certain pool size (diameter or depth) is inputted along with the pool temperature and the surface contacted by the pool (dirt or concrete). CHARM then calculates an evaporation rate for the compound of interest. In both cases the compounds are modeled separately; no multi-component modeling was done. The release duration is the total length of time the compound is being released. This number is used to calculate what are referred to as significant puffs. The significant puffs are spread evenly through time during the release. CHARM then interpolates between the significant puffs to obtain a seamless spatial concentration plot during the release. Finally, the input file requires the concentration values of three isopleths. The isopleths are the concentration contours, typically given in parts per million, laid over a horizontal (x,y), or vertical (y,z) spatial plot. An isopleth concentration value of 100 ppm, for example,

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(a) Radian Corporation, Austin, Texas, (512) 454-4797.

will show a region of the plume where the concentration is 100 ppm or greater. CHARM will calculate and display a three dimensional plume contour, but allows only one isopleth value to be input.

When the CHARM input file is completed and the program executed, the program asks what the snapshot time is. This number gives the time after initial release that the plume is to be examined. Typically a value of one hour was used for most releases, though in the cases of hot pool evaporations (burning ammunition or burning sarin) shorter times (ten minutes) were found to be necessary since many compounds have long since been volatilized and carried away in one hour's time for these scenarios. After CHARM has performed its calculation it displays a horizontal plot of the requested isopleths. The plot shows the isopleths at a given receptor height; that is, the height above the ground (z axis). This height can be changed and the plot redisplayed. A cursor can be run over the plot to determine a concentration at a particular location. At this point it is possible to have CHARM make vertical or three-dimensional plots (concentration cursor is not active for these plots) or generate tables of concentrations along centerlines at selected receptor heights. Unfortunately, CHARM does not have a facility for tabulating concentrations vertically or at some other off-normal surface angle. To determine the concentration pathlengths a distance from the source along the plume centerline was chosen; typically this is taken to be one hundred meters or greater to allow for sufficient turbulent mixing of air with the plume. Since the slant path of the laser light from the remotely piloted vehicle is approximately 45° (*vide infra*) a path through the plume, perpendicular to the plume centerline, was considered to go from the ground up through the plume at a 45° angle. From the vertical cross section of the plume, an estimate was made of the height above the ground at which the plume reached its maximum concentration. The slant path was then drawn through this point down to the ground at a 45° angle and extended upward an equal lateral distance on the other side of the plume. So, for example, if the plume's concentration was a maximum eight meters above the ground, the slant path was drawn down to the ground eight meters to the right of the plume centerline at an angle of 45° and extended upwards to an elevation of eight meters to the left of the plume centerline. Concentrations along this slant path were measured by plotting the horizontal plume contours at a minimum of five equally spaced receptor heights and using the concentration cursor to measure the concentration off the contour. The values were written down and later plotted as concentration (in ppm) vs. distance along the slant path and then numerically integrated to get the concentration pathlength.

As stated above CHARM does not have any utility for easily tabulating concentration pathlengths at different distances and angles with respect to the plume centerline. Calculating the concentration pathlengths is a time consuming and arduous task, so any future use of CHARM for calculating concentration pathlengths should be preceded with a reprogramming of the software to include this utility.

A gross test of the veracity of the CHARM model can be made by using the following formula:

$$C = \frac{Q}{u_{wc} H_{wc} W_{wc}}$$

where C is the concentration (kg/m^3), Q is the source emission rate (kg/s), u_{wc} is the worst case wind speed (assumed to be 1 m/s), H_{wc} is the worst case plume depth (assumed to be 50 m) and W_{wc} is the worst case plume width (assumed to equal $0.1x$, where x is the distance from the source). In the diesel electric generator exhaust scenario, carbon monoxide is assumed to be released at a rate of 3 g/s, so the above equation gives

$$C = \frac{0.003\ \mathrm{kg/s}}{(1\ \mathrm{m/s})(50\ \mathrm{m})(0.1 \times 274\ \mathrm{m})} = 2 \times 10^{-6}\ \mathrm{kg/m^3}$$

or 2000 μg of CO/m^3. CHARM calculates a value of 1140 μg of CO/m^3 at ground level at a distance of 274 meters from the source.

1.4 Spectroscopy

To determine if a target compound in a plume can be monitored remotely using infrared laser spectroscopy, the infrared absorption strength of the compound must be determined and the possibility of spectroscopic interference from the same or other compounds present in the atmosphere must also be considered.

Absorption of infrared radiation by gas phase molecules typically takes place when a vibrational motion (stretch, bend, torsion, etc) within a molecule is excited by electromagnetic radiation of a specific frequency from the ground (lowest energy) vibrational state to an excited (higher energy) vibrational state. Similar to the vibrational energy, the rotational energy is also quantized and a rotational fine structure is imposed upon the vibrational spectrum; that is, when a molecule absorbs an infrared photon the molecule is excited from a specific rotational state in the ground vibrational state to a specific rotational state in the excited vibrational state. The states involved are determined by quantum mechanical selection rules. The attenuation of infrared radiation traveling through a collection of absorbing molecules is given by the Beer-Lambert law (Measures 1988).

$$I(\tilde{\nu}, z) = I_0 \exp[-\kappa(\tilde{\nu}) z_D]$$

where I is the intensity of the light given as a function of light wavenumber $\tilde{\nu}$ (in cm^{-1}) pathlength z, I_0 is the intensity of the light incident upon the sample, κ is the absorption coefficient at light wavenumber $\tilde{\nu}$ and z_D is the concentration pathlength. The absorption coefficient for a particular molecule is dependent upon the transition moment at $\tilde{\nu}$, the molecule's partition functions, etc.

The Beer-Lambert law can be solved for the absorption coefficient as

$$\kappa(\tilde{\nu}) z = \ln(I_0/I) = 2.303 \log_{10}(I_0/I)$$

and absorbance is defined as

$$A = \ln(I_0/I) = 2.303\log_{10}(I_0/I)$$

Absorbances presented in this report are given as base e. Two other useful quantities related to spectroscopic intensities are defined as transmission (usually presented as % transmission)

$$T(\tilde{\nu}) = I(\tilde{\nu})/I_0(\tilde{\nu})$$

and the absorptance, which is given as

$$Ab(\tilde{\nu}) = [I_0(\tilde{\nu}) - I(\tilde{\nu})]/I_0(\tilde{\nu})$$

There are databases available, such as the Air Force's HITRAN Database (Rothman 1996), which can be used to tabulate line strengths and wavenumbers for rovibrational transitions of a molecule in its database over a particular wavenumber range as a function of temperature. The output file, which contains the aforementioned information for hundreds or hundreds of thousands of transitions for the molecule of interest, is used as the input of a program that convolves a linewidth for each transition and uses an input concentration-pathlength to calculate the absorption coefficient. The input linewidth parameters are the full width at half maximum for the air-broadened Lorentzian lineshape and the Doppler-broadened Gaussian lineshape. The input values to the program are summarized in the table in the Conclusion section. The program then plots the infrared spectrum in absorbance units as a function of wavenumber. The program is written for the Igor scientific plotting and analysis application, which is available for both the Mac and PC. The spectral plot data files are available upon request from the authors.

HITRAN's database is limited to only thirty-two molecules; these are small molecules found in the atmosphere or used as laboratory frequency standards, such as water, carbon dioxide, carbon monoxide, etc. Spectra of larger molecules shown in this report, such as benzene, *m*-xylene, acetonitrile, etc. come from the Hanst database (Hanst and Hanst 1993). This database gives experimental spectra of a larger selection of molecules at 20°C and 0.125 cm^{-1} resolution over a spectral range of 4000 to 500 cm^{-1}. Spectra from the Hanst database used in this report are rescaled in log base e absorbance units. The Hanst spectra will be marked "Hanst".

To see what atmospheric absorptions might interfere with the measurement of the spectrum of the target molecule, two programs were used to calculate the absorption spectrum of the atmosphere as a function of temperature, relative humidity, and pathlength. The two programs, MODTRAN (Ontar Corp. 1996) and FASCODE (Hanscom AFB 1996), differ in the algorithm details, but both can be used to calculate the absorption spectrum of the atmosphere. Both load transition information from HITRAN and, for the atmospheric spectra presented here, the "first seven" HITRAN molecules were used: water 1.88×10^4 ppm, carbon dioxide 350 ppm, ozone 0.0302 ppm, nitrous oxide 0.32 ppm, carbon monoxide 0.15 ppm, methane 1.7 ppm, and oxygen 21 percent. These numbers are for midlatitude, summer, 25°C,

transmission spectrum at pathlengths of 6.5, 13, 30, and 60 kilometers. The 6.5 km spectrum is overlaid with the complete spectrum of each target molecule to show regions where it may be possible to see target molecule spectra through atmospheric windows. Atmospheric spectra are typically shown in red and the target molecule spectra are shown in black. A plot of atmospheric transmission spectrum at all four pathlengths is shown below. FASCODE is capable of higher resolution and a 0.1 cm^{-1} resolution absorbance spectrum from 5000 to 500 cm^{-1} was calculated for a pathlength of 6.5 km. This calculation is expensive and so only one pathlength spectrum was calculated. This spectrum was overlaid with small portions (individual vibrational bands or portions of individual vibrational bands) of the absorbance spectrum of the target molecule.

The pathlengths that were chosen are based on the operational parameters of the unpiloted aerovehicles (UAVs) considered for remote sensing platforms. The two remotely piloted vehicles considered for performing active laser remote sensing are the Predator and the Global Hawk. The Predator typically operates at an altitude of 4.5 km with a slant range distance of 6.5 km (slant angle is approximately 44°). Its output optic diameter is 10 cm and the minimum spot size on the ground is 0.8 meter. For the Global Hawk a typical altitude is 20 km with a slant range distance of 30 km (slant angle is approximately 42°). Its output optic diameter is 20 cm and the minimum spot size on the ground is 1.8 meters. The ground laser spot diameter is given by

$$D_{spot} = \frac{4\lambda R}{\pi D_{optic}}$$

where D_{spot} is the laser spot diameter on the ground, λ is the laser wavelength, R is the slant range, and D_{optic} is the diameter of the output optic.

As shown in Figure 2, there are windows in the atmospheric infrared transmission spectrum centered at about 1000 cm^{-1}, 2700 cm^{-1}, and 4600 cm^{-1}. Water and carbon dioxide are the major obscurants in the spectrum. The goal is to find gaps in this spectrum where target molecules absorb strongly enough to be observed. When reading the atmosphere/analyte spectrum plots care should be taken to note the absorbance axes: atmospheric absorbance is on the left and analyte absorbance on the right. The scales for these may not be the same.

A table in Appendix D gives the concentrations of common atmospheric compounds along with their lifetimes, and a table in Appendix E gives Fourier transform infrared spectroscopy detection limits for a select group of compounds.

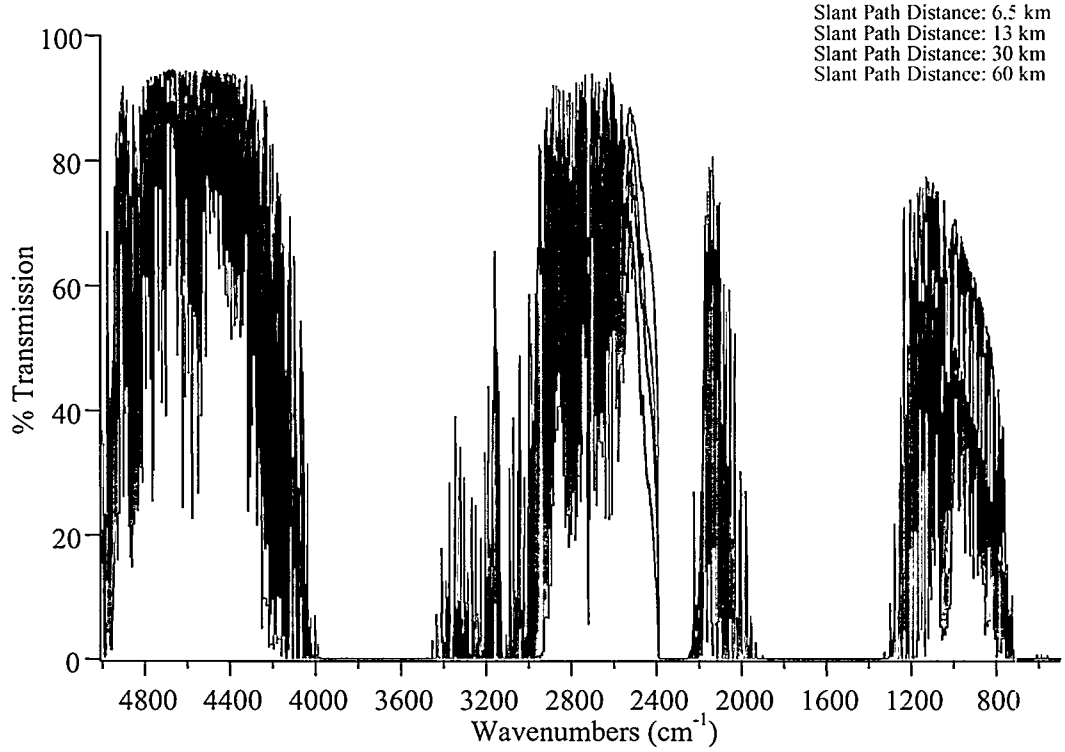


Figure 2. Transmission Through the Atmosphere, 50% Relative Humidity, 1 cm^{-1} Resolution, MODTRAN/HITRAN

1.5 Conclusions

A flow chart is presented in Figure 3 that summarizes the procedure for determining the concentration pathlengths. For each emission scenario there is a table listing the target chemicals and their emission rates. There is also a brief discussion of how the numbers were determined and a listing of any relevant references. The most abundant compounds for each scenario were modeled. For each compound, the CHARM input file is given on one page, followed by a page showing horizontal and vertical cross sections of the plume. A page follows showing a plot of the concentration down the centerline of the plume at a receptor height where the plume is most concentrated and a plot of the integrated concentration pathlength across the plume. Finally, a page showing the plots of the simulated spectra of the compound is given. The absorbance spectra were searched to find the most intense transitions of the target compounds that were not obscured by atmospheric absorptions. The results of the plume and spectral modeling are summarized in a table in the Conclusion section.

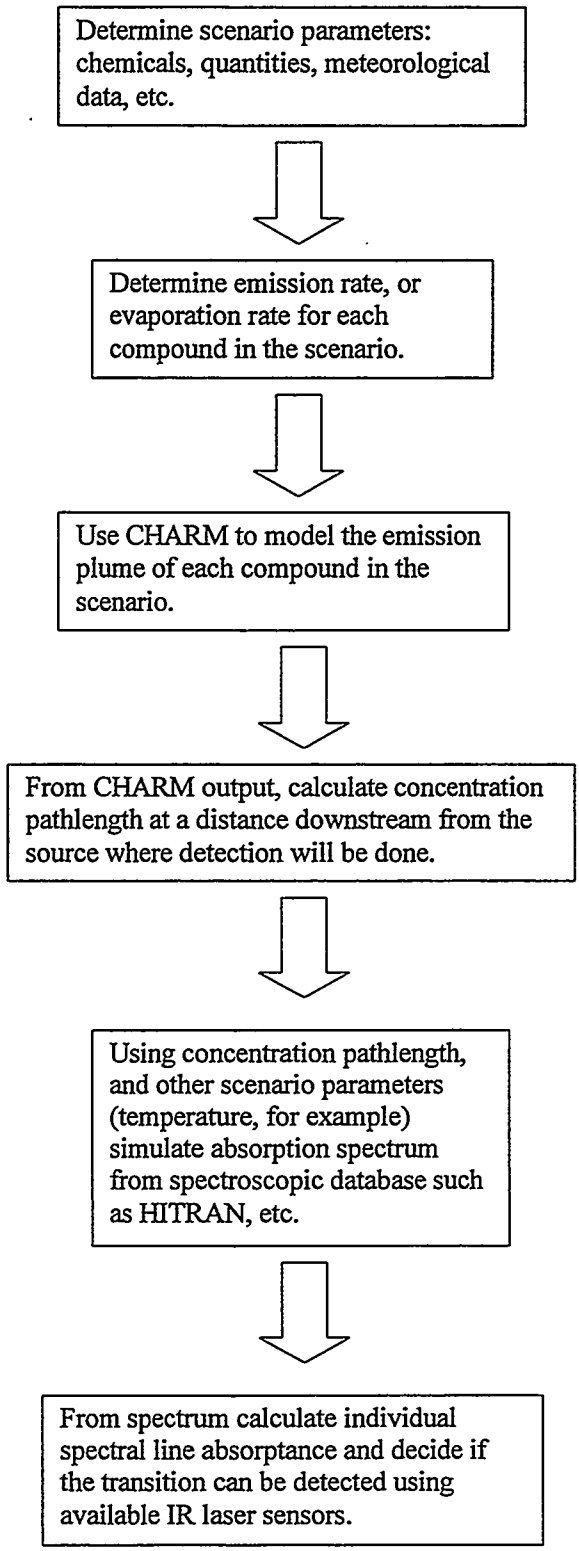


Figure 3. Flowchart for Determining Concentration Pathlengths

2.0 Operations

2.1 Diesel Electric Generator Exhaust

Compound	Normalized Emission Rate[a,b]	Emission rate (g/sec)
Carbon Dioxide	520 g/bhp-hr	600
NO_2	5 g/bhp-hr	6
Carbon Monoxide	2.3 g/bhp-hr	3
Sulfur Dioxide	0.58 g/bhp-hr	0.6
Formaldehyde	57 mg/bhp-hr	6×10^{-2}
Acetaldehyde	18 mg/bhp-hr	2×10^{-2}
Benzene	5.9 mg/bhp-hr	6×10^{-3}
Propionaldehyde	3.7 mg/bhp-hr	6×10^{-3}
Acrolein	2.1 mg/bhp-hr	3×10^{-3}
m-Xylene	2.0 mg/bhp-hr	3×10^{-3}
1,3-Butadiene	1.8 mg/bhp-hr	2×10^{-3}
Carbonyl sulfide	0.46 mg/bhp-hr	6×10^{-4}

(a) "Report to the Air Resources Board on the Proposed Identification of Diesel Exhaust as a Toxic Air Contaminant," Part A, Exposure Assessment, April 22, 1998. Robert K. Krieger, Project Manager, California Environmental Protection Agency, Air Resources Board.

(b) Brake horsepower (bhp) is a unit of power and it is the power delivered to the engine's drive shaft by the engine. Brake horsepower-hour is a unit of work; it is the work done when the engine's drive shaft exerts one horsepower for one hour. *Diesel Fuels Technical Review* (FTR-2), J. Bacha *et al.*, Chevron Products Company (1998).

Scenario: We assume here that four 500 kW diesel electric generators are used to power the underground facility. Each generator requires a diesel motor delivering 1000 bhp.[a] Multiplying 4000 bhp (for the four generators) by the normalized emission rate for the twelve most abundant compounds, excluding water, given in the second column and dividing by 3600 sec/hr gives the emission rate in grams/second in the third column. We also assume here that the exhaust from the diesel engines is vented through a 0.5 m diameter pipe and exits at a temperature of 50°C. Fuel is assumed to have a 0.5 wt% sulfur content.

Fuel consumption is calculated as follows: assuming that all the carbon in the exhaust exits as carbon dioxide, the number of grams of carbon exhausted per second is

$$(600 \text{ g/sec})(0.273) = 164 \text{ grams of carbon/sec}$$

(a) http://www.gov.on.ca/OMAFRA/english/engines/facts/99-005.htm Ontario Ministry of Agriculture Food and Rural Affairs, "Standby Electric Generators for Emergency Use."

where 0.273 is the mass fraction of carbon in CO_2. The mass fraction of carbon in diesel fuel is 0.87, so the mass of diesel fuel used per second is

$$(164 \text{ grams of carbon/sec})/0.87 = 188 \text{ grams of diesel/sec.}$$

The density of diesel fuel is approximately 0.85 g/cm^3, so the volume of diesel fuel consumed is

$$(188 \text{ grams of diesel/sec})/(0.85 \text{ g/cm}^3) = 222 \text{ cm}^3\text{/sec,}$$

or approximately 800 liters of diesel fuel consumed by all four generators per hour.

CHARM Version 9.3

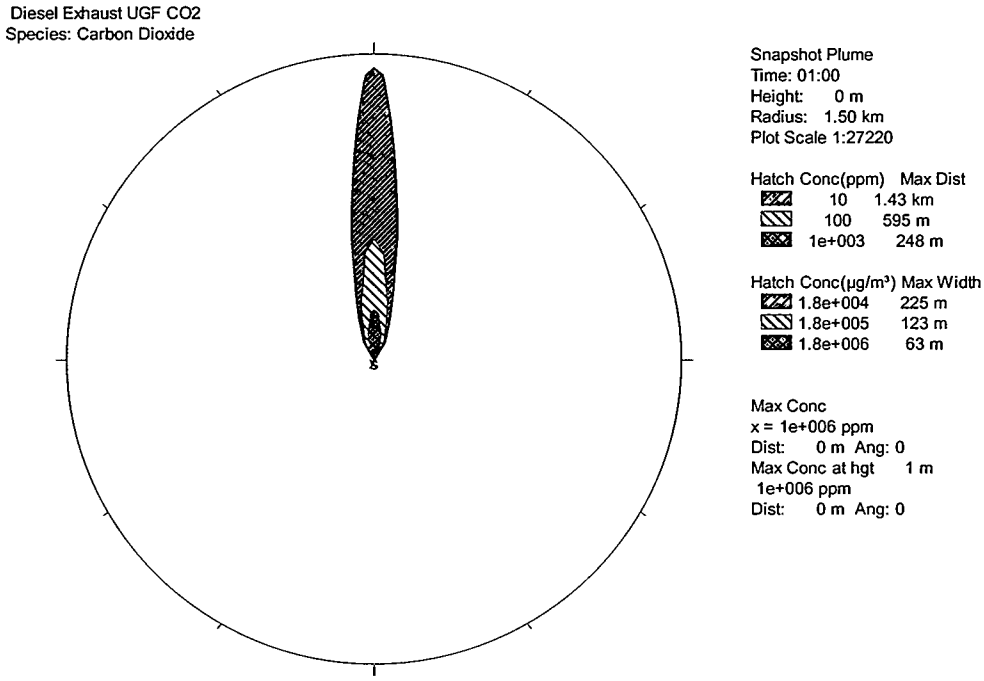
Title:	Generator Diesel Exhaust CO2
Species:	Carbon Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	10, 100, 1000
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	600 g/s
Release Duration:	24 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	1.841 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

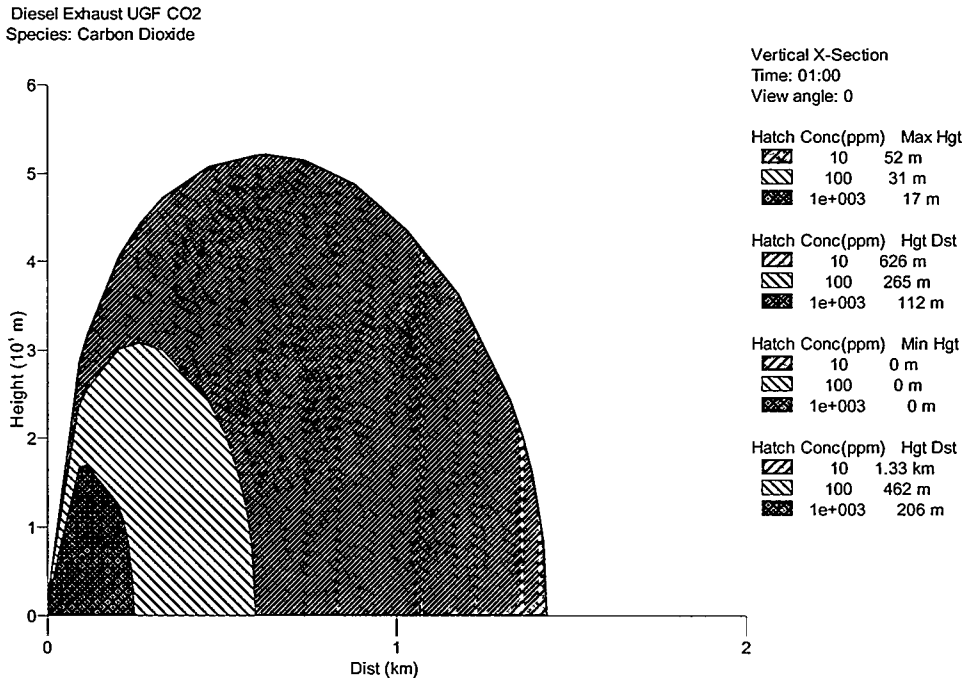
****

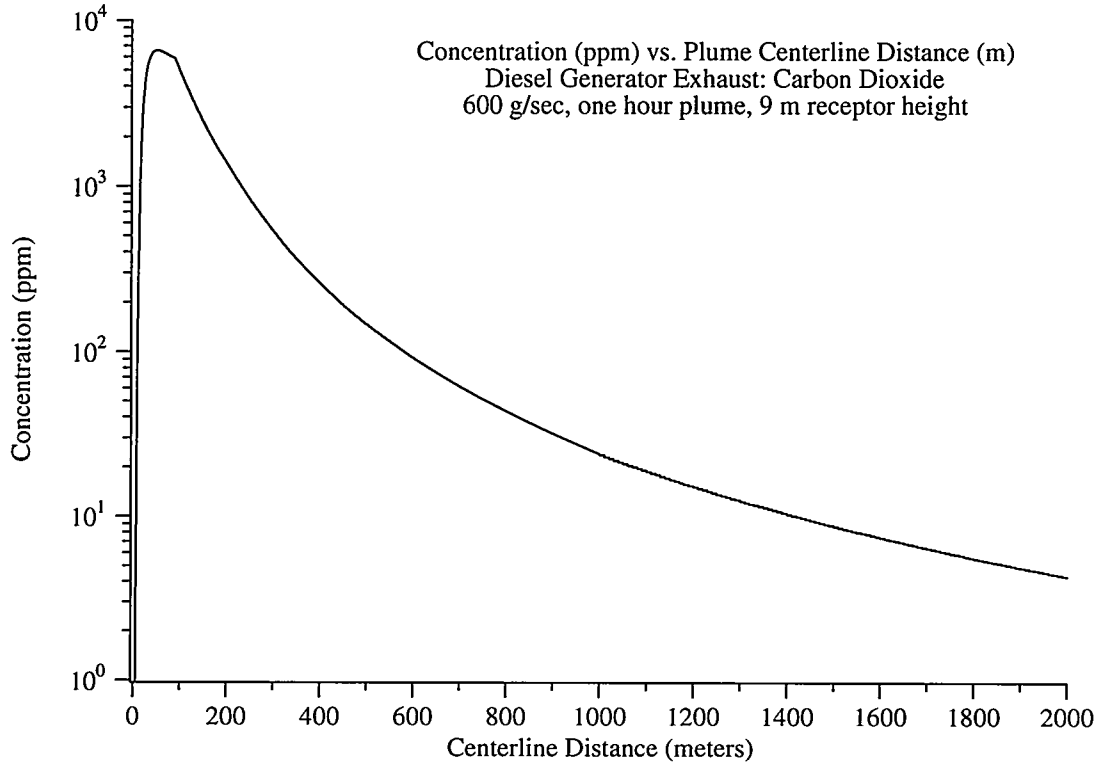
Met Data

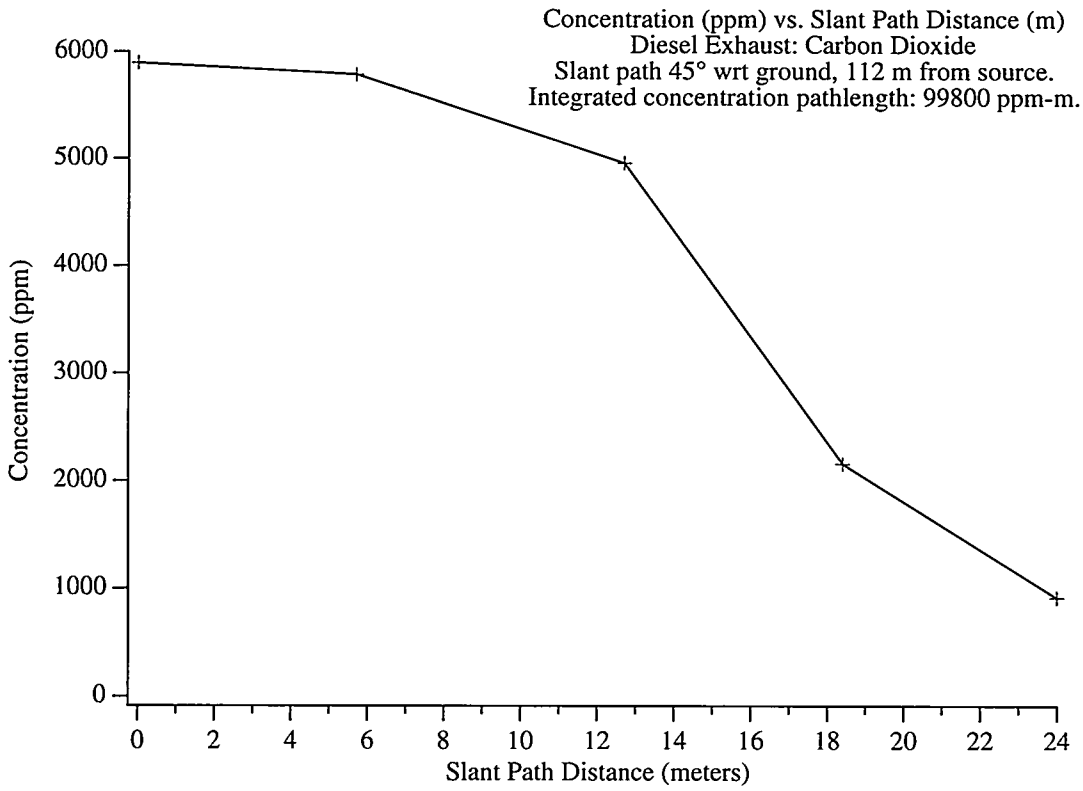
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Generator Exhaust: Carbon Dioxide, 600 g/sec, one-hour plume.



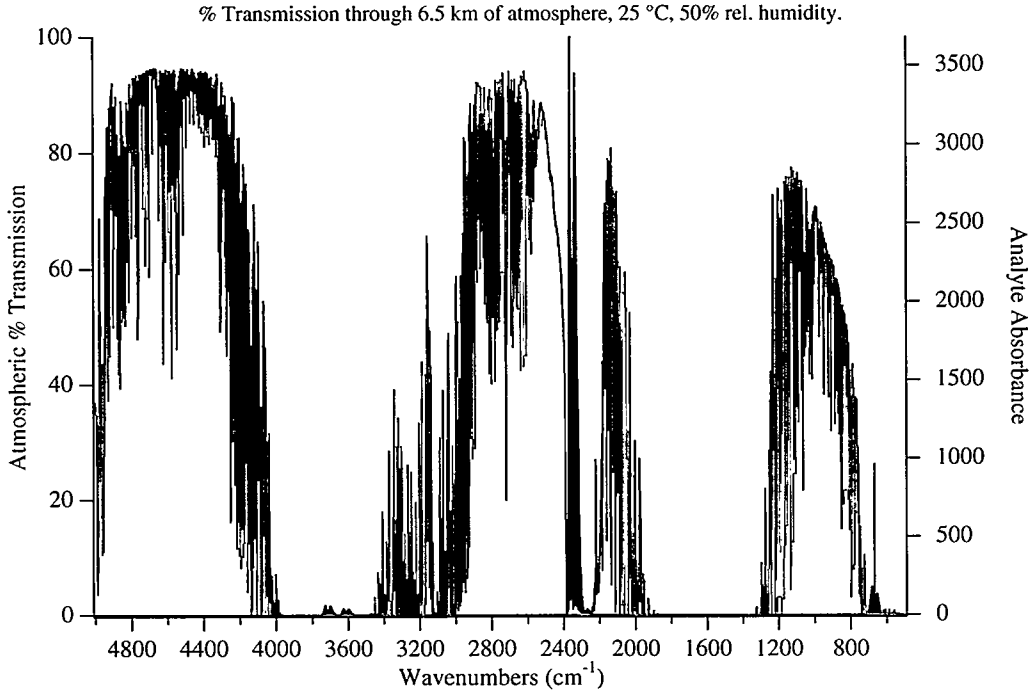



Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Generator Exhaust: Carbon Dioxide
600 g/sec, one hour plume, 9 m receptor height
Concentration (ppm)
10^4
10^3
10^2
10^1
10^0
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Exhaust: Carbon Dioxide
Slant path 45° wrt ground, 112 m from source.
Integrated concentration pathlength: 99800 ppm-m.
Concentration (ppm)
6000
5000
4000
3000
2000
1000
0
0
2
4
6
8
10
12
14
16
18
20
22
24
Slant Path Distance (meters)

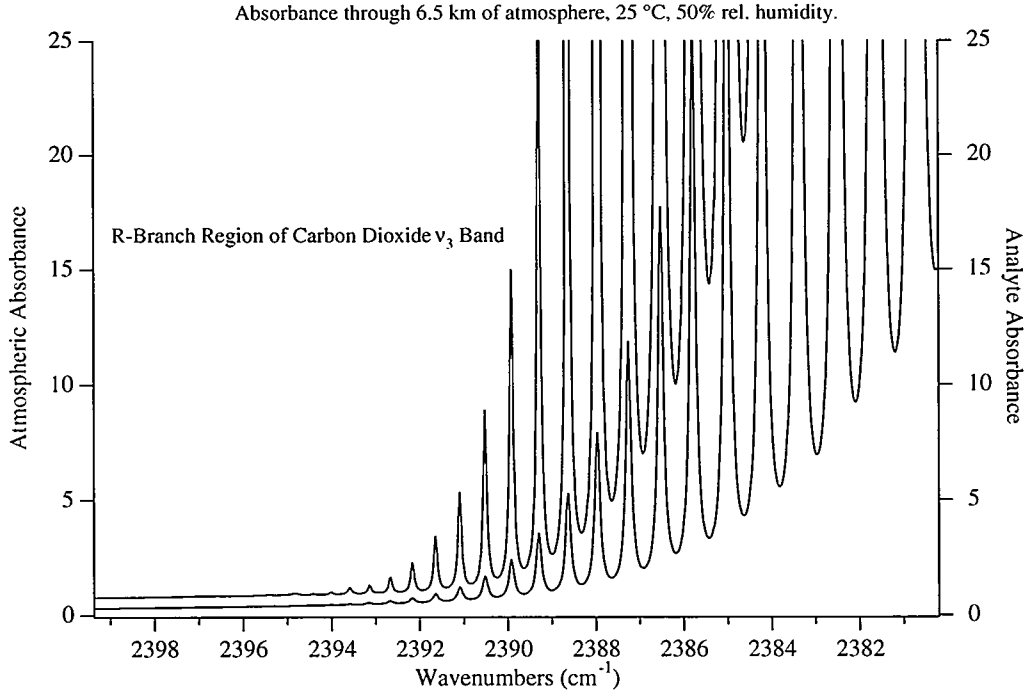
Carbon Dioxide from Diesel Electric Generator Exhaust
Carbon dioxide absorbance, 50 °C, 99,800 ppm-m, 112 m from vent.

% Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.

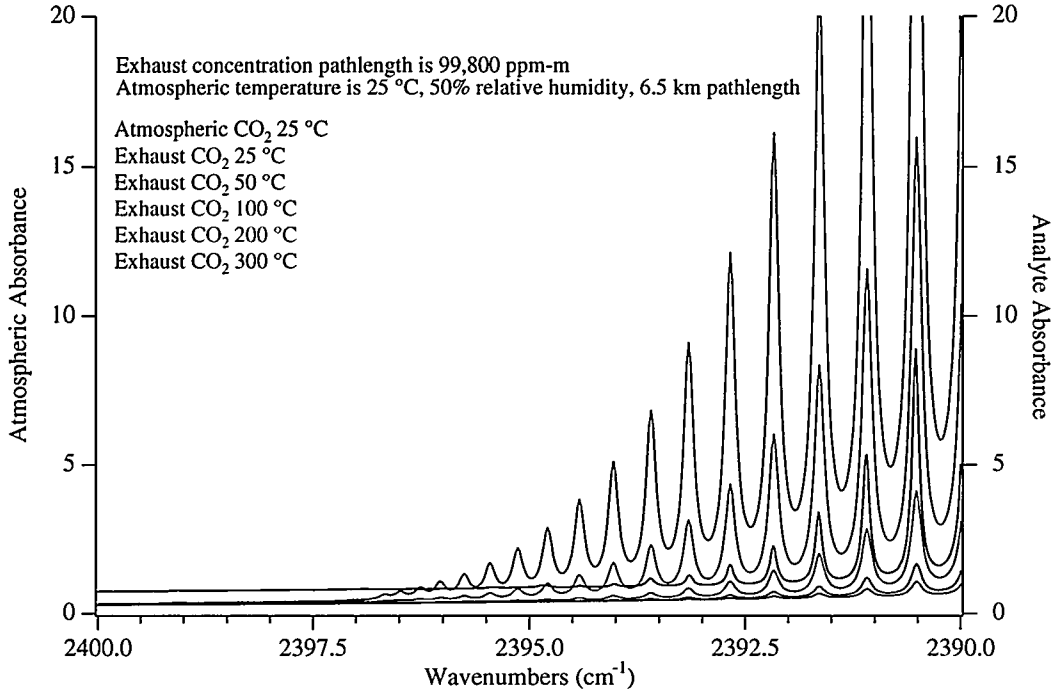


Carbon Dioxide from Diesel Electric Generator Exhaust
Carbon Dioxide absorbance 50 °C, 99,800 ppm-m, 112 m from vent.

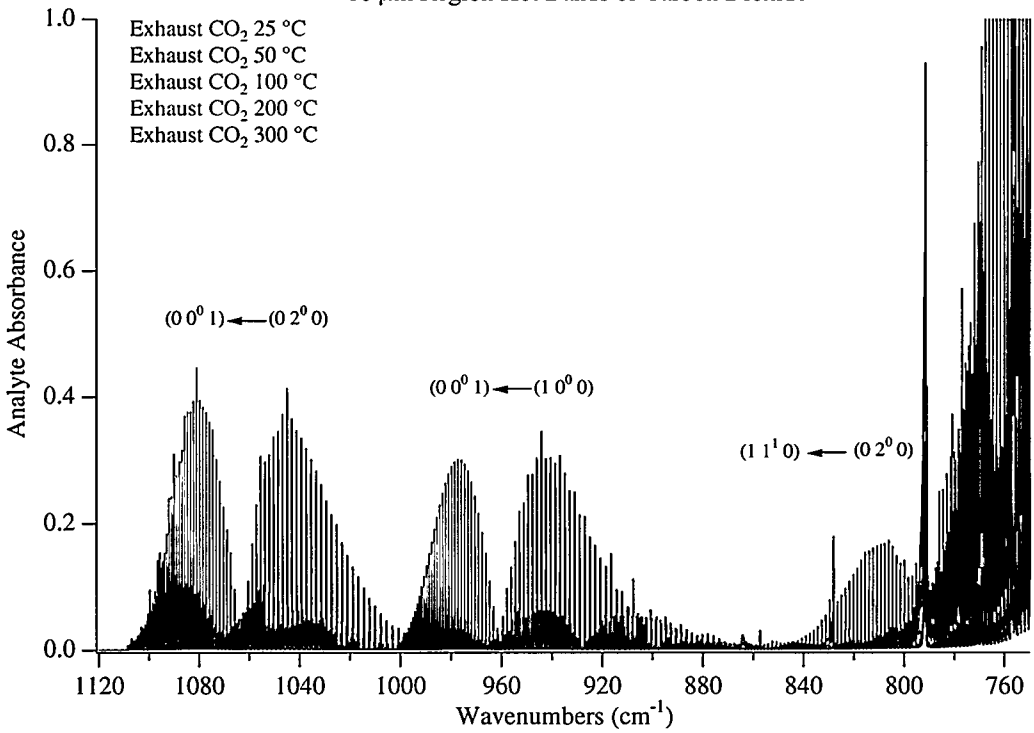
Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



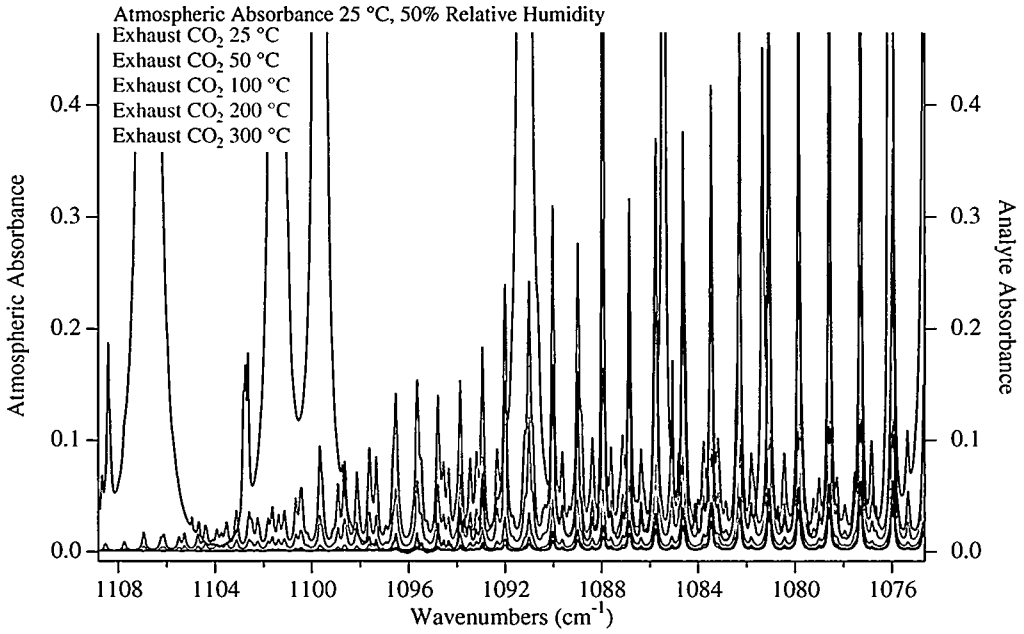
Carbon Dioxide from Diesel Electric Generator Exhaust:
Absorbance in R-Branch region of ν_3 Band at Various Temperatures



10 μm Region Hot Bands of Carbon Dioxide



R-Branch Region of the Carbon Dioxide (0 0^0 1) - (0 2^0 0) Hot Band



CHARM Version 9.3

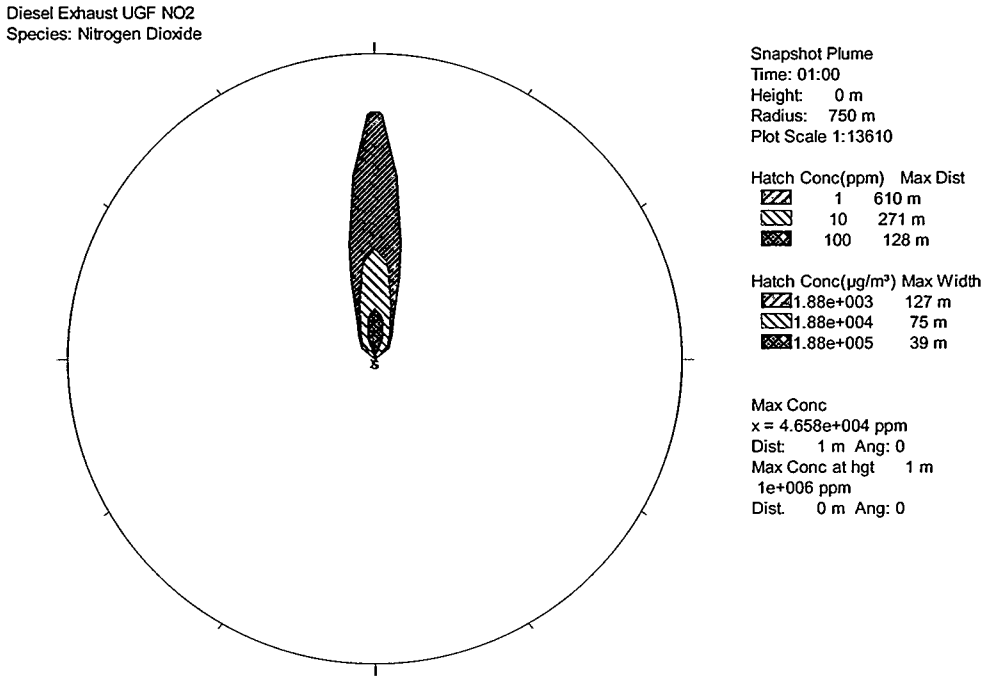
Title:	Generator Diesel Exhaust: NO2
Species:	Nitrogen Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	6 g/s
Release Duration:	24 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.01761 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

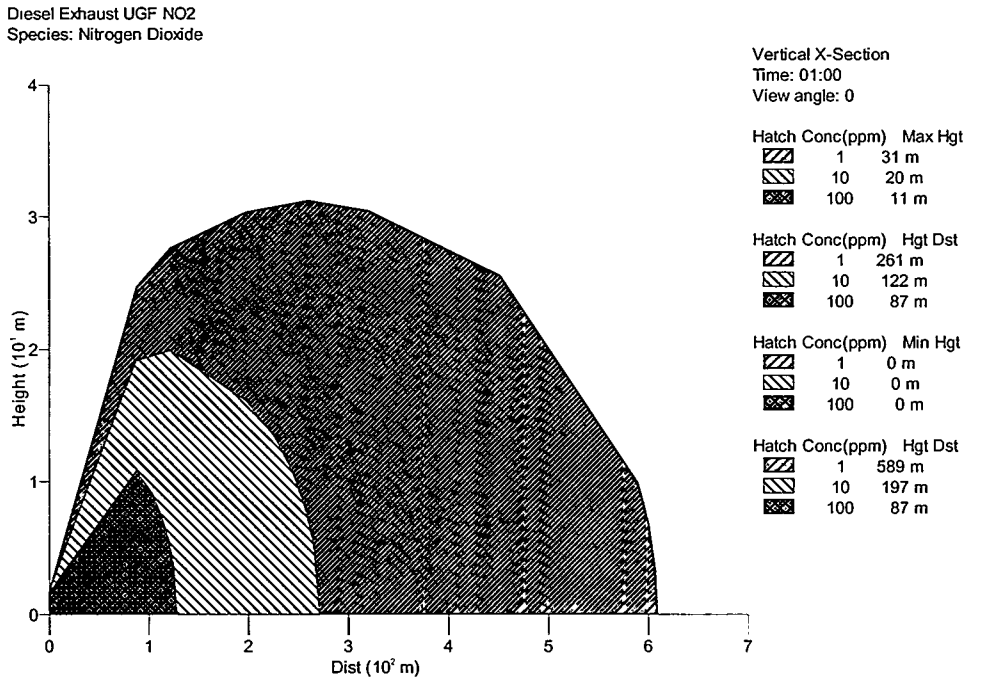
****

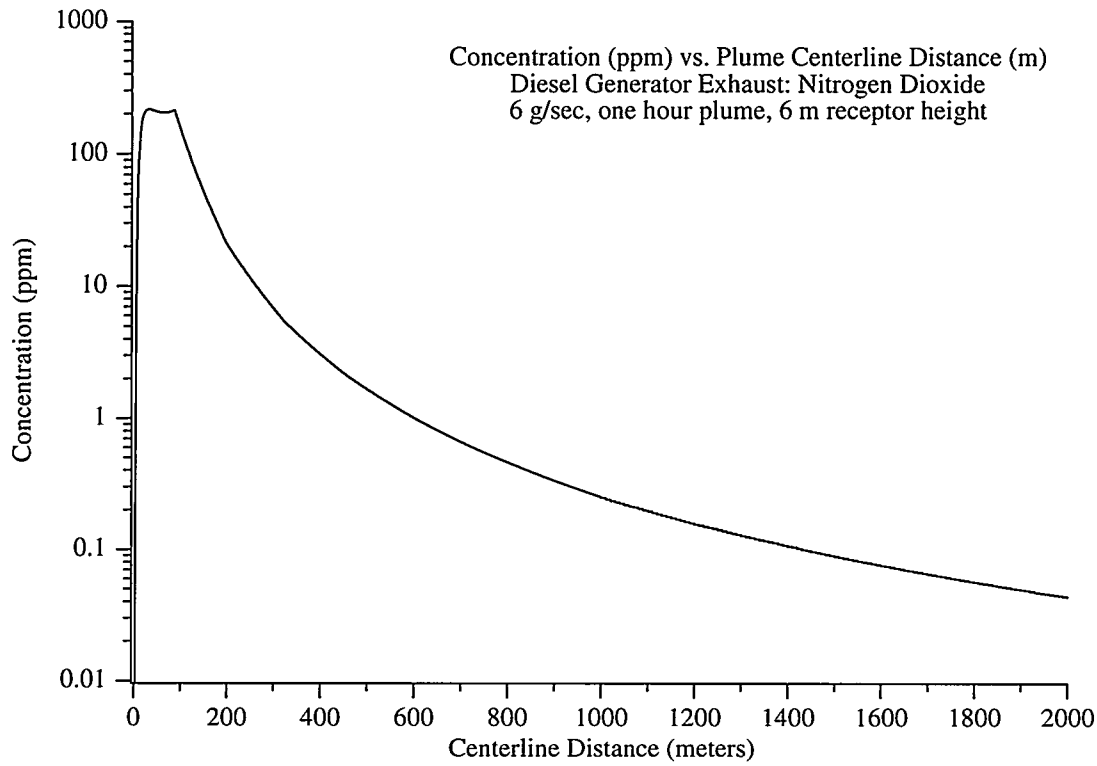
Met Data

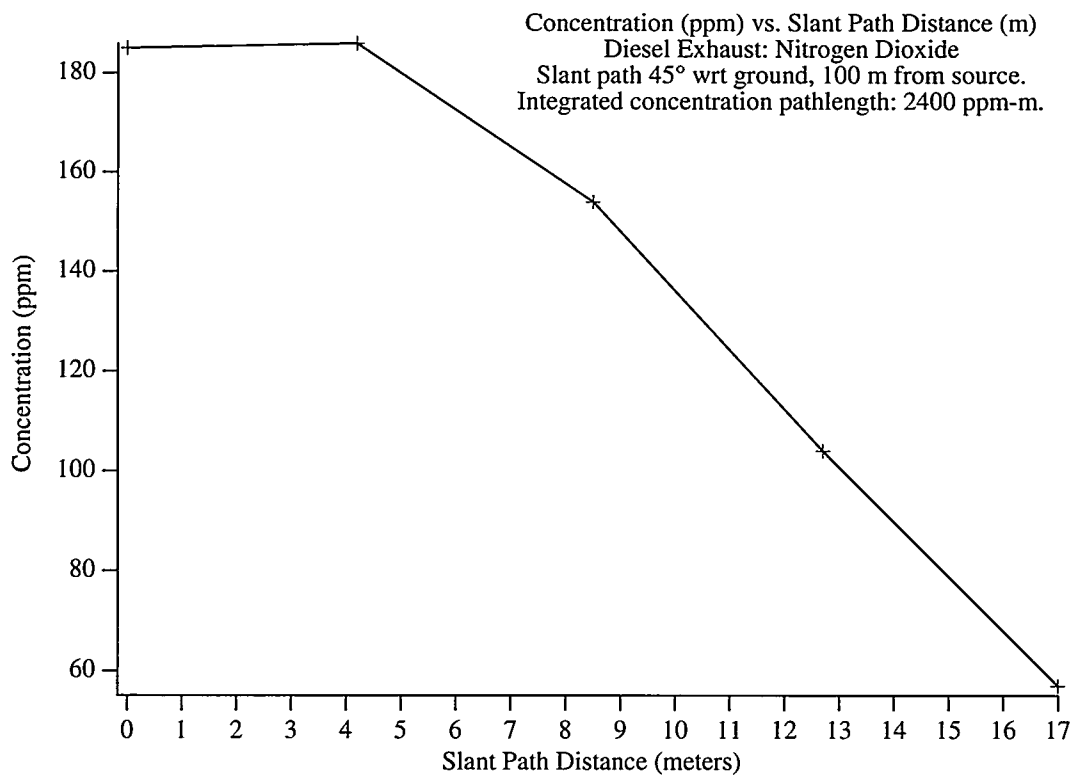
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Generator Exhaust: Nitrogen Dioxide, 6 g/sec, one-hour plume.

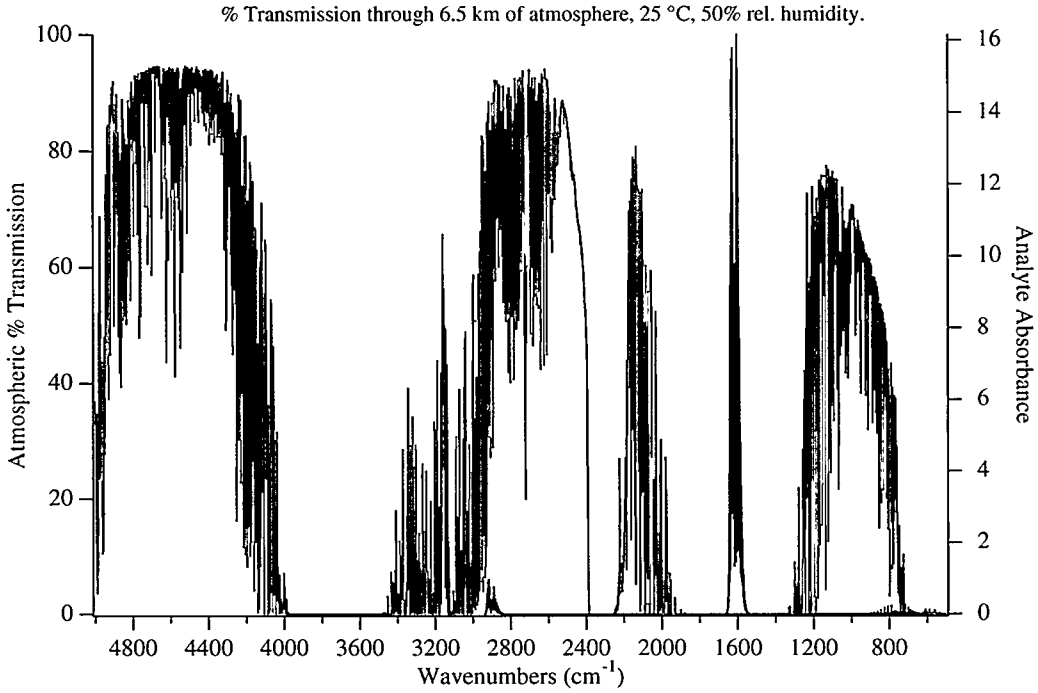




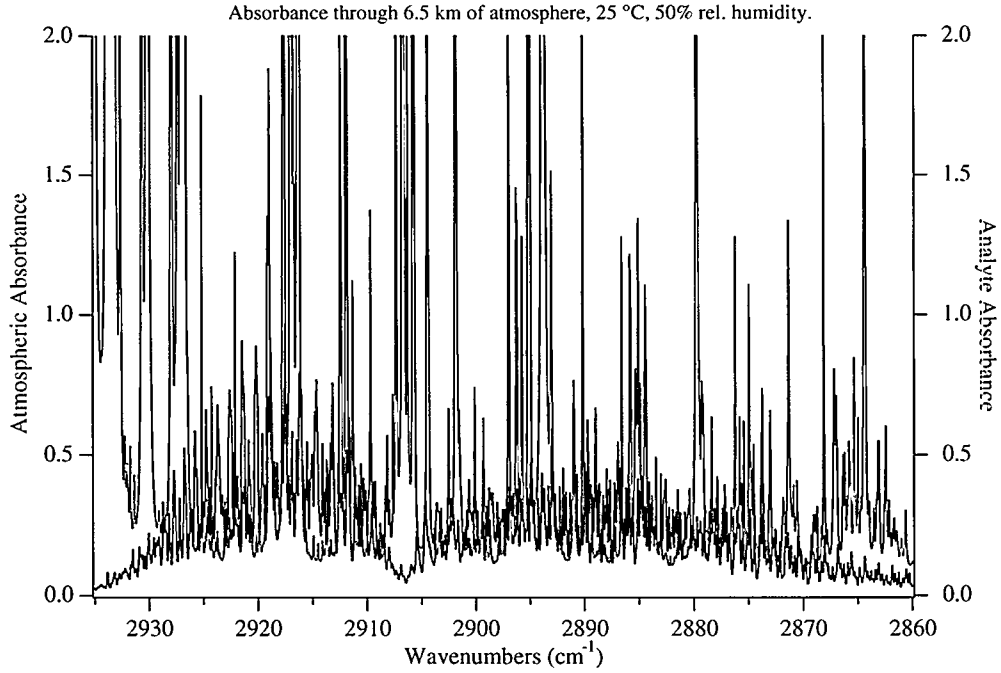

Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Generator Exhaust: Nitrogen Dioxide
6 g/sec, one hour plume, 6 m receptor height
Concentration (ppm)
1000
100
10
1
0.1
0.01
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Exhaust: Nitrogen Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 2400 ppm-m.
Concentration (ppm)
180
160
140
120
100
80
60
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
Slant Path Distance (meters)

Nitrogen Dioxide from Diesel Electric Generator Exhaust
Nitrogen dioxide absorbance, 50 °C, 2400 ppm-m, 100 m from vent.



Nitrogen Dioxide from Diesel Electric Generator Exhaust
Nitrogen dioxide absorbance, 50 °C, 2400 ppm-m, 100 m from vent.
Detail of $\nu_1 + \nu_3$ band



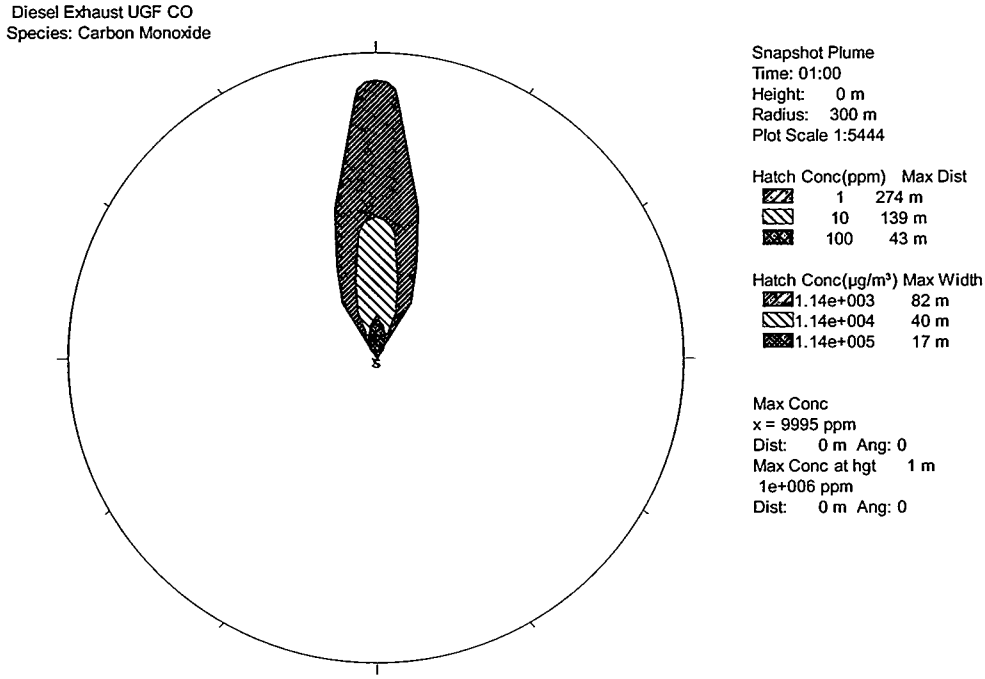
CHARM Version 9.3

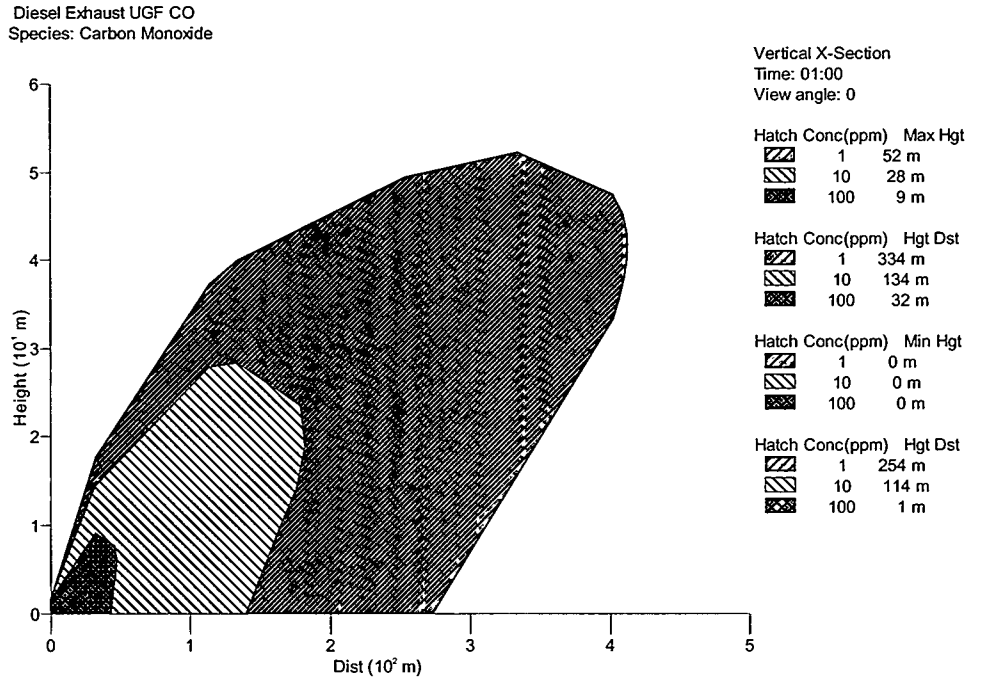
Title:	Generator Diesel Exhaust CO
Species:	Carbon Monoxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	3 g/s
Release Duration:	24 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.01446 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

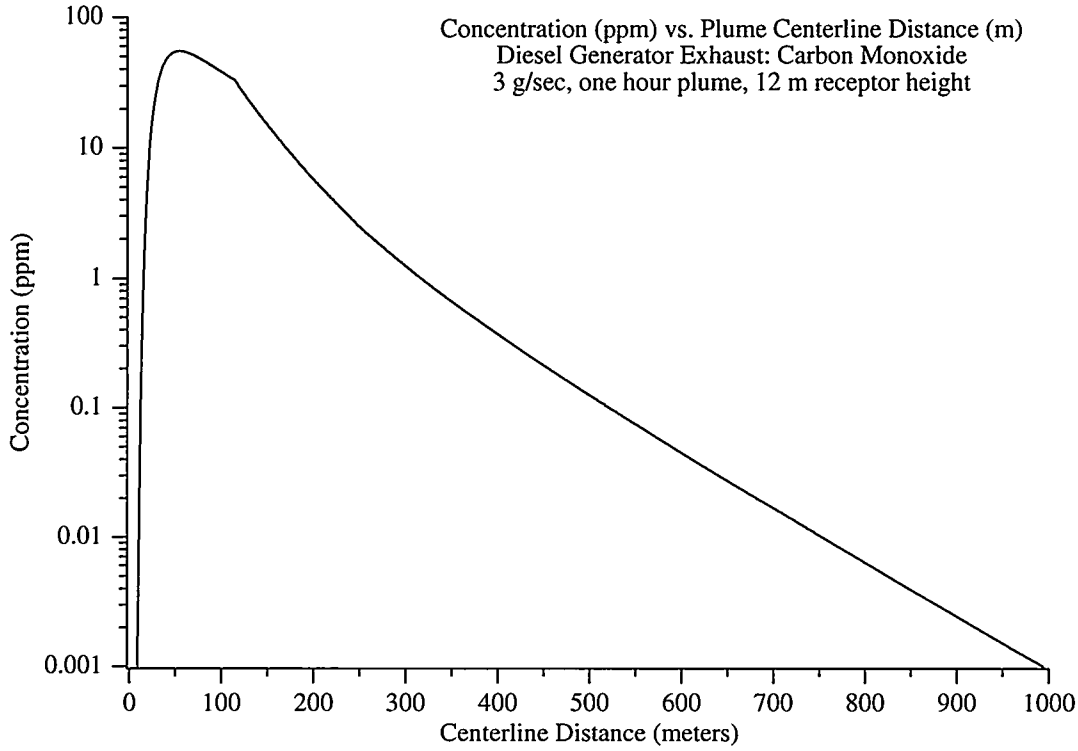
****

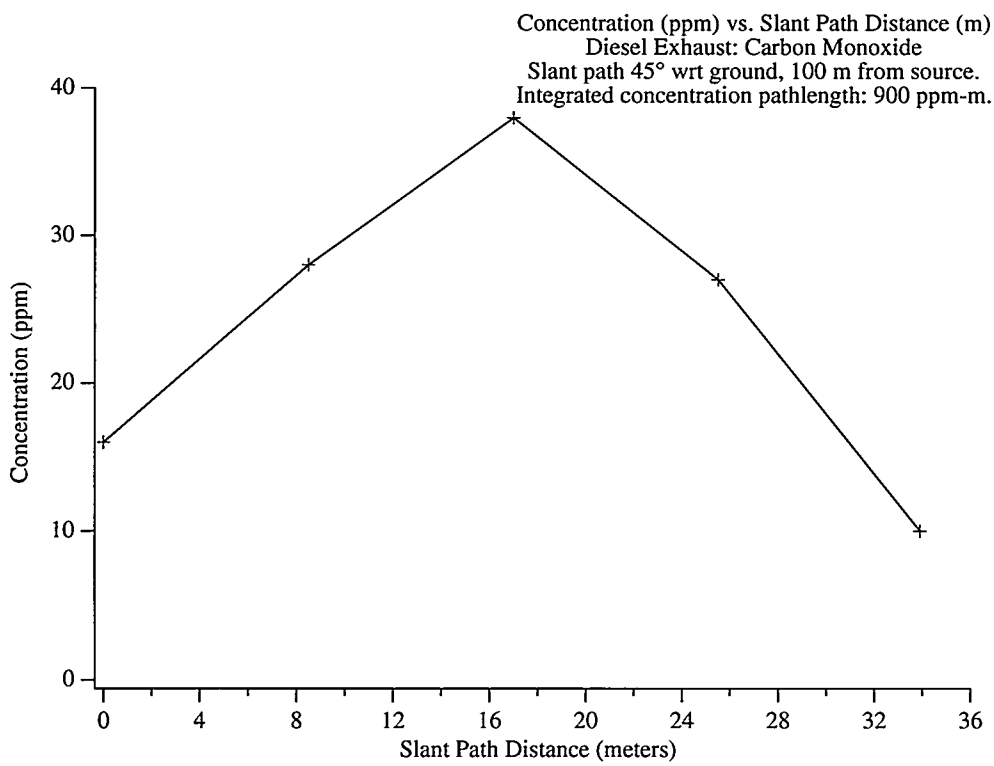
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Generator Exhaust: Carbon Monoxide, 3 g/sec, one-hour plume.

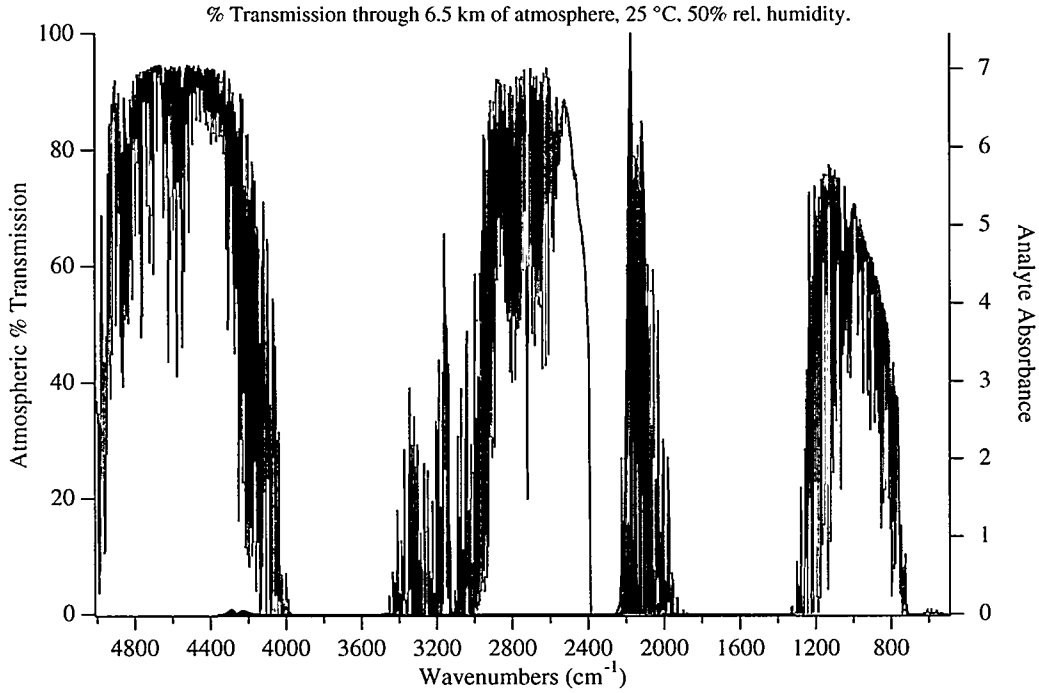




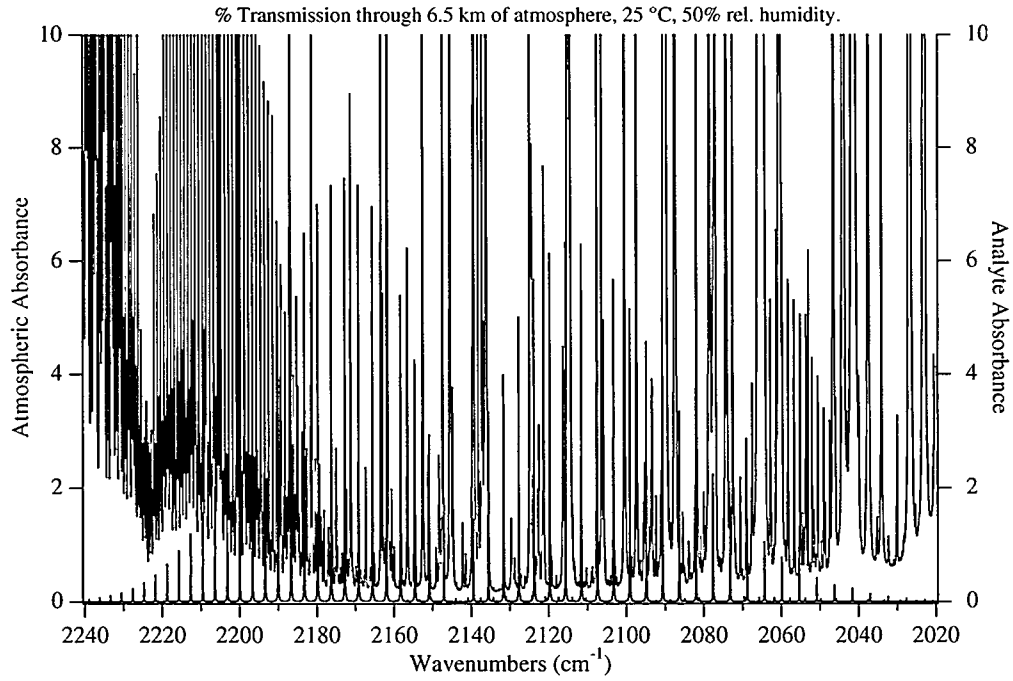

Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Generator Exhaust: Carbon Monoxide
3 g/sec, one hour plume, 12 m receptor height
Concentration (ppm)
100
10
1
0.1
0.01
0.001
0
100
200
300
400
500
600
700
800
900
1000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Exhaust: Carbon Monoxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 900 ppm-m.
Concentration (ppm)
40
30
20
10
0
0
4
8
12
16
20
24
28
32
36
Slant Path Distance (meters)

Carbon Monoxide from Diesel Electric Generator Exhaust
Carbon Monoxide absorbance, 50 °C, 900 ppm-m, 100 m from vent.



Carbon Monoxide from Diesel Electric Generator Exhaust
Carbon Monoxide absorbance, 50 °C, 2400 ppm-m, 100 m from vent.
Detail of fundamental band



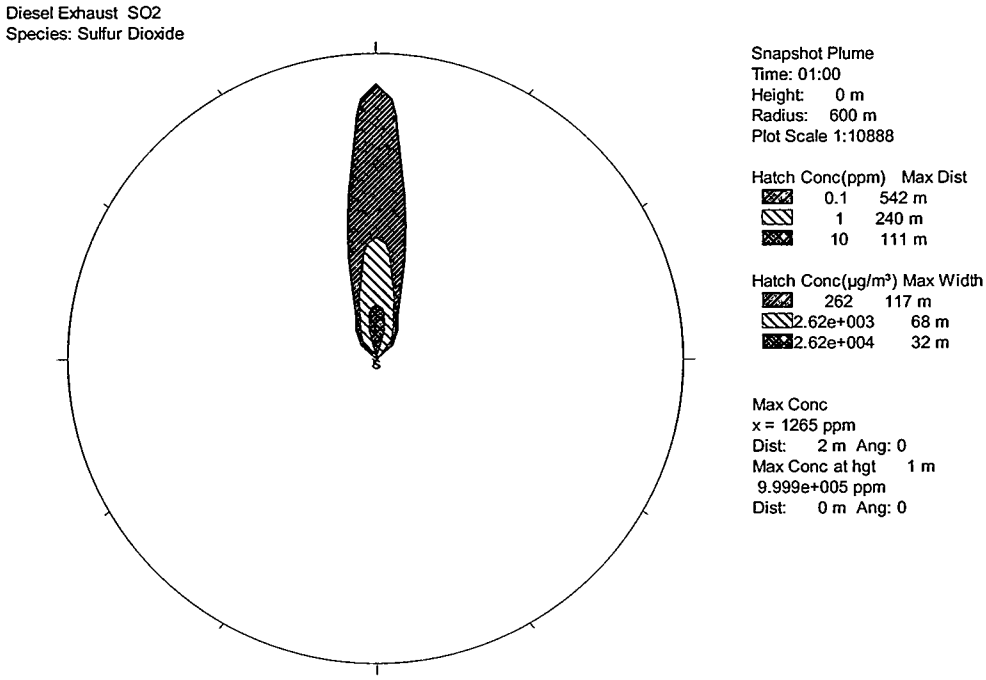
CHARM Version 9.3

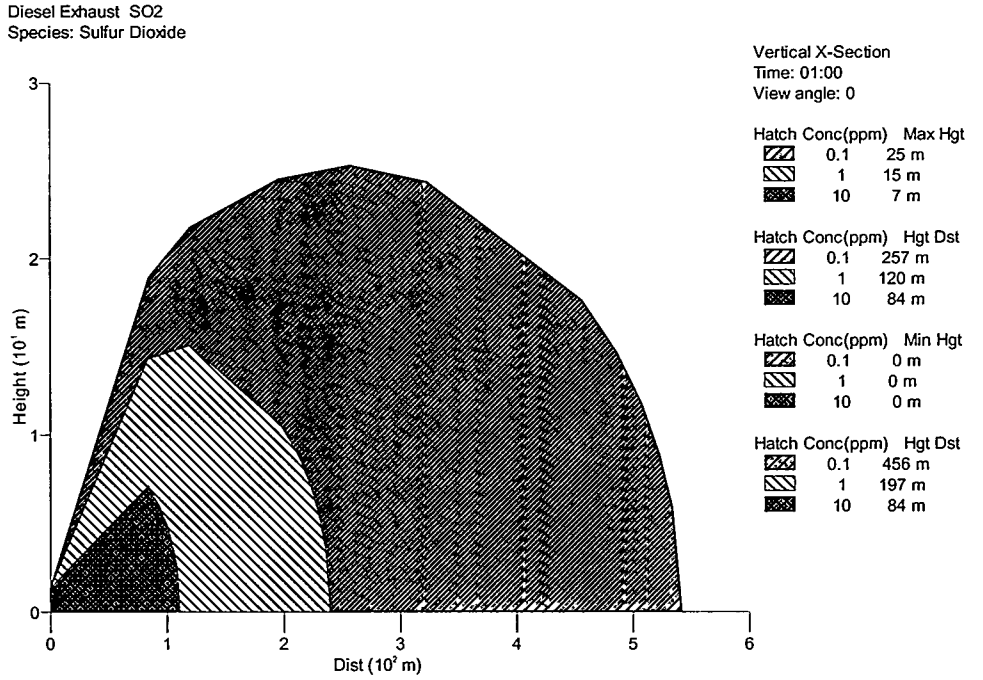
Title:	Generator Diesel Exhaust SO2
Species:	Sulfur Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 m
Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.6 g/s
Release Duration:	24 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.001265 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

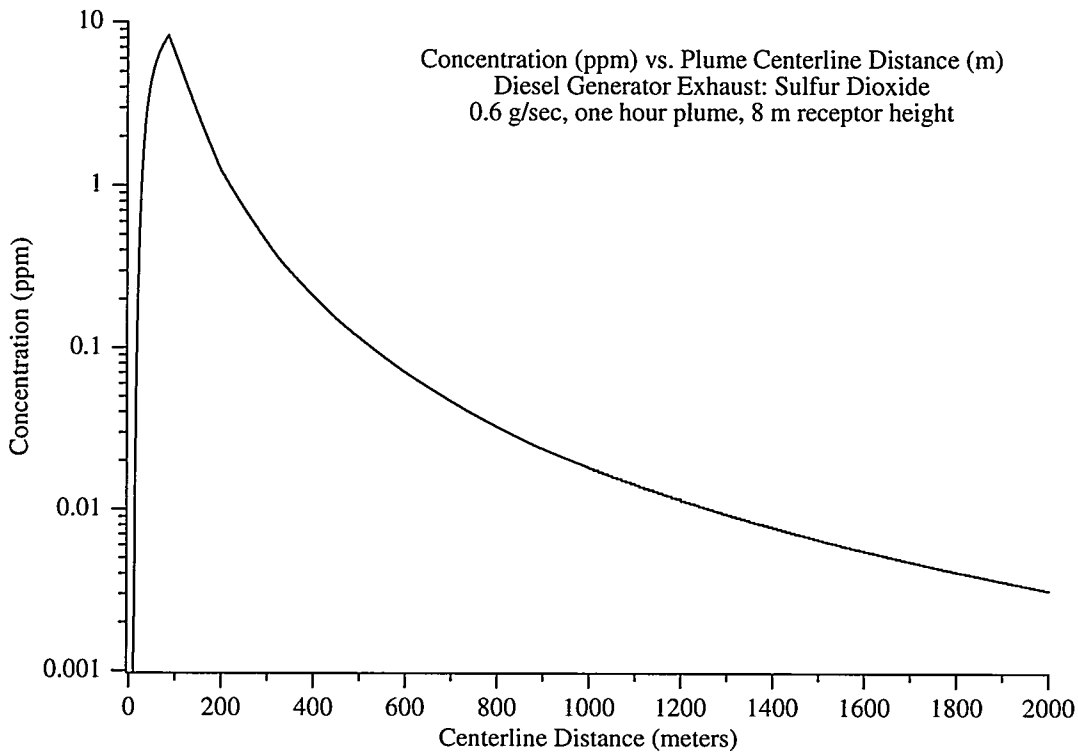
****

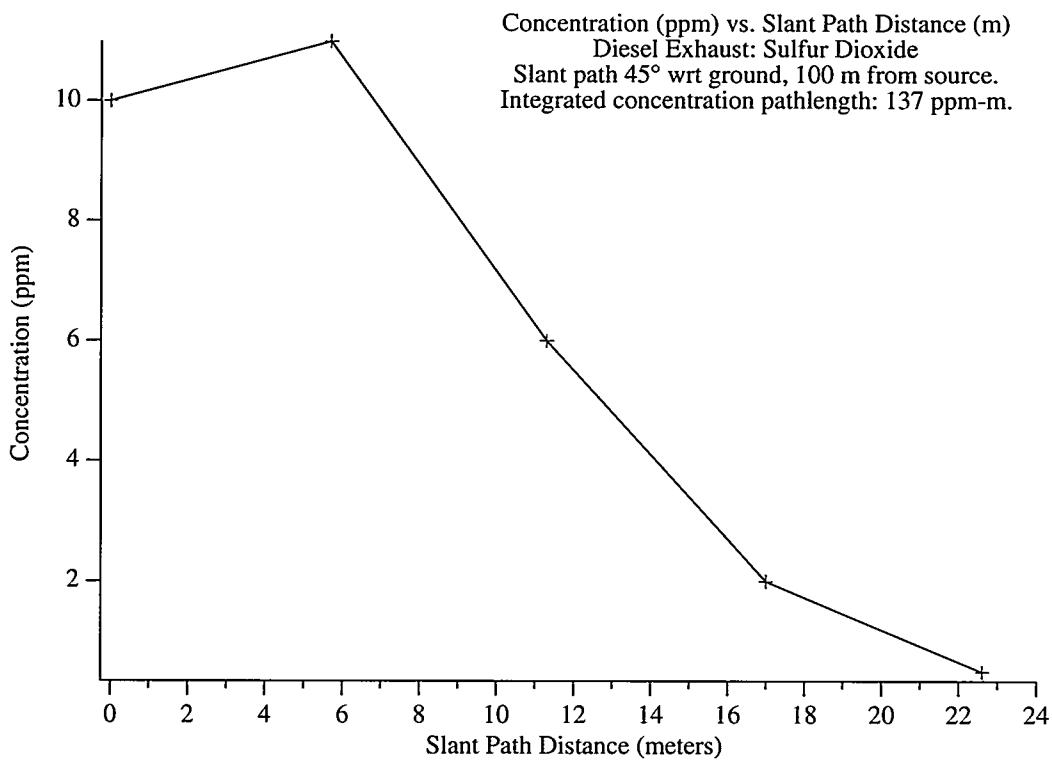
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Generator Exhaust: Sulfur Dioxide, 0.6 g/sec, one-hour plume.

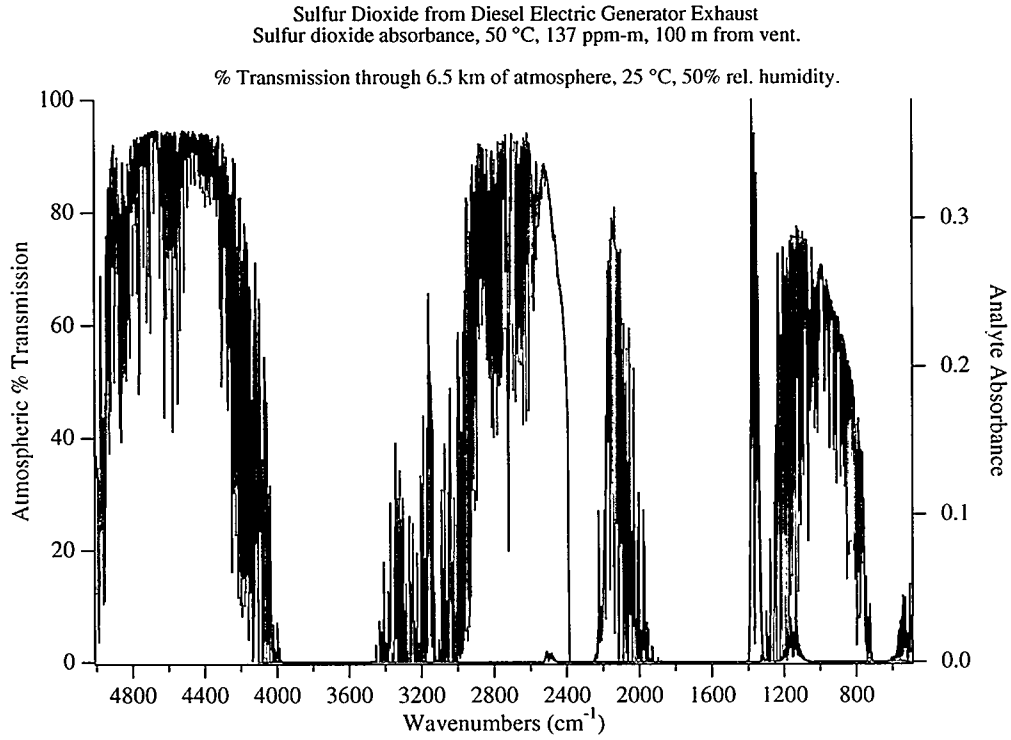


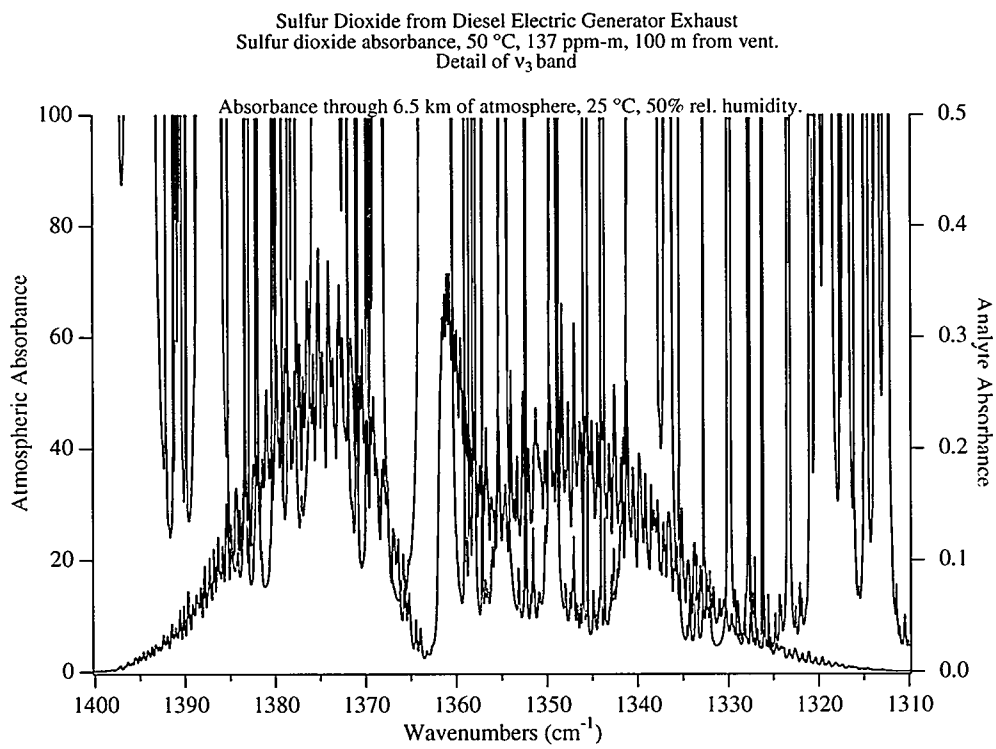



Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Generator Exhaust: Sulfur Dioxide
0.6 g/sec, one hour plume, 8 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Exhaust: Sulfur Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 137 ppm-m.
Concentration (ppm)
10
8
6
4
2
0
2
4
6
8
10
12
14
16
18
20
22
24
Slant Path Distance (meters)

(See also the SO_2 spectrum on p. 64.)





CHARM Version 9.3

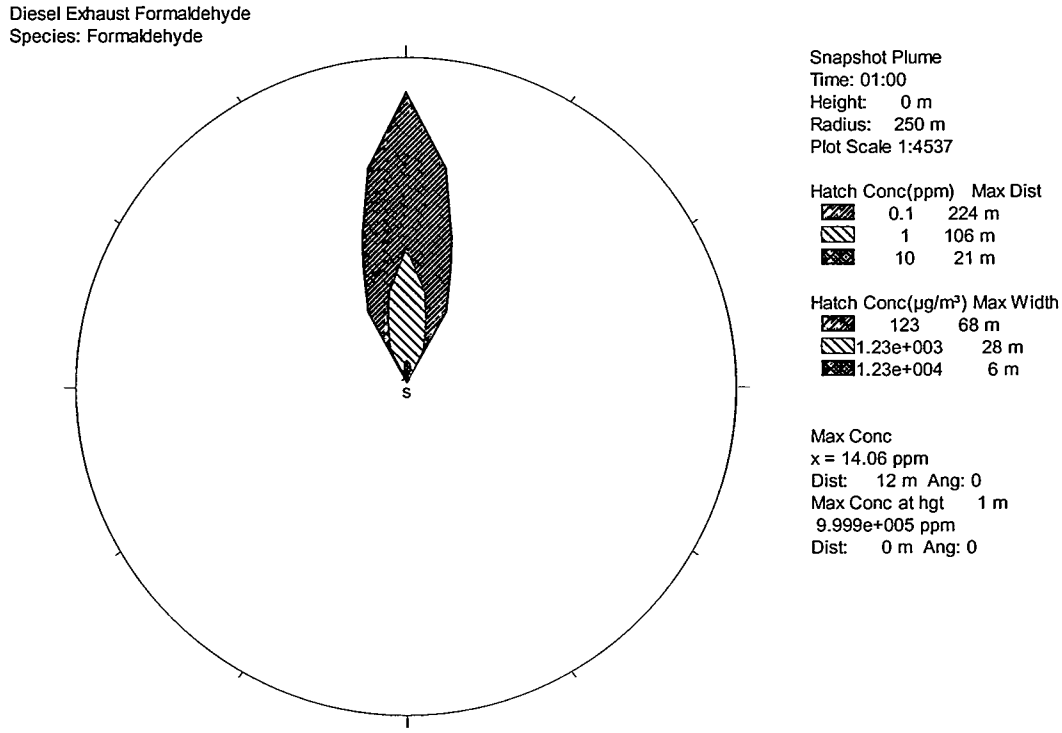
Title:	Generator Diesel Exhaust Formaldehyde
Species:	Formaldehyde
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.06 g/s
Release Duration:	24 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.0002698 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

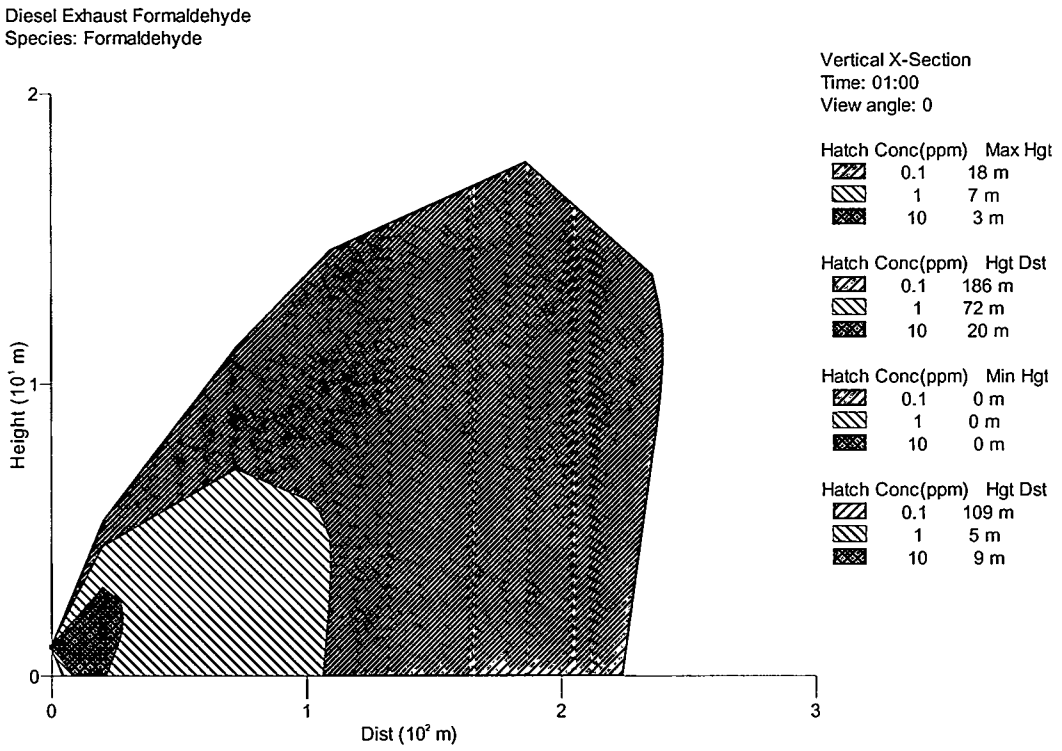
****

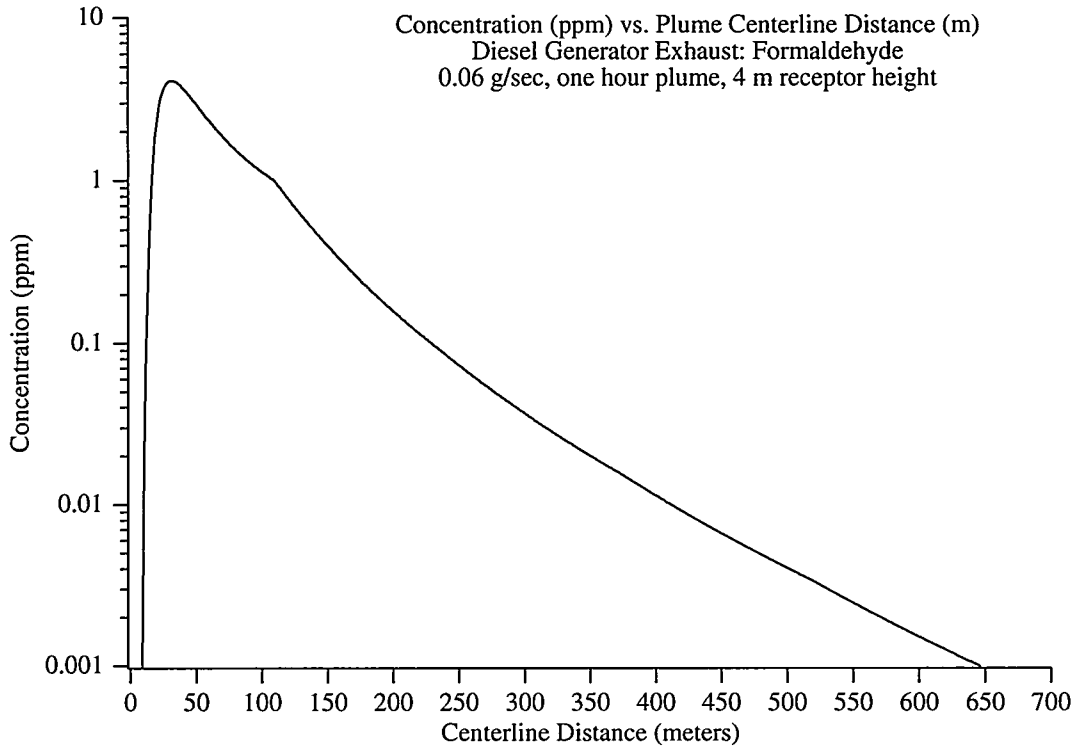
Met Data

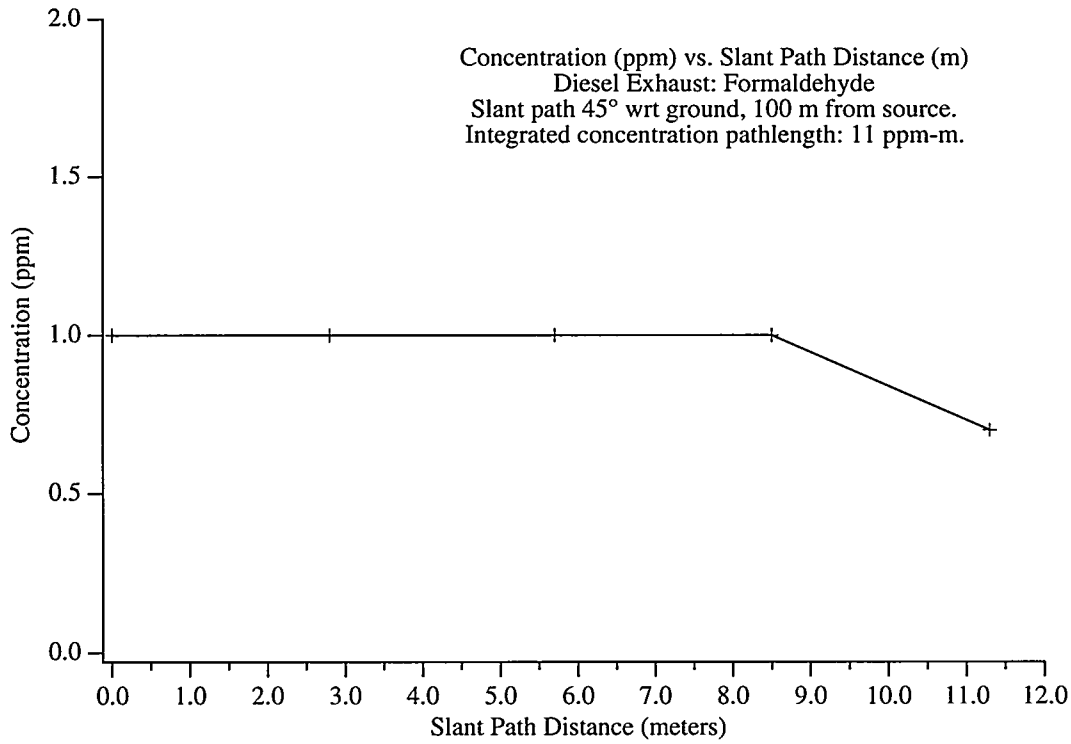
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

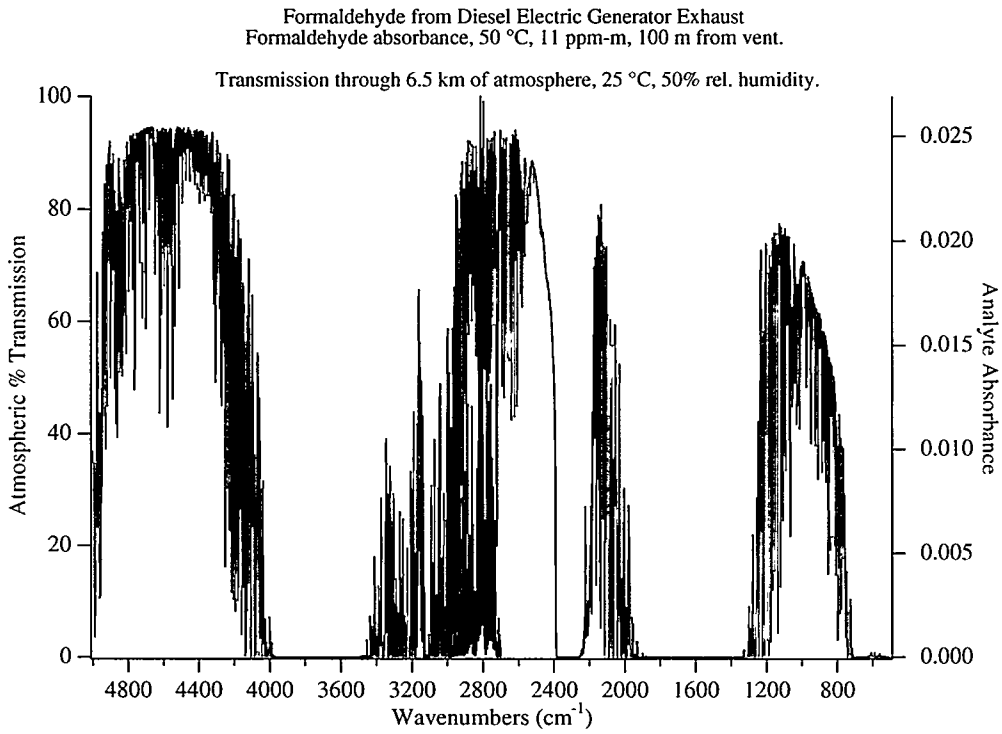
Diesel Generator Exhaust: Formaldehyde, 0.06 g/sec, one-hour plume.

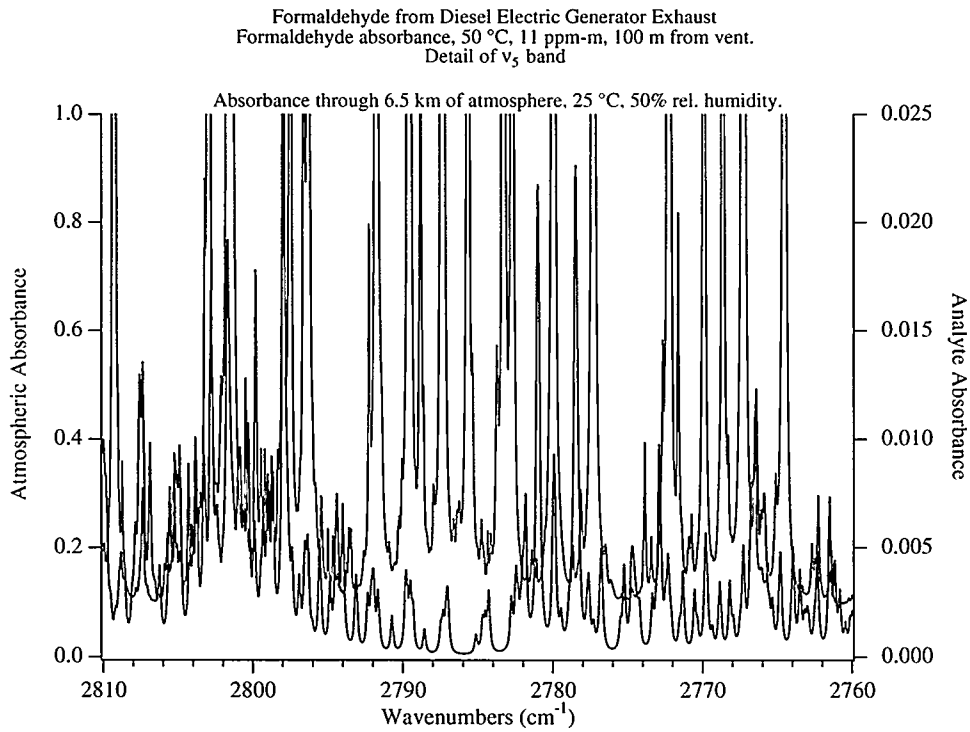





Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Generator Exhaust: Formaldehyde
0.06 g/sec, one hour plume, 4 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0
50
100
150
200
250
300
350
400
450
500
550
600
650
700
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Exhaust: Formaldehyde
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 11 ppm-m.
Concentration (ppm)
2.0
1.5
1.0
0.5
0.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
Slant Path Distance (meters)





There are also formaldehyde bands centered at 1167 and 1249 cm^{-1} that are not included in the HITRAN database. Apparently there is not good intensity information for these bands.

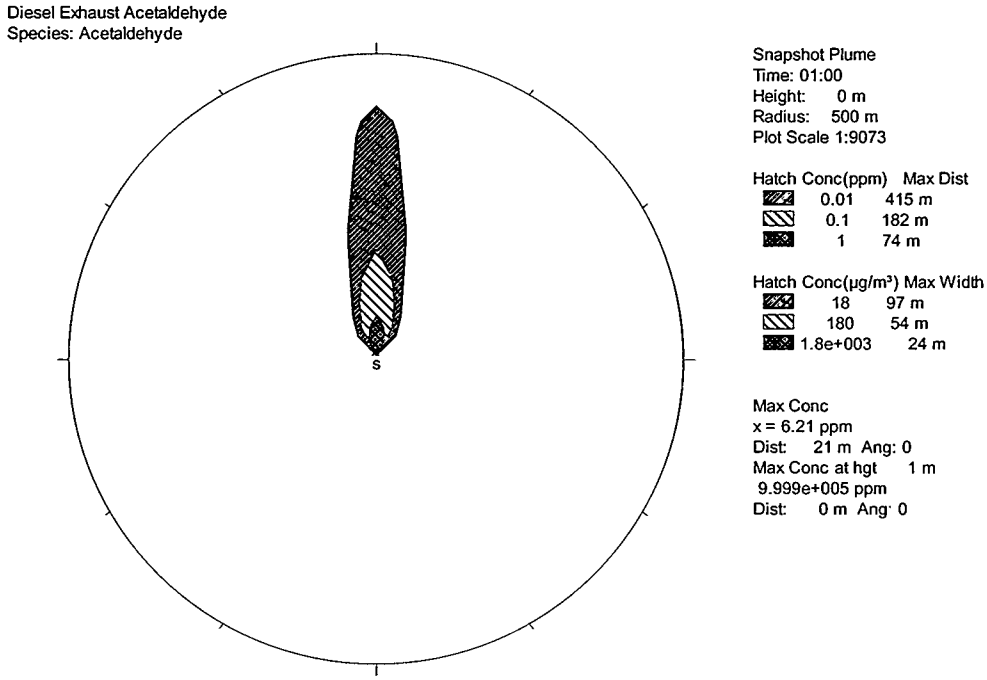
CHARM Version 9.3

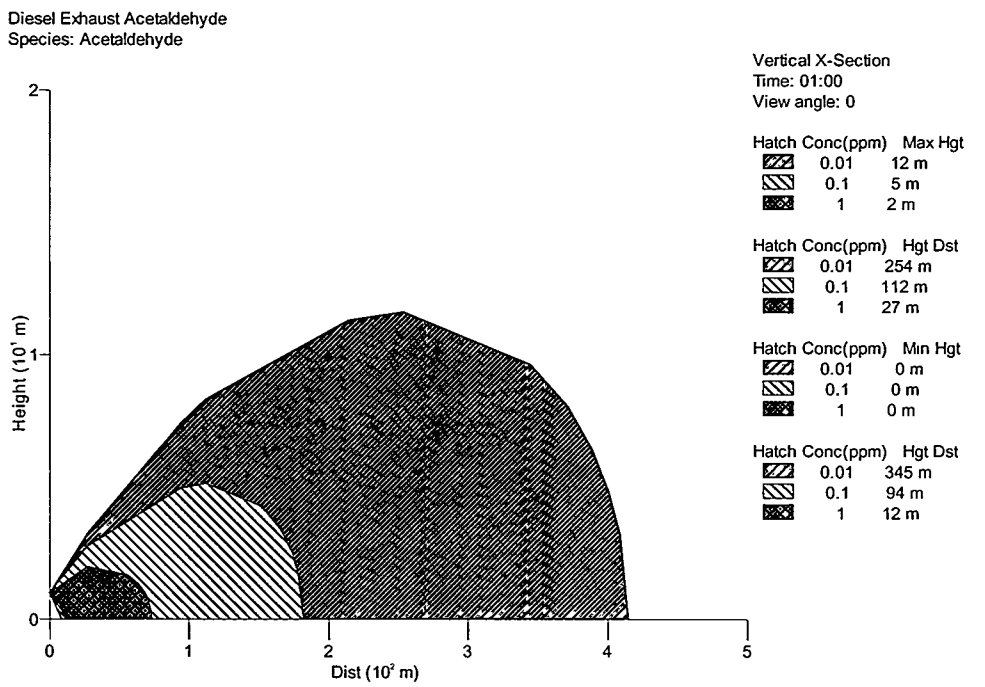
Title:	Generator Diesel Exhaust Acetaldehyde
Species:	Acetaldehyde
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.01, 0.1, 1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.02 g/s
Release Duration:	24 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	6.131e-005 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

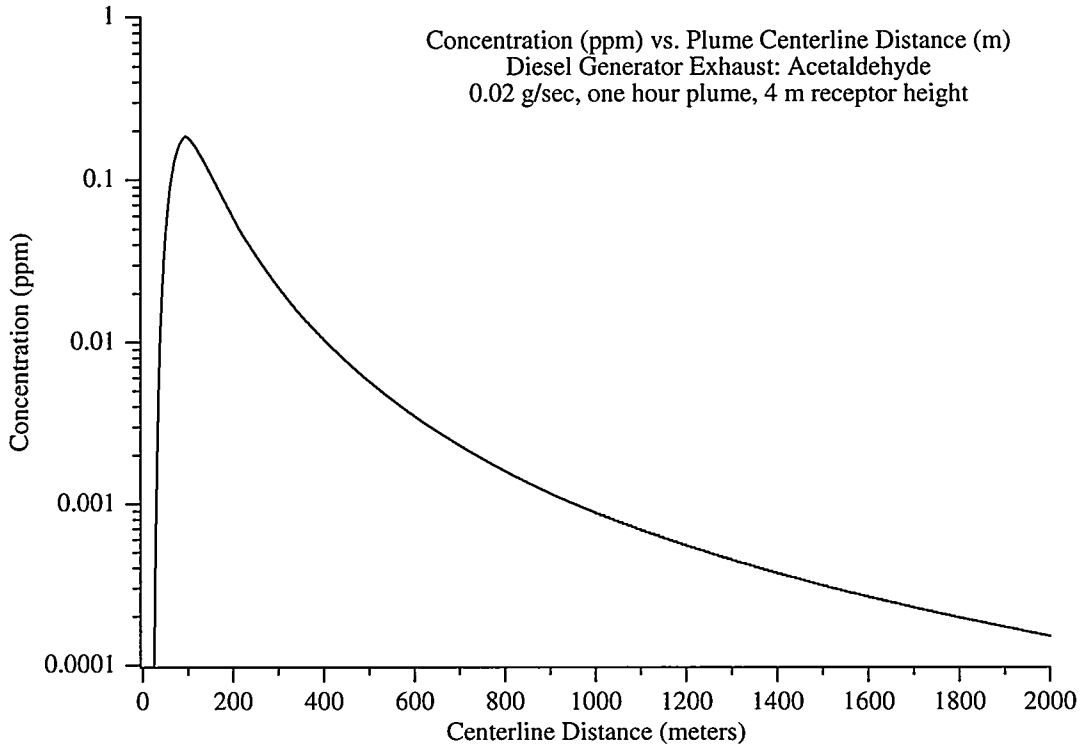
****

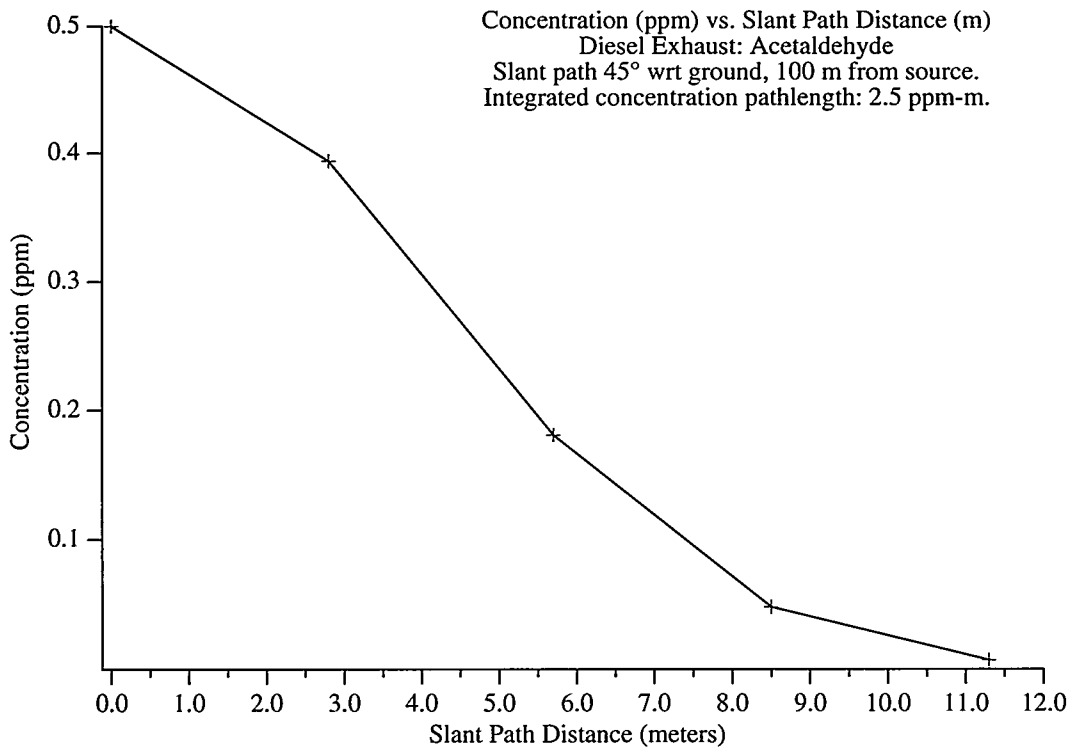
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Generator Exhaust: Acetaldehyde, 0.02 g/s, one-hour plume.

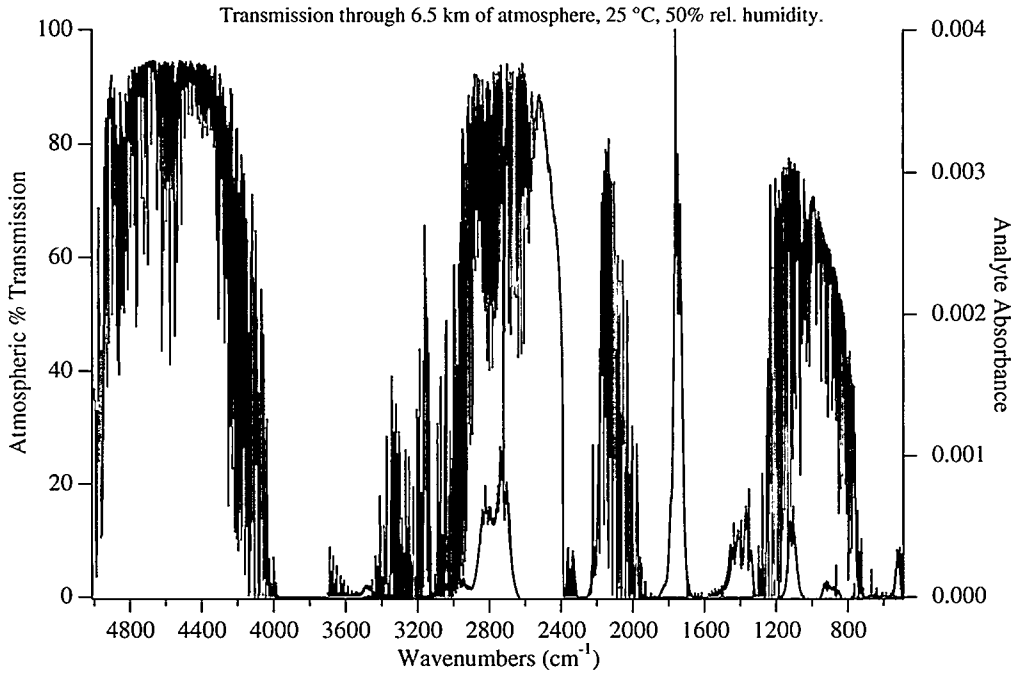




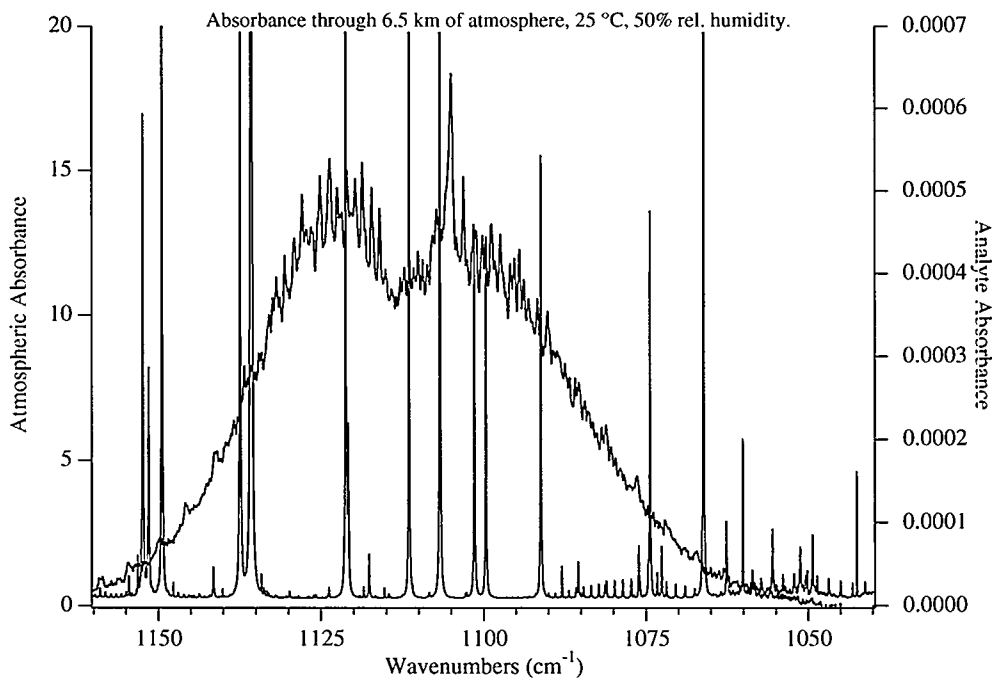

Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Generator Exhaust: Acetaldehyde
0.02 g/sec, one hour plume, 4 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Exhaust: Acetaldehyde
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 2.5 ppm-m.
Concentration (ppm)
0.5
0.4
0.3
0.2
0.1
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
Slant Path Distance (meters)

Acetaldehyde from Diesel Electric Generator Exhaust
Acetaldehyde absorbance, 20 °C, 2.5 ppm-m, 100 m from vent.
Hanst database.

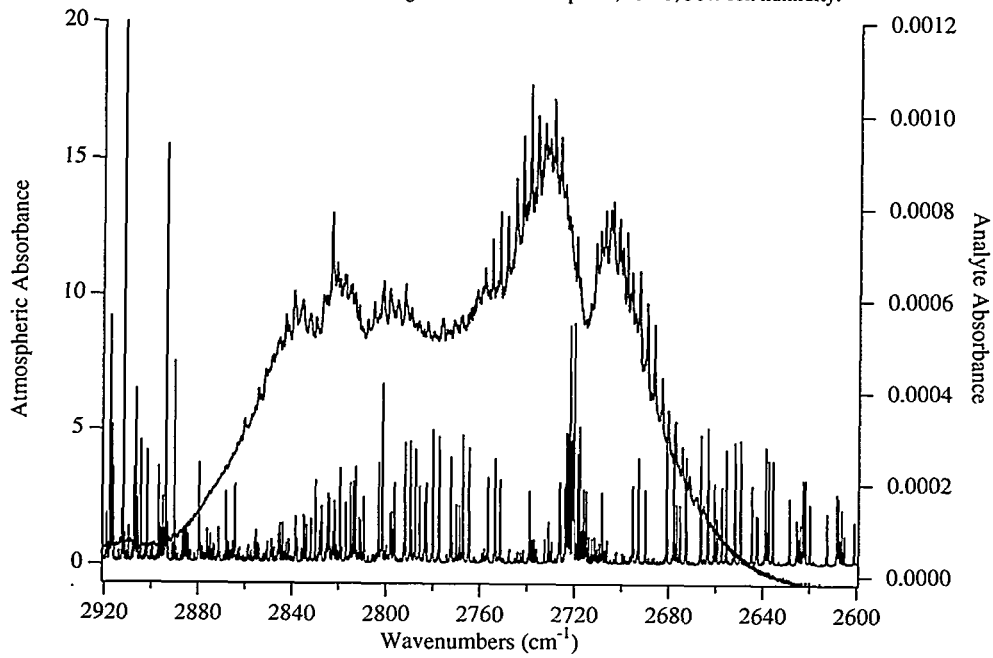


Acetaldehyde from Diesel Electric Generator Exhaust
Acetaldehyde absorbance, 20 °C, 2.5 ppm-m, 100 m from vent.
ν_8 band, Hanst database.



Acetaldehyde from Diesel Electric Generator Exhaust
Acetaldehyde absorbance, 20 °C, 2.5 ppm-m, 100 m from vent.
ν_2 and ν_3 region, Hanst database.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



2.2 TEL Diesel Exhaust

Compound	Normalized Emission Rate[a,b]	Engine Emission Rate (g/sec)	Emission Rate from One Vent (g/sec)
Carbon Dioxide	520 g/bhp-hr	300	75
NO_2	5 g/bhp-hr	3	0.8
Carbon Monoxide	2.3 g/bhp-hr	1	0.3
Sulfur Dioxide	0.58 g/bhp-hr	0.3	0.08
Formaldehyde	57 mg/bhp-hr	0.03	0.008
Acetaldehyde	18 mg/bhp-hr	0.01	0.003
Benzene	5.9 mg/bhp-hr	0.003	0.0008
Propionaldehyde	3.7 mg/bhp-hr	0.002	0.0005
Acrolein	2.1 mg/bhp-hr	0.001	0.0003
m-Xylene	2.0 mg/bhp-hr	0.001	0.0003
1,3-Butadiene	1.8 mg/bhp-hr	0.001	0.0003
Carbonyl sulfide	0.46 mg/bhp-hr	0.0003	0.00008

(a) "Report to the Air Resources Board on the Proposed Identification of Diesel Exhaust as a Toxic Air Contaminant," Part A, Exposure Assessment, April 22, 1998. Robert K. Krieger, Project Manager, California Environmental Protection Agency, Air Resources Board.

(b) Brake horsepower (bhp) is a unit of power and it is the power delivered to the engine's drive shaft by the engine. Brake horsepower-hour is a unit of work; it is the work done when the engine's drive shaft exerts one horsepower for one hour. *Diesel Fuels Technical Review* (FTR-2), J. Bacha *et al.*, Chevron Products Company (1998).

Scenario: We assume here that four transporter erector launchers (TEL) are running and moving in the tunnel. The TEL is modeled after the Russian MAZ-543 TEL, which has a combat weight of 42,150 kg, a length of 9.4 m, width of 3.1 m, and height of 3.7 m. The MAZ-543 TEL has a maximum speed of 60 km/hr, maximum range of 650 km, and uses a D12A-525 V-12 water cooled engine that delivers 525 horse power at 2100 RPM.[a] We also assume that the stated horse power is the brake horse power. Fuel is assumed to have a 0.5 wt% sulfur content.

The four TELs are running in the tunnel at one time, and the vehicles are running continuously. The emission rate given in the third column is the total rate for the twelve most abundant exhaust compounds for all four engines, and is calculated by multiplying the engine horsepower by four and then multiplying by the normalized emission rate given in the second column. The emission rate given in the fourth column is the emission rate coming out of one of the four main tunnel vents. Each vent is 2 meters in diameter, the ventilation rate is 2000 m^3/min (2×10^6 liter/min) for each vent, which gives a linear vent speed of 10.6 m/sec. The tunnel volume is 2×10^6 m^3, or 2×10^9 liters so the ventilation rate of tunnel air can be expressed as (8×10^6 l/min)/(24.45 l/mole) = 3.27×10^5 moles/min, where 24.45 l/mole is the

(a) http://www.hawk.dk/russian.asp

molar volume of air at 25°C. To exchange all of the tunnel air once requires (2×10^6 m^3)/(8000 m^3/min) = 250 minutes (four hours and ten minutes).

The above analysis assumes that the vehicles have been running continuously, but given an engine emission rate and a tunnel ventilation rate it is possible to calculate the concentration of a particular exhaust component before it has reached a steady state concentration after 250 minutes of running; during engine startup, for example. This is done as follows. Let x(t) be the number of moles of, for example, carbon dioxide at time t. Then the rate of change of the number of moles of carbon dioxide is given by (Derrick and Grossman 1976)

$$\frac{dx}{dt} = A - Bx$$

where A is the engine emission rate and B is the tunnel ventilation rate. The solution of this differential equation is given as,

$$x(t) = e^{-Bt}\left[\int Ae^{Bt}dt + C\right]$$

For carbon dioxide from the TEL exhaust, A = 409 moles/min, and B = 0.004 min^{-1} and solving for t = 0 gives C = -1.0225×10^5 moles,

$$x(t) = 1.0225 \times 10^5 - 1.0225 \times 10^5 e^{-0.004t}$$

Similar equations can be written for the other compounds.

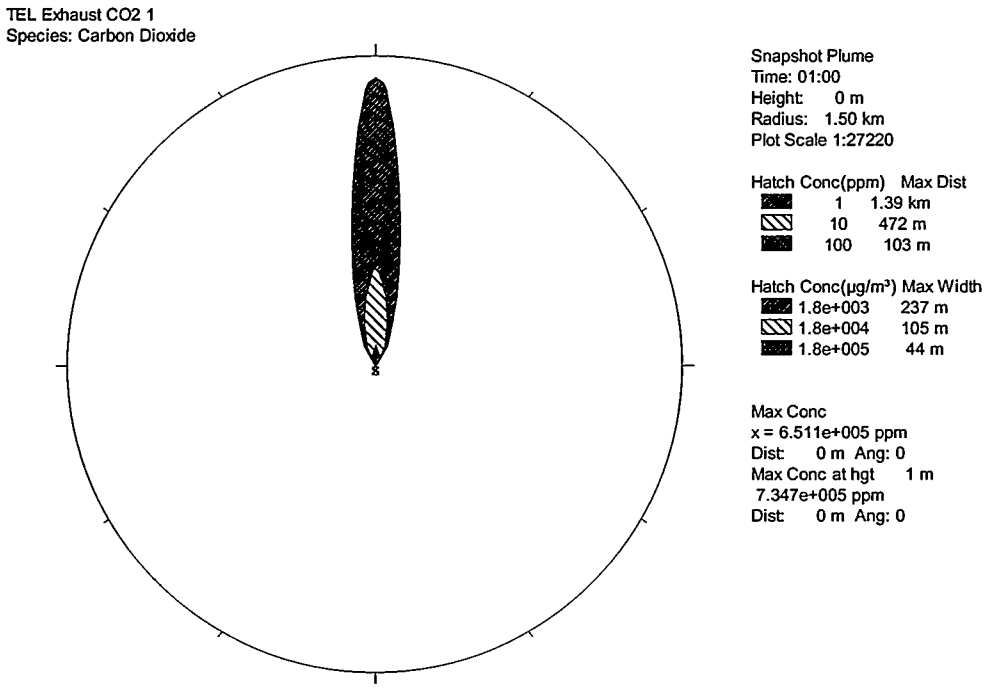
CHARM Version 9.3

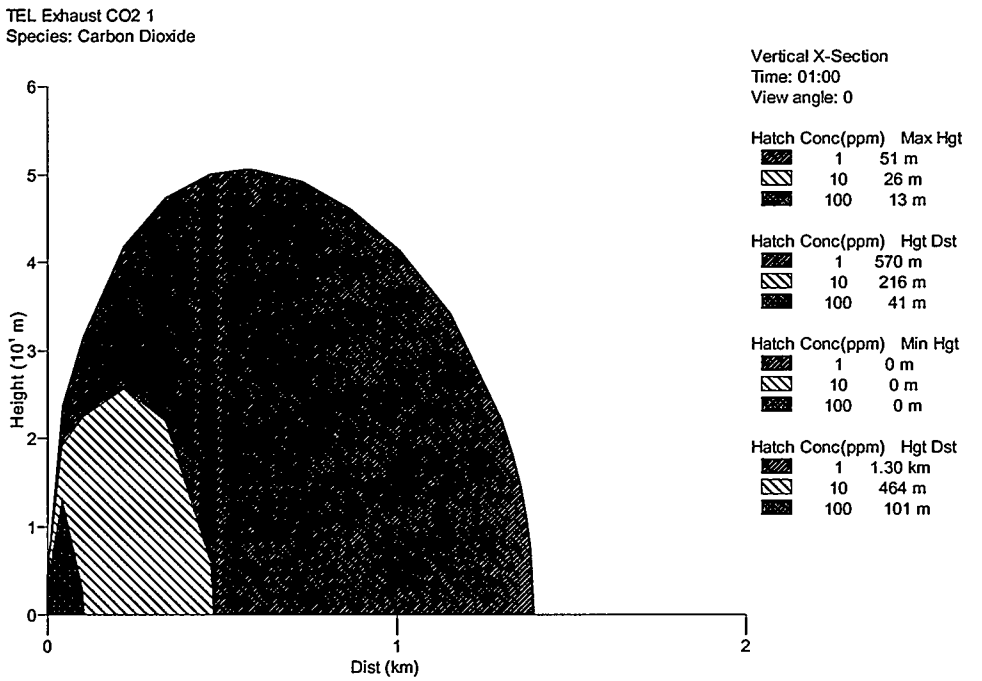
Title:	TEL Diesel Exhaust CO2
Species:	Carbon Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	75 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	10.62 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0.9987

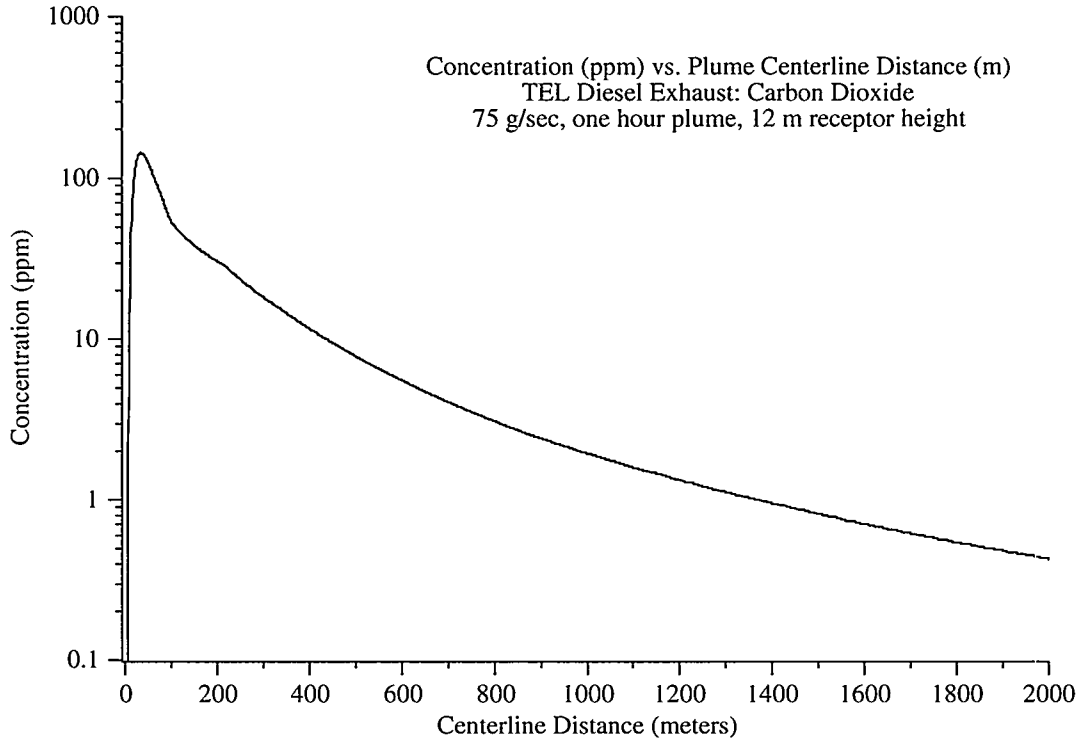
****

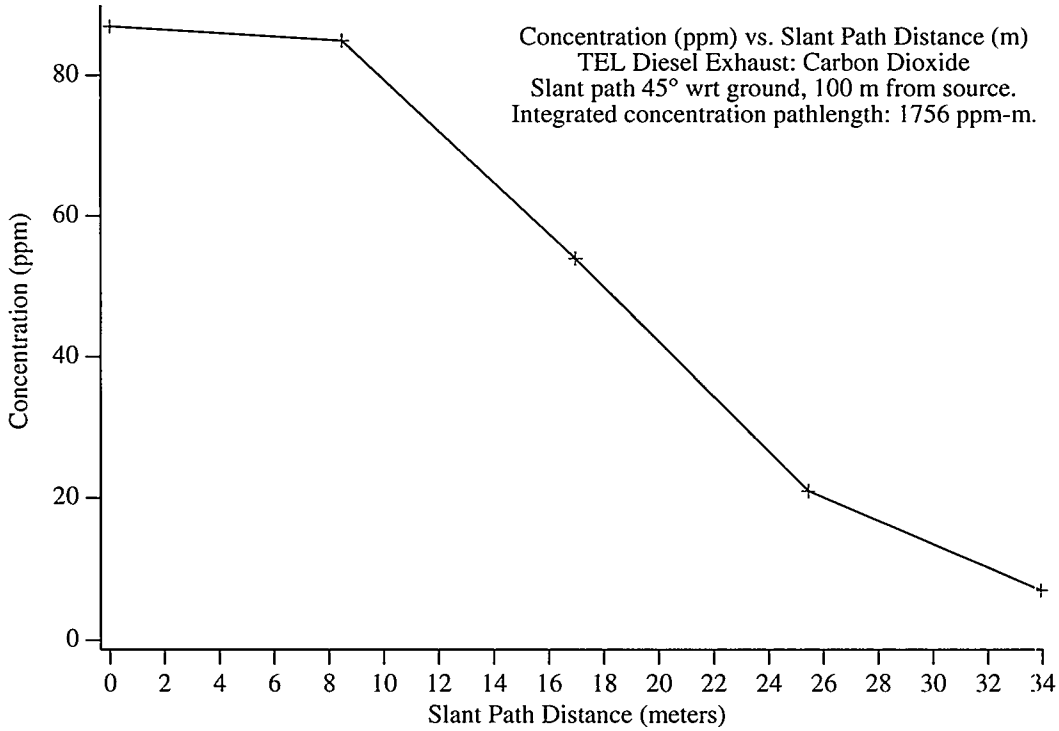
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

TEL Diesel Exhaust: Carbon Dioxide, 75 g/sec, one vent, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
TEL Diesel Exhaust: Carbon Dioxide
75 g/sec, one hour plume, 12 m receptor height
Concentration (ppm)
1000
100
10
1
0.1
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
TEL Diesel Exhaust: Carbon Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 1756 ppm-m.
Concentration (ppm)
80
60
40
20
0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
34
Slant Path Distance (meters)

CHARM Version 9.3

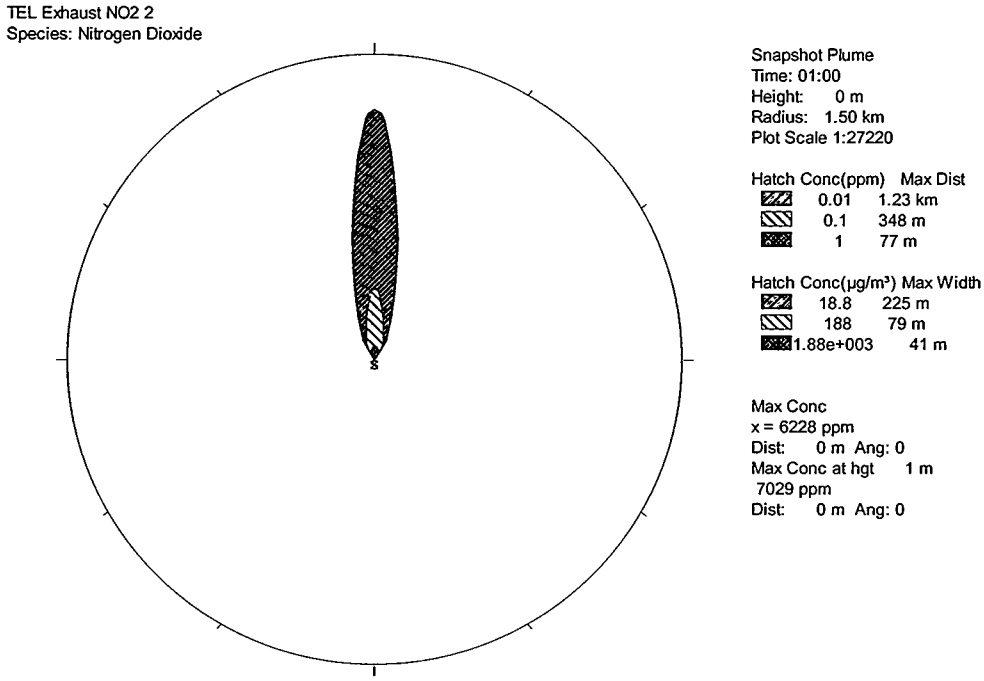
Title:	TEL Diesel Exhaust NO2
Species:	Nitrogen Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.01, 0.1, 1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.75 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	10.6 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

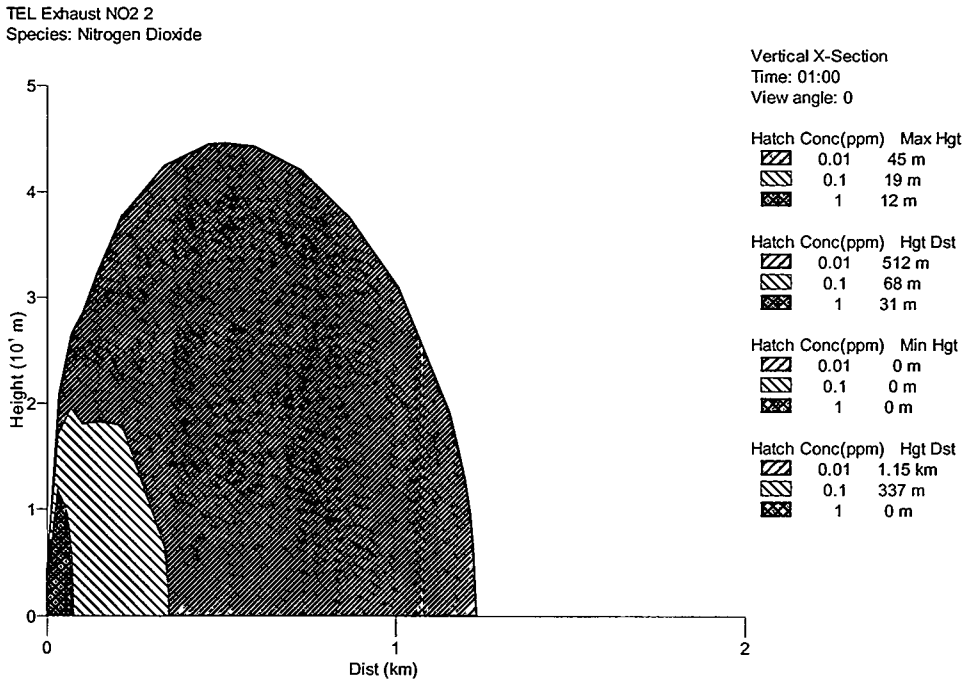
****

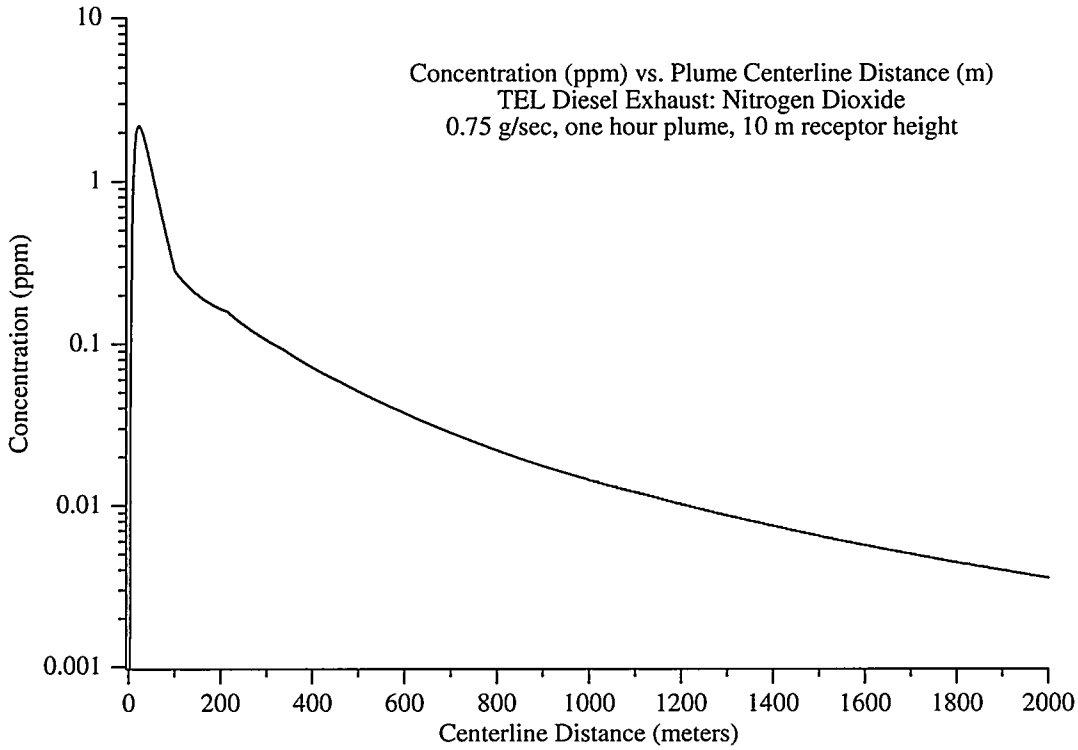
Met Data

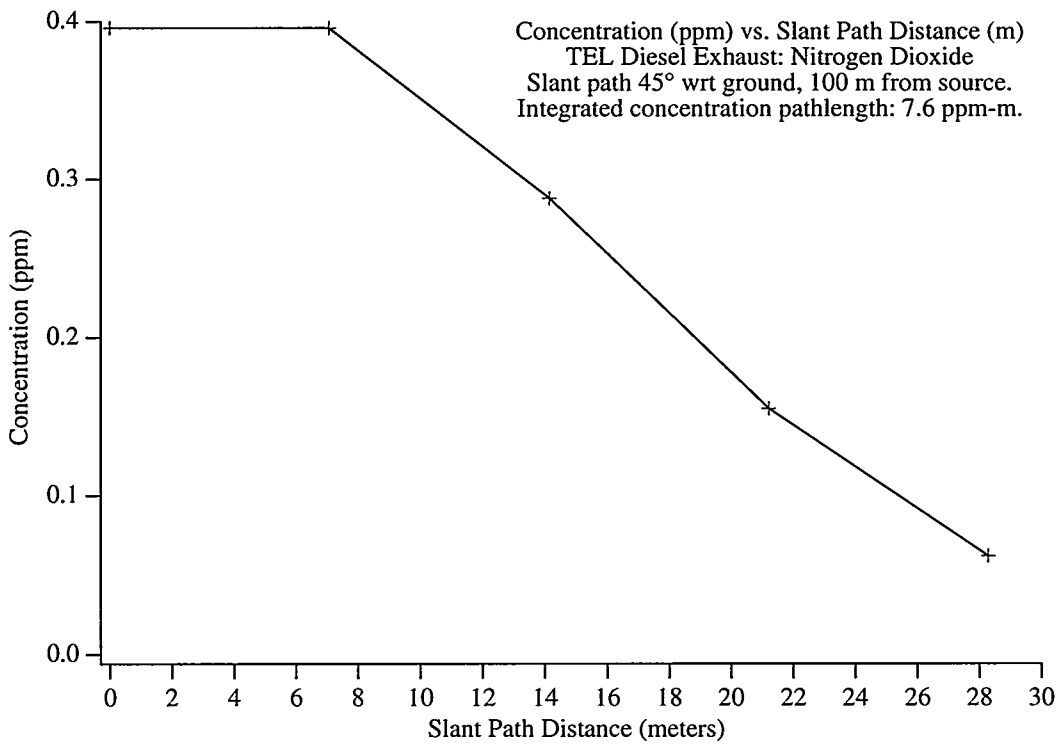
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

TEL Diesel Exhaust: Nitrogen Dioxide, 0.75 g/sec, one vent, one-hour plume.

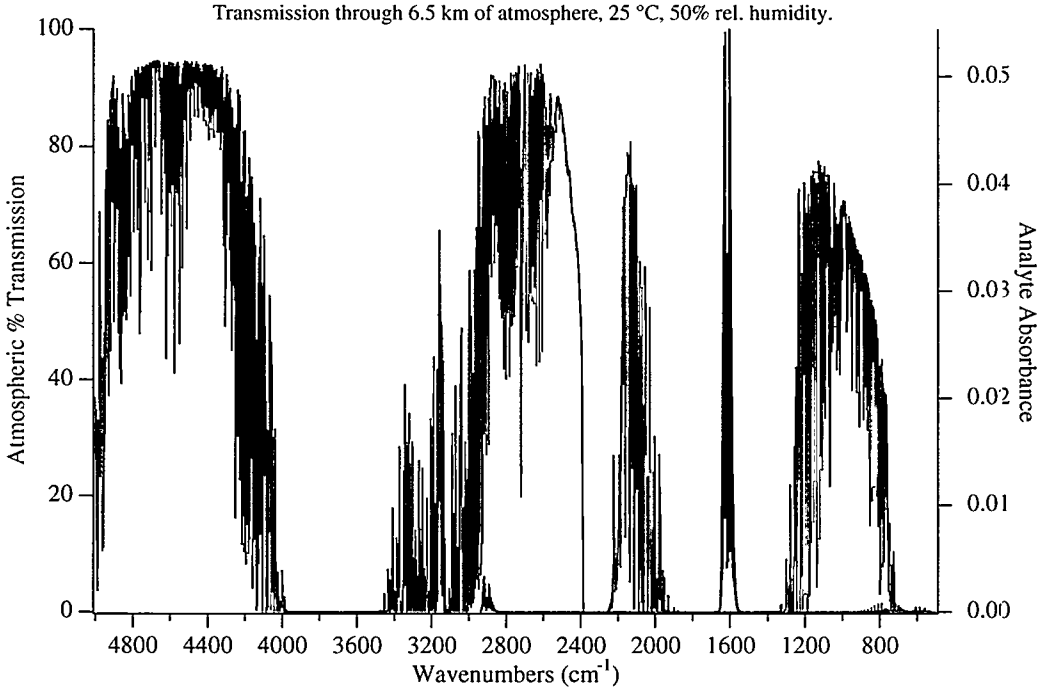




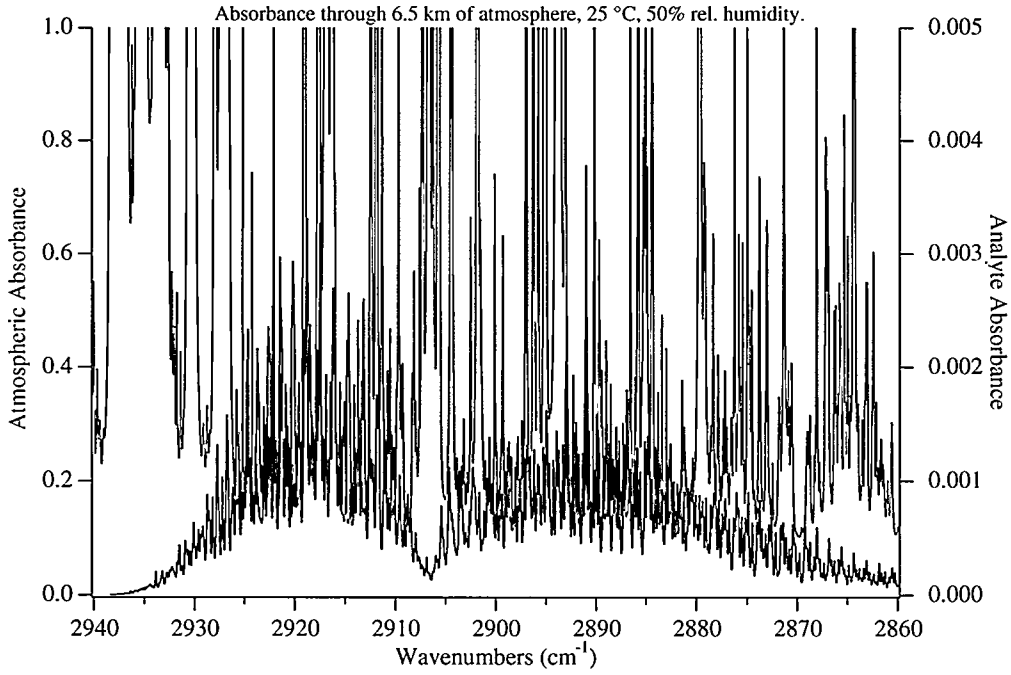

Concentration (ppm) vs. Plume Centerline Distance (m)
TEL Diesel Exhaust: Nitrogen Dioxide
0.75 g/sec, one hour plume, 10 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
TEL Diesel Exhaust: Nitrogen Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 7.6 ppm-m.
Concentration (ppm)
0.4
0.3
0.2
0.1
0.0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
Slant Path Distance (meters)

Nitrogen Dioxide from TEL Diesel Exhaust
Nitrogen dioxide absorbance, 25 °C, 7.6 ppm-m, 100 m from vent.



Nitrogen Dioxide from TEL Diesel Exhaust
Nitrogen dioxide absorbance, 25 °C, 7.6 ppm-m, 100 m from vent.
Detail of $\nu_1 + \nu_3$ band



CHARM Version 9.3

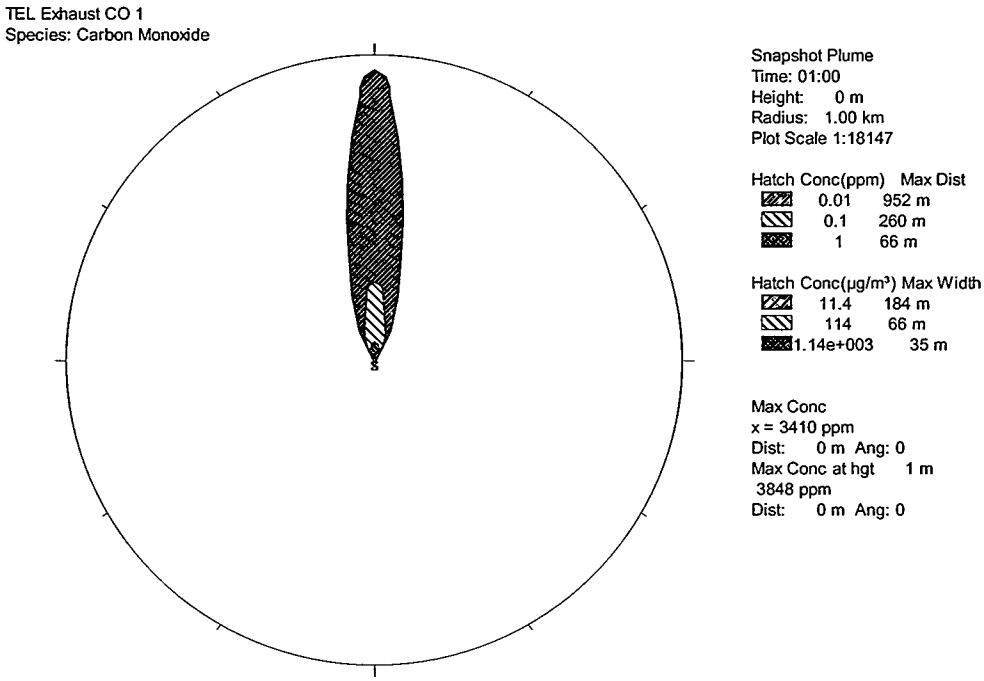
Title:	TEL Diesel Exhaust CO
Species:	Carbon Monoxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.01, 0.1, 1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.25 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	10.5 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

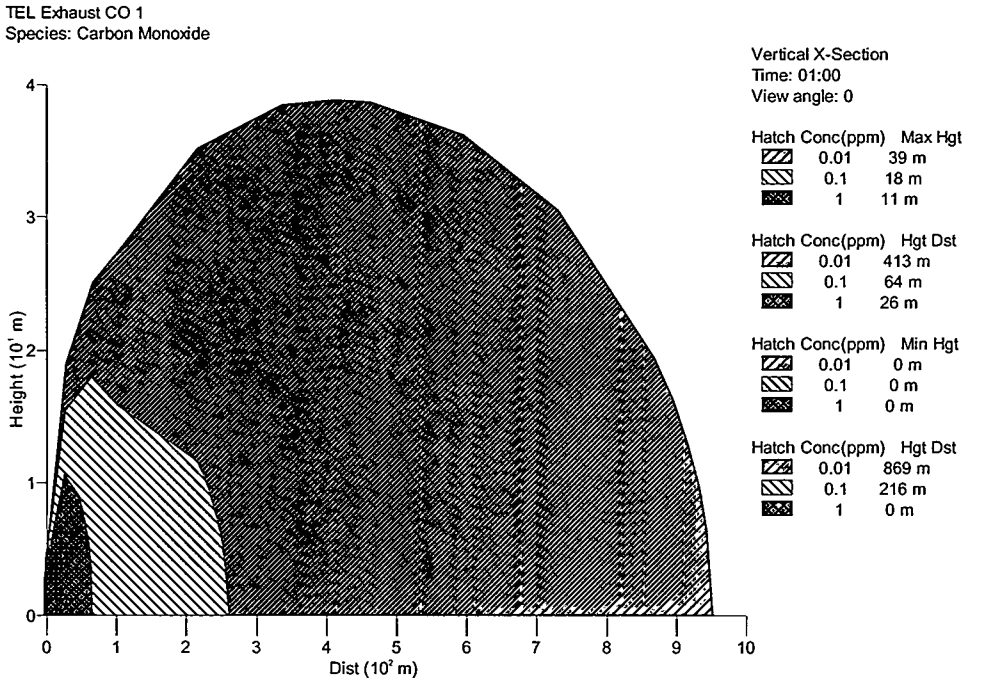
****

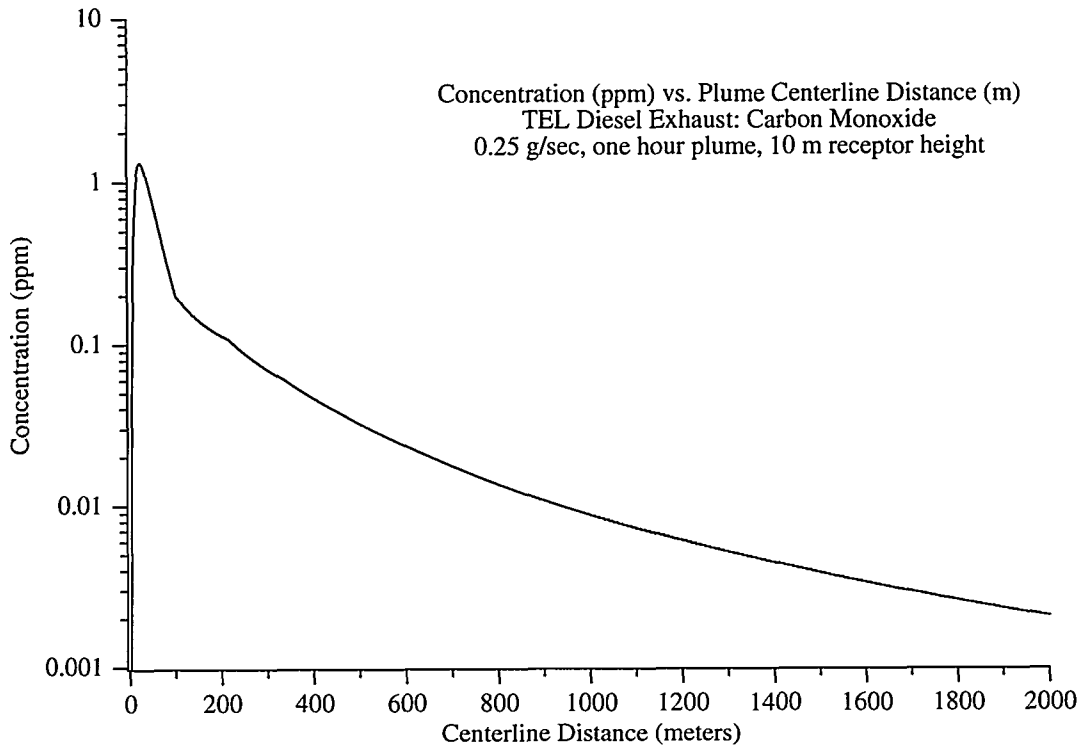
Met Data

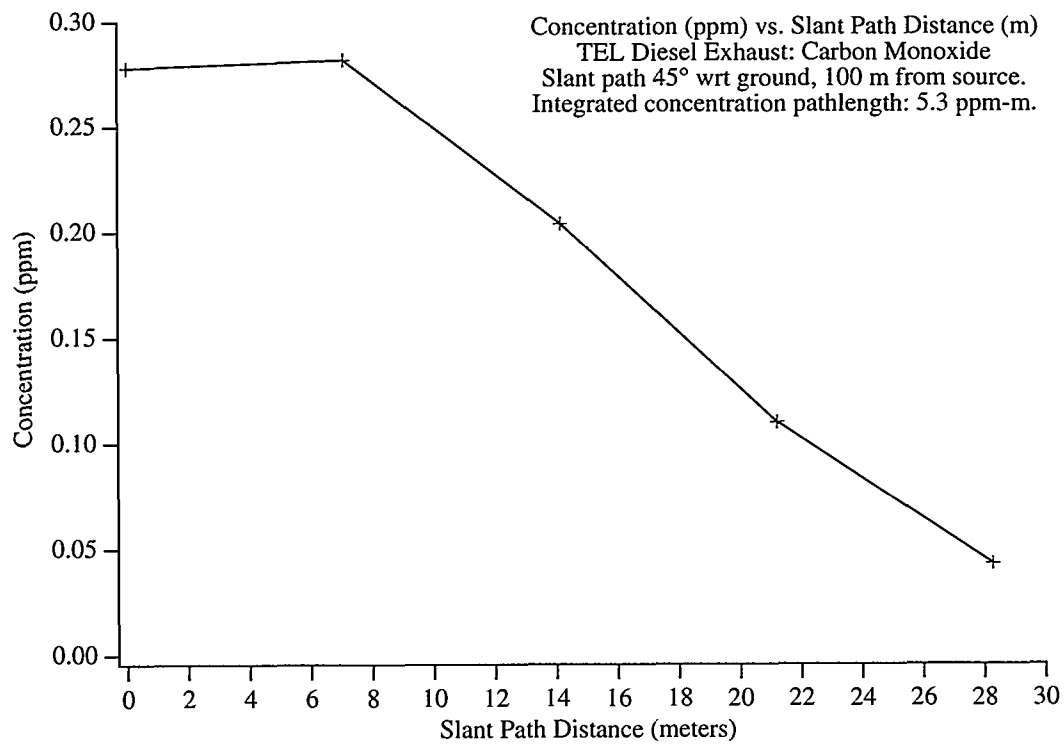
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

TEL Diesel Exhaust: Carbon Monoxide, 0.25 g/sec, one vent, one-hour plume.

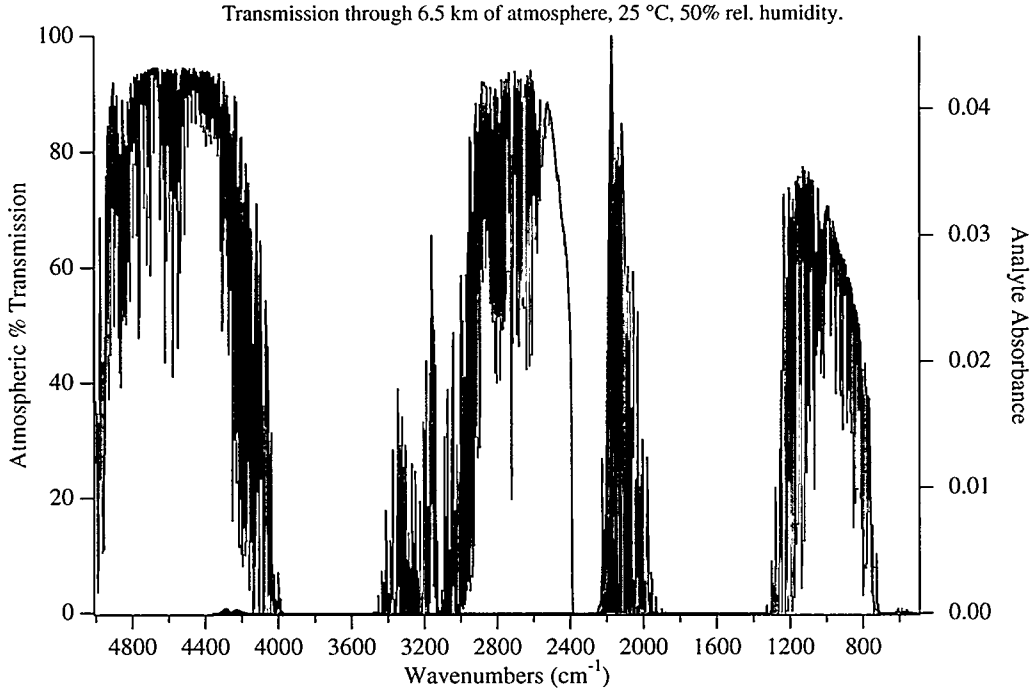




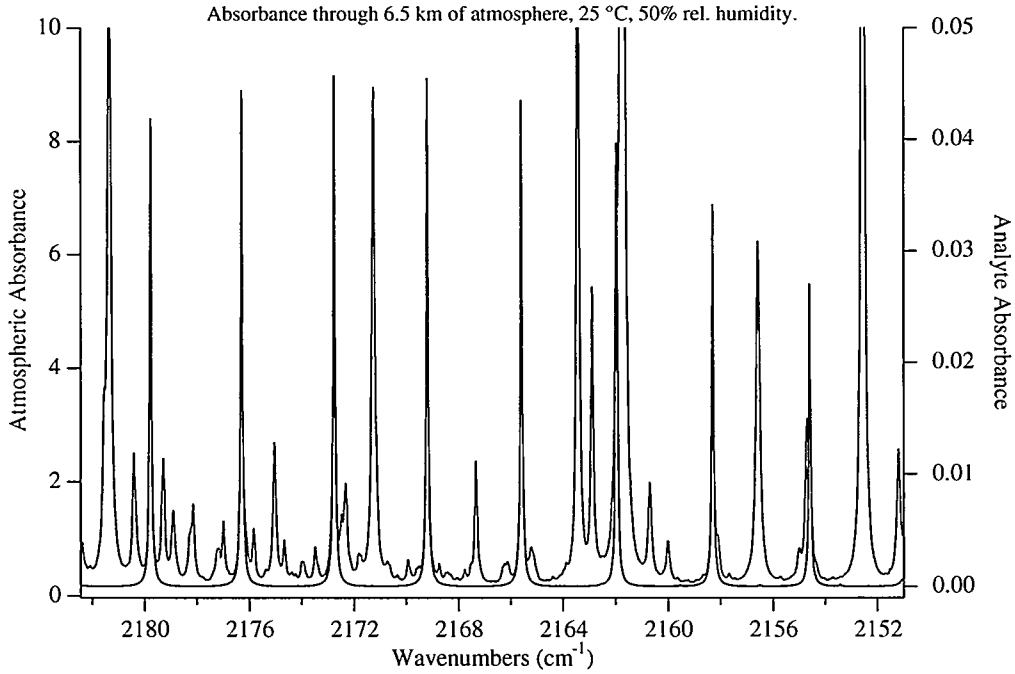

Concentration (ppm) vs. Plume Centerline Distance (m)
TEL Diesel Exhaust: Carbon Monoxide
0.25 g/sec, one hour plume, 10 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
TEL Diesel Exhaust: Carbon Monoxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 5.3 ppm-m.
Concentration (ppm)
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
Slant Path Distance (meters)

Carbon Monoxide from TEL Diesel Exhaust
Carbon Monoxide absorbance, 25 °C, 5.3 ppm-m, 100 m from vent.



Carbon Monoxide from TEL Diesel Exhaust
Carbon monoxide absorbance, 25 °C, 5.3 ppm-m, 100 m from vent.
Detail of R-branch region of fundamental band.



CHARM Version 9.3

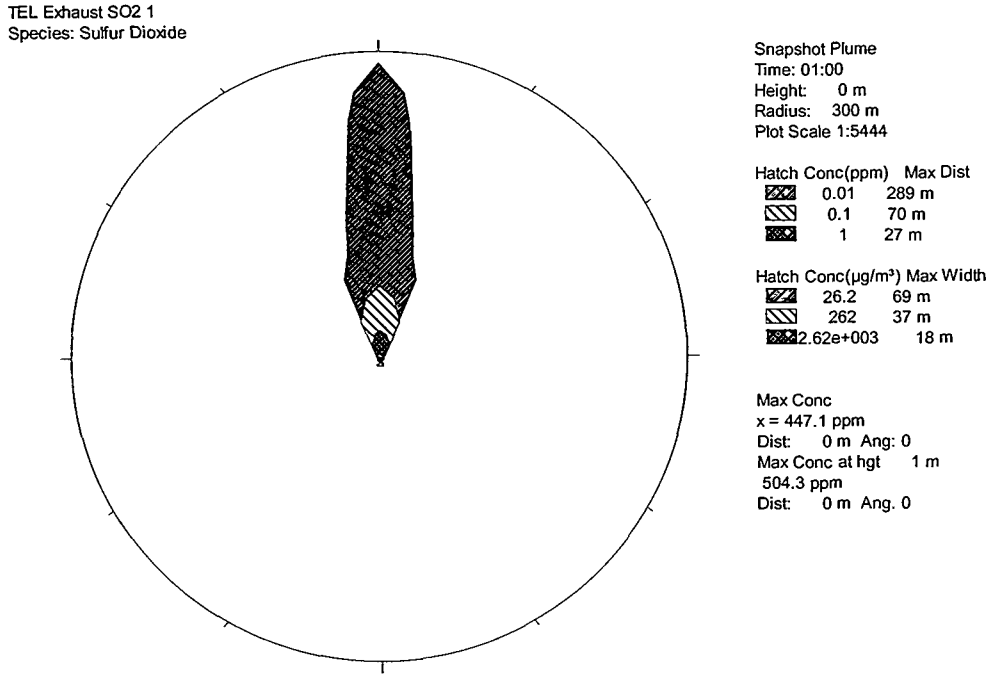
Title:	TEL Diesel Exhaust SO2
Species:	Sulfur Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.01, 0.1, 1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.075 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

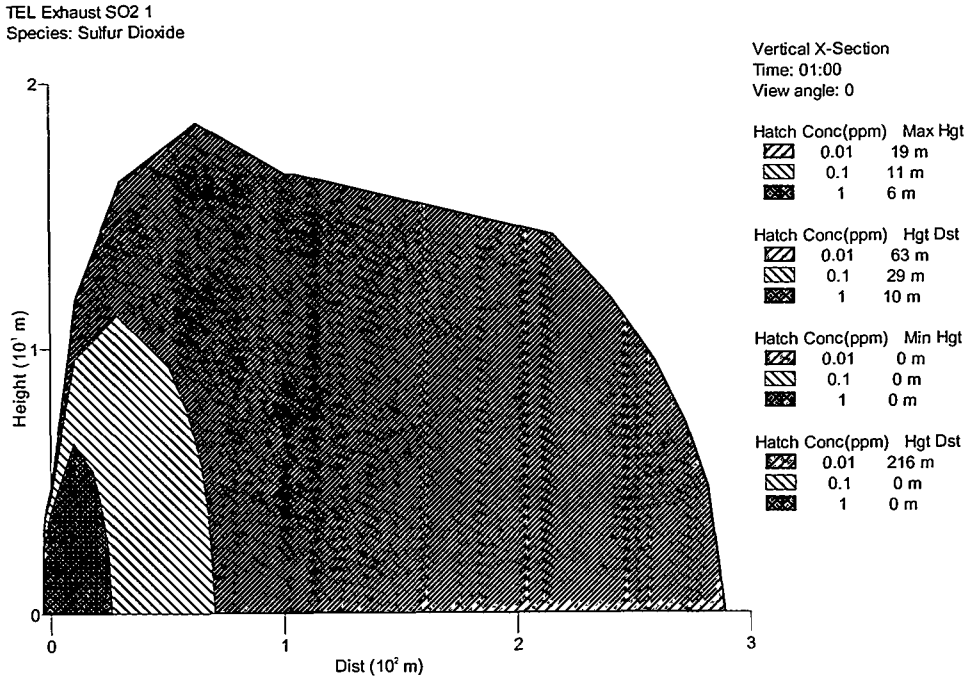
****

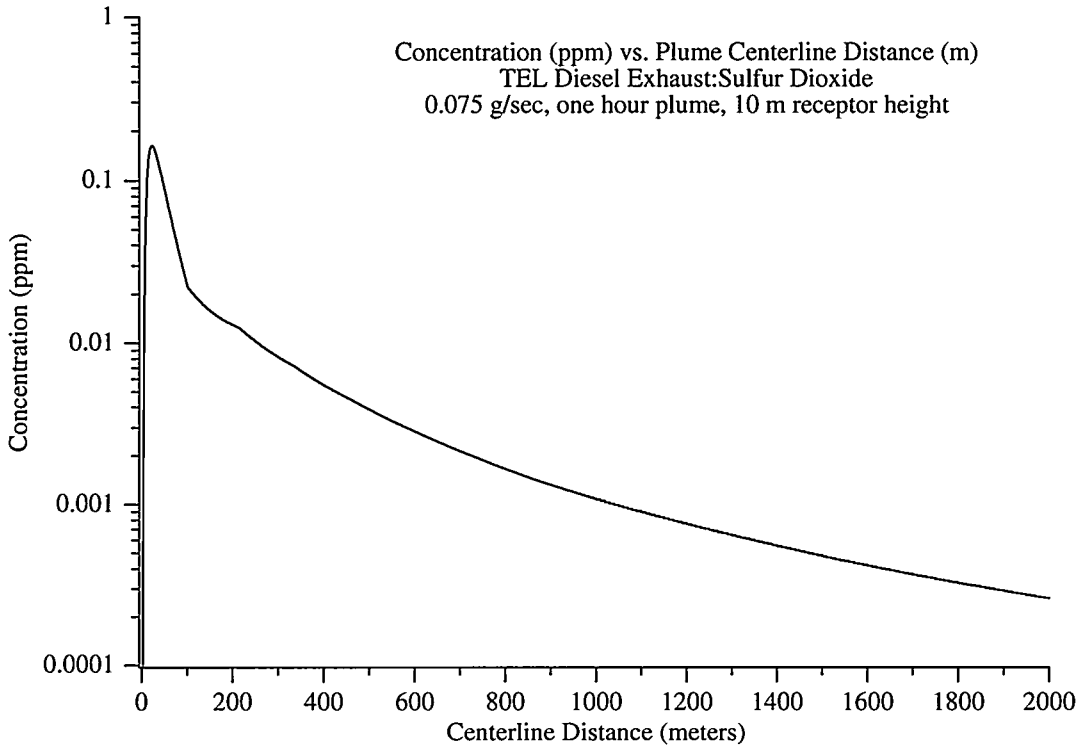
Met Data

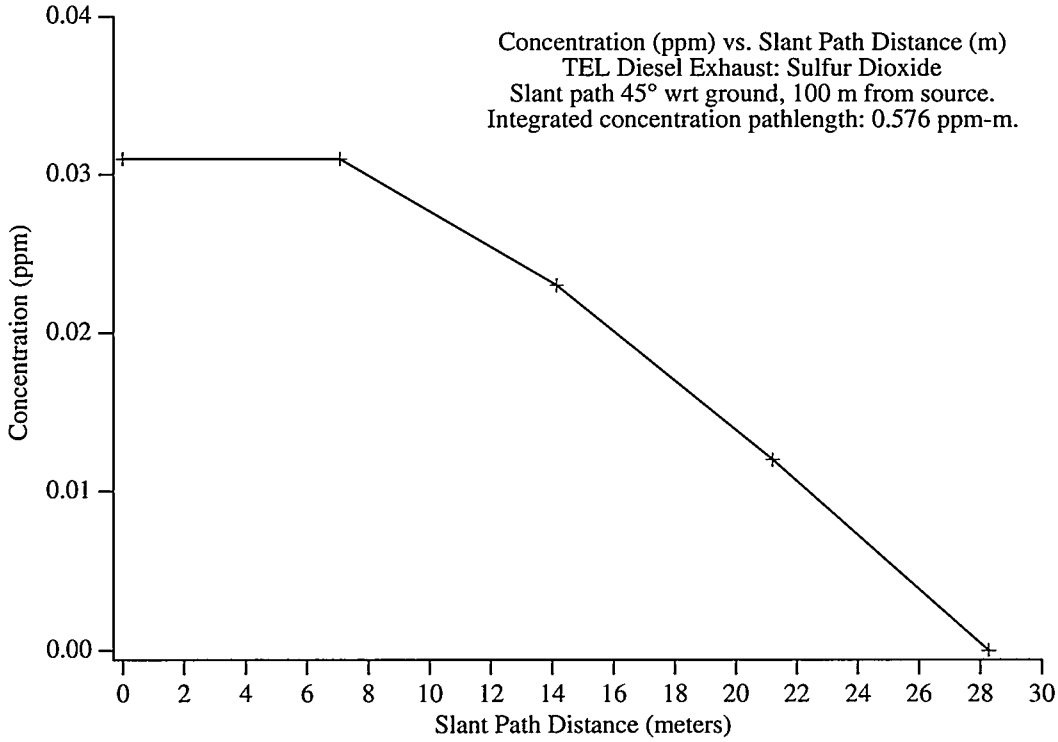
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m²
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

TEL Diesel Exhaust: Sulfur Dioxide, 0.075 g/sec, one vent, one-hour plume.

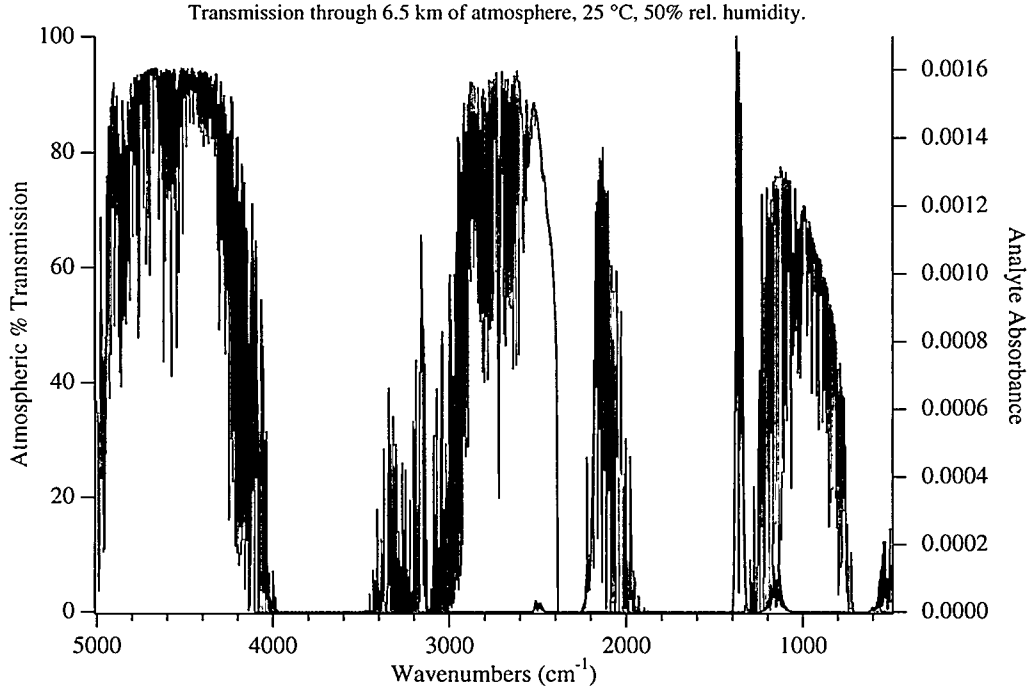




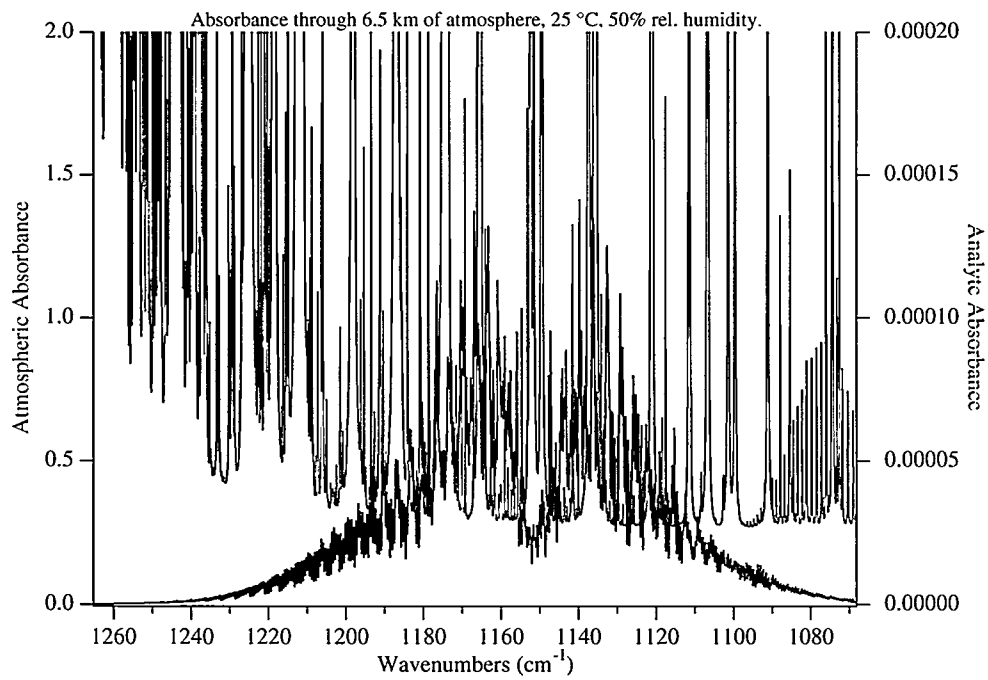

Concentration (ppm) vs. Plume Centerline Distance (m)
TEL Diesel Exhaust:Sulfur Dioxide
0.075 g/sec, one hour plume, 10 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
TEL Diesel Exhaust: Sulfur Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 0.576 ppm-m.
Concentration (ppm)
0.04
0.03
0.02
0.01
0.00
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
Slant Path Distance (meters)

Sulfur Dioxide from TEL Diesel Exhaust
Sulfur dioxide absorbance, 25 °C, 0.576 ppm-m, 100 m from vent.



Sulfur Dioxide from TEL Diesel Exhaust
Sulfur dioxide absorbance, 25 °C, 0.576 ppm-m, 100 m from vent.
Detail of ν_1 band



CHARM Version 9.3

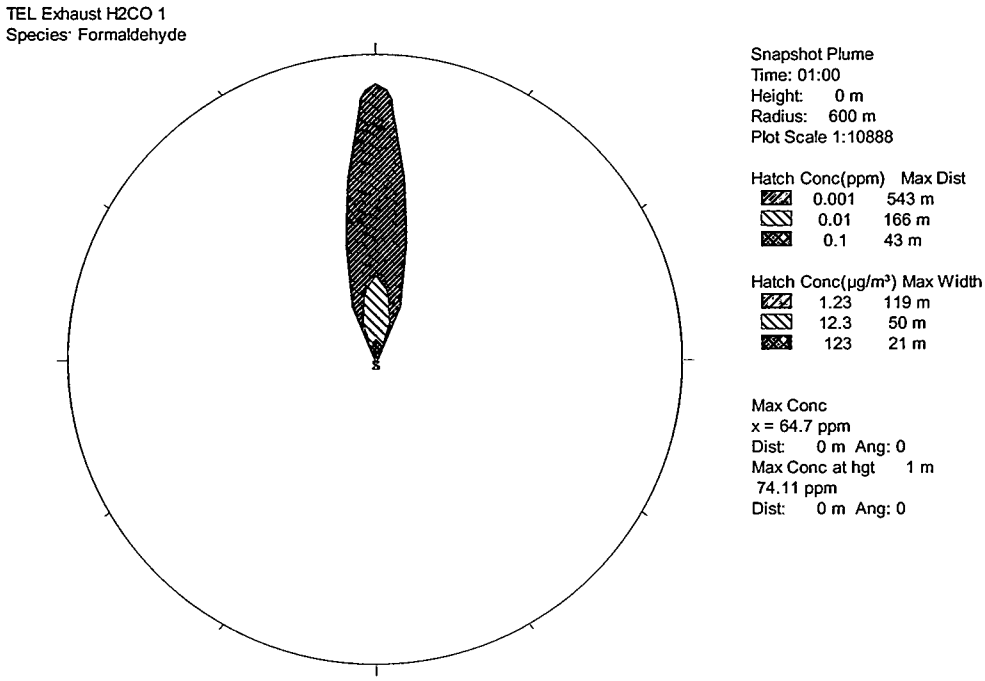
Title:	TEL Diesel Exhaust H2CO
Species:	Formaldehyde
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.005 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

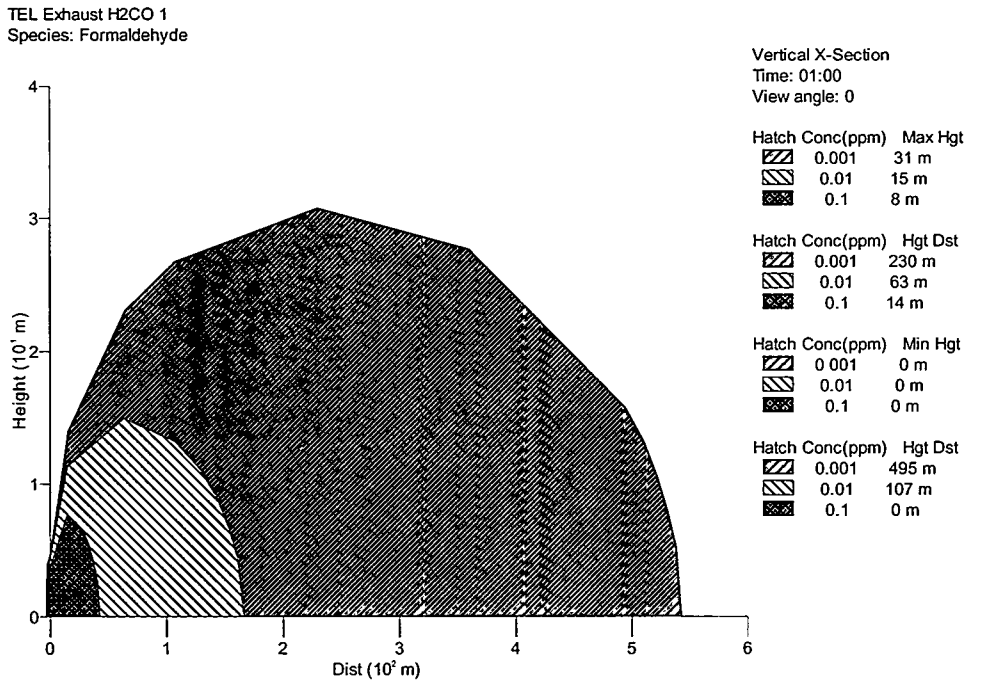
****

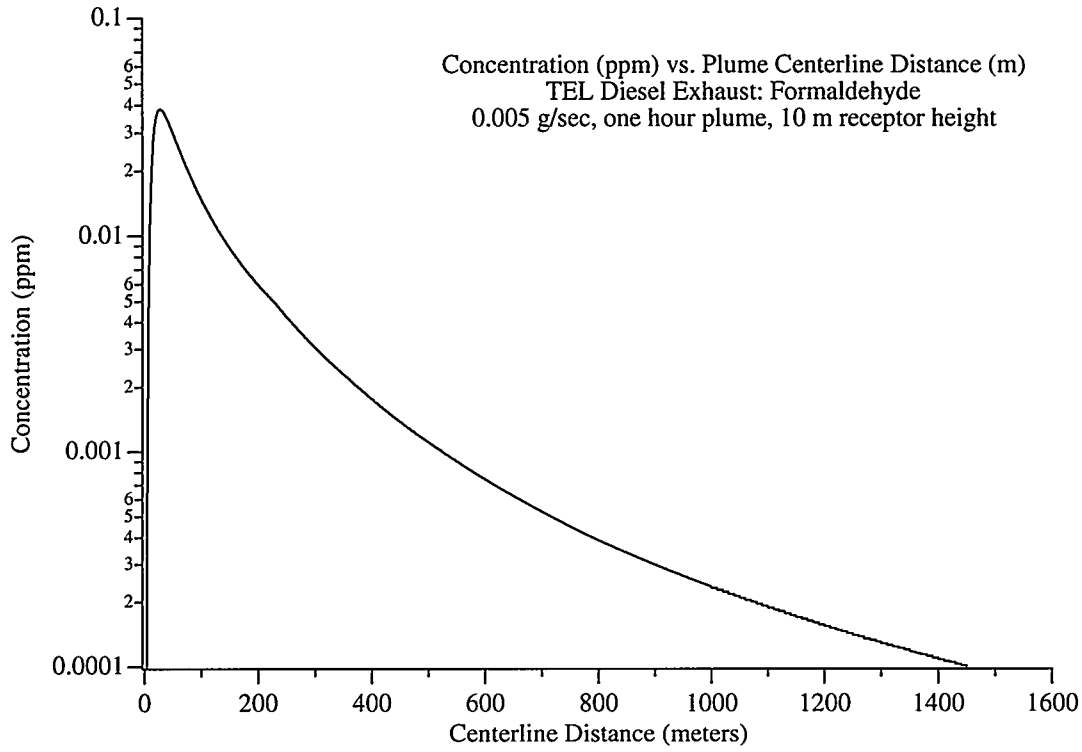
Met Data

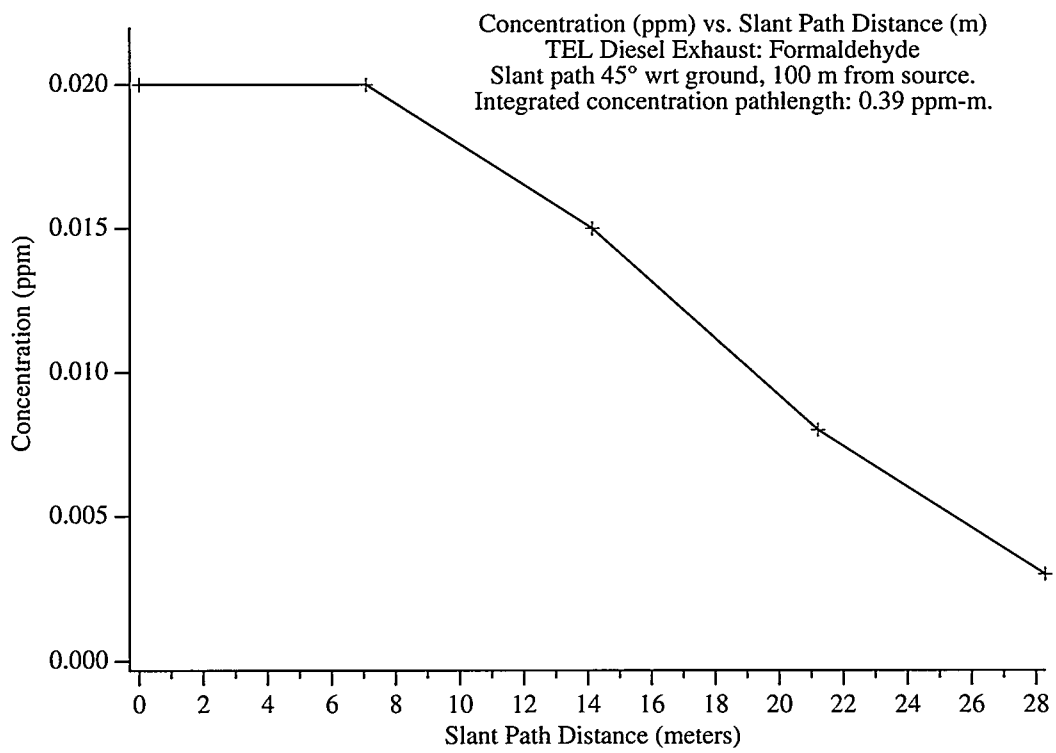
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

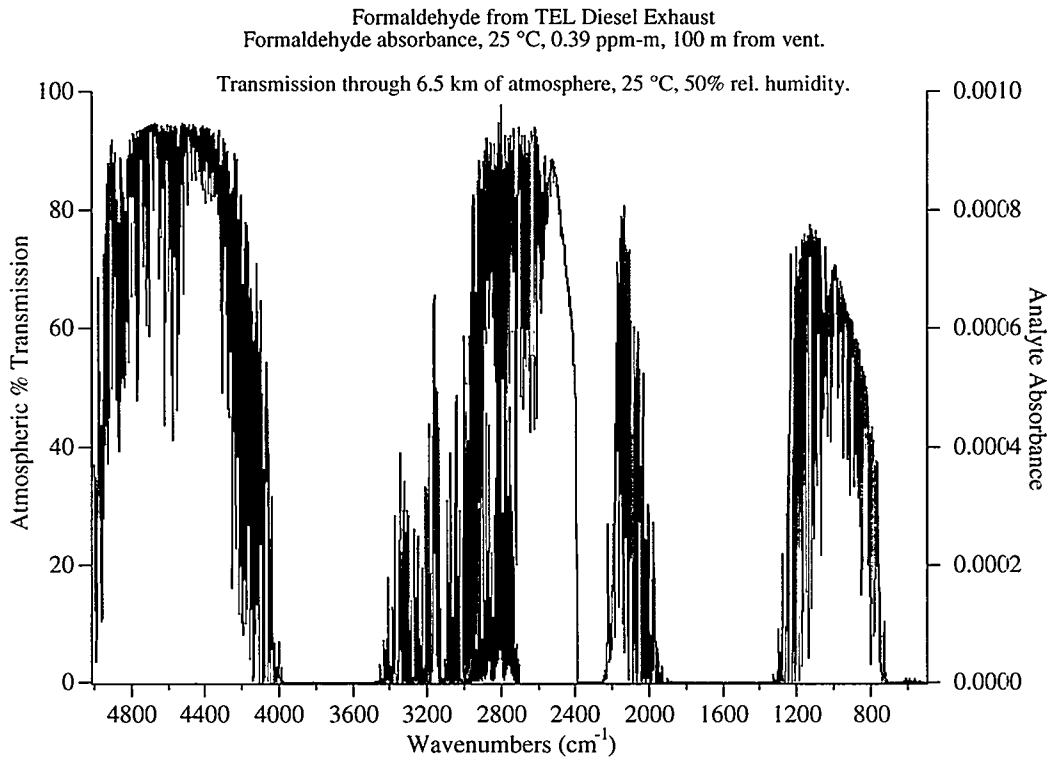
TEL Diesel Exhaust: Formaldehyde, 0.005 g/sec, one vent, one-hour plume.

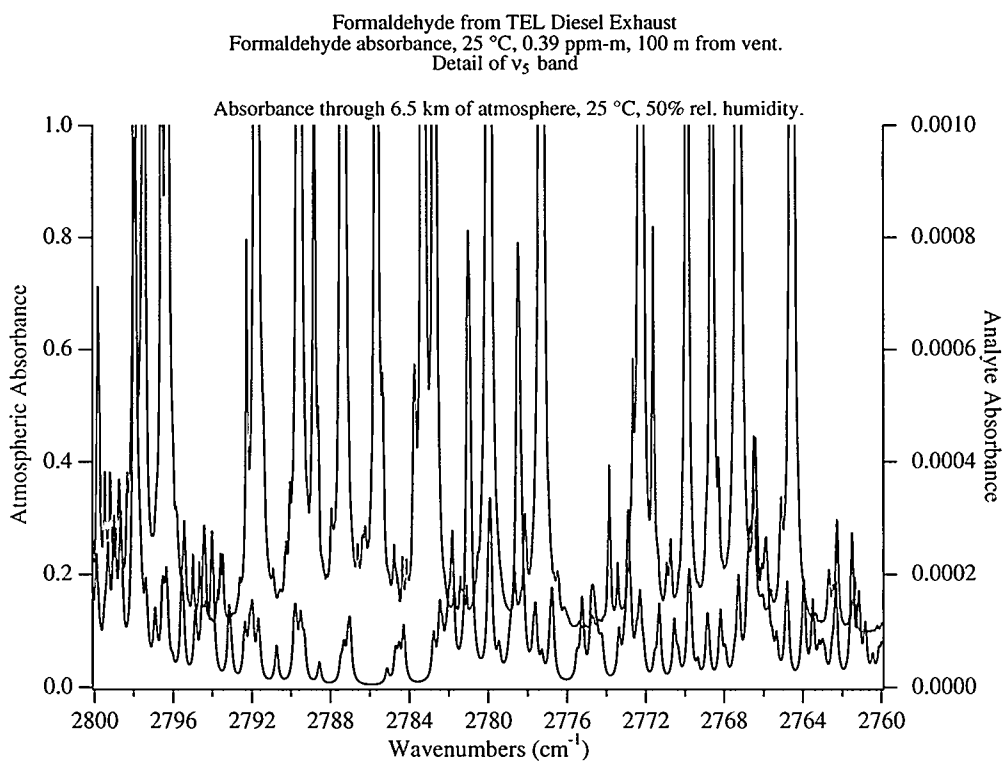





Concentration (ppm) vs. Plume Centerline Distance (m)
TEL Diesel Exhaust: Formaldehyde
0.005 g/sec, one hour plume, 10 m receptor height
Concentration (ppm)
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
TEL Diesel Exhaust: Formaldehyde
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 0.39 ppm-m.
Concentration (ppm)
0.020
0.015
0.010
0.005
0.000
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
Slant Path Distance (meters)


Formaldehyde from TEL Diesel Exhaust
Formaldehyde absorbance, 25 °C, 0.39 ppm-m, 100 m from vent.
Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric % Transmission
Analyte Absorbance
Wavenumbers (cm-1)
100
80
60
40
20
0
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
4800 4400 4000 3600 3200 2800 2400 2000 1600 1200 800


Formaldehyde from TEL Diesel Exhaust
Formaldehyde absorbance, 25 °C, 0.39 ppm-m, 100 m from vent.
Detail of ν5 band
Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric Absorbance
Analyte Absorbance
Wavenumbers (cm-1)
1.0
0.8
0.6
0.4
0.2
0.0
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
2800 2796 2792 2788 2784 2780 2776 2772 2768 2764 2760

CHARM Version 9.3

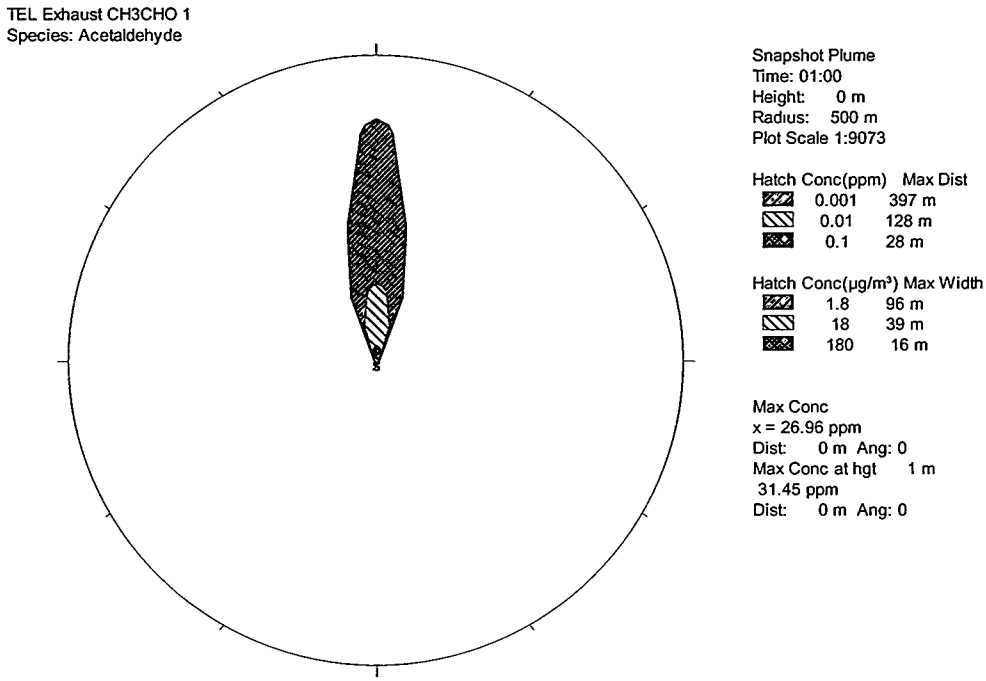
Title:	TEL Diesel Exhaust CH3CHO
Species:	Acetaldehyde
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.003 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

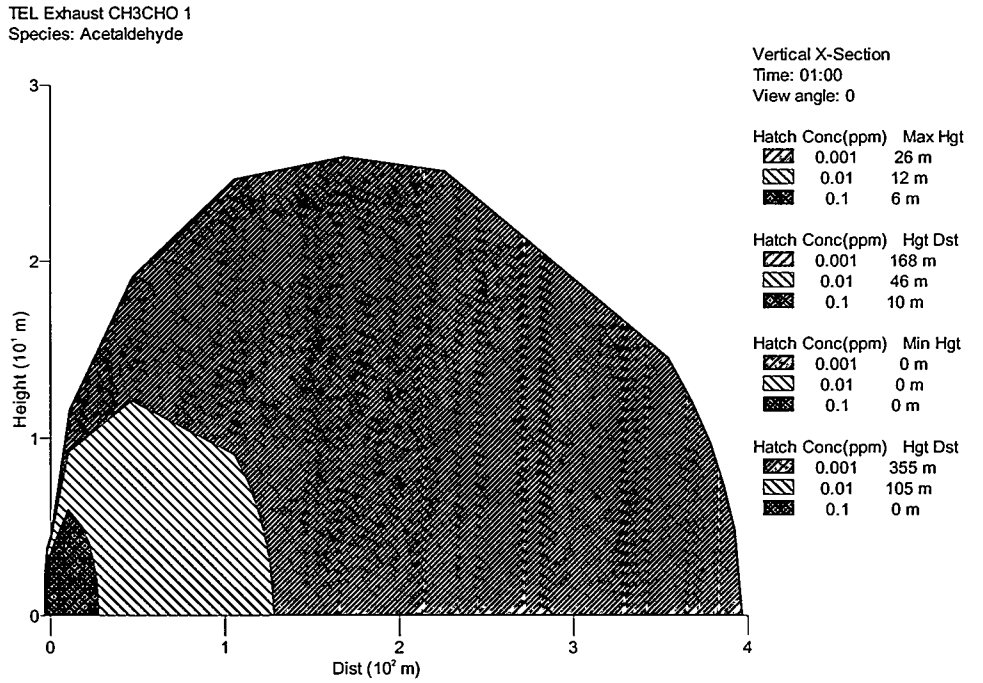
****

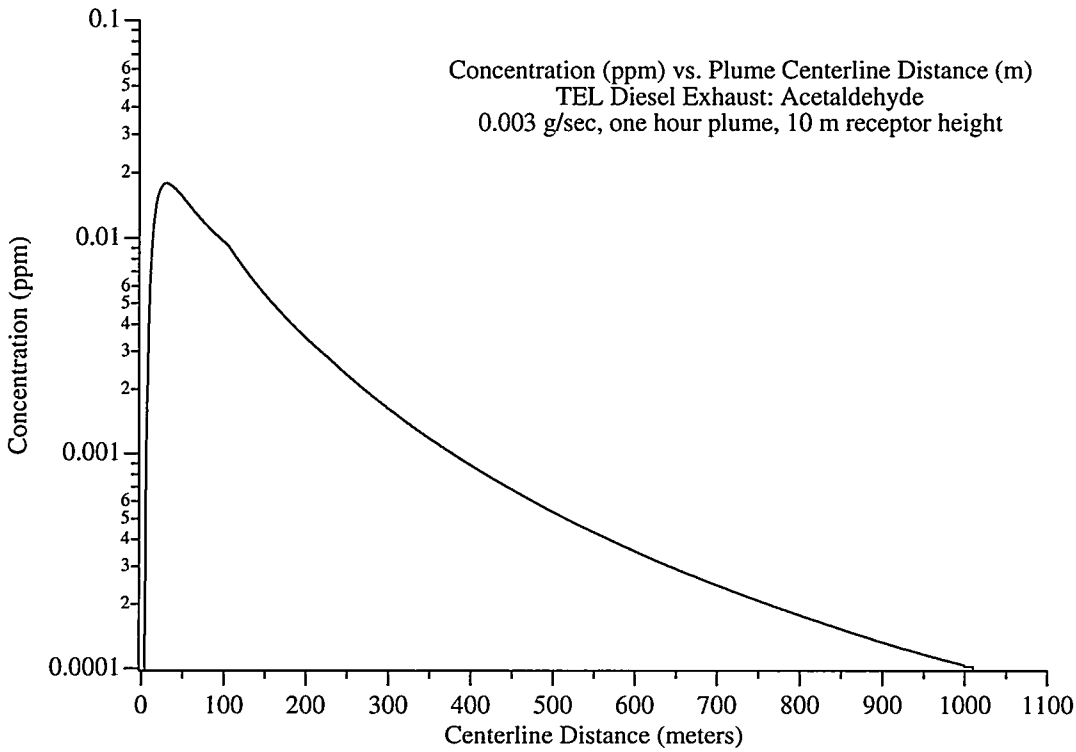
Met Data

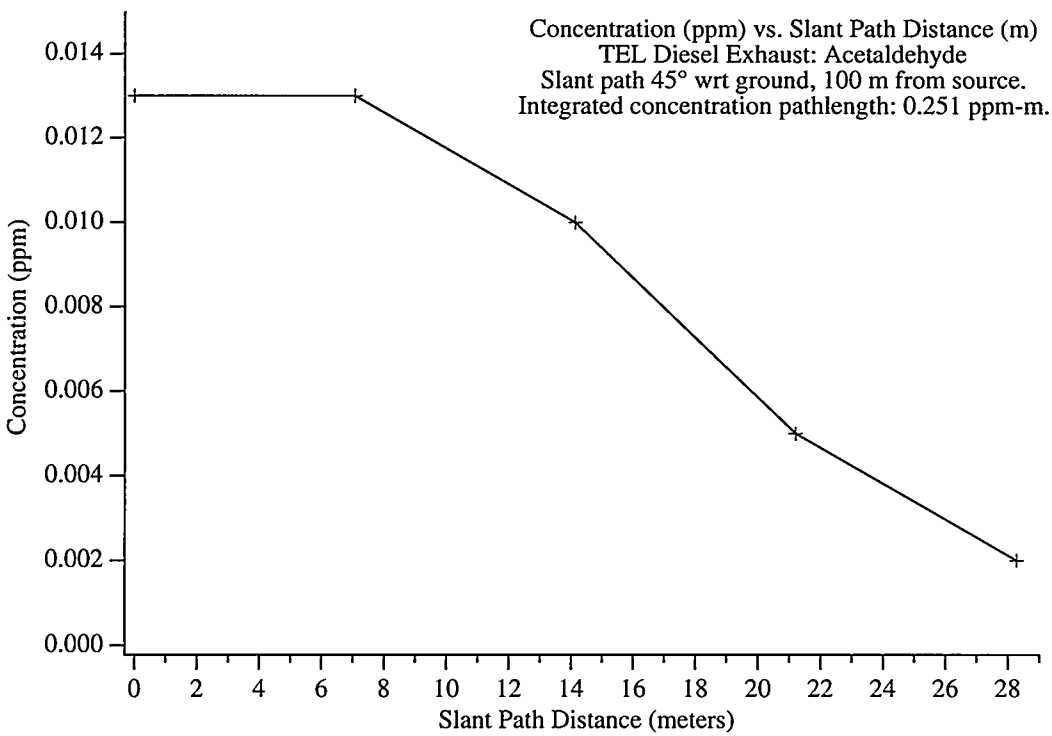
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

TEL Diesel Exhaust: Acetaldehyde, 0.003 g/sec, one vent, one-hour plume.

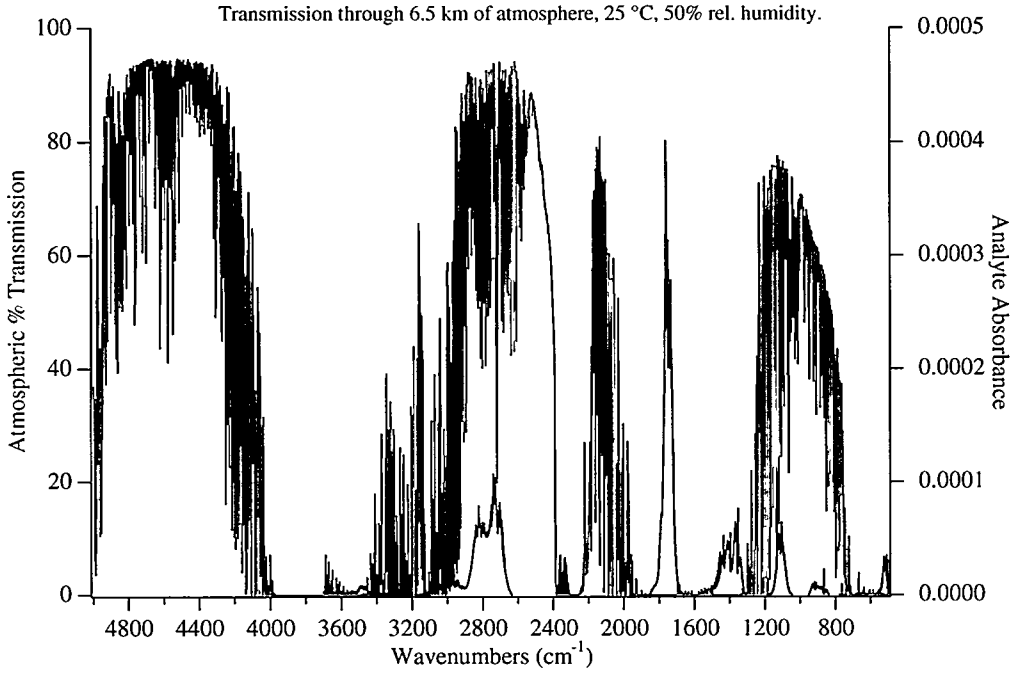




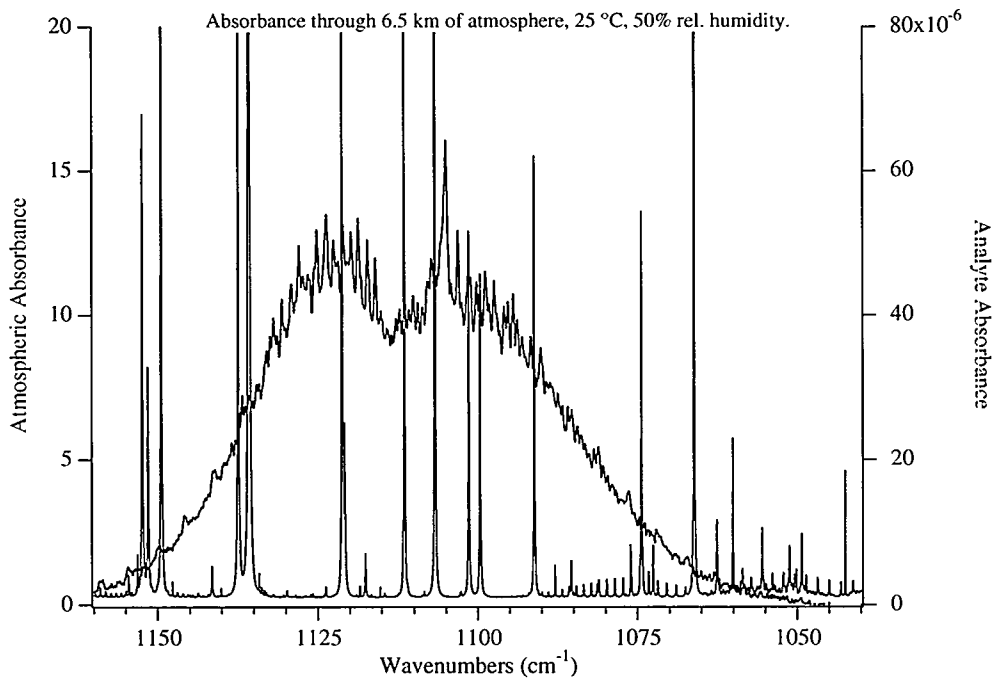

Concentration (ppm) vs. Plume Centerline Distance (m)
TEL Diesel Exhaust: Acetaldehyde
0.003 g/sec, one hour plume, 10 m receptor height
Concentration (ppm)
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
900
1000
1100
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
TEL Diesel Exhaust: Acetaldehyde
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 0.251 ppm-m.
Concentration (ppm)
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
Slant Path Distance (meters)

Acetaldehyde from TEL Diesel Exhaust
Acetaldehyde absorbance, 20 °C, 0.251 ppm-m, 100 m from vent.
Hanst database.

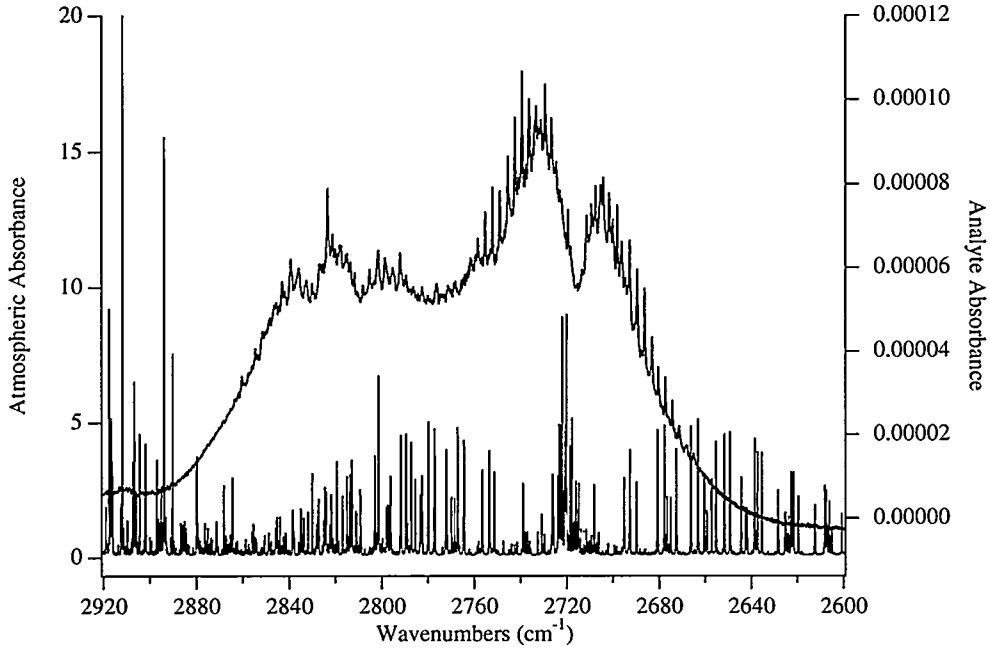


Acetaldehyde from TEL Diesel Exhaust
Acetaldehyde absorbance, 20 °C, 0.251 ppm-m, 100 m from vent.
ν_8 band, Hanst database.



Acetaldehyde from TEL Diesel Exhaust
Acetaldehyde absorbance, 20 °C, 0.251 ppm-m, 100 m from vent.
ν_2 and ν_3 region, Hanst database.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



2.3 Diesel Storage Evaporation

Compound	Emission rate (g/sec)
Octane	0.003
Cyclooctane	0.003
2,2,4-Trimethylpentane	0.003
Xylene	0.003
Hexane	0.002
Cyclohexane	0.002
2,2-Dimethylbutane	0.002
Benzene	0.002
Heptane	0.002
Cycloheptane	0.002
2,2-Dimethylpentane	0.002
2,4-Dimethylpentane	0.002
Toluene	0.002

Scenario: Assume a diesel storage volume of 800,000 liters and a volume evaporation rate of 0.1 volume%/month (Becker *et al.* 1995; Fingas 1997). This is an underground tank with snorkel venting. Assuming a fuel density of 0.85 g/cm^3, this gives an evaporation rate of about 0.1 g/sec.

Diesel fuel consists of thousands of compounds with a mass% distribution of compounds peaked at carbon number sixteen (C16) (Bacha *et al.* 1998). The most volatile compounds are those with C10 or less. Though these compounds comprise less than 2 mass% of the fuel, they account for approximately half the vapor pressure over the liquid at 25 °C. To obtain a list of relatively simple spectral signature molecules, we consider here the diesel vapor to be comprised of unbranched, branched, and cycloalkanes and aromatics between C6 and C10 (Woodrow and Seiber 1988; EST 1982).

CHARM Version 9.3

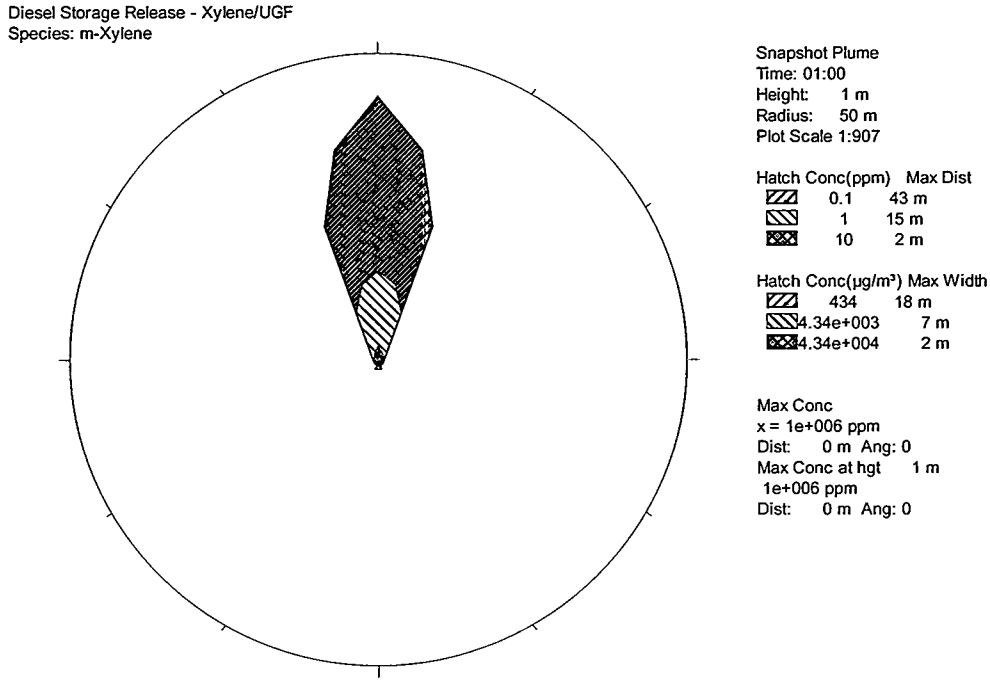
Title:	Diesel Storage Release - Xylene/UGF
Species:	m-Xylene
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Direction:	0°
Release Height Above Ground	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.003 g/s
Release Duration:	24 hrs
Puff Temperature:	30°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 mph
Vertical Puff Speed (Calculated):	3.58e-006 m/s
Exit state assumed:	vapor
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

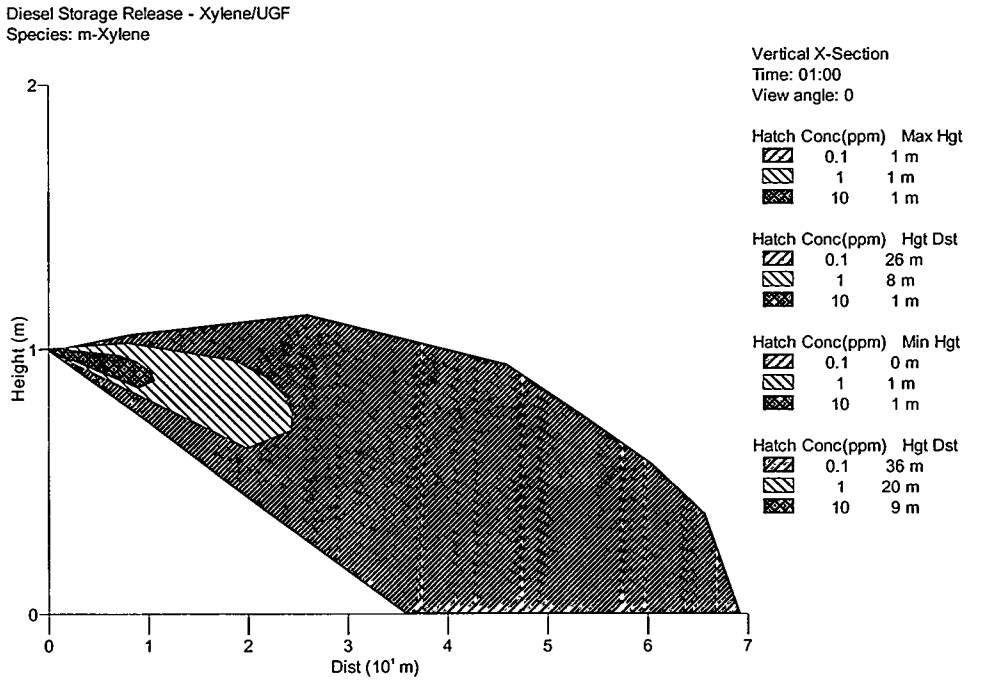
****

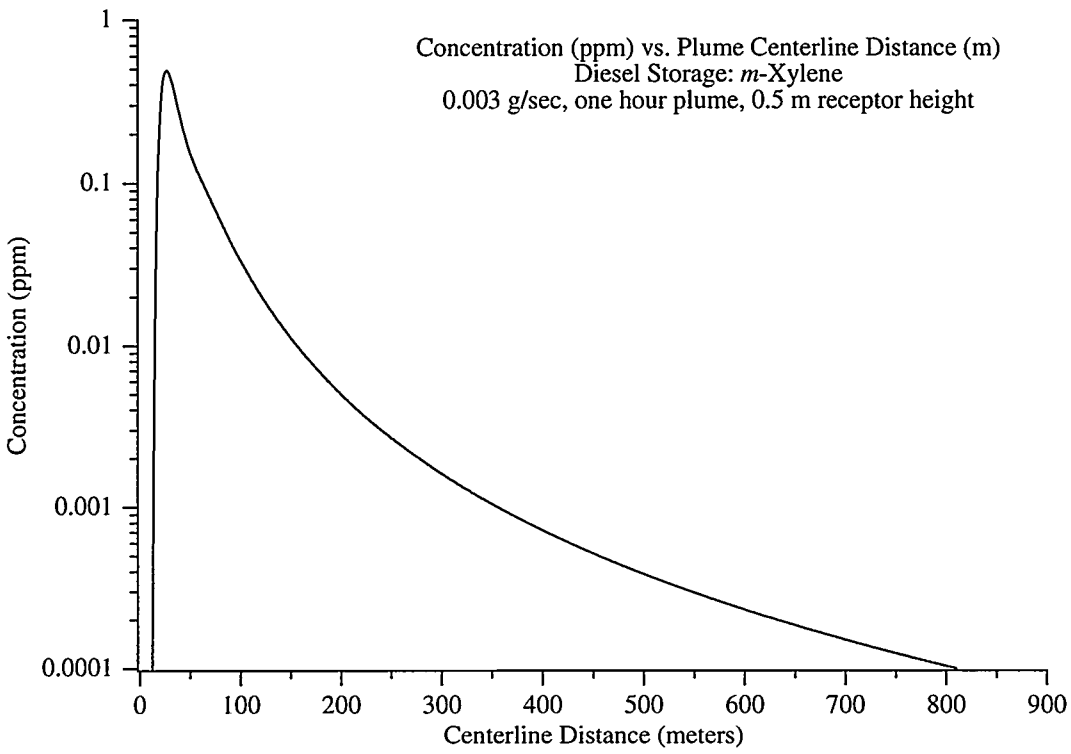
Met Data

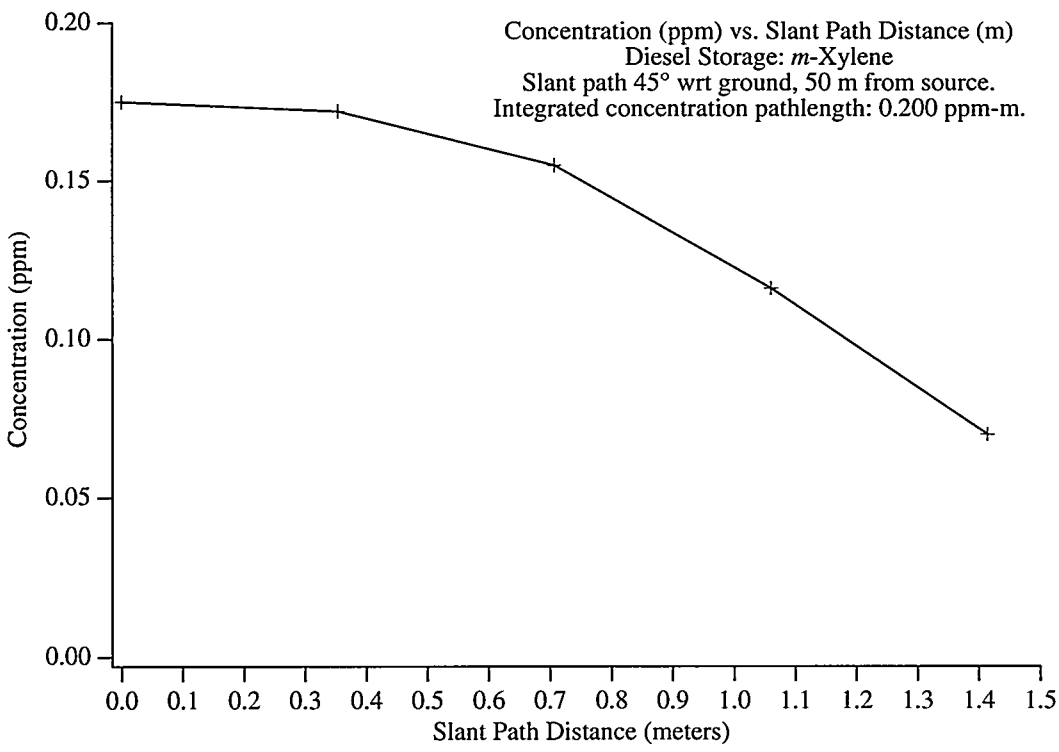
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	10
Stability Class:	D (Calculated, Sunshine = high)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Winds Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Storage Evaporation: *m*-Xylene, 0.003 g/sec, one-hour plume.

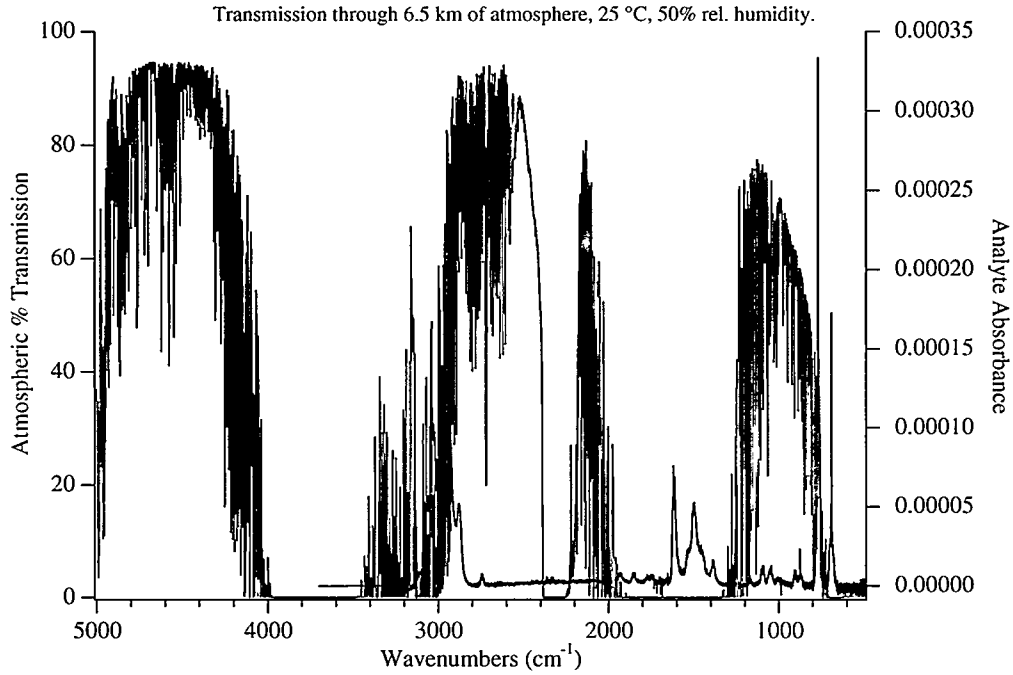




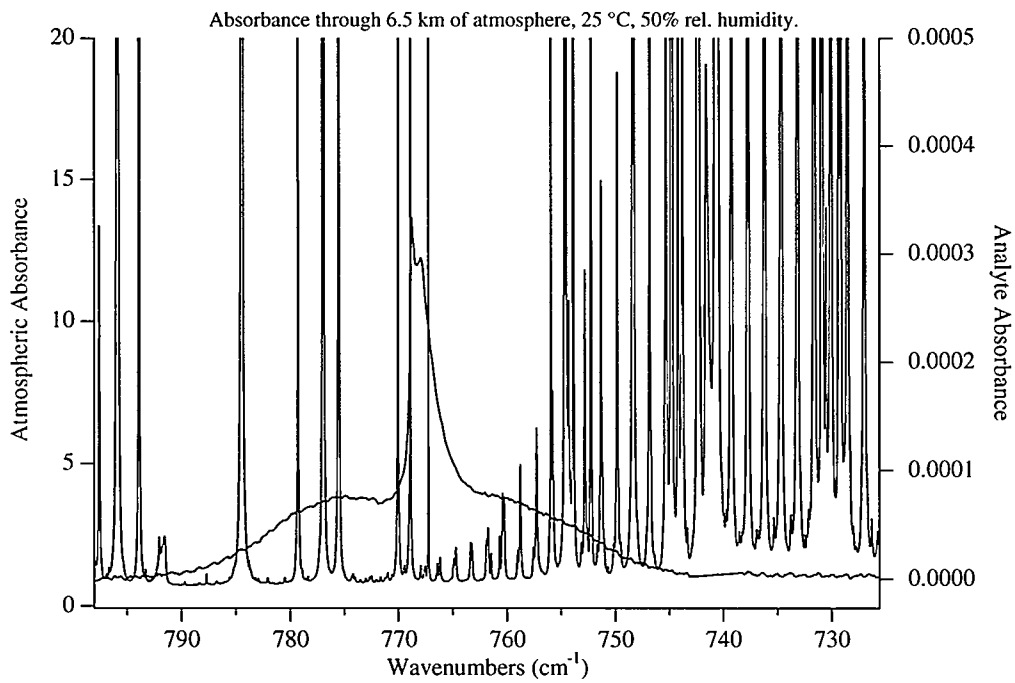

Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Storage: m-Xylene
0.003 g/sec, one hour plume, 0.5 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
900
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Storage: m-Xylene
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 0.200 ppm-m.
Concentration (ppm)
0.20
0.15
0.10
0.05
0.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
Slant Path Distance (meters)

m-Xylene from Diesel Fuel Storage Evaporation
m-Xylene absorbance, 20 °C, 0.2 ppm-m, 50 m from vent.
Hanst database.



m-Xylene from Diesel Fuel Storage Evaporation
m-Xylene absorbance, 20 °C, 0.2 ppm-m, 50 m from vent.
Hanst database.



CHARM Version 9.3

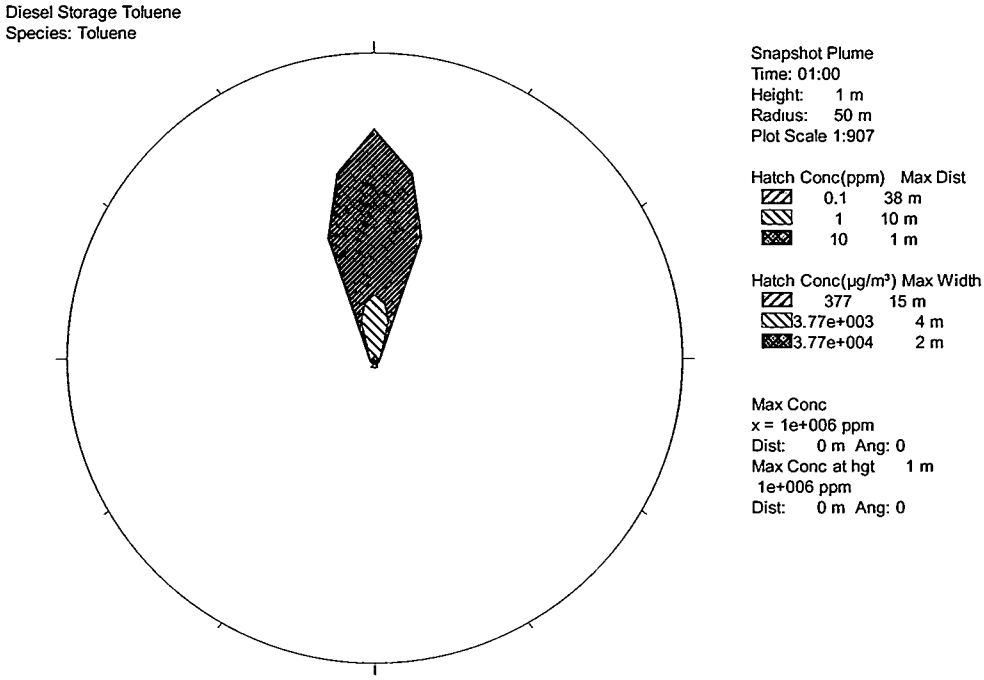
Title:	Diesel Storage Toluene
Species:	Toluene
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Direction:	0°
Release Height Above Ground	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.002 g/s
Release Duration:	24 hrs
Puff Temperature:	30°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 mph
Vertical Puff Speed (Calculated):	2.75e-006 m/s
Exit state assumed:	vapor
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

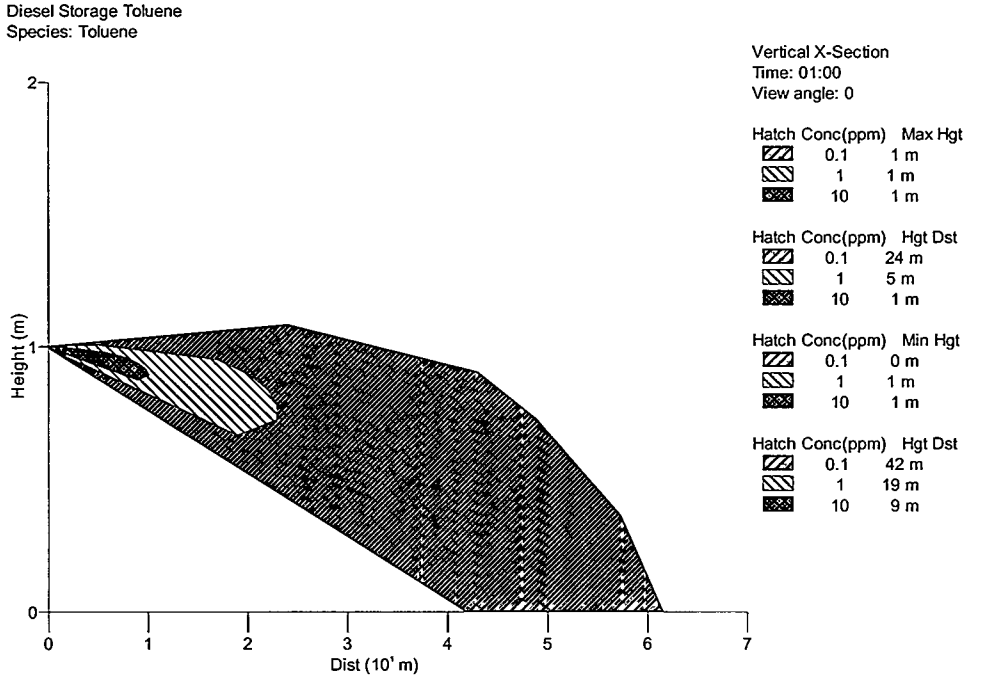
****

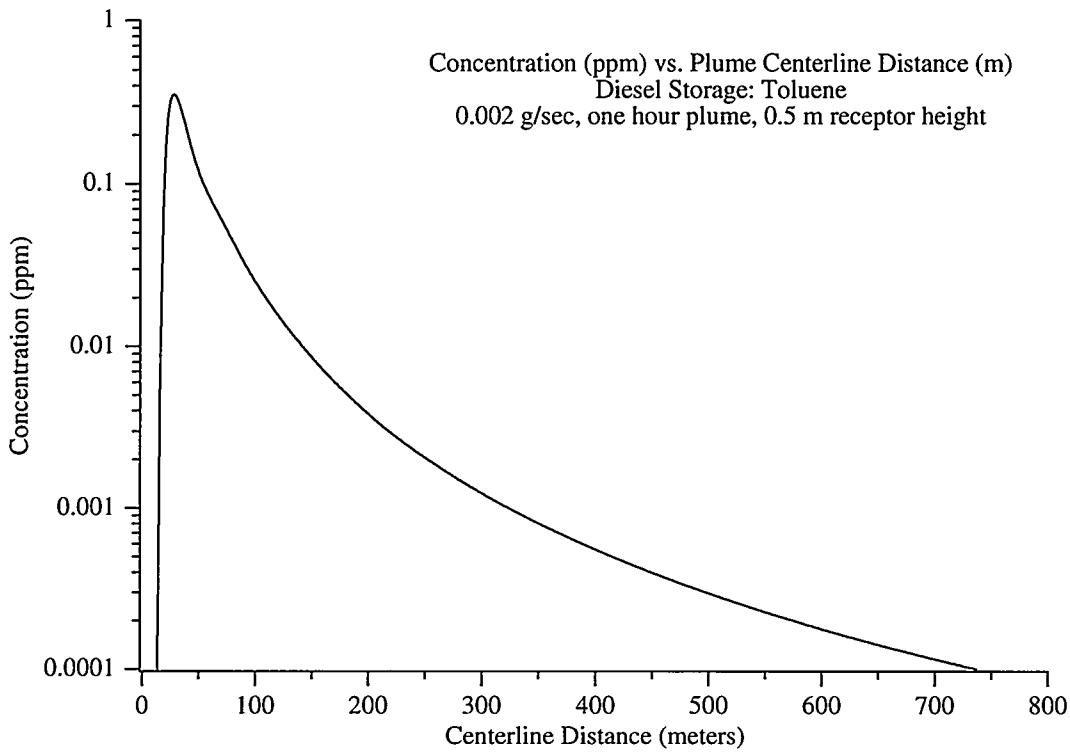
Met Data

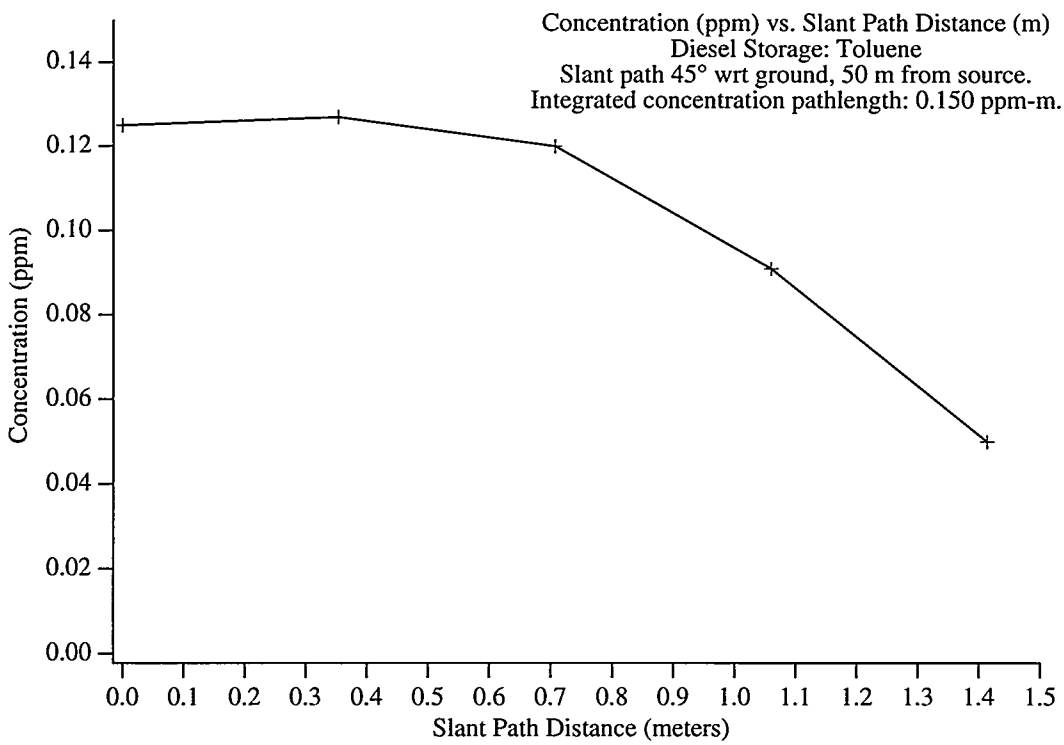
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Winds Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Storage Evaporation: Toluene, 0.002 g/sec, one-hour plume.

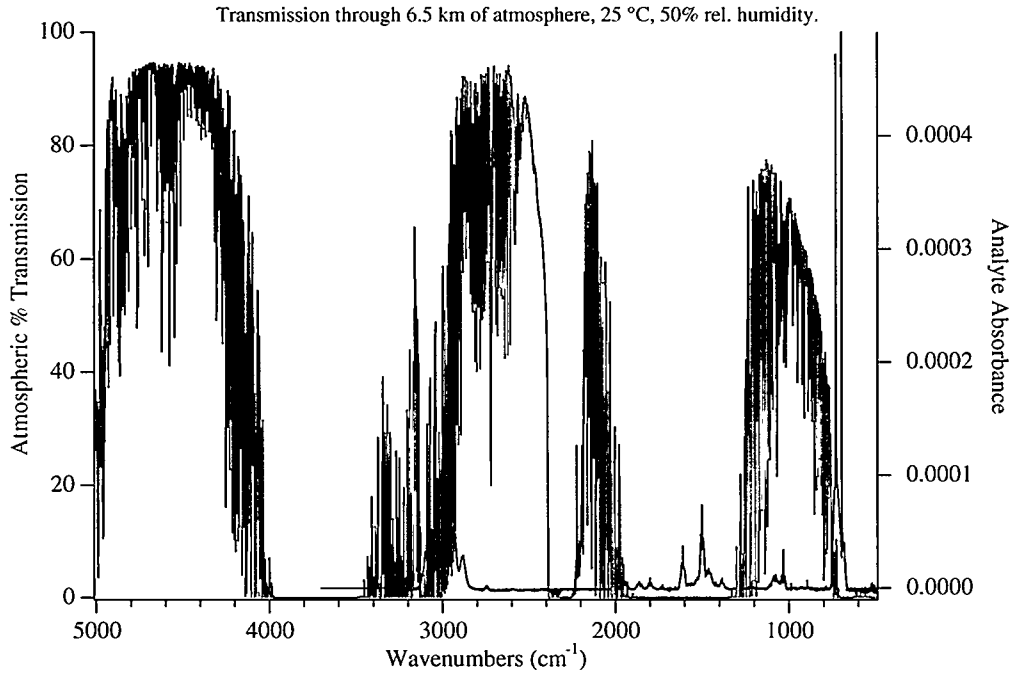




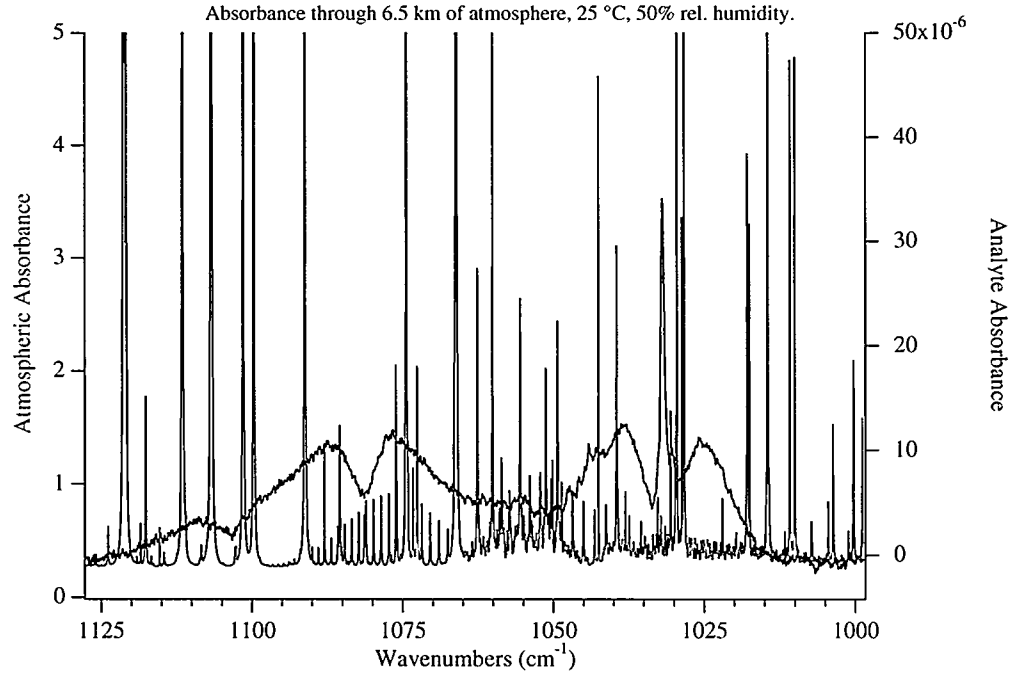

Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Storage: Toluene
0.002 g/sec, one hour plume, 0.5 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Storage: Toluene
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 0.150 ppm-m.
Concentration (ppm)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
Slant Path Distance (meters)

Toluene from Diesel Fuel Storage Evaporation
Toluene absorbance, 20 °C, 0.15 ppm-m, 50 m from vent.
Hanst database.



Toluene from Diesel Fuel Storage Evaporation
Toluene absorbance, 20 °C, 0.15 ppm-m, 50 m from vent.
Hanst database.



CHARM Version 9.3

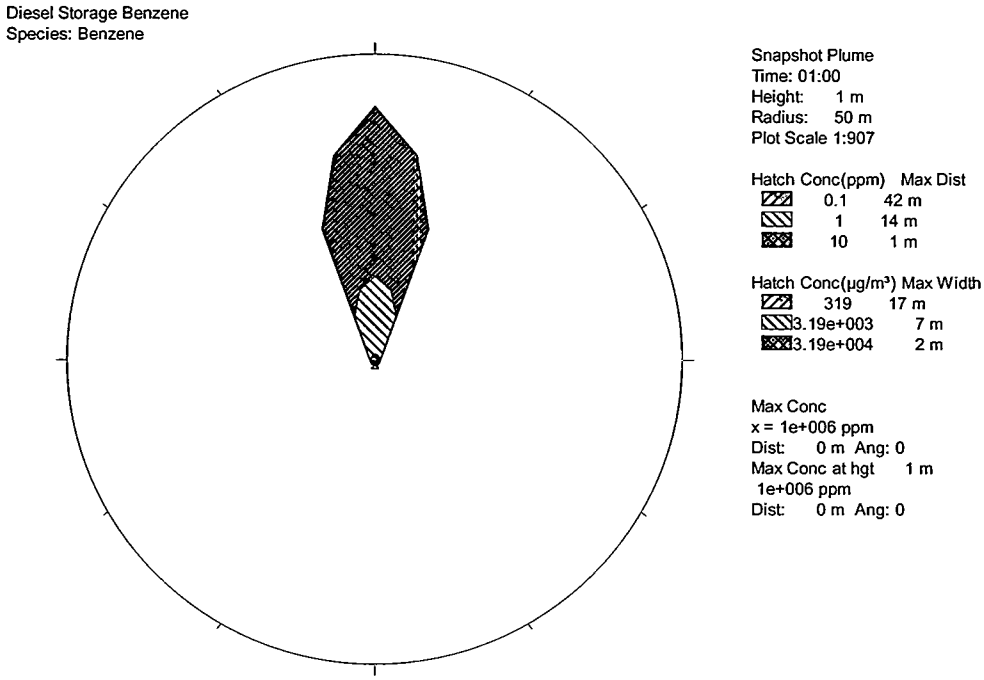
Title:	Diesel Storage Benzene
Species:	Benzene
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	0.1 , 1 , 10
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.002 g/s
Release Duration:	24 hrs
Puff Temperature:	30°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 mph
Vertical Puff Speed (Calculated):	3.244e-006 m/s
Exit State Assumed:	vapor
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

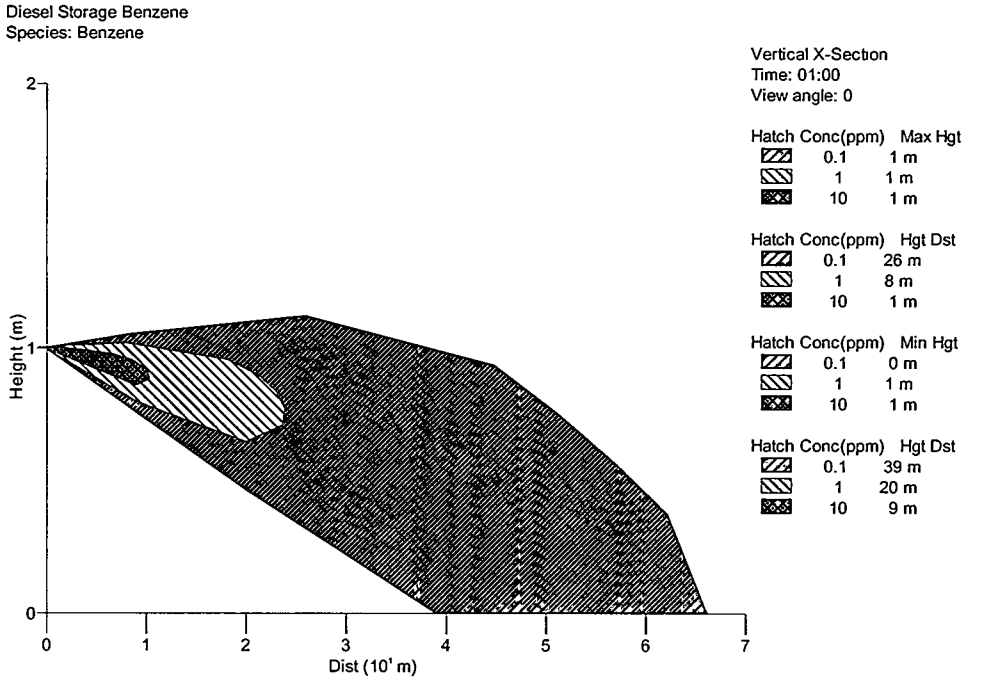
****

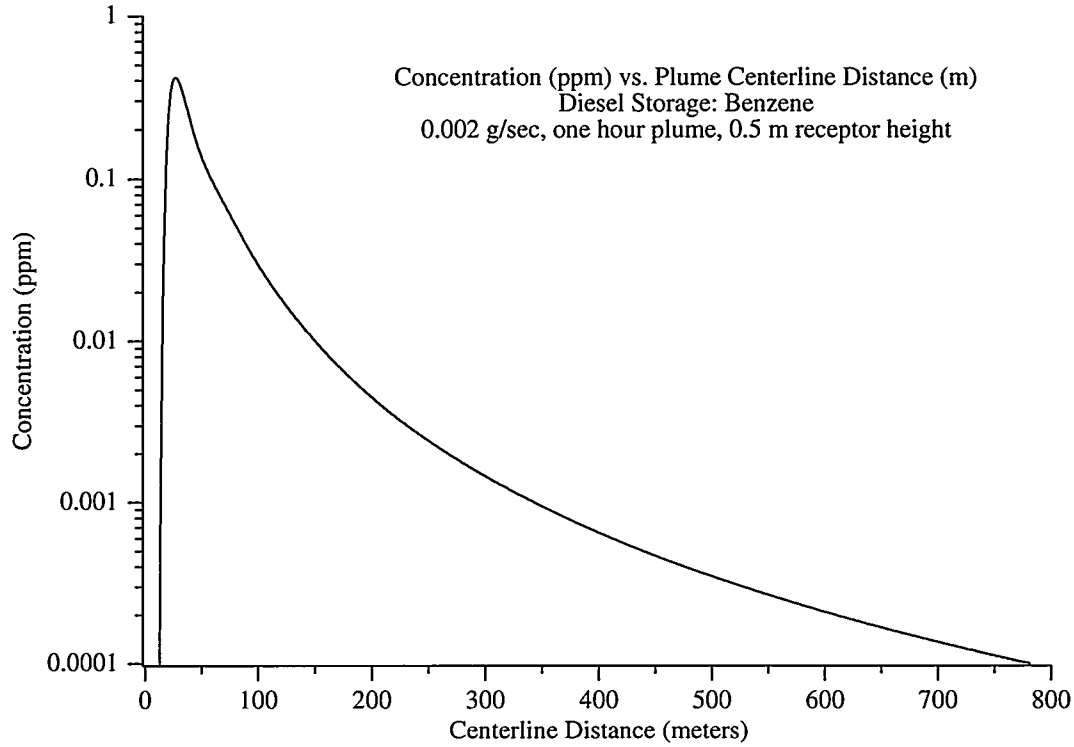
Met Data

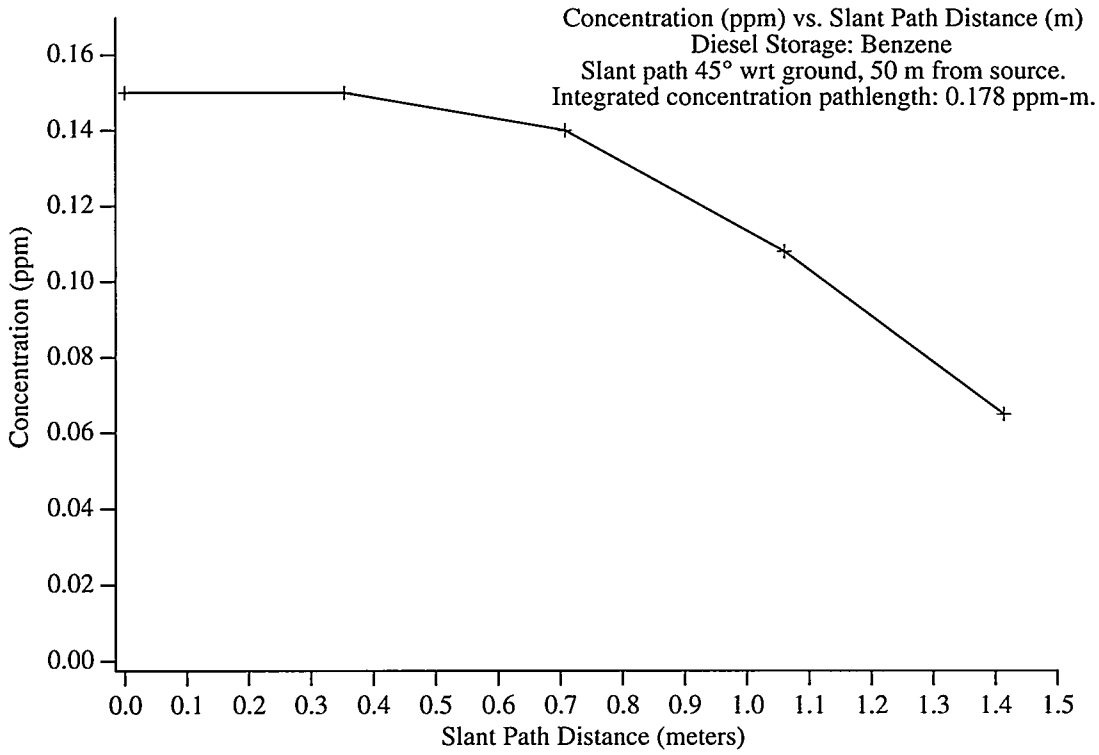
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m²
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

Diesel Storage Evaporation: Benzene, 0.002 g/sec, one-hour plume.



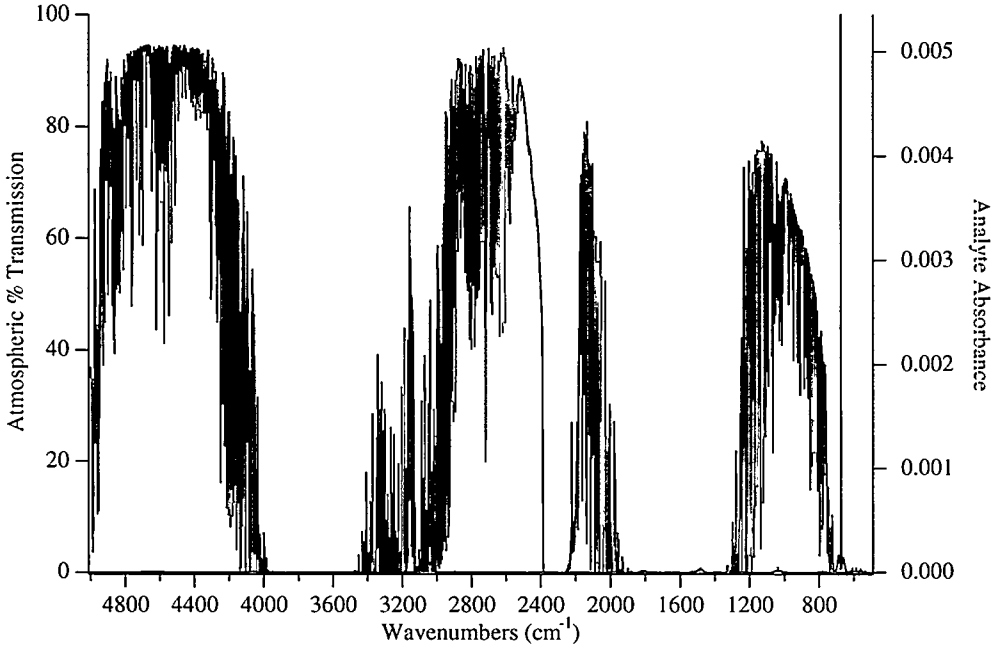



Concentration (ppm) vs. Plume Centerline Distance (m)
Diesel Storage: Benzene
0.002 g/sec, one hour plume, 0.5 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Diesel Storage: Benzene
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 0.178 ppm-m.
Concentration (ppm)
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
Slant Path Distance (meters)

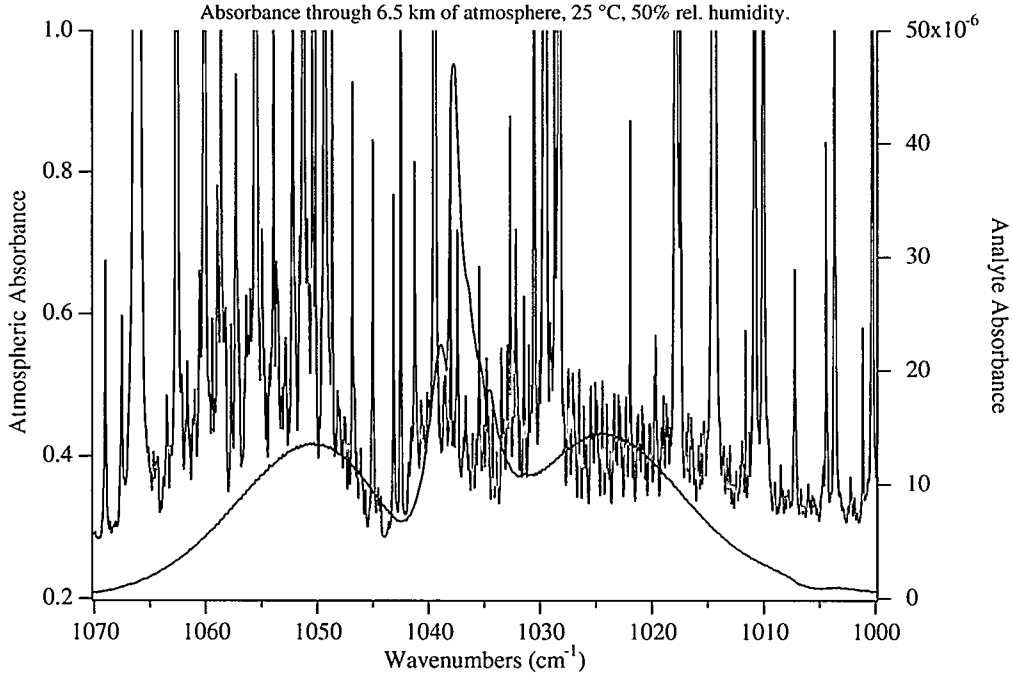
Benzene from Diesel Fuel Storage Evaporation
Benzene absorbance, 20 °C, 0.18 ppm-m, 50 m from vent.
Hanst database.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Benzene from Diesel Fuel Storage Evaporation
Benzene absorbance, 20 °C, 0.18 ppm-m, 50 m from vent.
Hanst database.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



2.4 SCUD Missile Fueling

Compound	Mass Spilled (kg)
Nitric acid	30
Dinitrogen tetroxide	2
Water	2
Nitrogen dioxide	1
Hydrogen fluoride	0.4

Scenario: One SCUD missile fueled with 1000 kg of kerosene and 3500 kg of inhibited red fuming nitric acid (IRFNA) (Lennox 1991). Assume a 1 wt% spill of the IRFNA. A spill of the kerosene is ignored since this would produce a very low concentration plume of hydrocarbons.

Red fuming nitric acid is 85% HNO_3, approximately 10% NO_x and 5% water. The acid is "inhibited" by adding approximately 1% hydrogen fluoride. The HF acts as a getter for water in the stainless steel fuel tanks. The vapor composition over 85% nitric acid at 30°C is 36 Torr HNO_3 and 1.3 Torr water. At 30°C, approximately 70% of the NO_x is N_2O_4 and 30% is NO_2. It is assumed that all of the NO_x is immediately volatilized (Perry and Green 1997).

To simulate the spectra of the nitric acid portion of the IRFNA plume, the concentration-pathlength of the total plume was multiplied by 85% to obtain a concentration-pathlength for the nitric acid.

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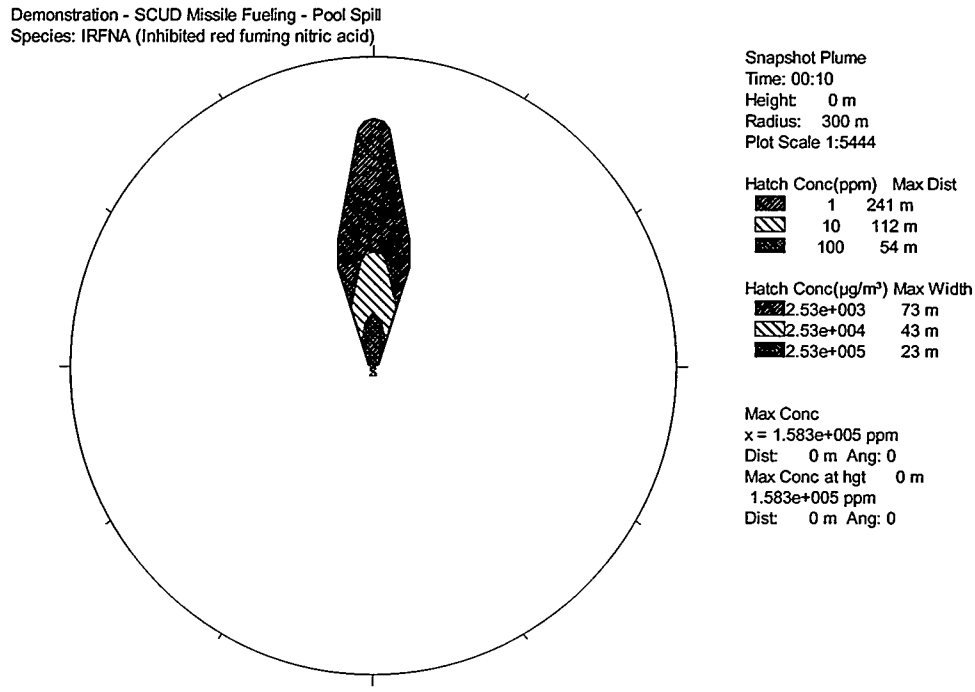
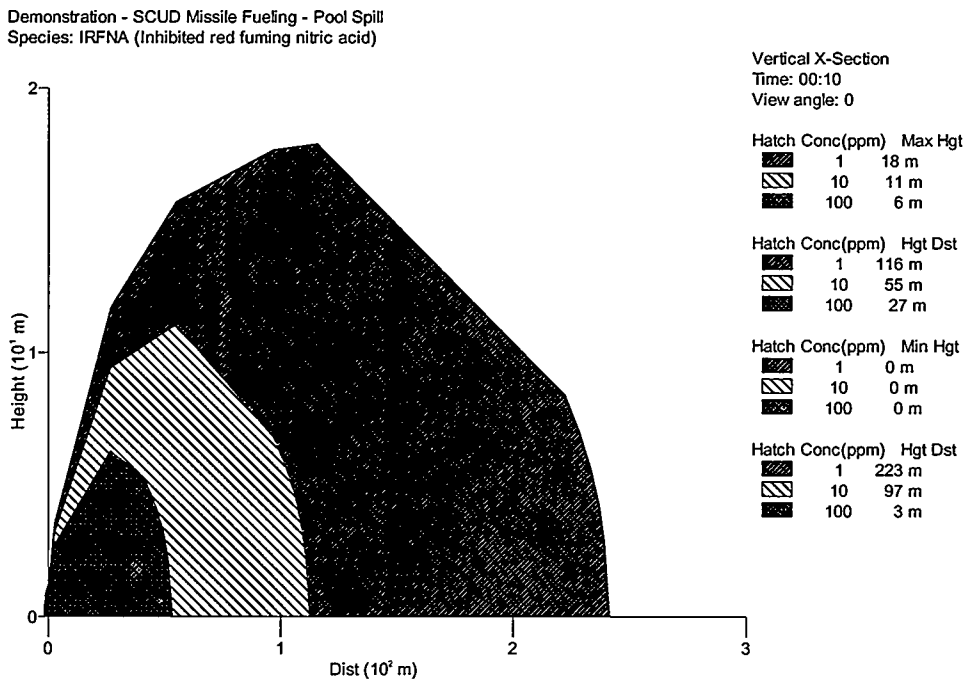
Title:	Demo - SCUD Missile Fueling - Pool Spill
Species:	IRFNA (Inhibited red fuming nitric acid)
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 ft
Amount Released:	35 kilograms
Pool Diameter (Calculated):	0.7582 m
Pool Depth:	0.05 m
Pool Temperature assumed to be ambient or boiling pt.	
No Pool Mitigation Time	
Solar radiation pool evaporation efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be	concrete
Surface Specific Heat:	900 joules/kg K
Surface Thermal Conductivity:	1.2 w/m K
Surface Density:	2100 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.16
Darcy Constant of Surface:	0 m

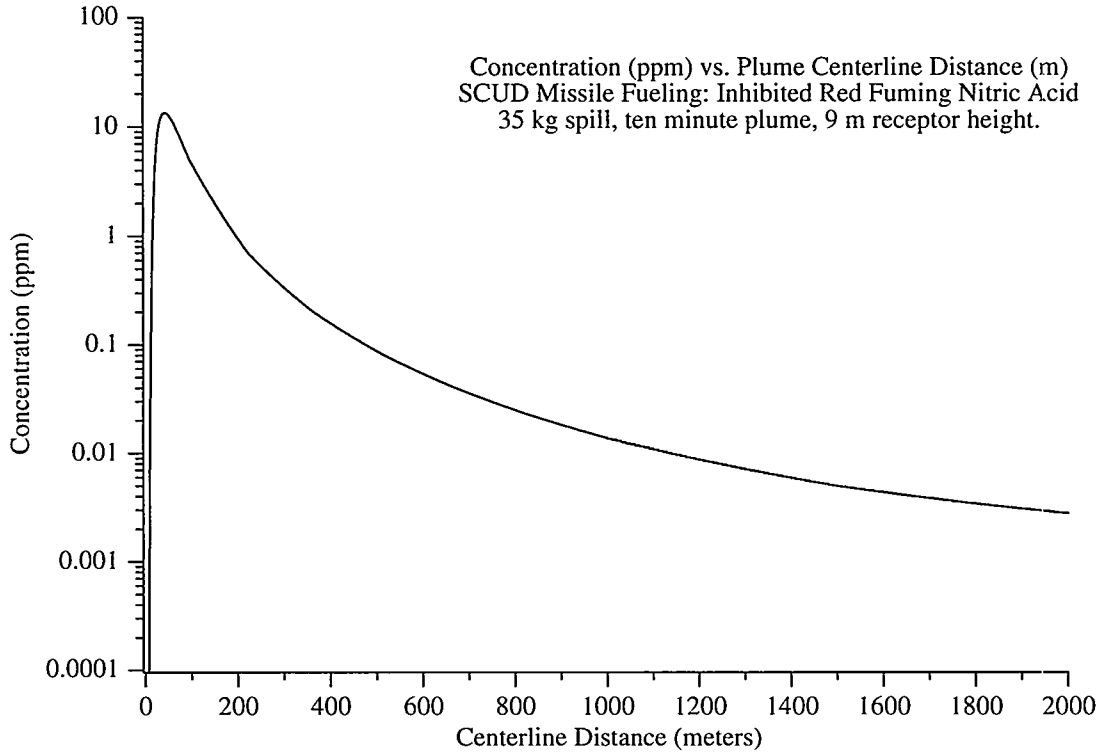
****

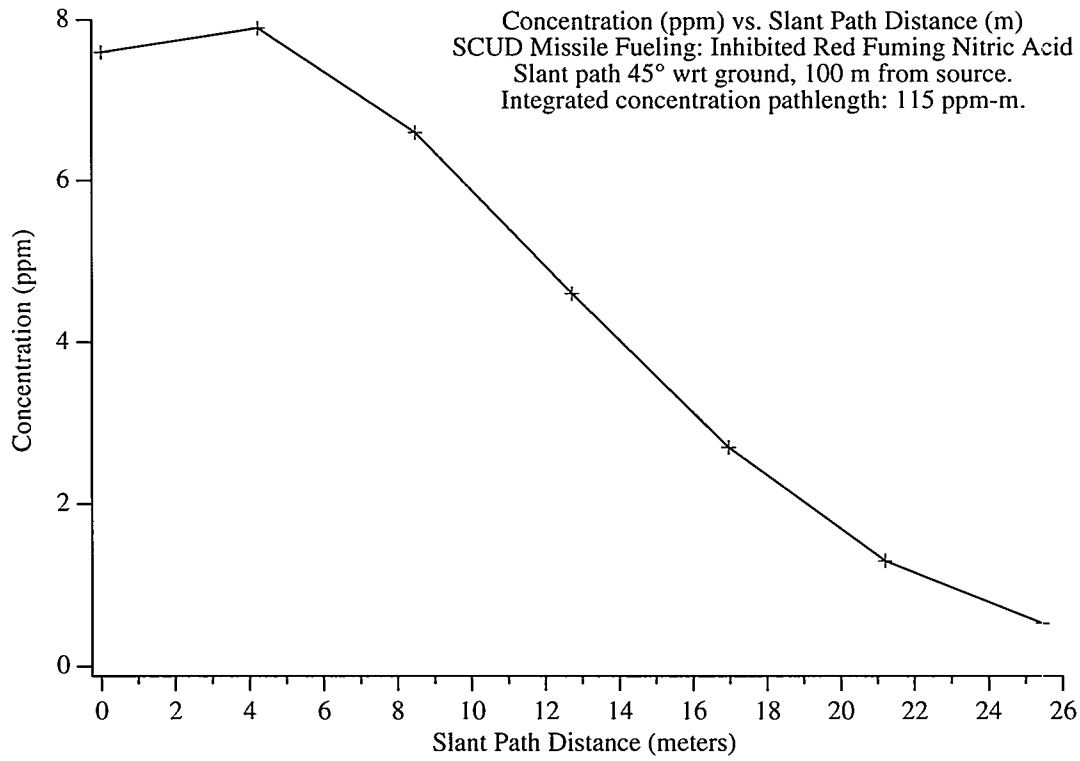
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	30°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	10
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:00:00	
Wind Direction:	180°
Wind Speed:	5 m/s

SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid, 35 kg, ten-minute plume.

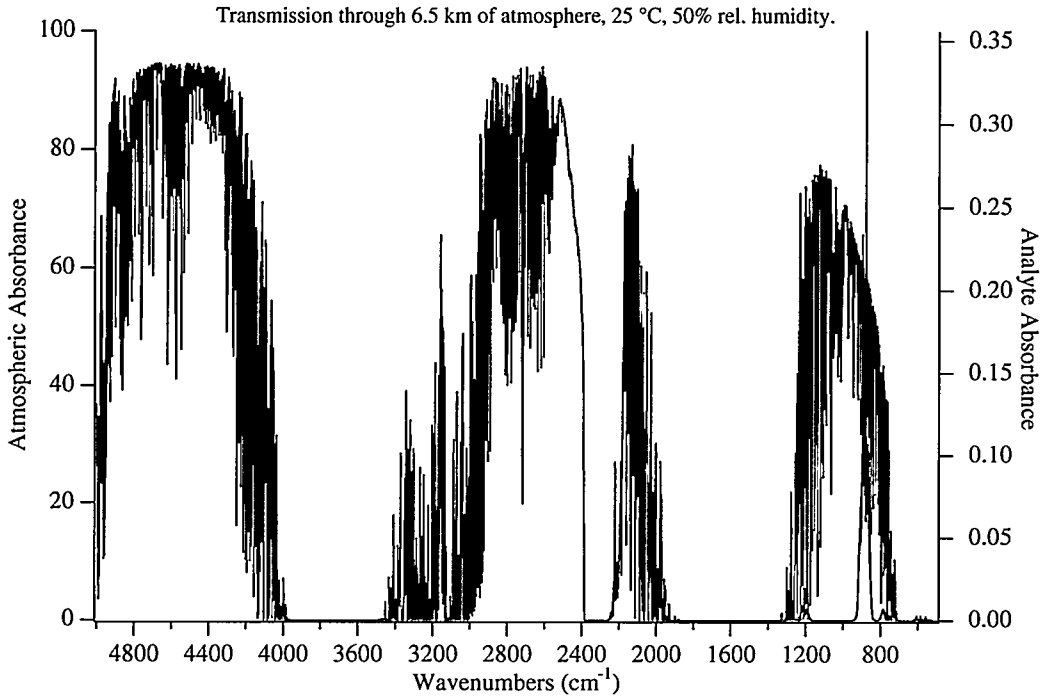




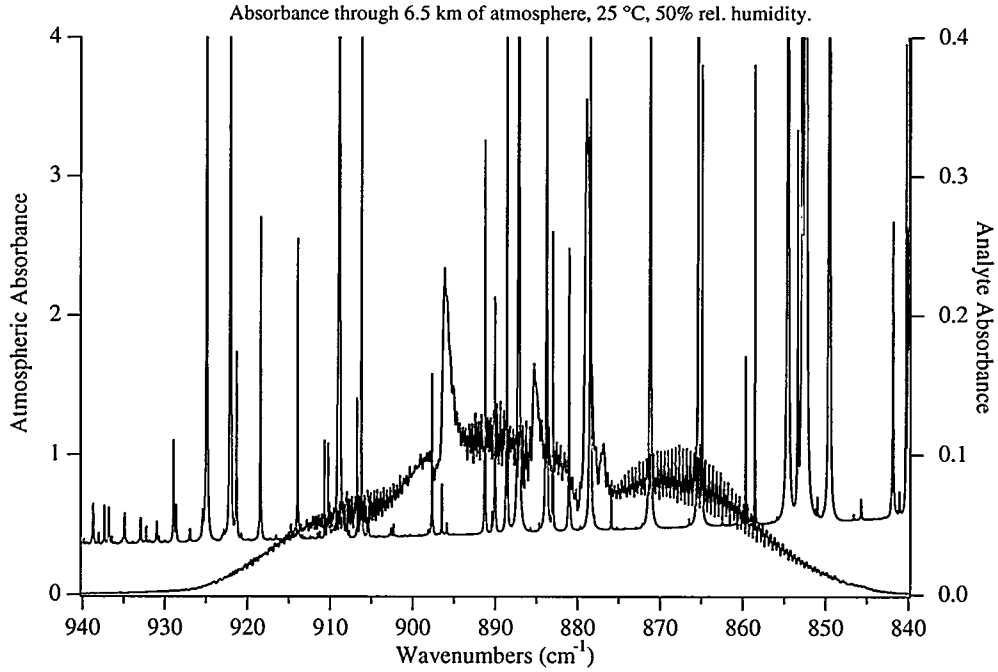

Concentration (ppm) vs. Plume Centerline Distance (m)
SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid
35 kg spill, ten minute plume, 9 m receptor height.
Concentration (ppm)
100
10
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 115 ppm-m.
Concentration (ppm)
8
6
4
2
0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
Slant Path Distance (meters)

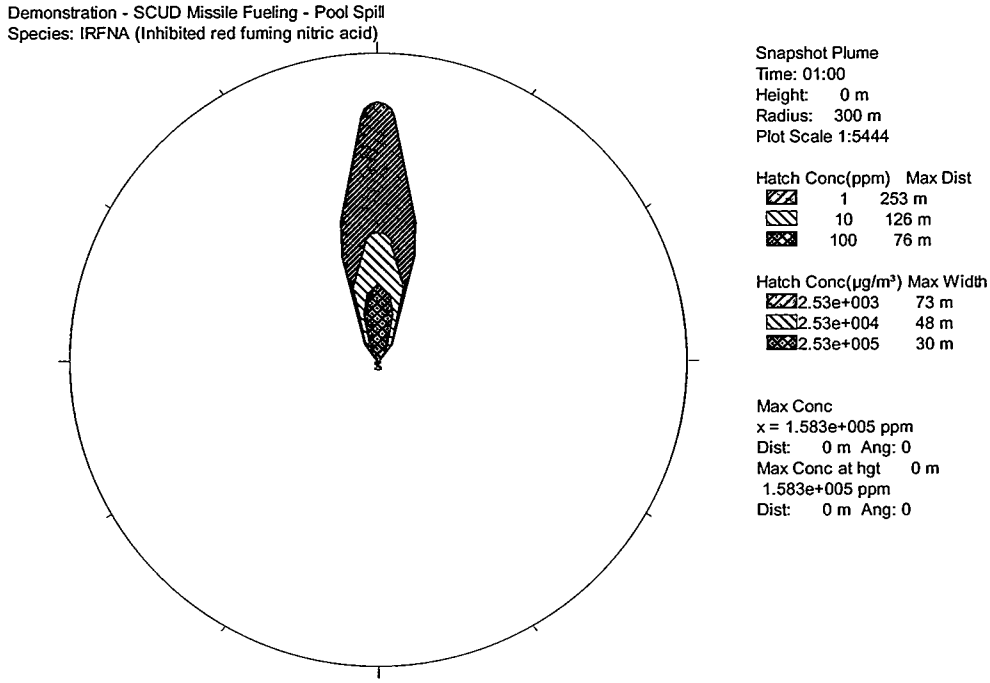
Nitric Acid from SCUD Missile Fueling
Nitric acid absorbance, 25 °C, 98 ppm-m, 100 m from vent.

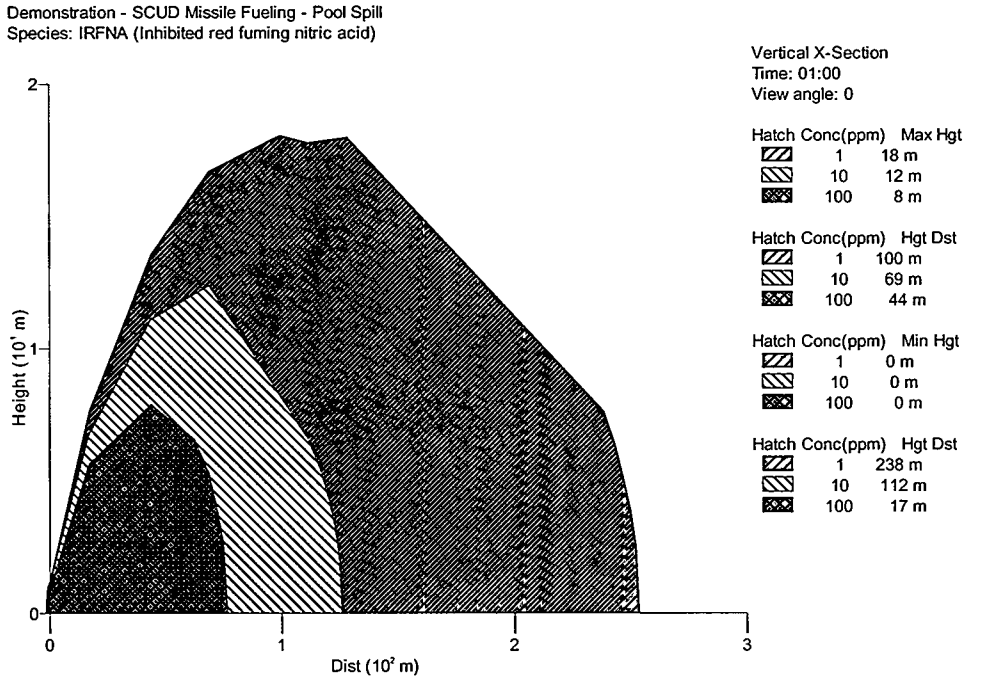


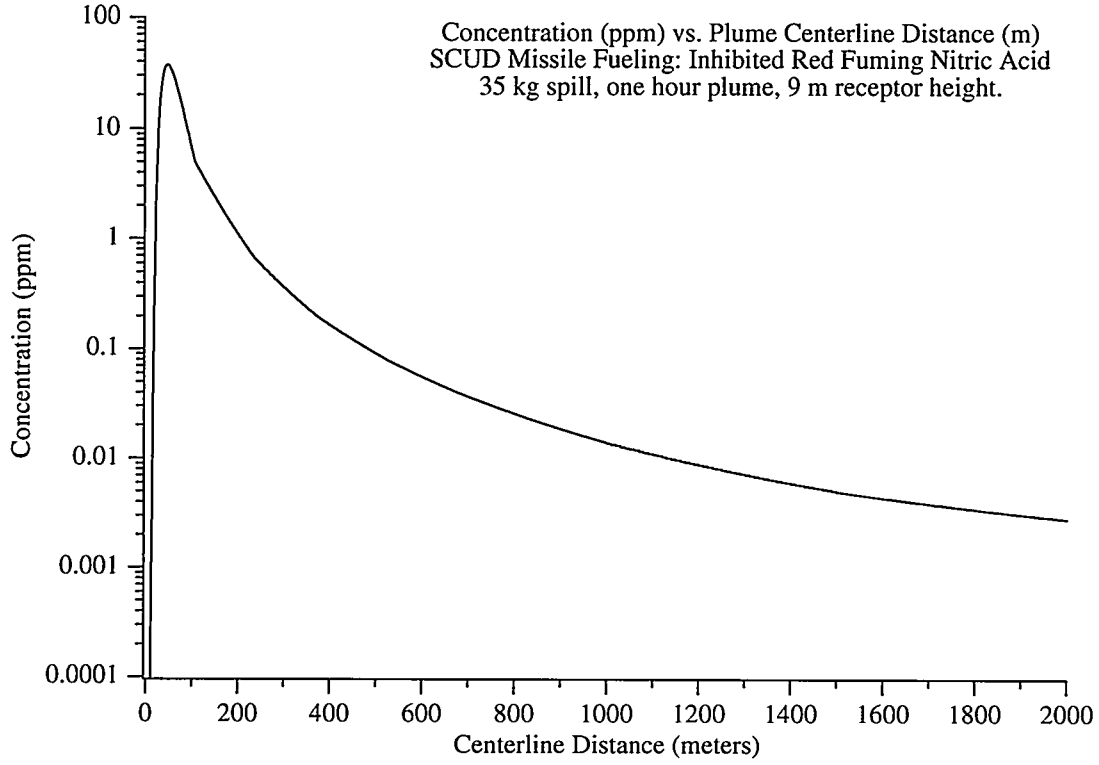
Nitric Acid from SCUD Missile Fueling
Nitric acid absorbance, 25 °C, 98 ppm-m, 100 m from vent.
Detail of ν_5 Band

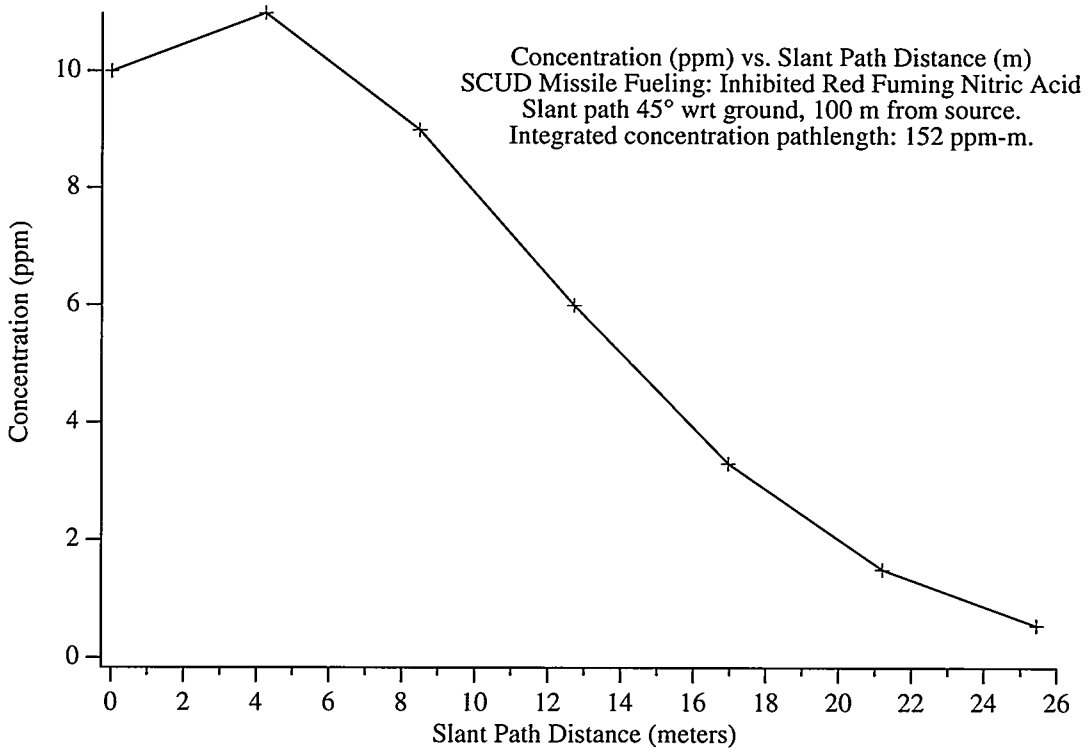


SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid, 35 kg, one-hour plume.

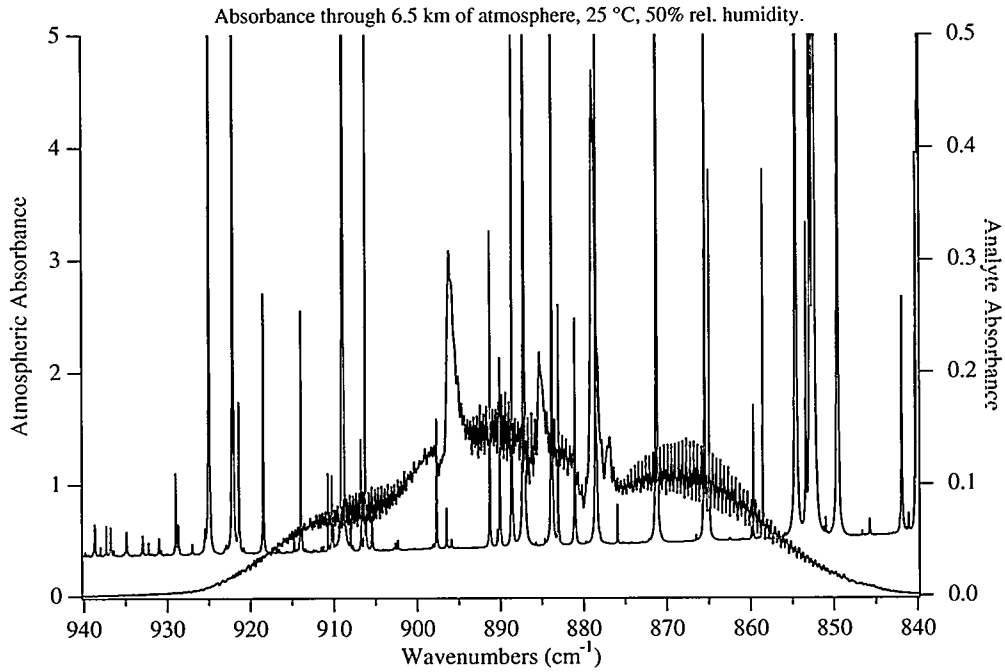





Concentration (ppm) vs. Plume Centerline Distance (m)
SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid
35 kg spill, one hour plume, 9 m receptor height.
Concentration (ppm)
100
10
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)

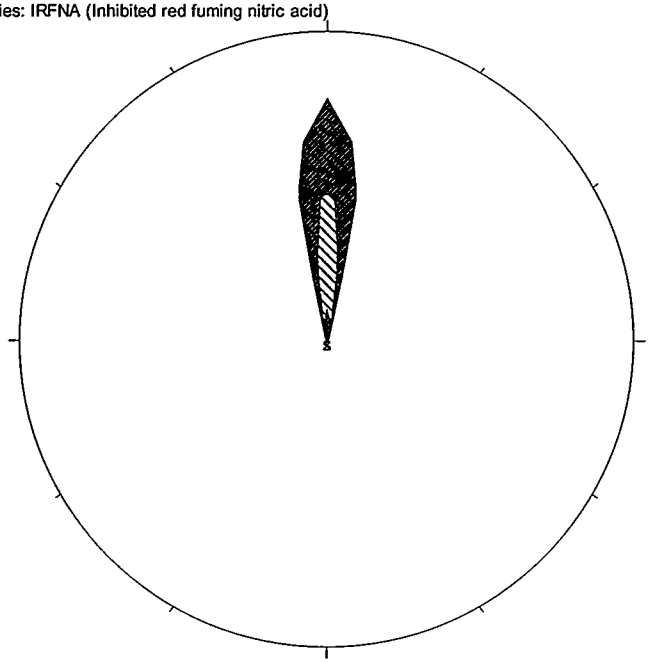

Concentration (ppm) vs. Slant Path Distance (m)
SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 152 ppm-m.
Concentration (ppm)
10
8
6
4
2
0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
Slant Path Distance (meters)

Nitric Acid from SCUD Missile Fueling
Nitric acid absorbance, 25 °C, 129 ppm-m, 100 m from vent.
Detail of ν_5 Band



SCUD Missile Fueling: Inhibited Red Fuming Nitric Acid, 35 kg, five-hour plume.

Demonstration - SCUD Missile Fueling - Pool Spill
Species: IRFNA (Inhibited red fuming nitric acid)



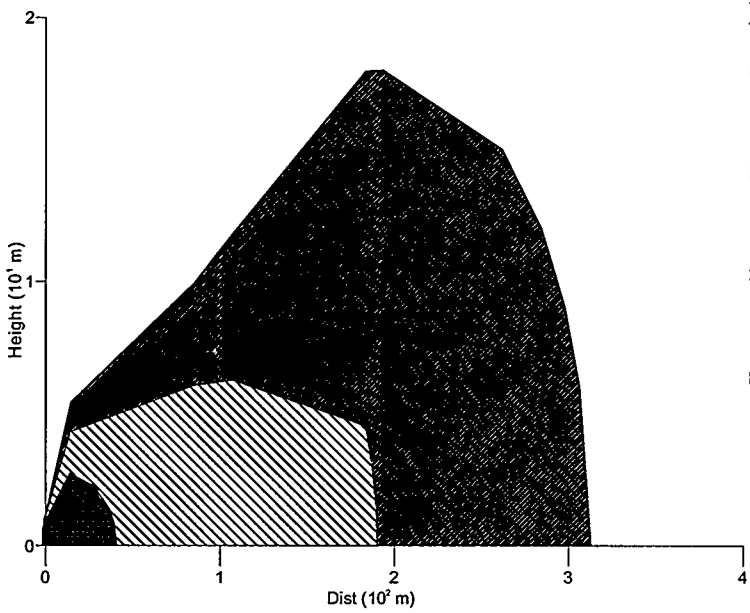
Snapshot Plume
Time: 05:00
Height: 0 m
Radius: 400 m
Plot Scale 1:7259

Hatch	Conc(ppm)	Max Dist
	1	313 m
	10	190 m
	100	41 m

Hatch	Conc(μg/m³)	Max Width
	2.53e+003	75 m
	2.53e+004	24 m
	2.53e+005	9 m

Max Conc
x = 1.583e+005 ppm
Dist: 0 m Ang: 0
Max Conc at hgt 0 m
1.583e+005 ppm
Dist: 0 m Ang: 0

Demonstration - SCUD Missile Fueling - Pool Spill
Species: IRFNA (Inhibited red fuming nitric acid)



Vertical X-Section
Time: 05:00
View angle: 0

Hatch	Conc(ppm)	Max Hgt
	1	18 m
	10	6 m
	100	3 m

Hatch	Conc(ppm)	Hgt Dst
	1	193 m
	10	107 m
	100	14 m

Hatch	Conc(ppm)	Min Hgt
	1	0 m
	10	0 m
	100	0 m

Hatch	Conc(ppm)	Hgt Dst
	1	183 m
	10	183 m
	100	0 m

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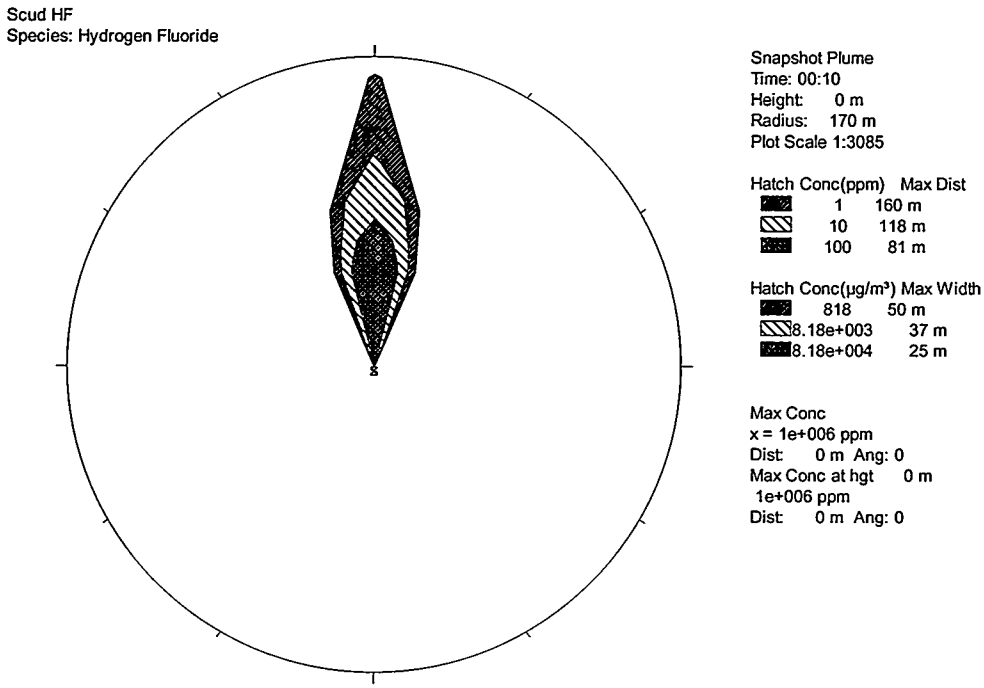
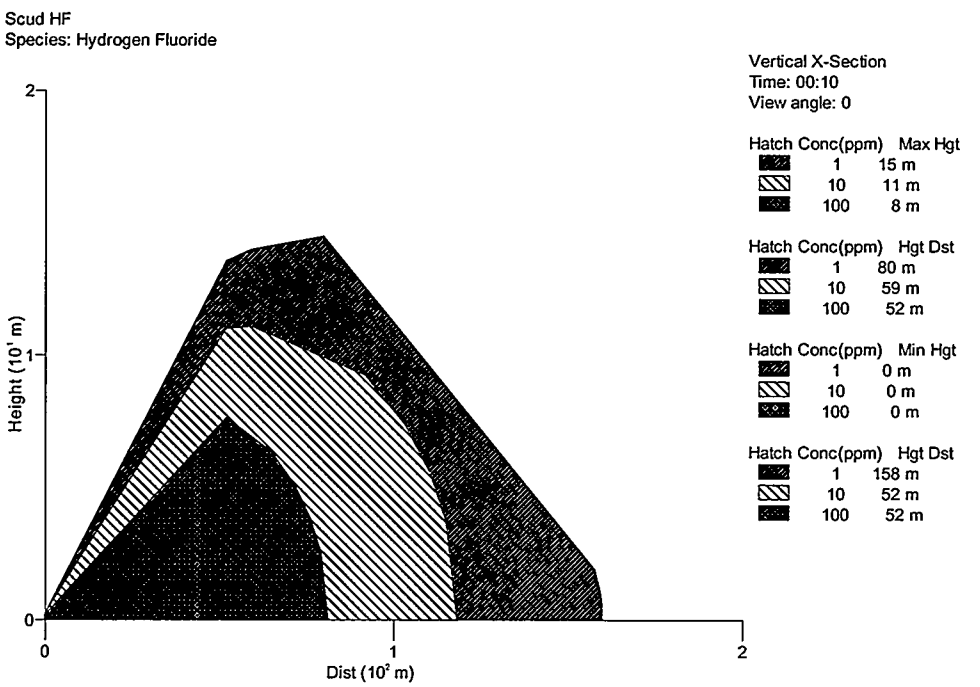
Title:	Scud HF
Species:	Hydrogen Fluoride
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 ft
Amount Released:	0.4 kilograms
Pool Diameter (Calculated):	0.3388 ft
Pool Depth:	0.05 m
Pool Temperature assumed to be ambient or boiling pt.	
No Pool Mitigation Time	
Solar radiation pool evaporation efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be concrete	
Surface Specific Heat:	900 joules/kg K
Surface Thermal Conductivity:	1.2 w/m K
Surface Density:	2100 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.16
Darcy Constant of Surface:	0 m

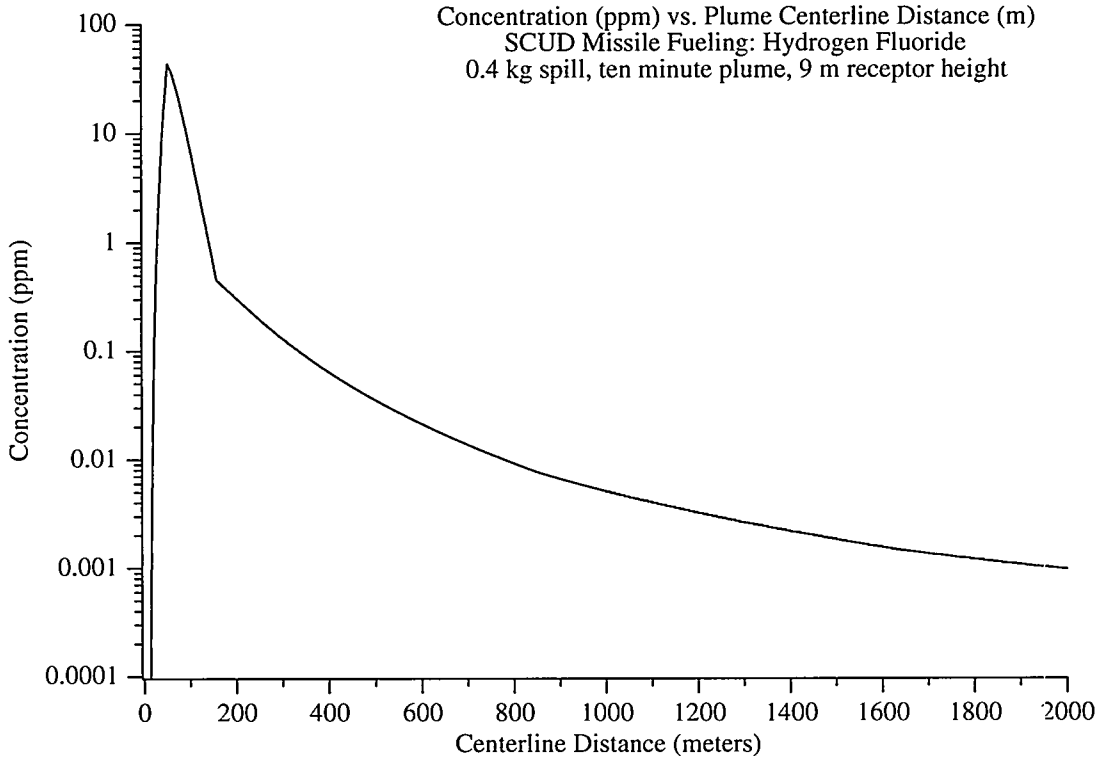
****

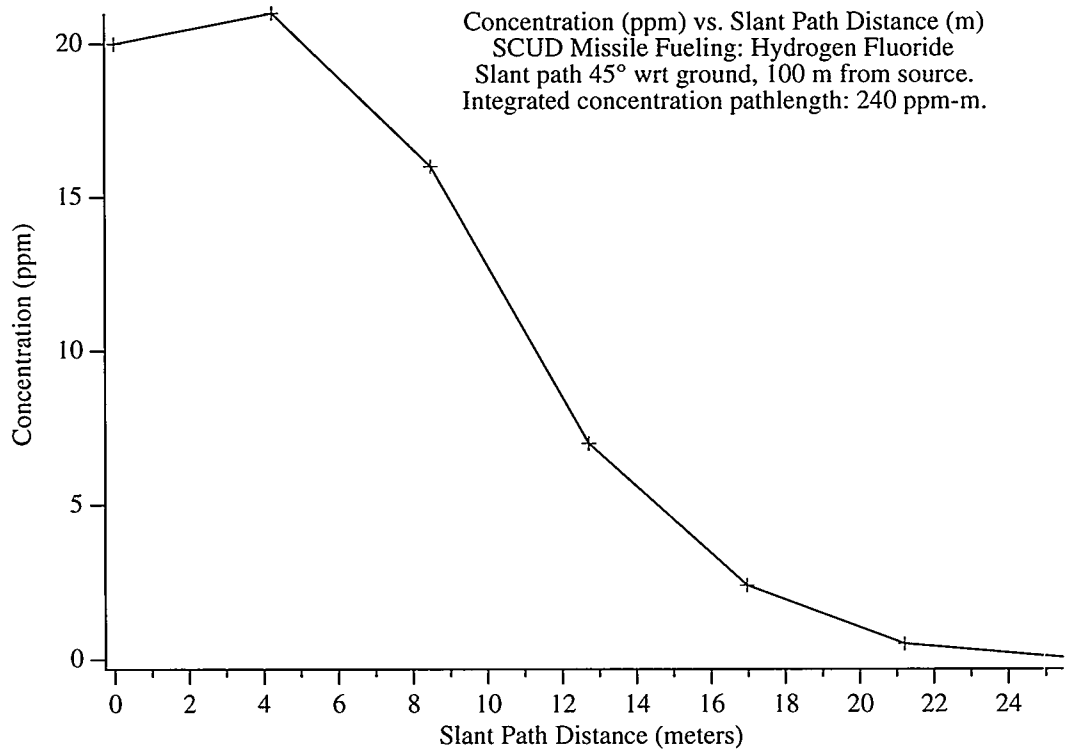
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

SCUD Missile Fueling: Hydrogen Fluoride, 0.4 kg, ten-minute plume.



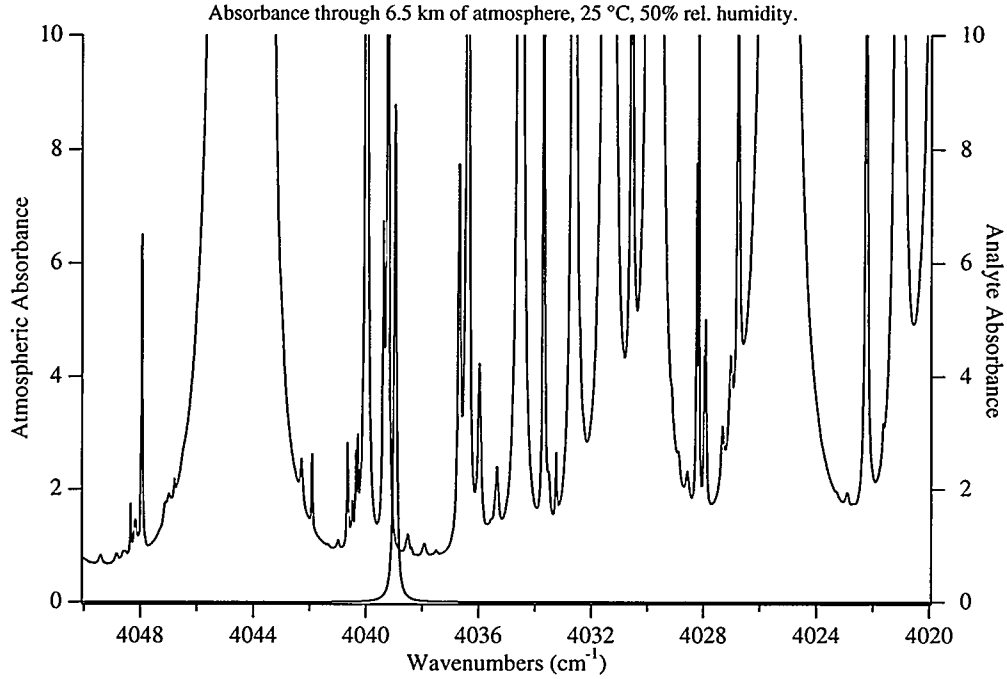



Concentration (ppm) vs. Plume Centerline Distance (m)
SCUD Missile Fueling: Hydrogen Fluoride
0.4 kg spill, ten minute plume, 9 m receptor height
Concentration (ppm)
100
10
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
SCUD Missile Fueling: Hydrogen Fluoride
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 240 ppm-m.
Concentration (ppm)
20
15
10
5
0
0
2
4
6
8
10
12
14
16
18
20
22
24
Slant Path Distance (meters)

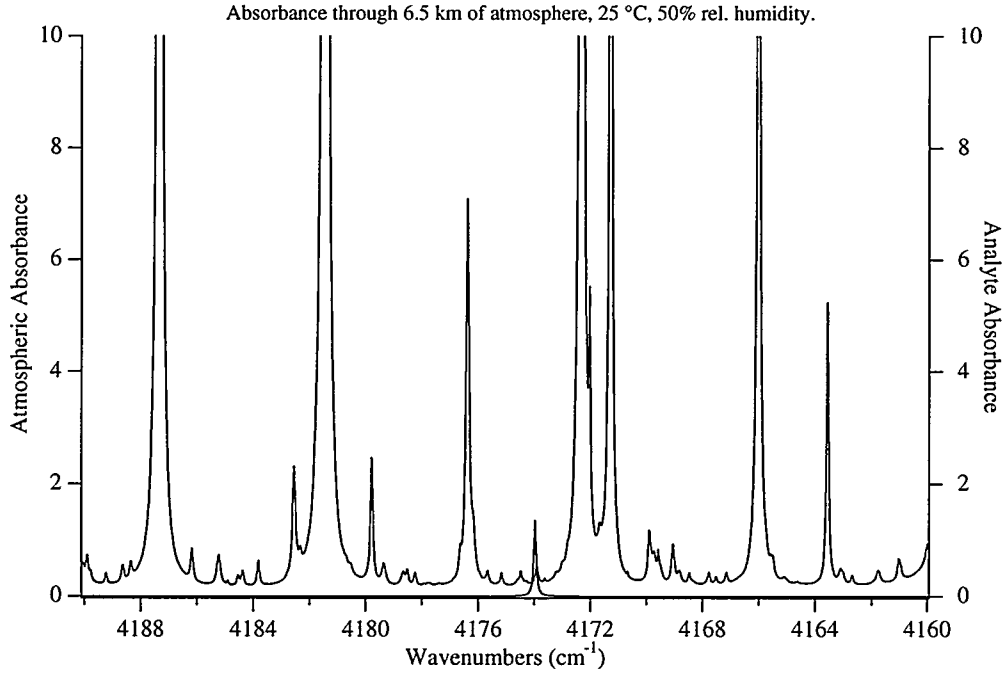
Hydrogen Fluoride from SCUD Missile Fueling
Hydrogen fluoride absorbance, 25 °C, 240 ppm-m, 100 m from vent.
Detail of R(1) fundamental transition.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.

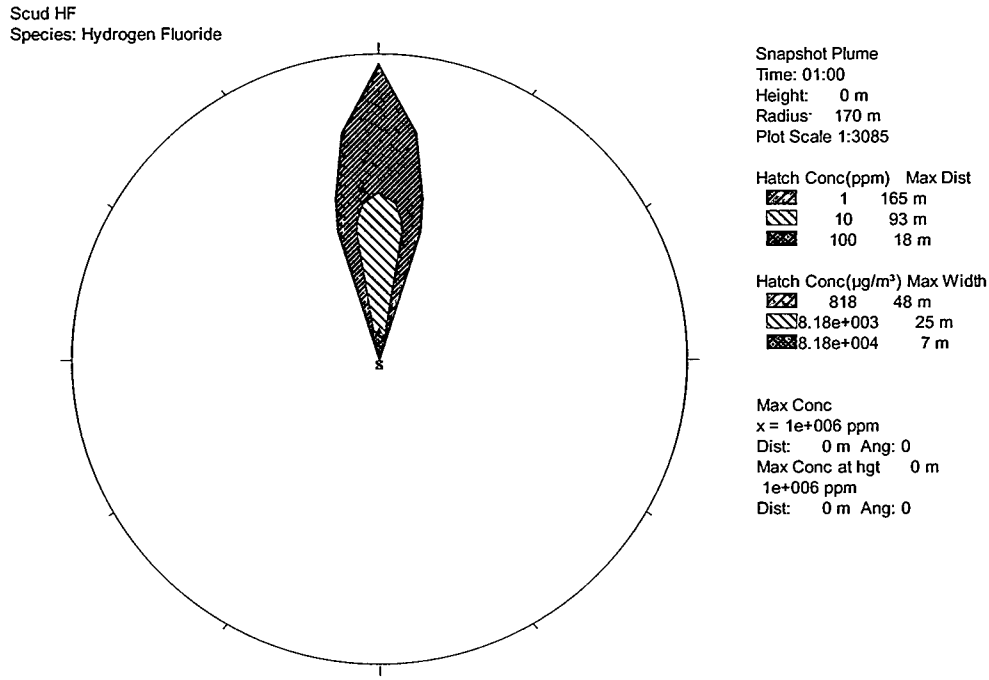


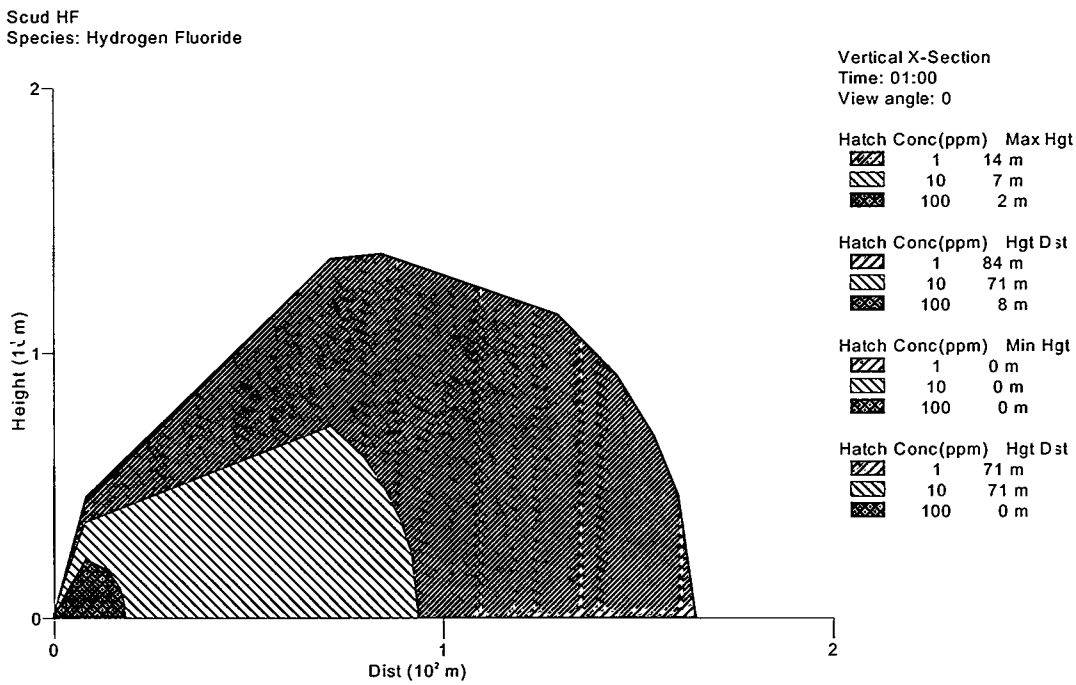
Hydrogen Fluoride from SCUD Missile Fueling
Hydrogen fluoride absorbance, 25 °C, 240 ppm-m, 100 m from vent.
Detail of R(5) fundamental transition.

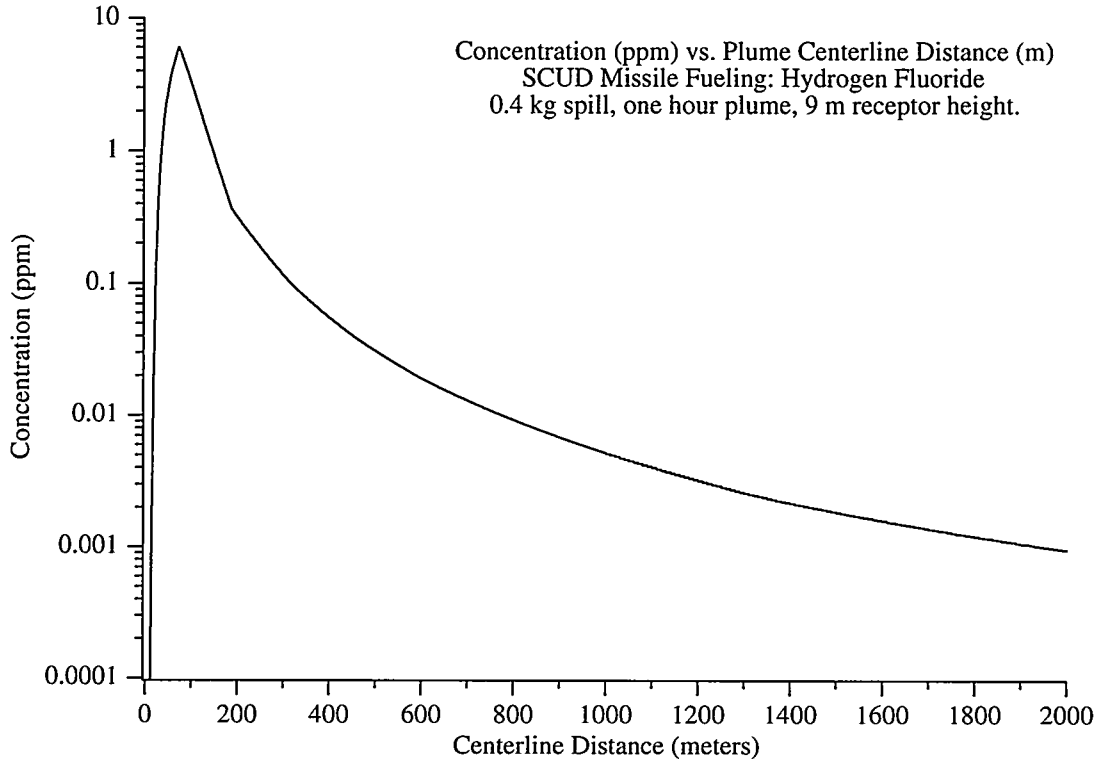
Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.

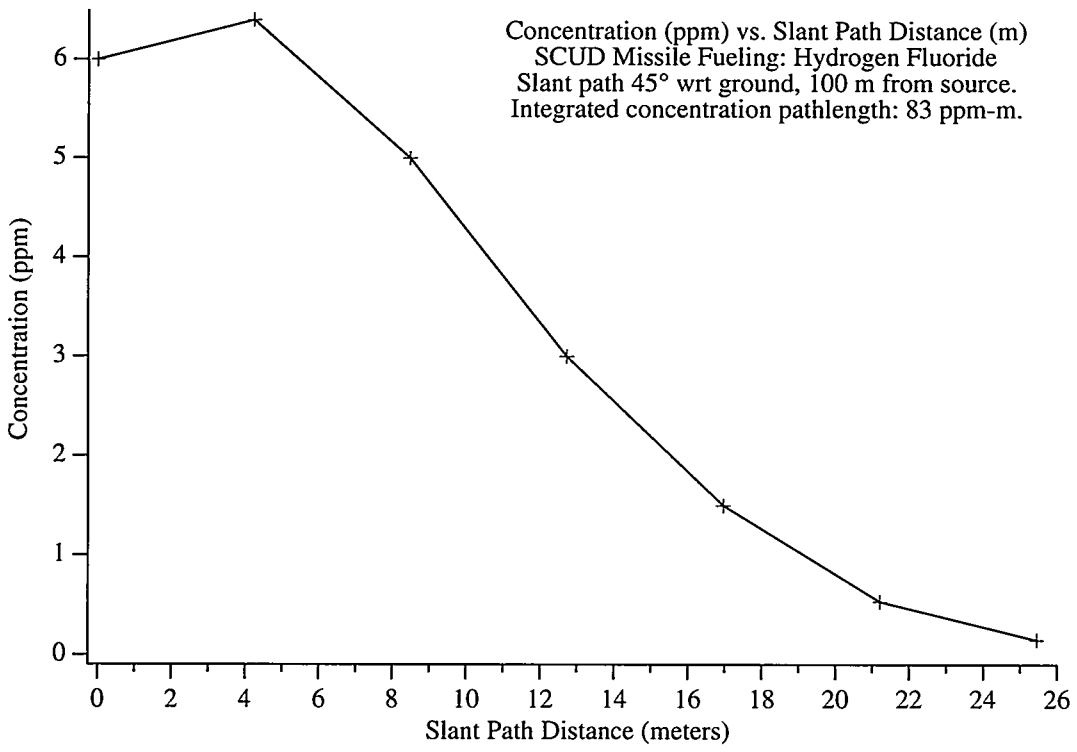


SCUD Missile Fueling: Hydrogen Fluoride, 0.4 kg, one-hour plume.

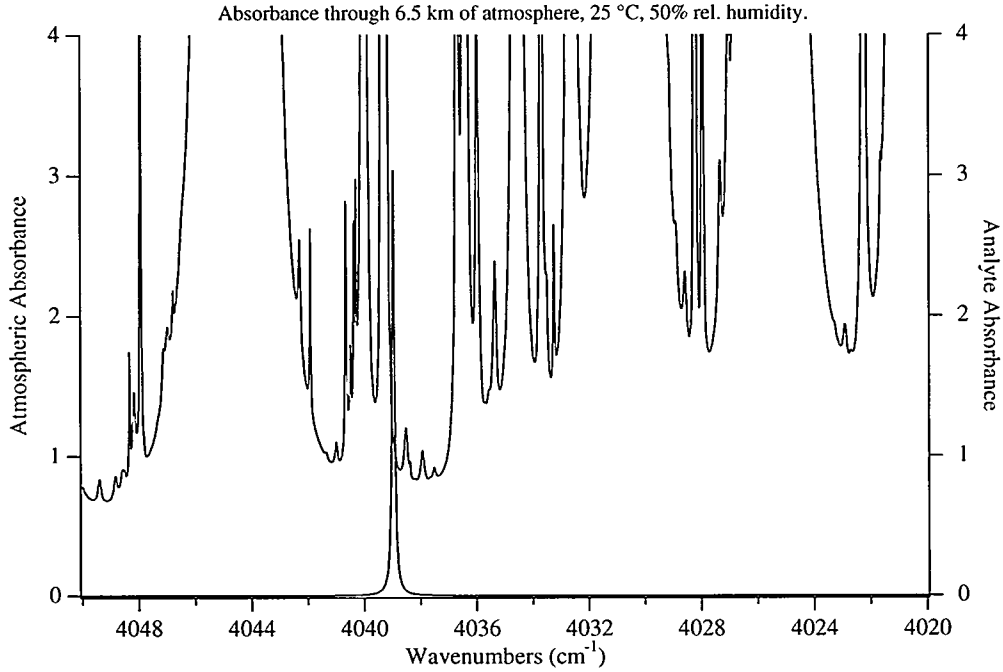




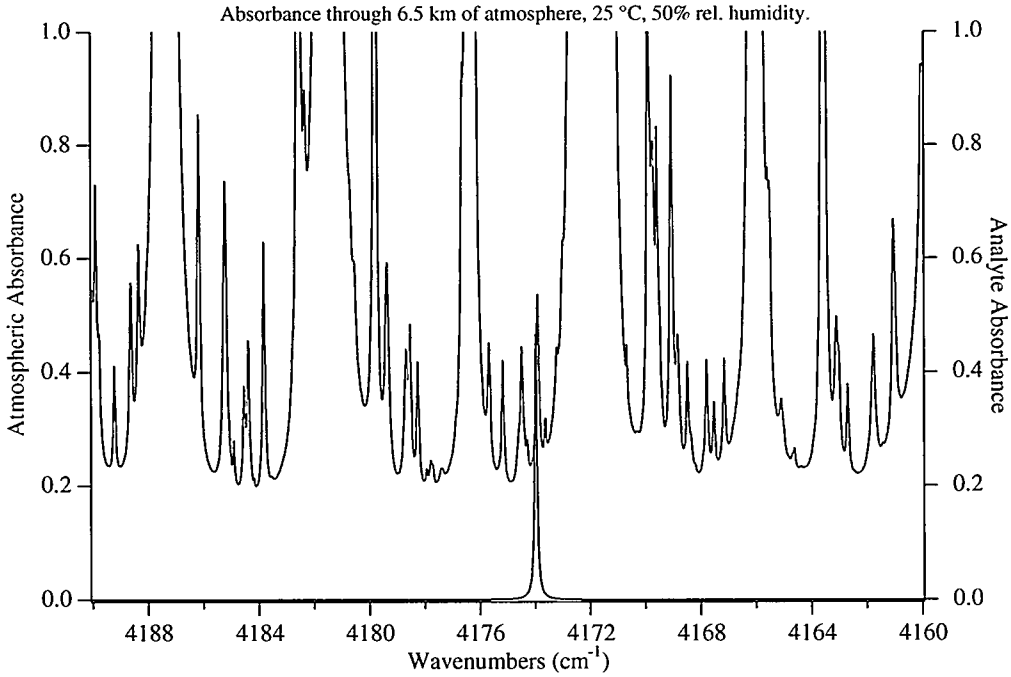

Concentration (ppm) vs. Plume Centerline Distance (m)
SCUD Missile Fueling: Hydrogen Fluoride
0.4 kg spill, one hour plume, 9 m receptor height.
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
SCUD Missile Fueling: Hydrogen Fluoride
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 83 ppm-m.
Concentration (ppm)
6
5
4
3
2
1
0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
Slant Path Distance (meters)

Hydrogen Fluoride from SCUD Missile Fueling
Hydrogen fluoride absorbance, 25 °C, 83 ppm-m, 100 m from vent.
Detail of R(1) fundamental transition.



Hydrogen Fluoride from SCUD Missile Fueling
Hydrogen fluoride absorbance, 25 °C, 83 ppm-m, 100 m from vent.
Detail of R(5) fundamental transition.



3.0 Battle Damage Assessment

3.1 Burning Ammunition

Compound	Total Emission (kg)
Carbon monoxide	23,000
Nitric oxide	16,000
Carbon dioxide	11,000
Hydrogen cyanide	500
Formaldehyde	300
Nitrous acid	300

Scenario: One hundred tons of artillery shells containing 20% nitro cellulous propellant, 40% explosives (TNT), and the balance as metal casings. Burning pool temperature is assumed to be 1500 K. Not all effluents, such as nitrogen, hydrogen, water, metal, etc., are listed. See Bernecker and Smith (1966), Adams and Shaw (1992), Brill *et al.* (1996), and Yinon (1999).

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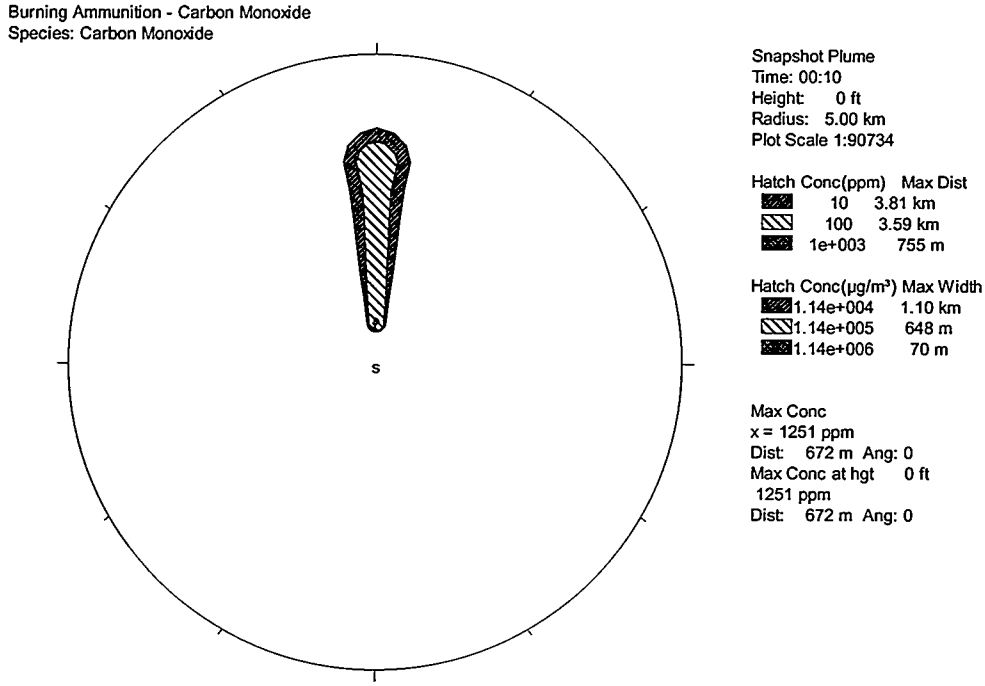
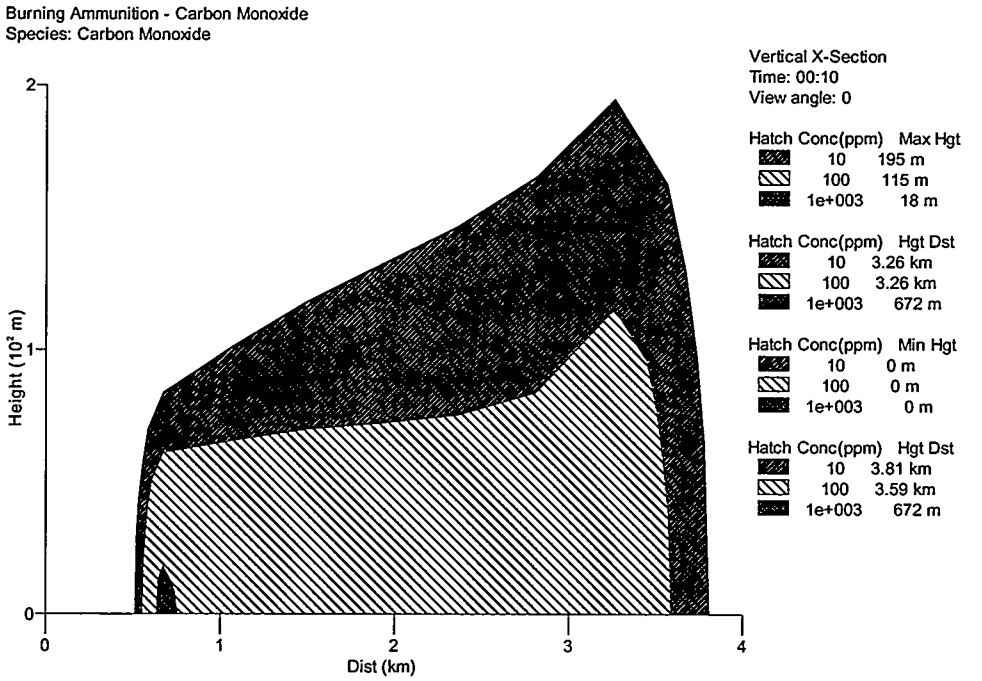
Title:	Burning Ammunition - Carbon Monoxide
Species:	Carbon Monoxide
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	10, 100, 1000
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 ft
Amount Released:	2.3e+004 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	39.12 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be	dirt
Surface Specific Heat:	800 joules/kg K
Surface Thermal Conductivity:	0.32 w/m K
Surface Density:	1640 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.34
Darcy Constant of Surface:	2.8e-007 m

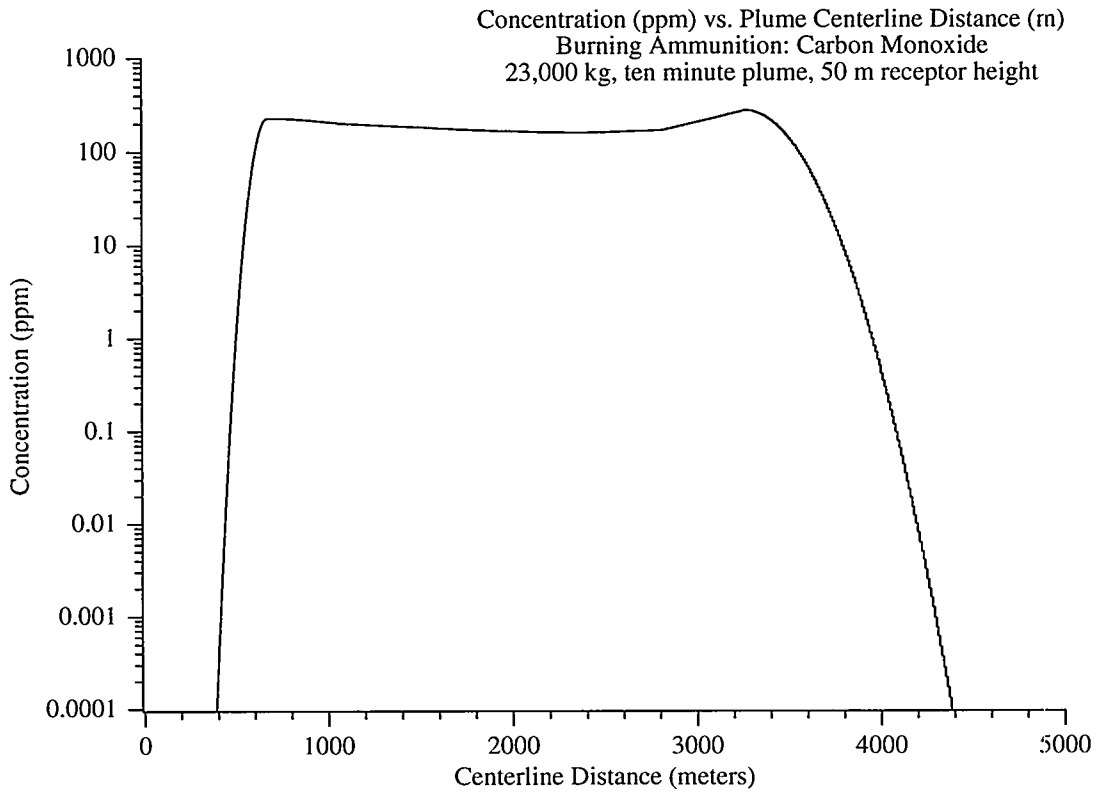
****

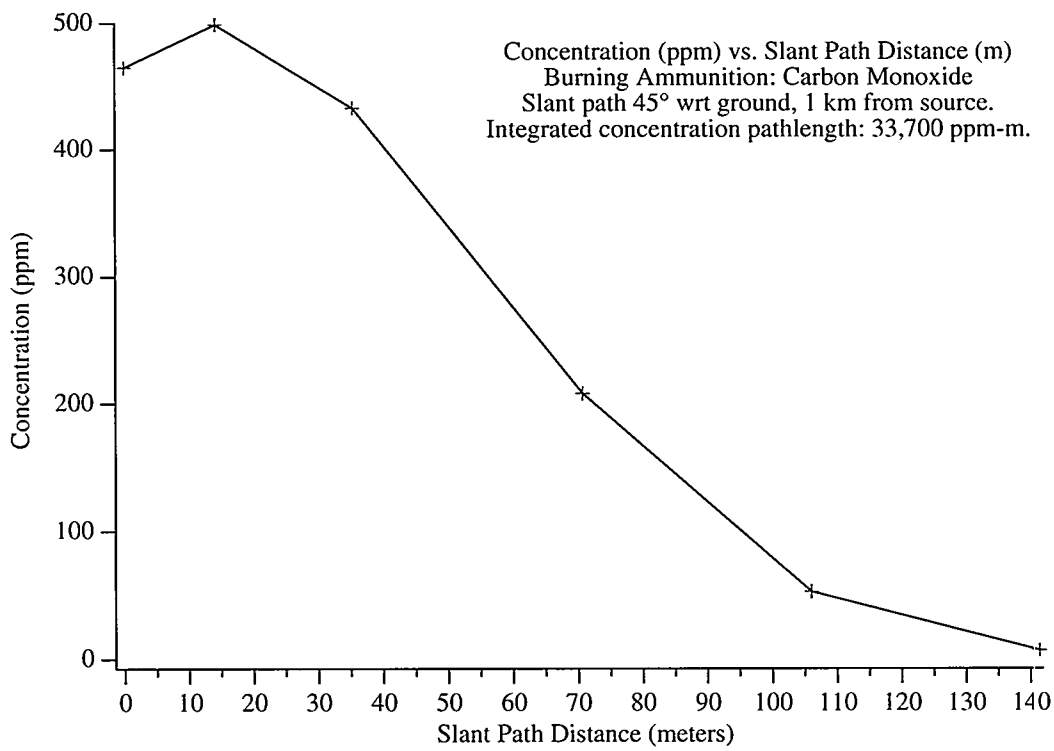
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind measurement altitude	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Ammunition: Carbon Monoxide, 23,000 kg, ten-minute plume.



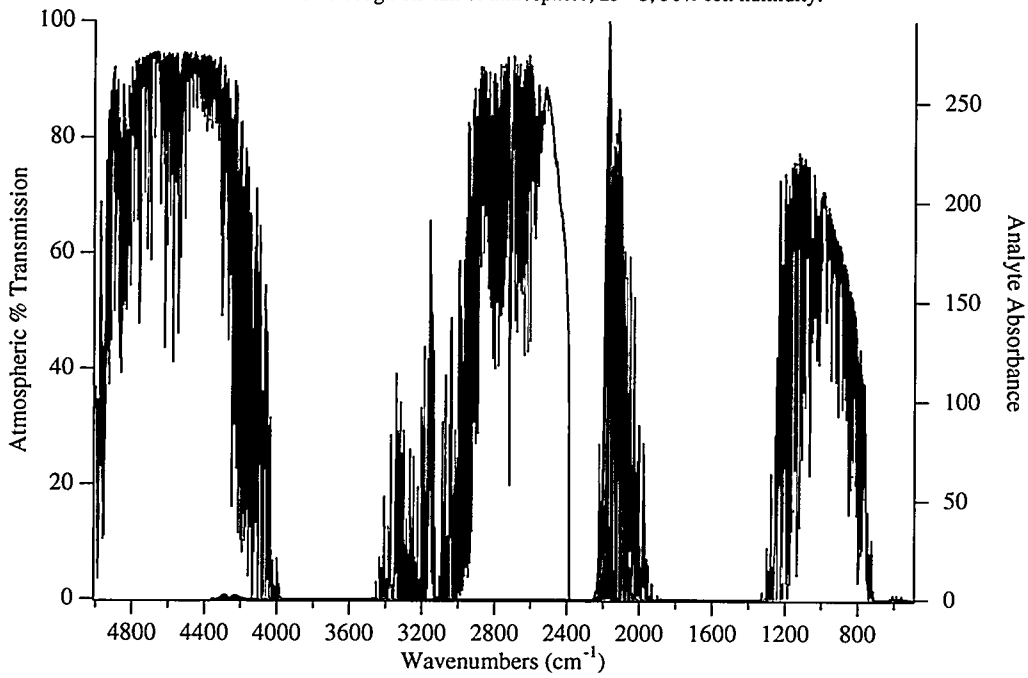



Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Ammunition: Carbon Monoxide
23,000 kg, ten minute plume, 50 m receptor height
Concentration (ppm)
1000
100
10
1
0.1
0.01
0.001
0.0001
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Ammunition: Carbon Monoxide
Slant path 45° wrt ground, 1 km from source.
Integrated concentration pathlength: 33,700 ppm-m.
Concentration (ppm)
500
400
300
200
100
0
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
Slant Path Distance (meters)

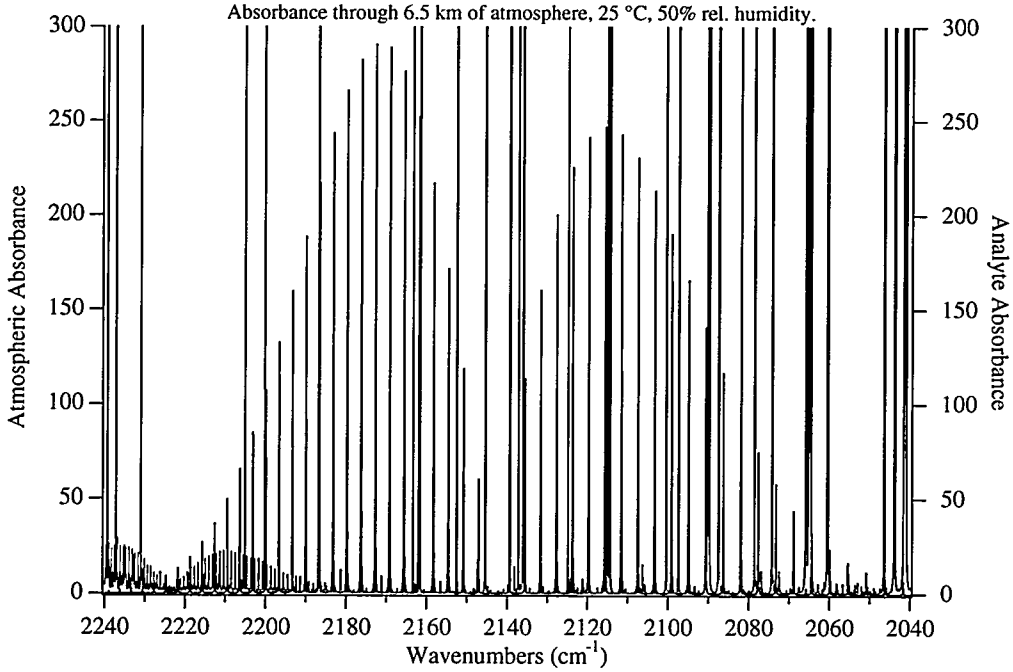
Carbon Monoxide from Burning Ammunition
Carbon monoxide absorbance, 25 °C, 33,700 ppm-m, 1000 m from fire.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Carbon Monoxide from Burning Ammunition
Carbon monoxide absorbance, 25 °C, 33,700 ppm-m, 1000 m from fire.
Detail of fundamental band.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



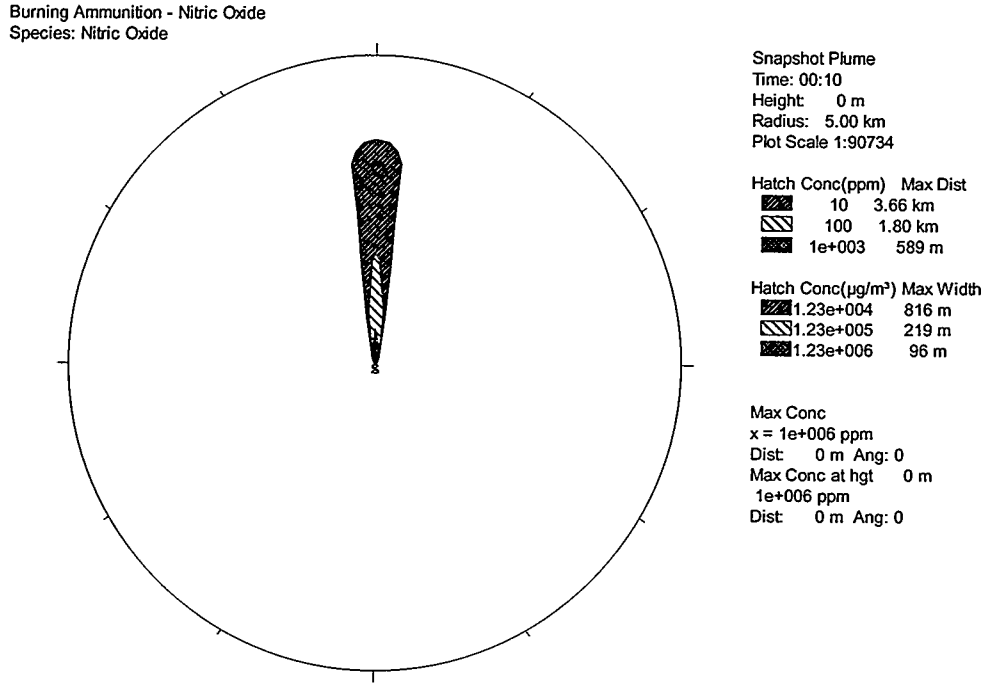
CHARM Version 9.3

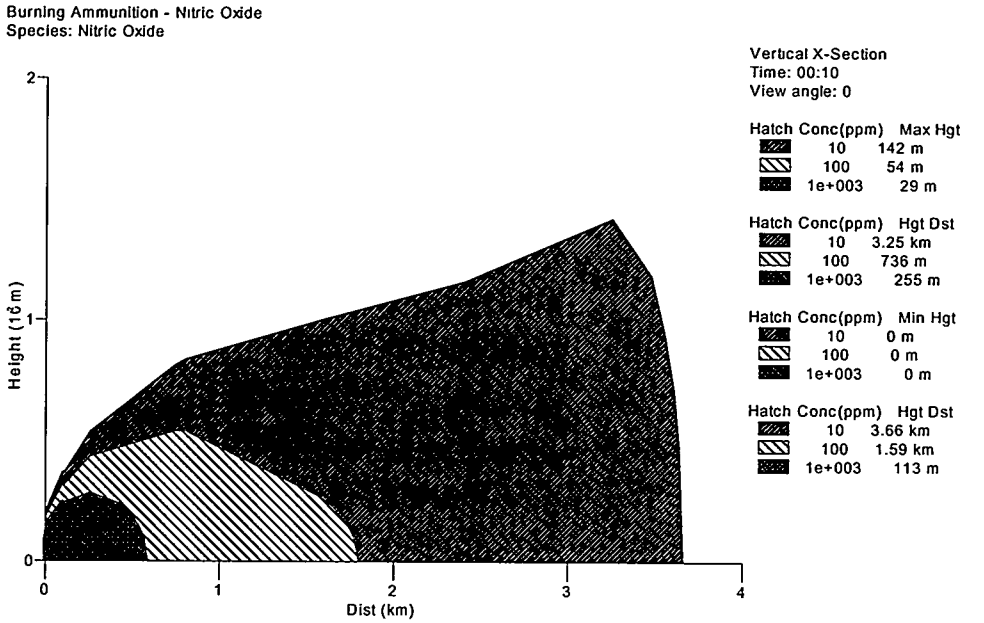
Title:	Burning Ammunition - Nitric Oxide
Species:	Nitric Oxide
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	10, 100, 1000
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	1.6e+004 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	15.51 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be	concrete
Surface Specific Heat:	900 joules/kg K
Surface Thermal Conductivity:	1.2 w/m K
Surface Density:	2100 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.16
Darcy Constant of Surface:	0 m

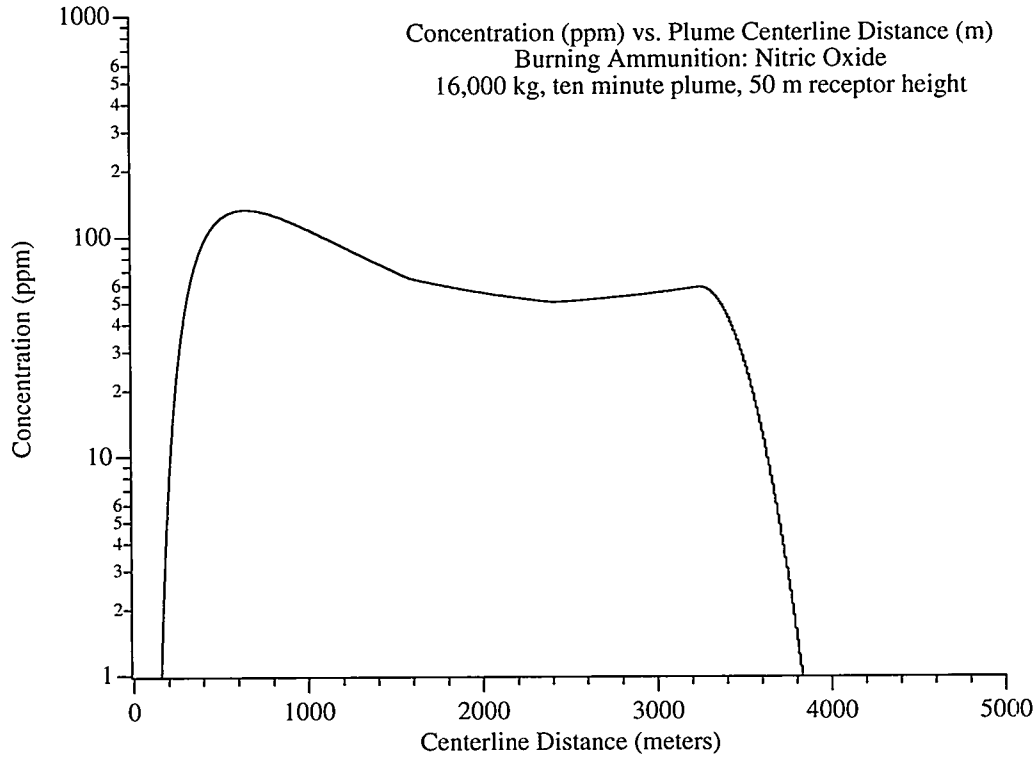
****

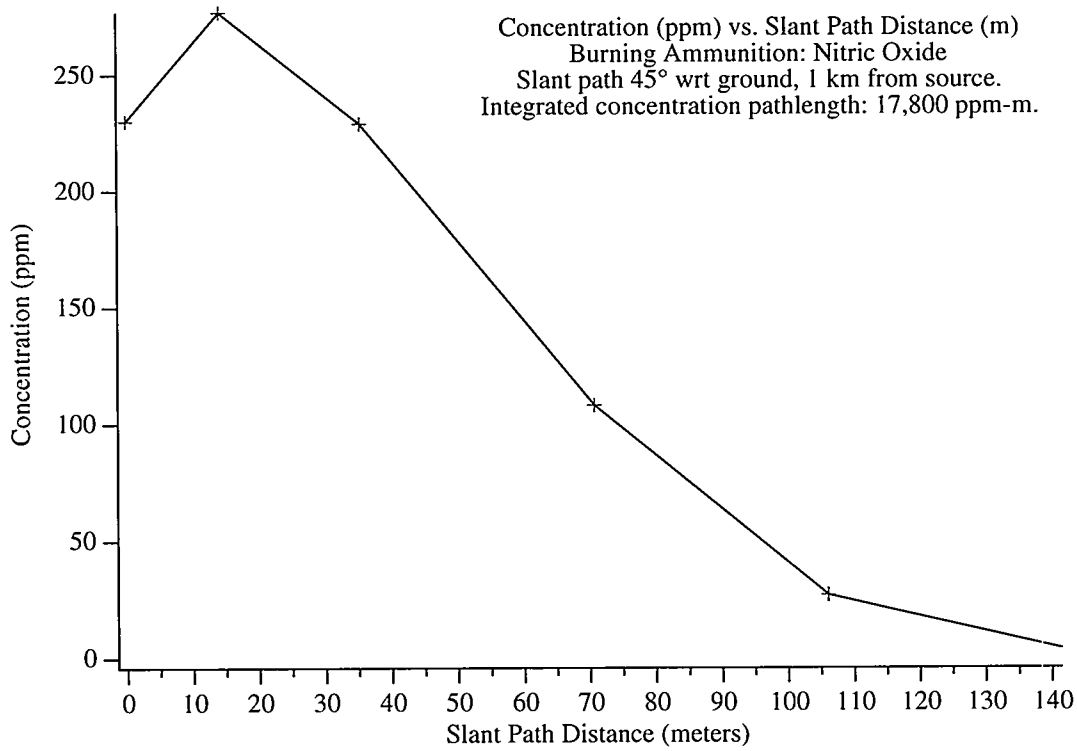
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Ammunition: Nitric Oxide, 16,000 kg, ten-minute plume.



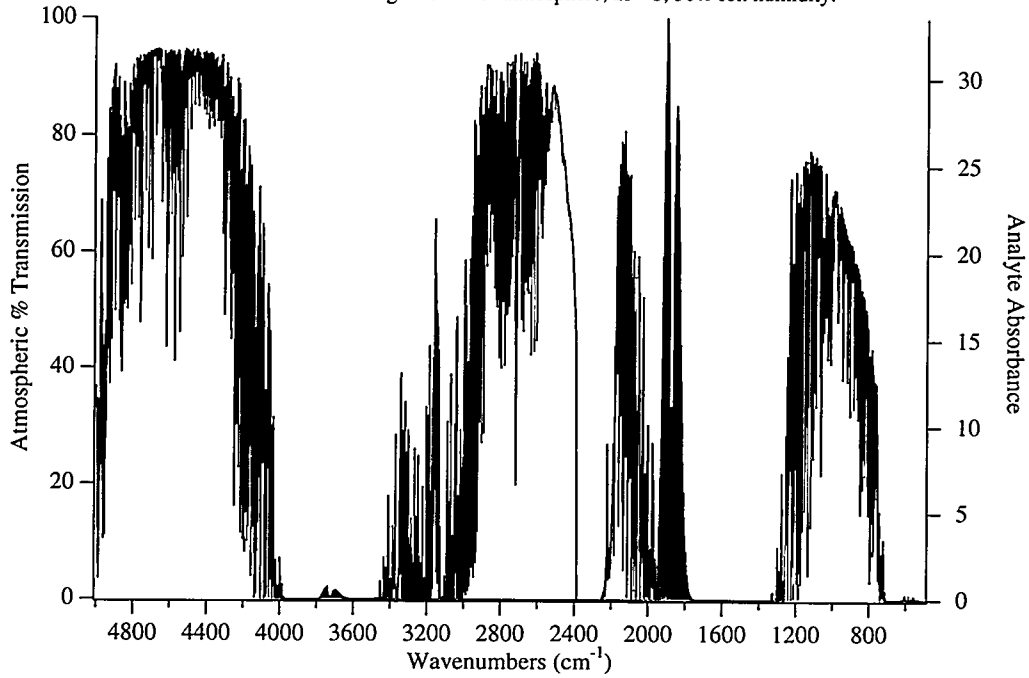



Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Ammunition: Nitric Oxide
16,000 kg, ten minute plume, 50 m receptor height
Concentration (ppm)
1000
100
10
1
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Ammunition: Nitric Oxide
Slant path 45° wrt ground, 1 km from source.
Integrated concentration pathlength: 17,800 ppm-m.
Concentration (ppm)
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
Slant Path Distance (meters)

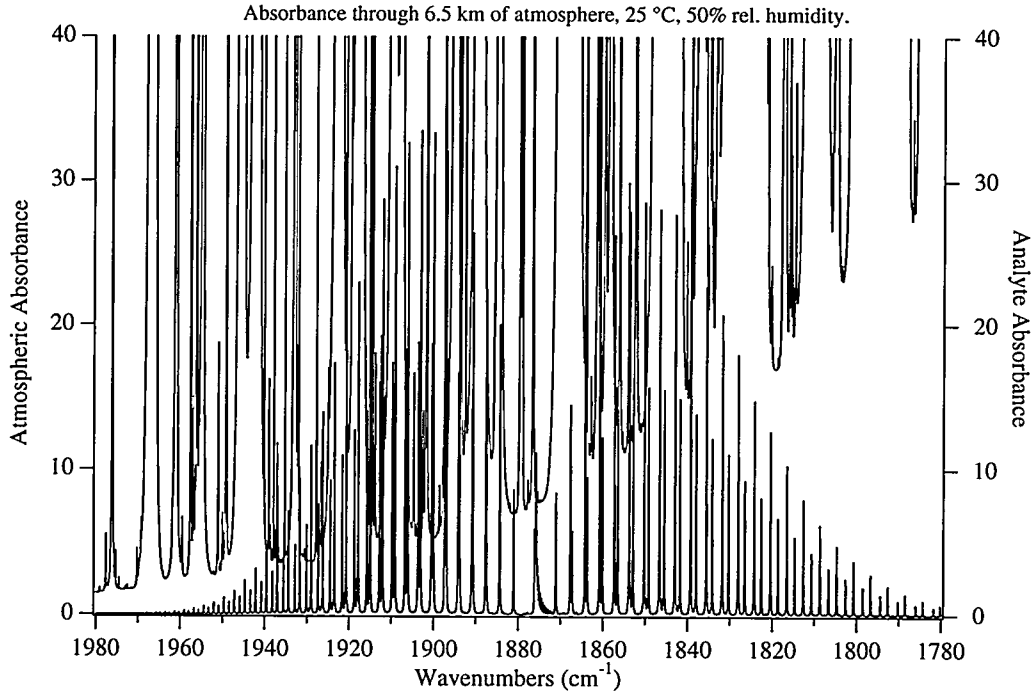
Nitric Oxide from Burning Ammunition
Nitric Oxide absorbance, 25 °C, 17,800 ppm-m, 1000 m from fire.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Nitric Oxide from Burning Ammunition
Nitric oxide absorbance, 25 °C, 17,800 ppm-m, 1000 m from fire.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



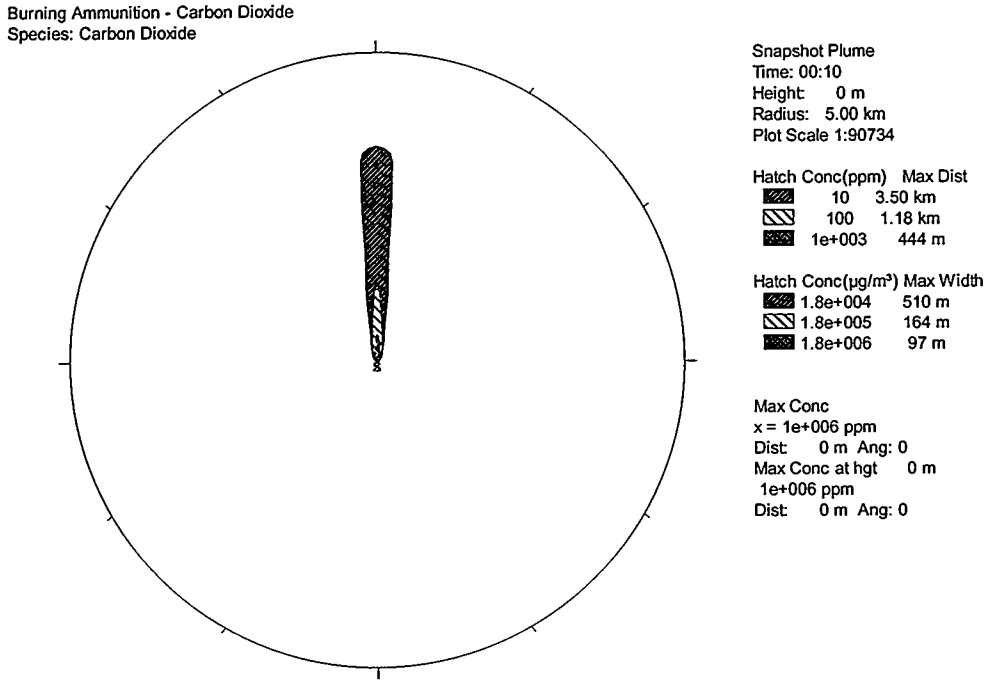
CHARM Version 9.3

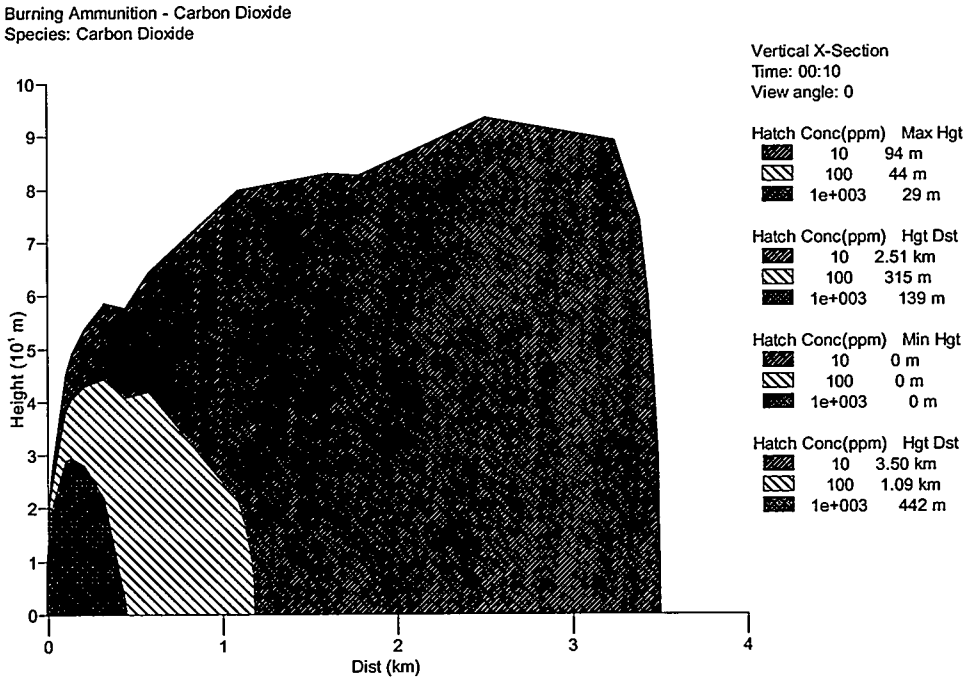
Title:	Burning Ammunition - Carbon Dioxide
Species:	Carbon Dioxide
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	10, 100, 1000
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	1.1e+004 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	11.86 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be:	concrete
Surface Specific Heat:	900 joules/kg K
Surface Thermal Conductivity:	1.2 w/m K
Surface Density:	2100 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.16
Darcy Constant of Surface:	0 m

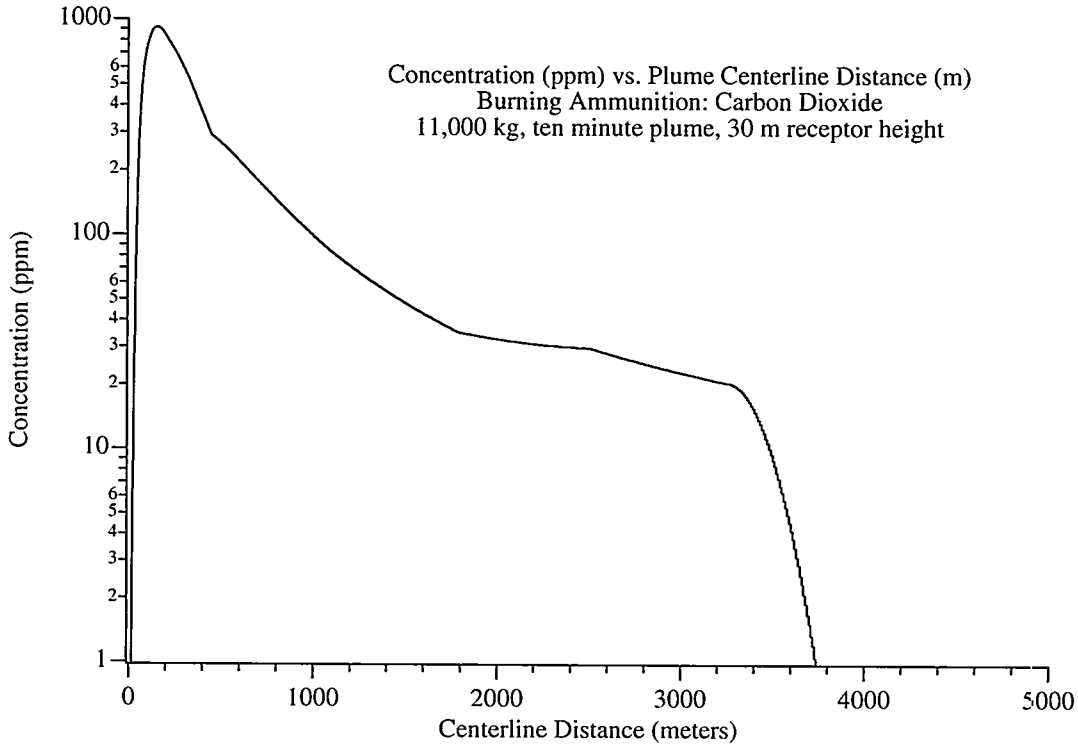
****

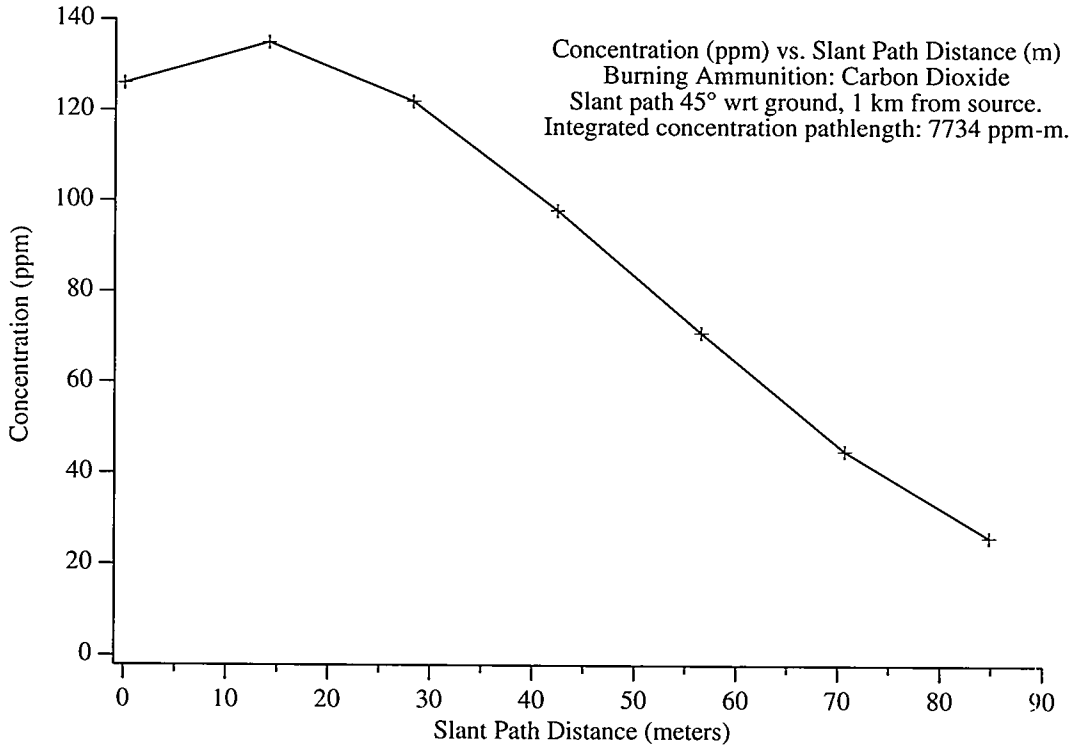
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Ammunition: Carbon Dioxide, 11,000 kg, ten-minute plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Ammunition: Carbon Dioxide
11,000 kg, ten minute plume, 30 m receptor height
Concentration (ppm)
1000
100
10
1
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Ammunition: Carbon Dioxide
Slant path 45° wrt ground, 1 km from source.
Integrated concentration pathlength: 7734 ppm-m.
Concentration (ppm)
140
120
100
80
60
40
20
0
0
10
20
30
40
50
60
70
80
90
Slant Path Distance (meters)

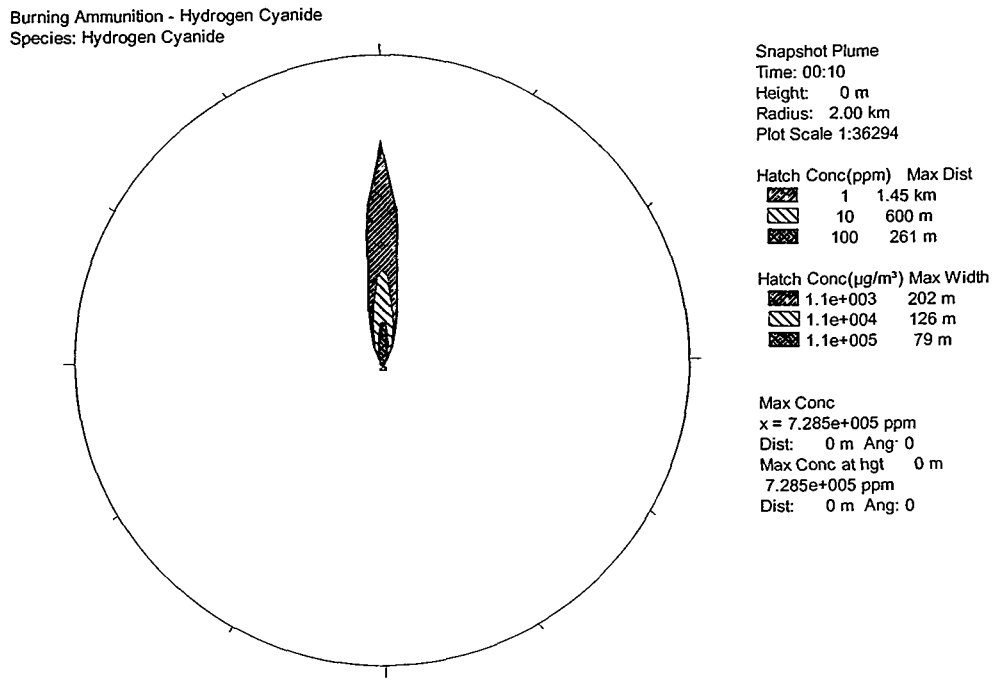
CHARM Version 9.3

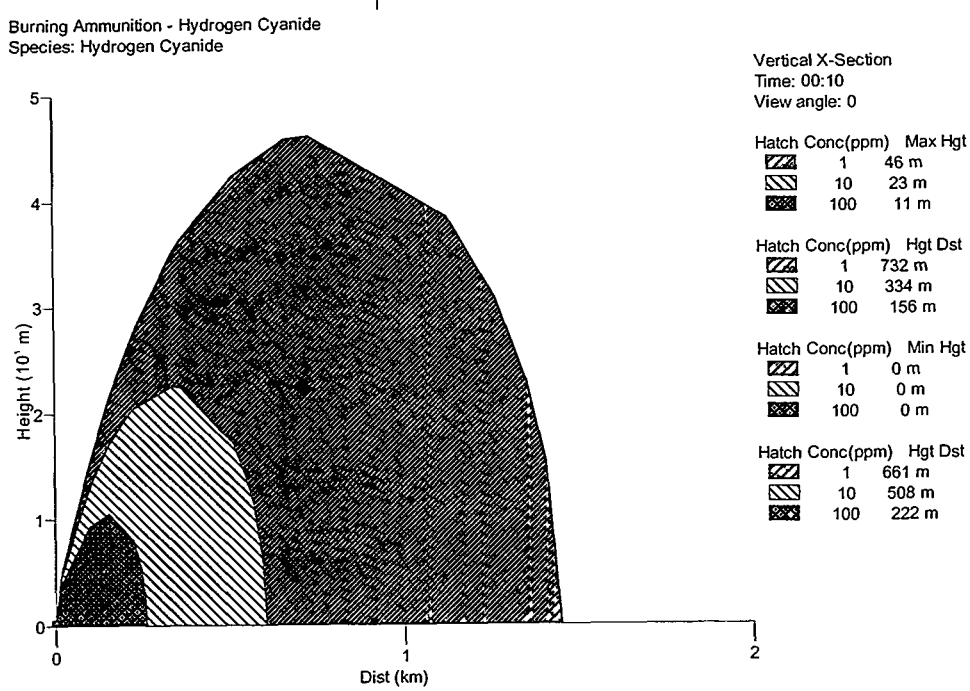
Title:	Burning Ammunition - Hydrogen Cyanide
Species:	Hydrogen Cyanide
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	500 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	1.285 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar radiation pool evaporation efficiency	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be:	concrete
Surface Specific Heat:	900 joules/kg K
Surface Thermal Conductivity:	1.2 w/m K
Surface Density:	2100 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.16
Darcy Constant of Surface:	0 m

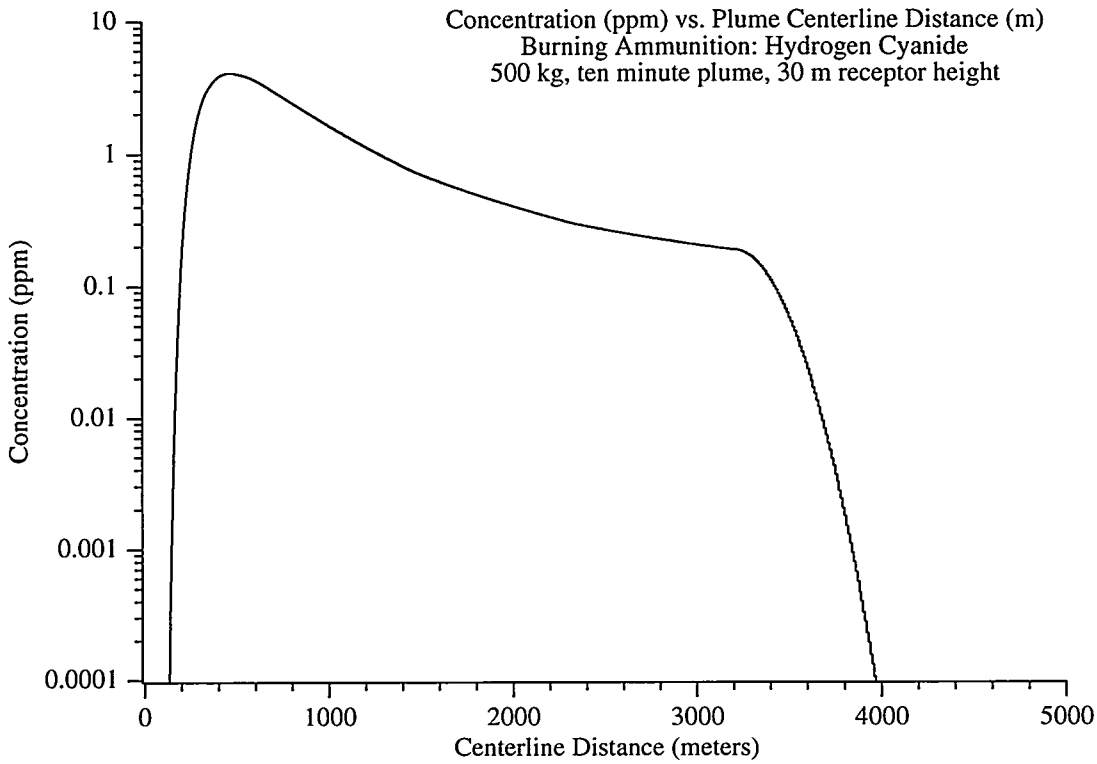
****

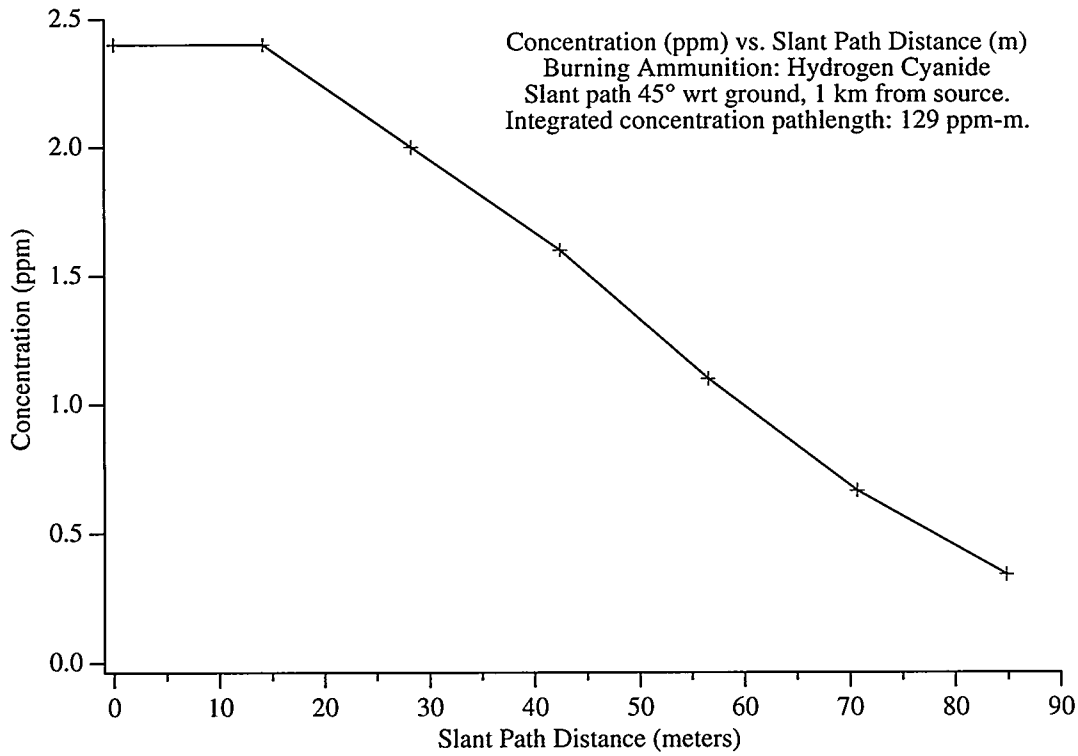
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Ammunition: Hydrogen Cyanide, 500 kg, ten-minute plume.

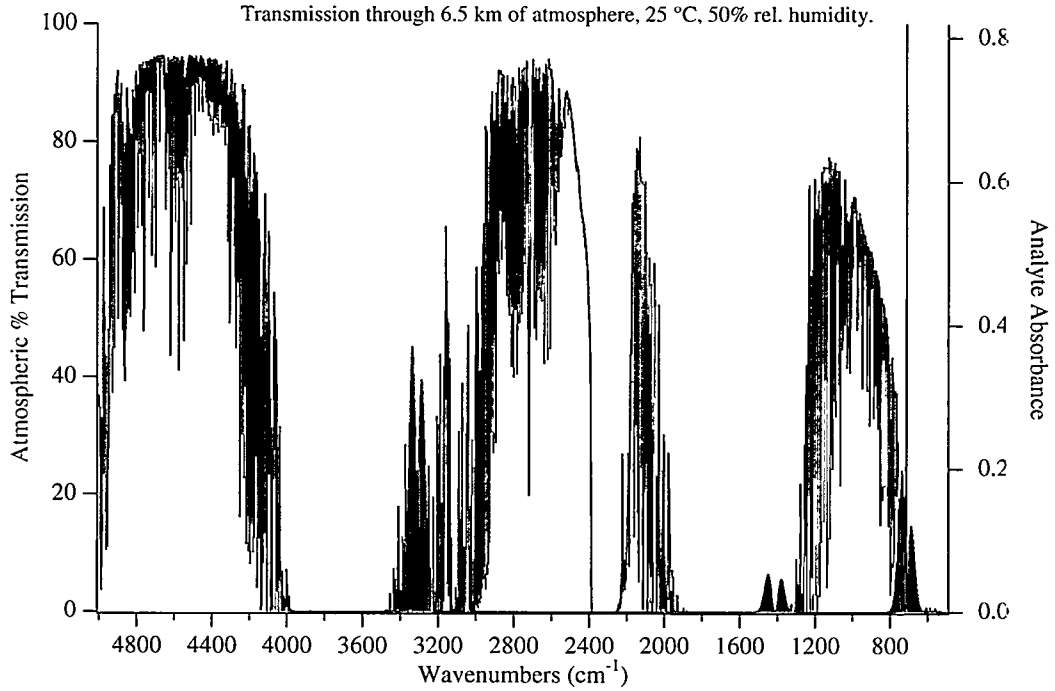




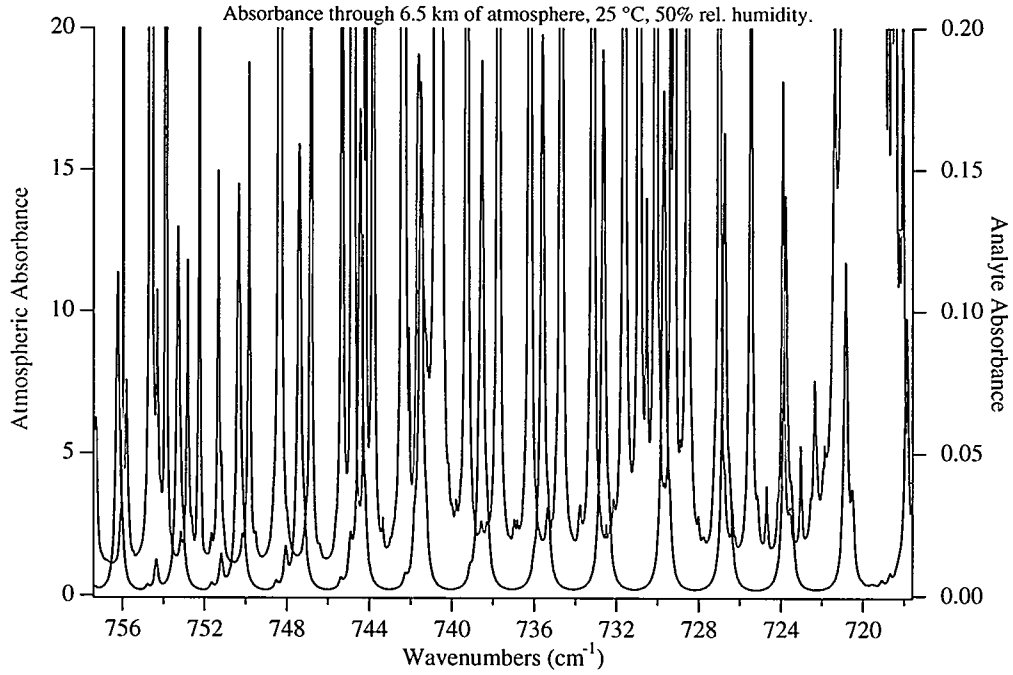

Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Ammunition: Hydrogen Cyanide
500 kg, ten minute plume, 30 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Ammunition: Hydrogen Cyanide
Slant path 45° wrt ground, 1 km from source.
Integrated concentration pathlength: 129 ppm-m.
Concentration (ppm)
2.5
2.0
1.5
1.0
0.5
0.0
0
10
20
30
40
50
60
70
80
90
Slant Path Distance (meters)

Hydrogen Cyanide from Burning Ammunition
Hydrogen cyanide absorbance, 25 °C, 129 ppm-m, 1000 m from fire.



Hydrogen Cyanide from Burning Ammunition
Hydrogen cyanide absorbance, 25 °C, 129 ppm-m, 1000 m from fire.
Detail of the R-branch of the ν_2 band.



CHARM Version 9.3

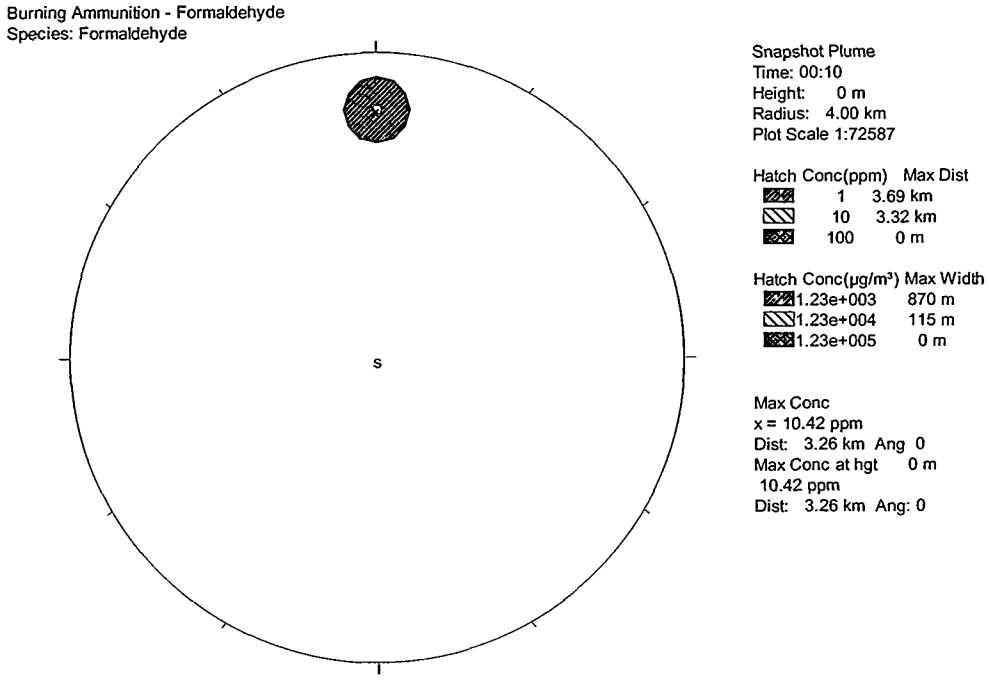
Title:	Burning Ammunition - Formaldehyde
Species:	Formaldehyde
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	300 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	0.5755 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 ft^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be:	concrete
Surface Specific Heat:	900 joules/kg K
Surface Thermal Conductivity:	1.2 w/m K
Surface Density:	2100 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.16
Darcy Constant of Surface:	0 m

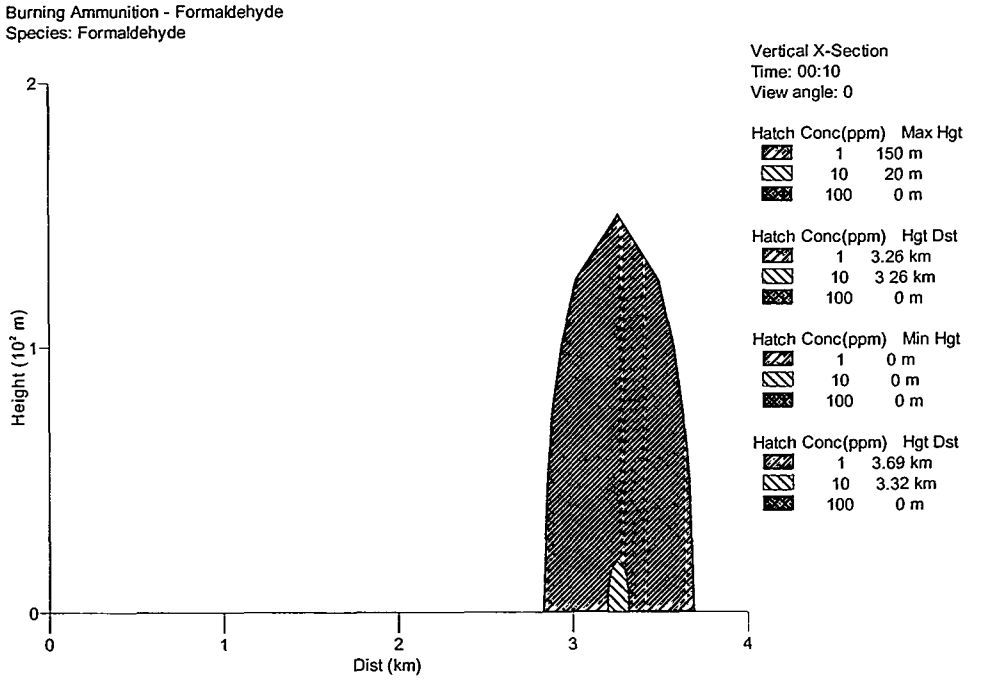
****

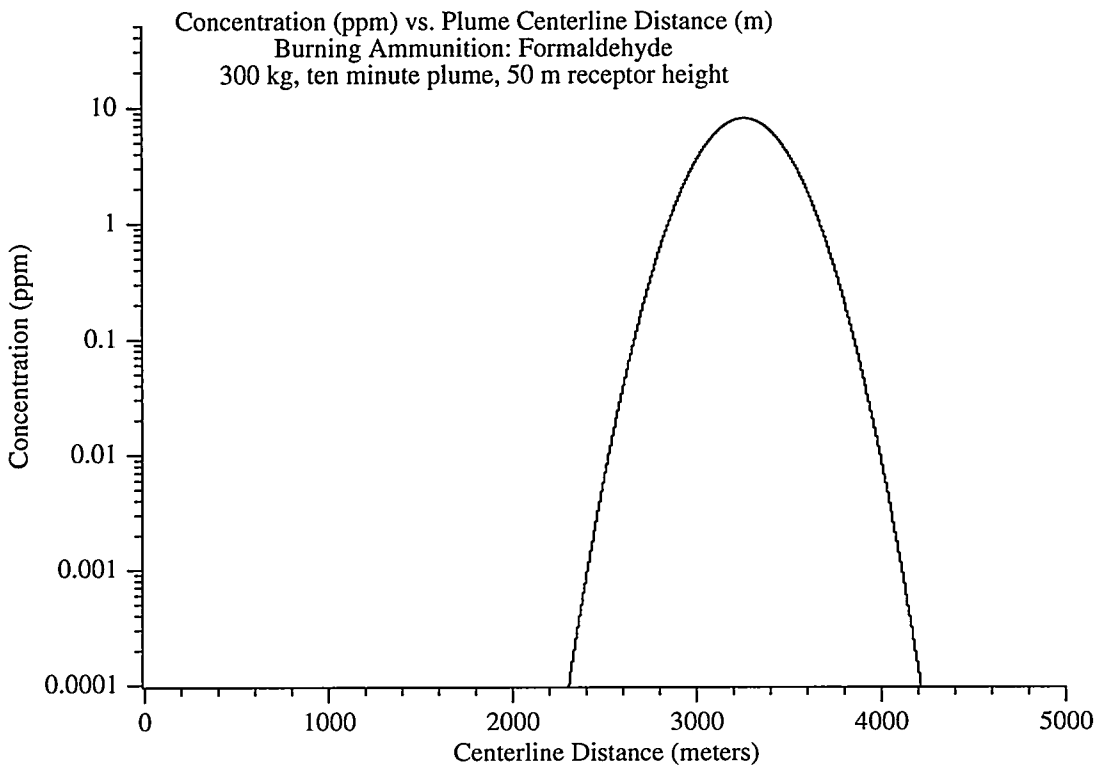
Met Data

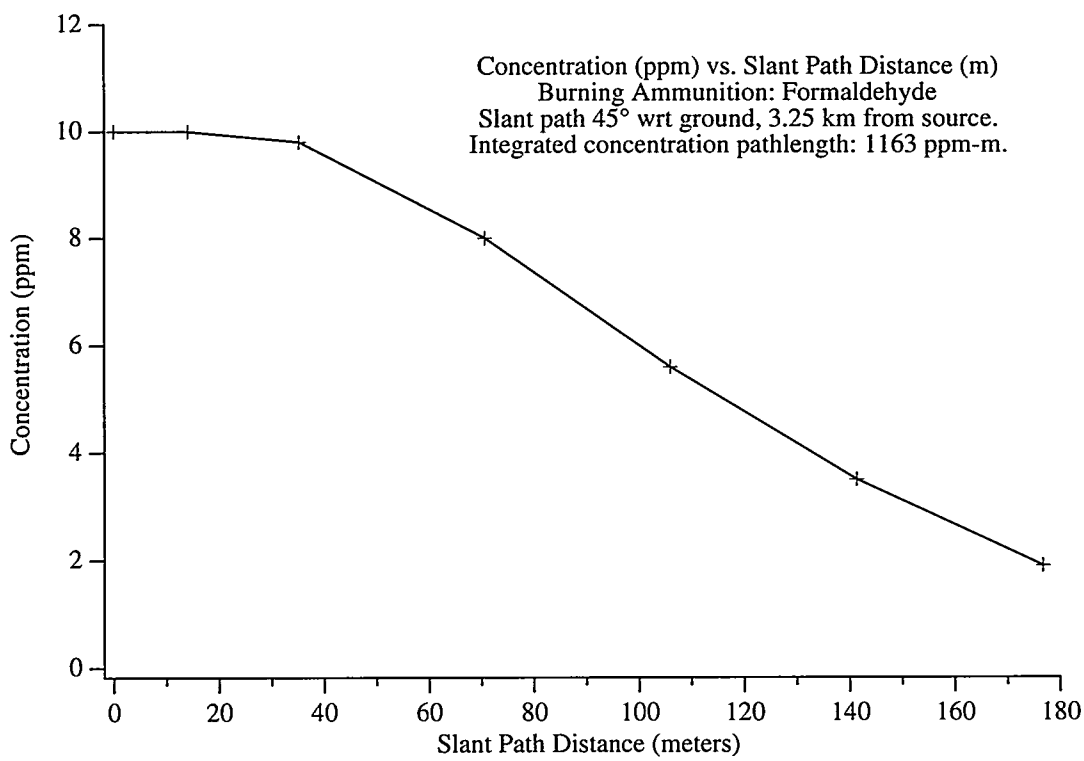
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Ammunition: Formaldehyde, 300 kg, ten-minute plume.



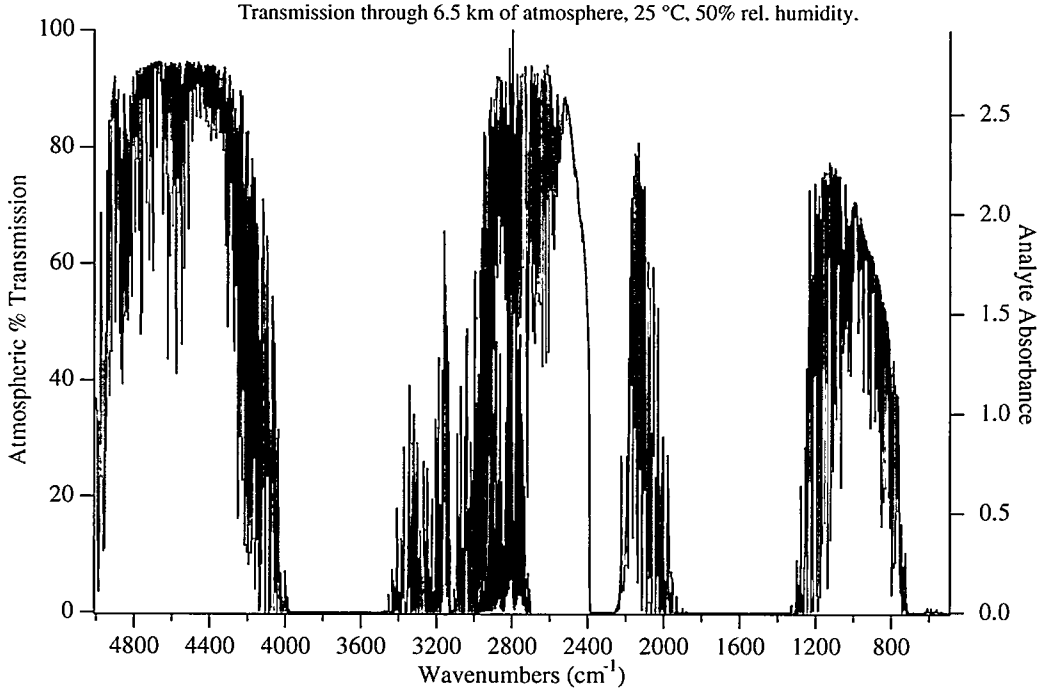



Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Ammunition: Formaldehyde
300 kg, ten minute plume, 50 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Ammunition: Formaldehyde
Slant path 45° wrt ground, 3.25 km from source.
Integrated concentration pathlength: 1163 ppm-m.
Concentration (ppm)
12
10
8
6
4
2
0
0
20
40
60
80
100
120
140
160
180
Slant Path Distance (meters)

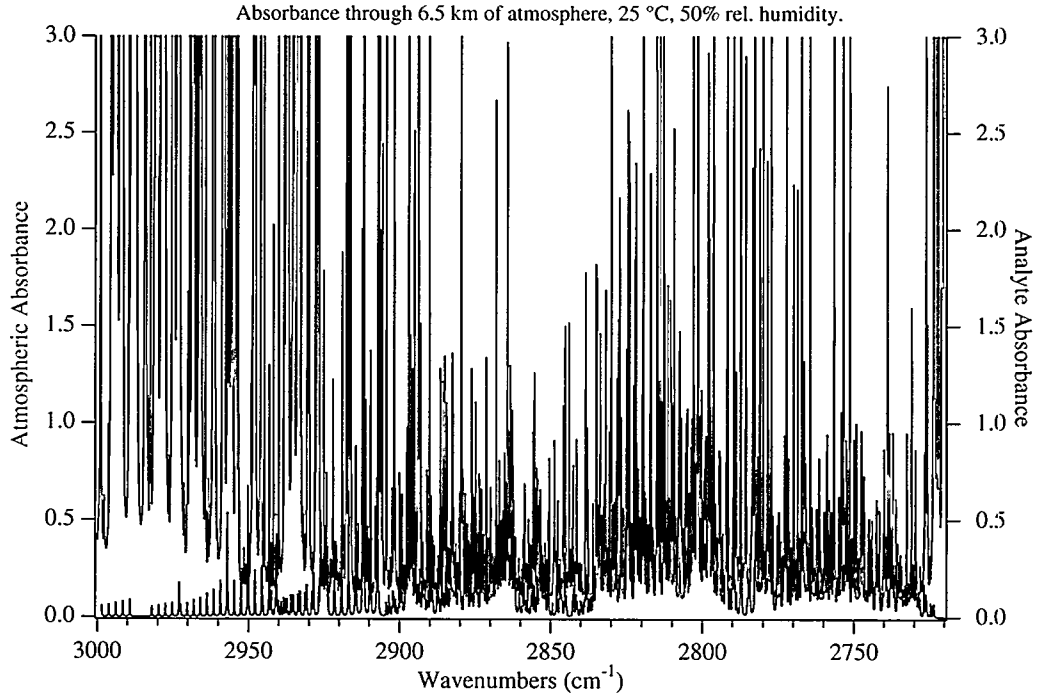
Formaldehyde from Burning Ammunition
Formaldehyde absorbance, 25 °C, 1163 ppm-m, 3250 m from fire.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Formaldehyde from Burning Ammunition
Formaldehyde absorbance, 25 °C, 1163 ppm-m, 3250 m from fire.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



3.2 Burning Sarin (GB)

Compound[a]	Total Emission (kg)[a]
Carbon dioxide	1141
Water	525
Phosphorous pentoxide[b]	460
Hydrogen fluoride	130

(a) Pugh, D. L., J. A. Baker, T. R. Gervasoni, and H. F. Hilderbrandt. October 1970. "Incineration of GB and Containment of Gaseous Products," Edgewood Arsenal Technical Report #4463.
(b) Phosphorous pentoxide is rapidly converted to phosphoric acid down stream of the burning pool.

Scenario: One ton (909 kg) of stored sarin (GB, isopropyl methylphosphonofluoridate) is burned in an explosion at a temperature of 1500 K. The quantities of the compounds are calculated from the stoichiometry of the combustion reaction:

$$2CH_3\text{-}P(O)(F)\text{-}OC_3H_7 + 13CO_2 \rightarrow 8CO_2 + 9H_2O + P_2O_5 + 2HF$$

This scenario assumes complete combustion of material; in fact some material may be volatilized without destruction (Pugh *et al.* 1970; Rapp *et al.* 1997; Cool *et al.* 1998).

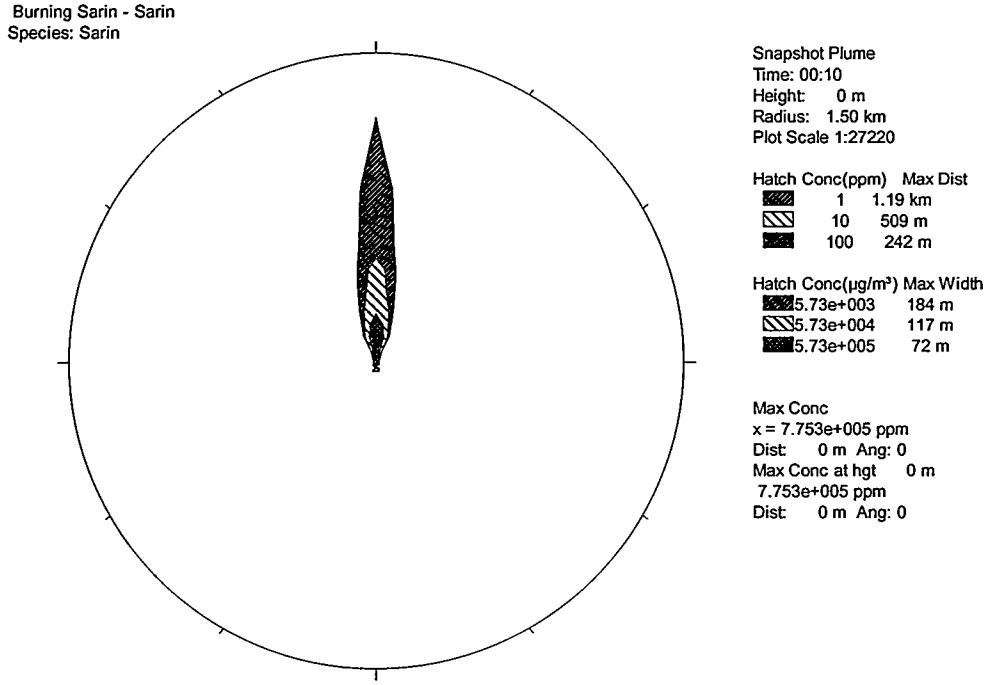
CHARM Version 9.3

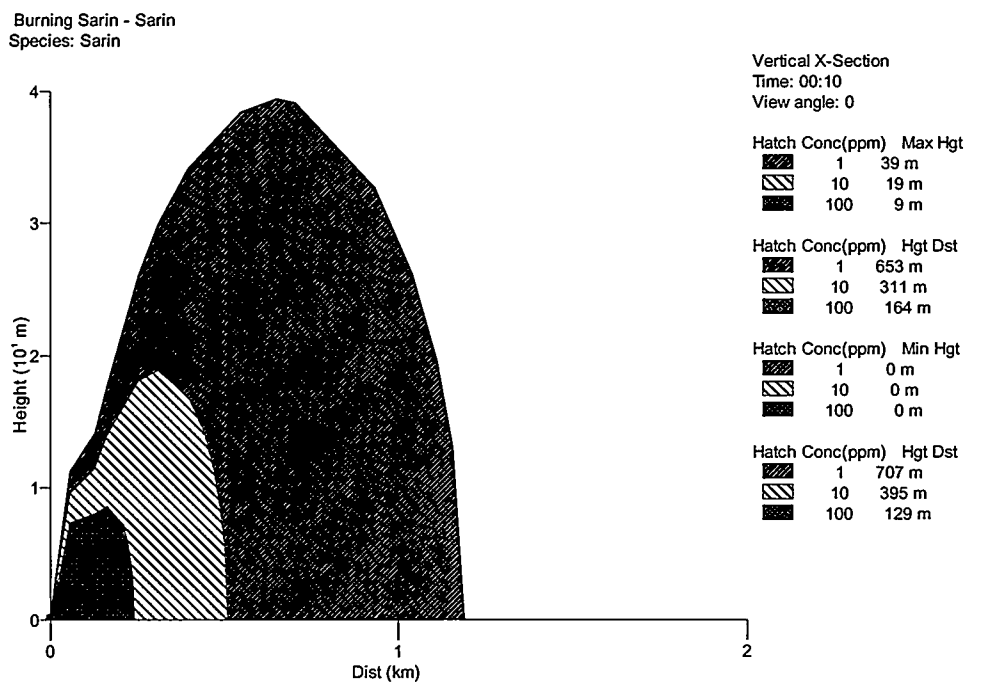
Title:	Burning Sarin - Sarin
Species:	Sarin
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	909 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	1.088 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 m^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be	dirt
Surface Specific Heat:	800 joules/kg K
Surface Thermal Conductivity:	0.32 w/m K
Surface Density:	1640 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.34
Darcy Constant of Surface:	2.8e-007 m

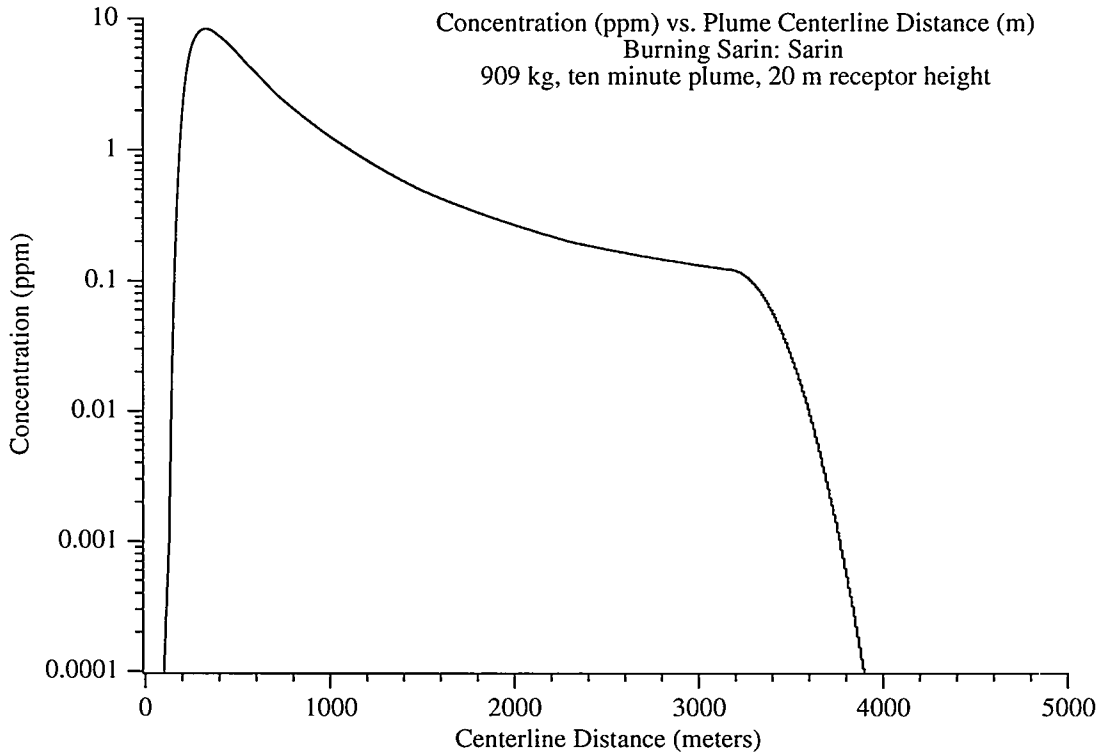
****

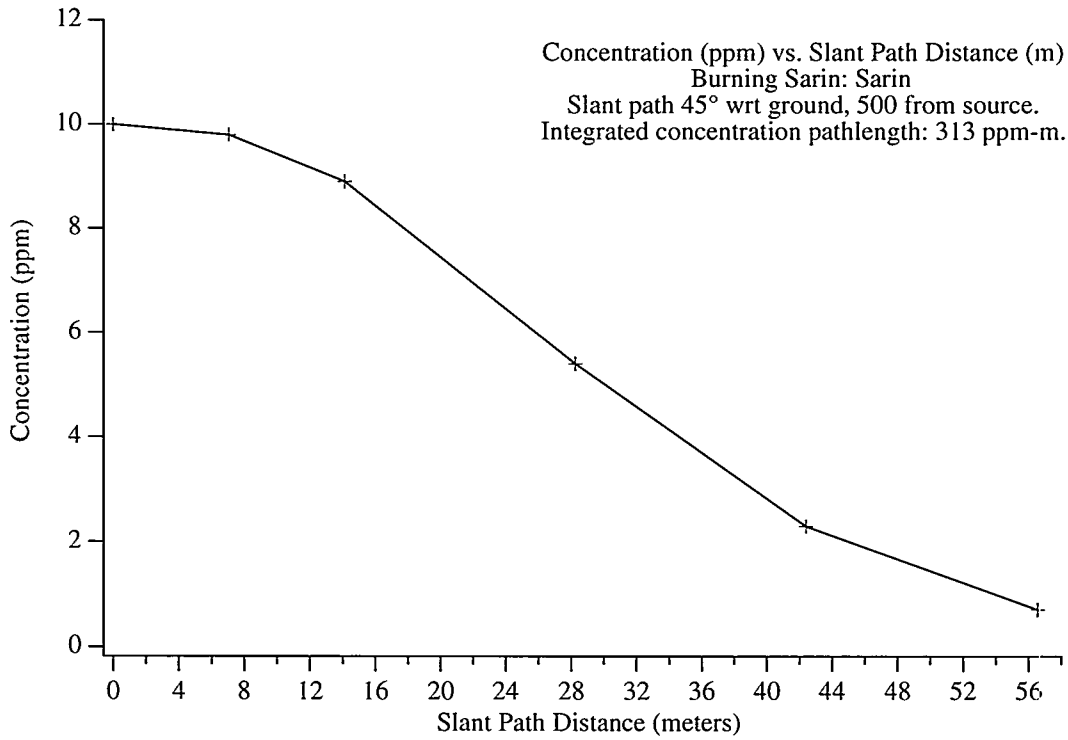
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No Inversion Present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Sarin: Sarin, 909 kg, ten-minute plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Sarin: Sarin
909 kg, ten minute plume, 20 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Sarin: Sarin
Slant path 45° wrt ground, 500 from source.
Integrated concentration pathlength: 313 ppm-m.
Concentration (ppm)
12
10
8
6
4
2
0
0
4
8
12
16
20
24
28
32
36
40
44
48
52
56
Slant Path Distance (meters)

CHARM Version 9.3

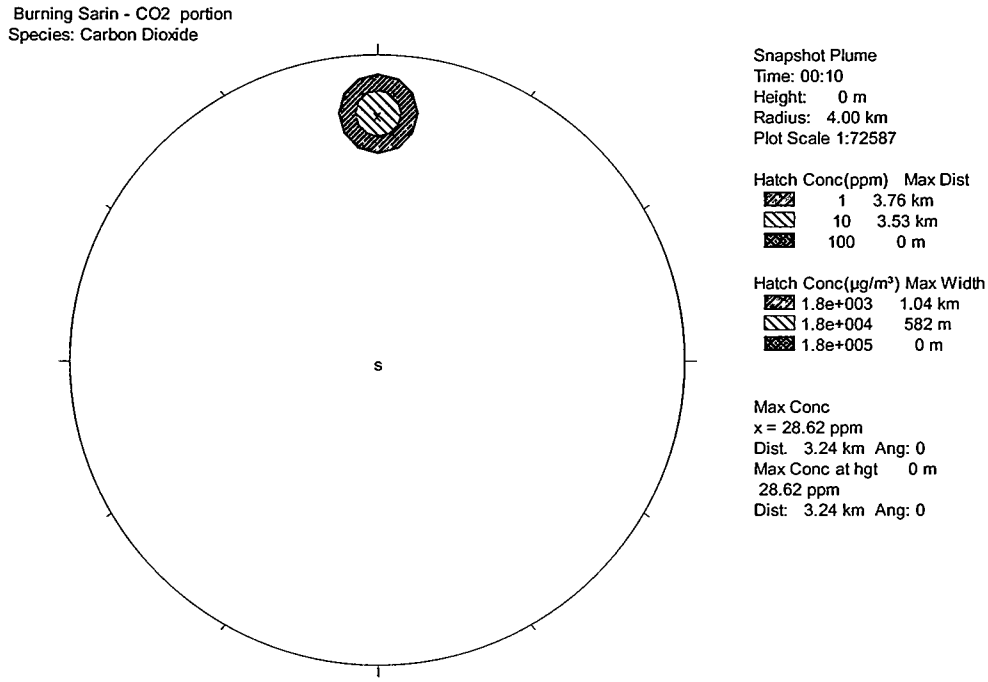
Title:	Burning Sarin - CO2 portion
Species:	Carbon Dioxide
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 ft
Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	1141 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	1.231 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 m^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be	dirt
Surface Specific Heat:	800 joules/kg K
Surface Thermal Conductivity:	0.32 w/m K
Surface Density:	1640 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.34
Darcy Constant of Surface:	2.8e-007 m

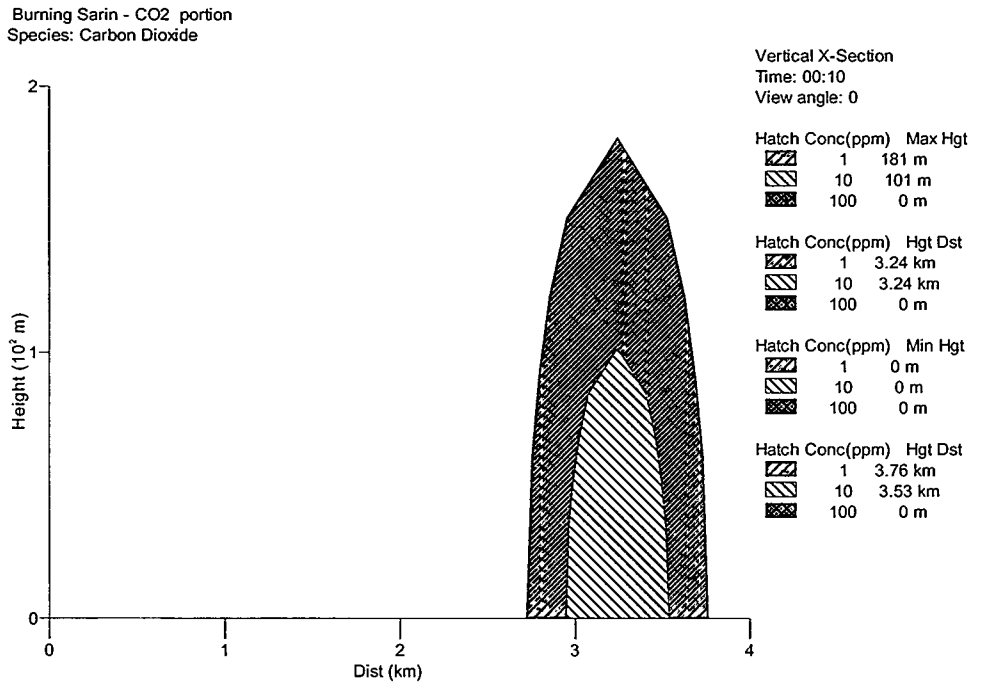
****

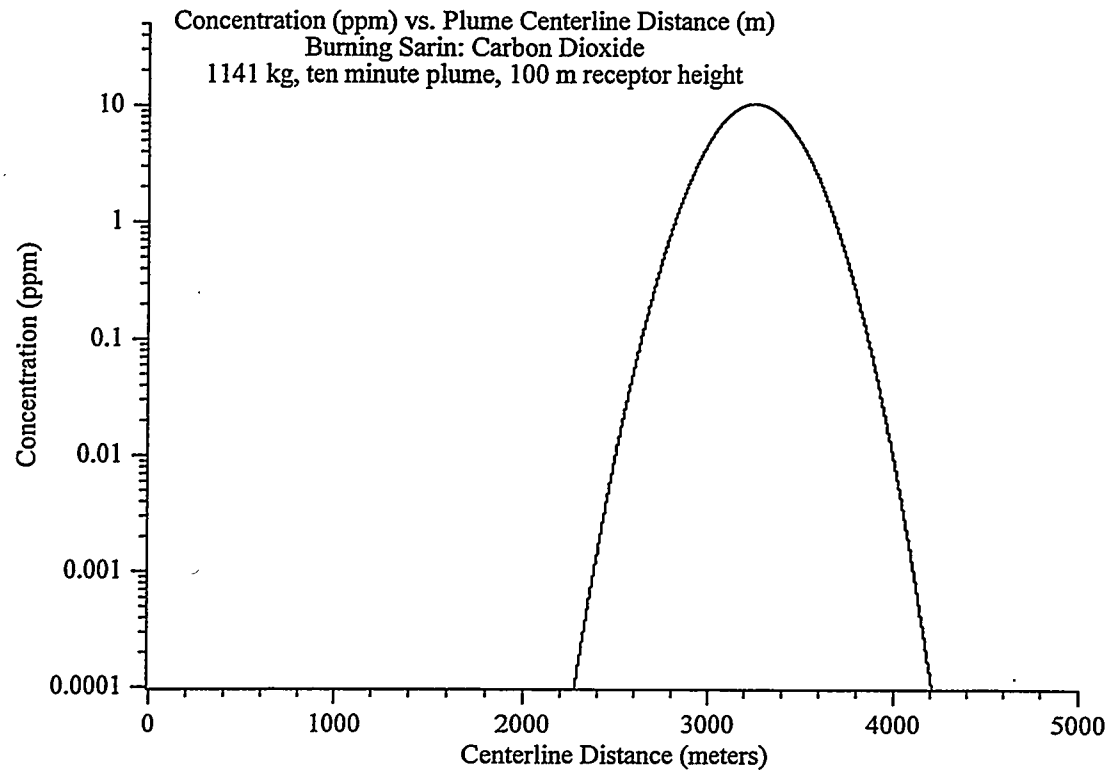
Met Data

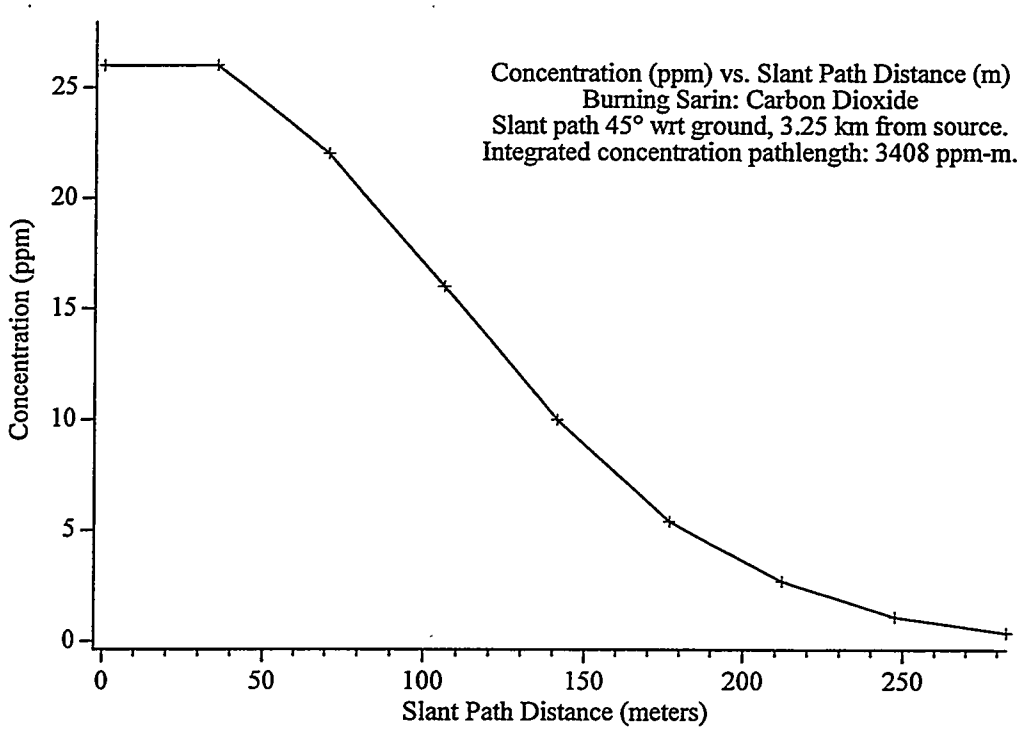
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Burning Sarin: Carbon Dioxide, 1141 kg, ten-minute plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Sarin: Carbon Dioxide
1141 kg, ten minute plume, 100 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Sarin: Carbon Dioxide
Slant path 45° wrt ground, 3.25 km from source.
Integrated concentration pathlength: 3408 ppm-m.
Concentration (ppm)
25
20
15
10
5
0
0
50
100
150
200
250
Slant Path Distance (meters)

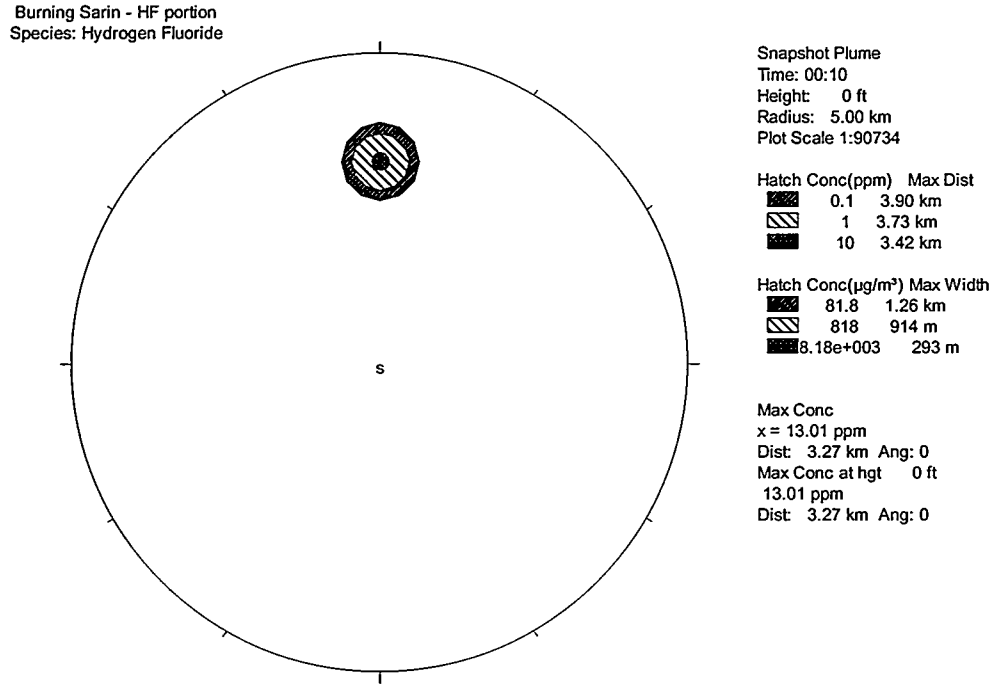
CHARM Version 9.3

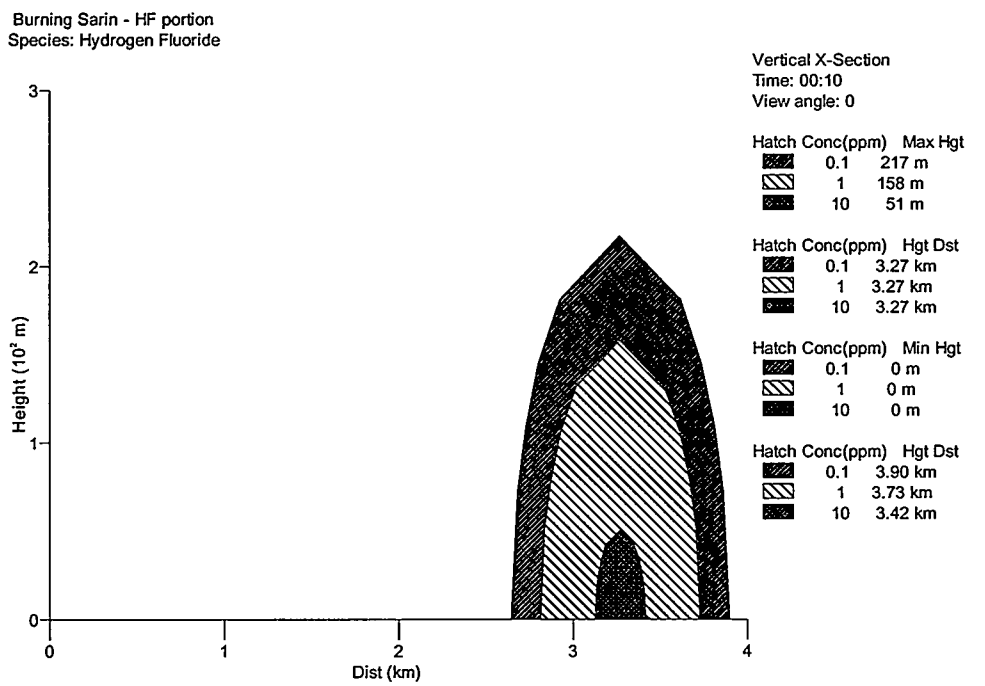
Title:	Burning Sarin - HF portion
Species:	Hydrogen Fluoride
Release Type:	Pool/Lagoon Description
Emergency Response Output:	Plume
X location:	0 ft
Y location:	0 ft
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 ft
Building Width:	0 ft
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Liquid Pool Surface Height Above Ground:	0 m
Amount Released:	130 kilograms
Pool Diameter:	10 m
Pool Depth (Calculated):	0.2244 in
Pool Temperature:	1500 K
No Pool Mitigation Time	
Solar Radiation Pool Evaporation Efficiency:	1
Wetted Tank Surface Area (liquid pool fire):	0 m^2
Water Fraction of Spill Surface (0 -> 1):	0.15
Surface is assumed to be	dirt
Surface Specific Heat:	800 joules/kg K
Surface Thermal Conductivity:	0.32 w/m K
Surface Density:	1640 kg/m^3
Relative Pore Volume of Surface (0 ->1):	0.34
Darcy Constant of Surface:	2.8e-007 m

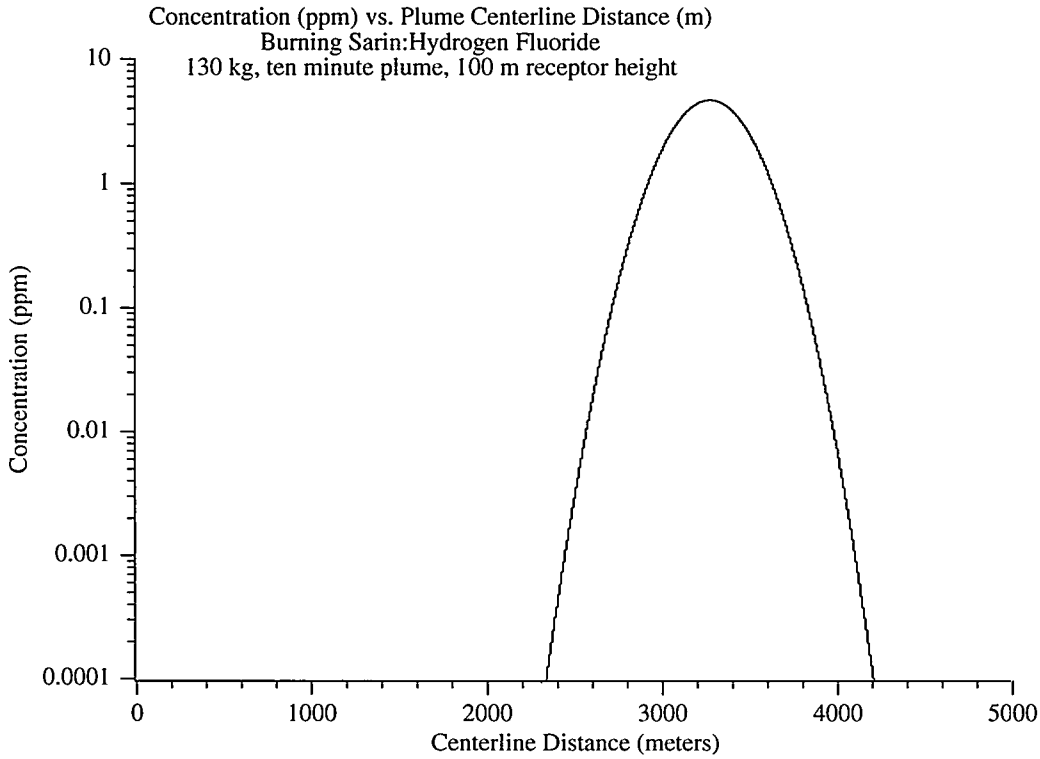
****

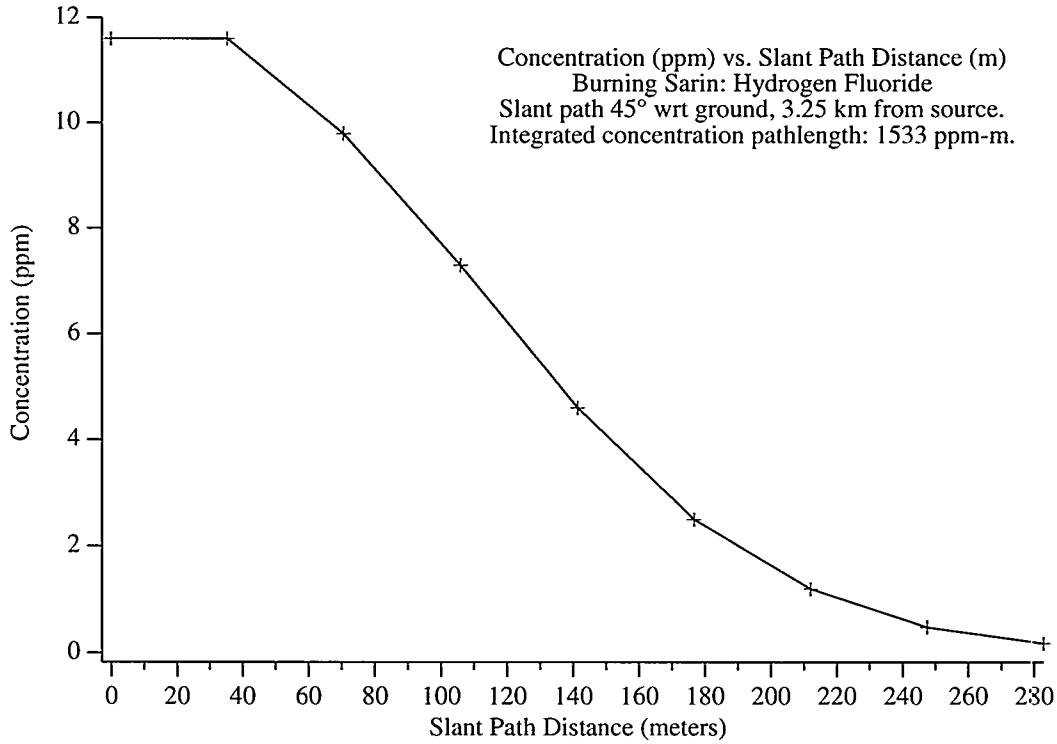
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

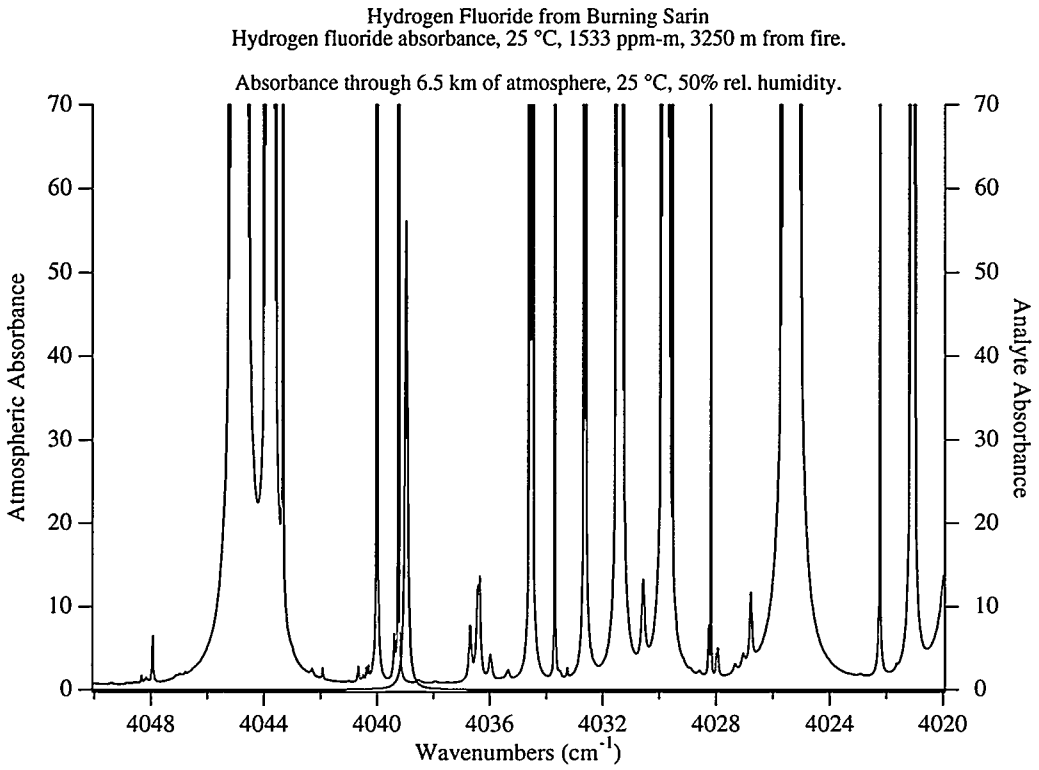
Burning Sarin: Hydrogen Fluoride, 130 kg, ten-minute plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Burning Sarin:Hydrogen Fluoride
130 kg, ten minute plume, 100 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
1000
2000
3000
4000
5000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Burning Sarin: Hydrogen Fluoride
Slant path 45° wrt ground, 3.25 km from source.
Integrated concentration pathlength: 1533 ppm-m.
Concentration (ppm)
12
10
8
6
4
2
0
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
Slant Path Distance (meters)


Hydrogen Fluoride from Burning Sarin
Hydrogen fluoride absorbance, 25 °C, 1533 ppm-m, 3250 m from fire.
Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric Absorbance
Analyte Absorbance
Wavenumbers (cm-1)
0
10
20
30
40
50
60
70
4048
4044
4040
4036
4032
4028
4024
4020

4.0 Human Activities

4.1 Exhaled Human Breath

Compound	Emission Rate (g/sec) for 1000 People	Emission Rate (g/sec) from One Vent
Carbon Dioxide[a]	9	2
Water[b]	4	1
Methane[c]	2×10^{-3}	5×10^{-4}
Carbon monoxide[c]	4×10^{-4}	1×10^{-5}
Ammonia[d]	4×10^{-5}	1×10^{-5}
Acetone[e,f,g,h]	2×10^{-5}	5×10^{-6}
Acetonitrile[i]	8×10^{-6}	2×10^{-6}
Isoprene[e,g,h,i]	6×10^{-6}	2×10^{-6}
p-Tolualdehyde[e,g,h]	3×10^{-6}	8×10^{-7}
Ethylene	3×10^{-6}	8×10^{-7}
Toluene[e,g,h]	2×10^{-6}	5×10^{-7}
2,3-Dimethylhexane[e,g,h]	2×10^{-6}	5×10^{-7}
Acetaldehyde[e,g,h]	1×10^{-6}	3×10^{-7}
Ethyl Alcohol[e,g,h]	1×10^{-6}	3×10^{-7}

(a) Phillips (1992)
(b) Assumes equimolar output with carbon dioxide
(c) Moskalenko *et al.* (1996)
(d) Hunt and Williams (1977)
(e) Krotoszynski *et al.* (1977)
(f) Phillips and Greenberg (1987)
(g) Phillips and Greenberg (1992)
(h) Conkle *et al.* (1975)
(i) Gelmont *et al.* (1981)

Scenario: One-thousand people performing sedentary and light-duty activities in an underground facility. Assumes a breath ventilation rate of 5 liters/minute; 70% alveolar air, 30% dead space air.

CHARM Version 9.3

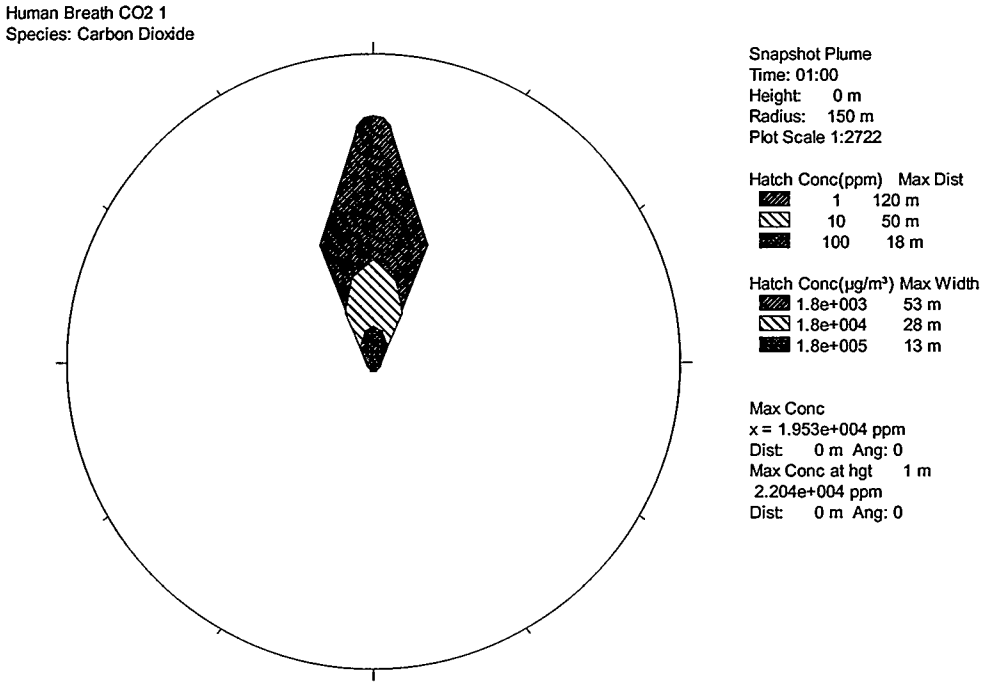
Title:	Human Breath CO2
Species:	Carbon Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	2.25 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

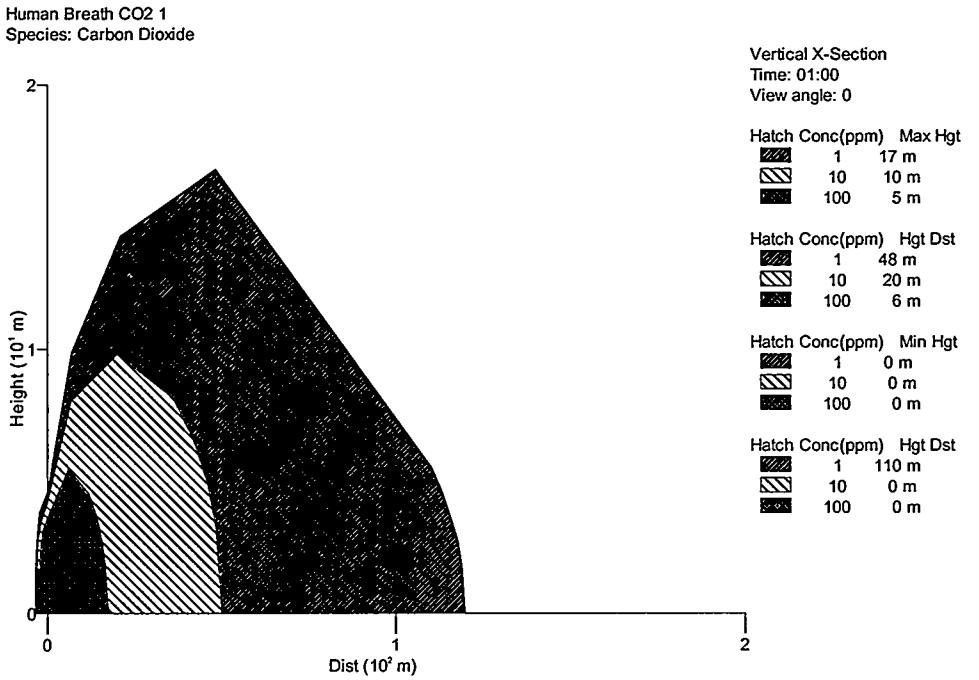
****

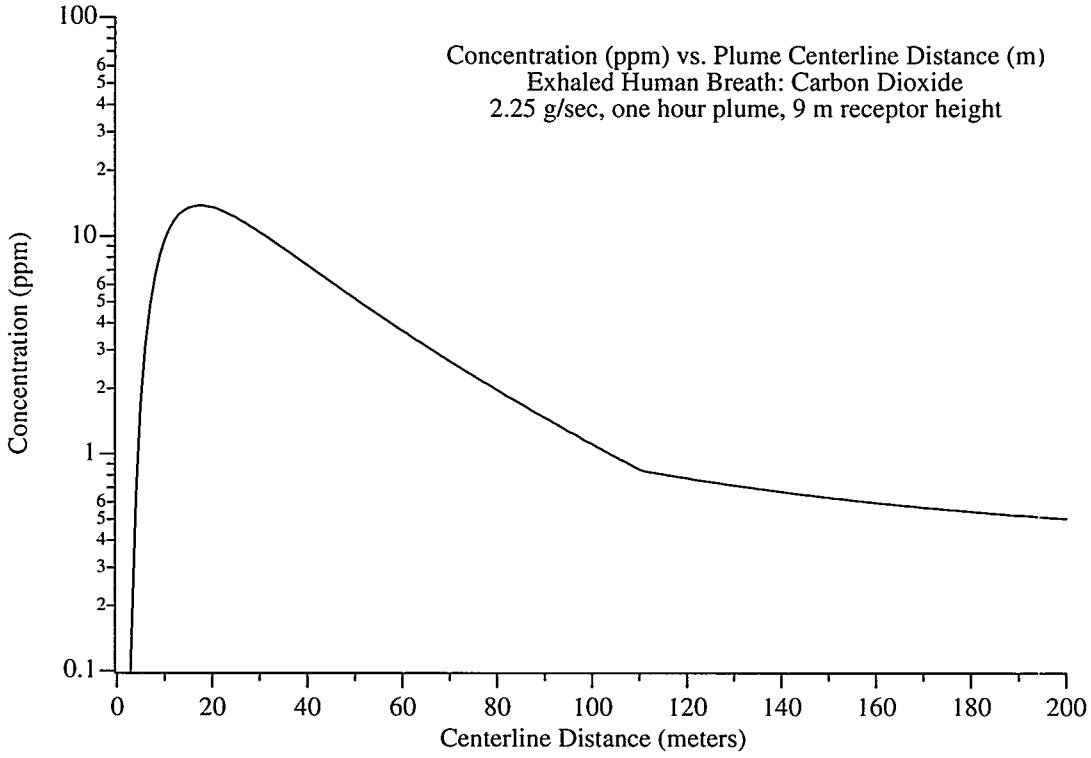
Met Data

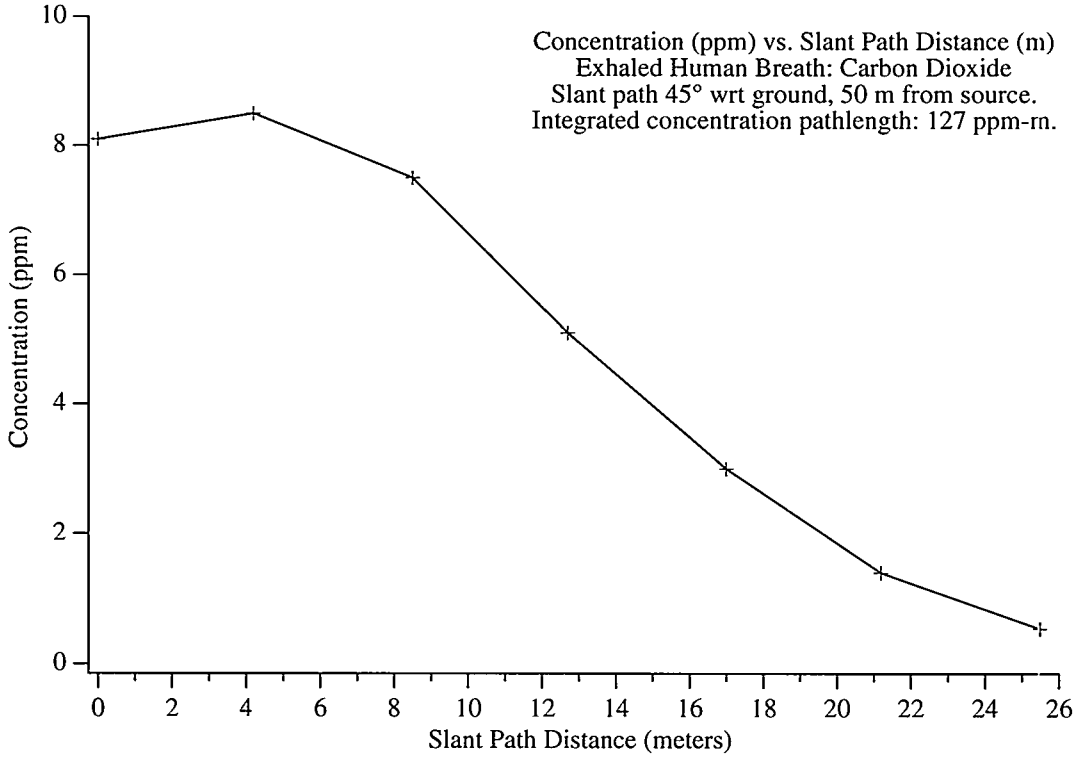
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Human Breath: Carbon Dioxide, 2.25 g/sec, one vent, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Exhaled Human Breath: Carbon Dioxide
2.25 g/sec, one hour plume, 9 m receptor height
Concentration (ppm)
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Exhaled Human Breath: Carbon Dioxide
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 127 ppm-m.
Concentration (ppm)
Slant Path Distance (meters)

CHARM Version 9.3

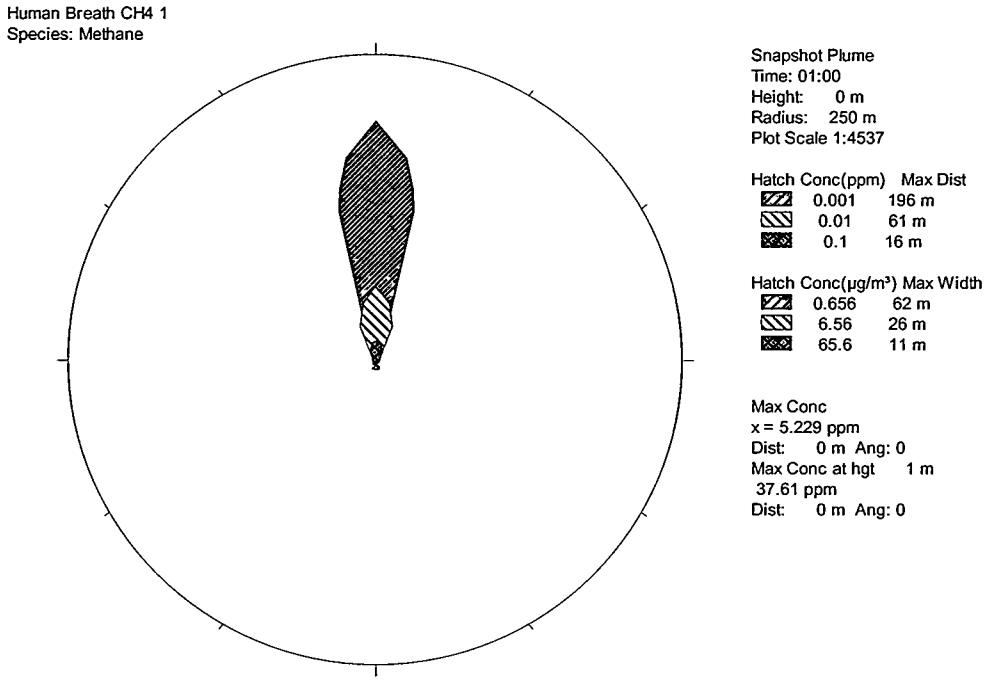
Title:	Human Breath CH4
Species:	Methane
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.0005 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

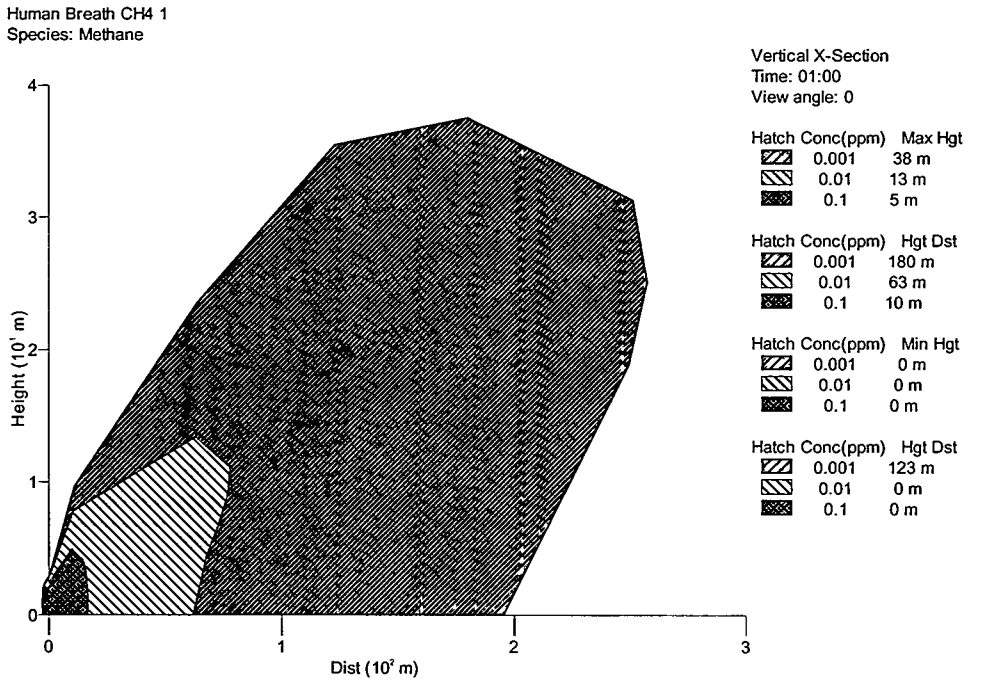
****

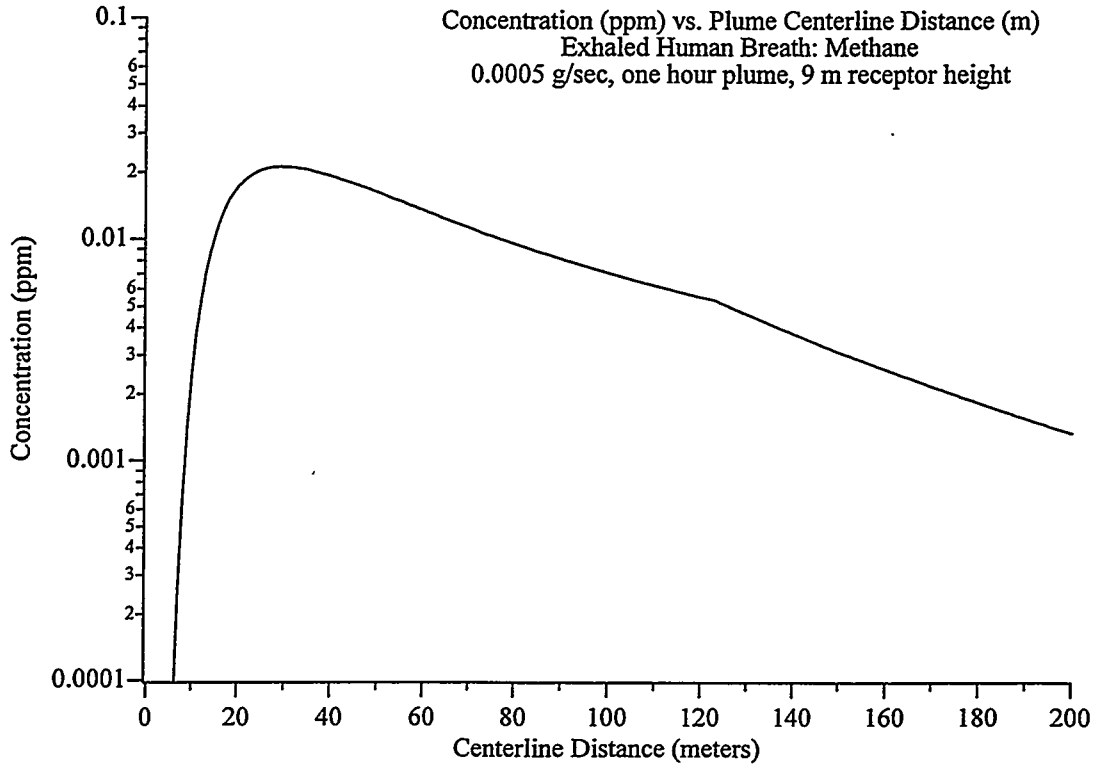
Met Data

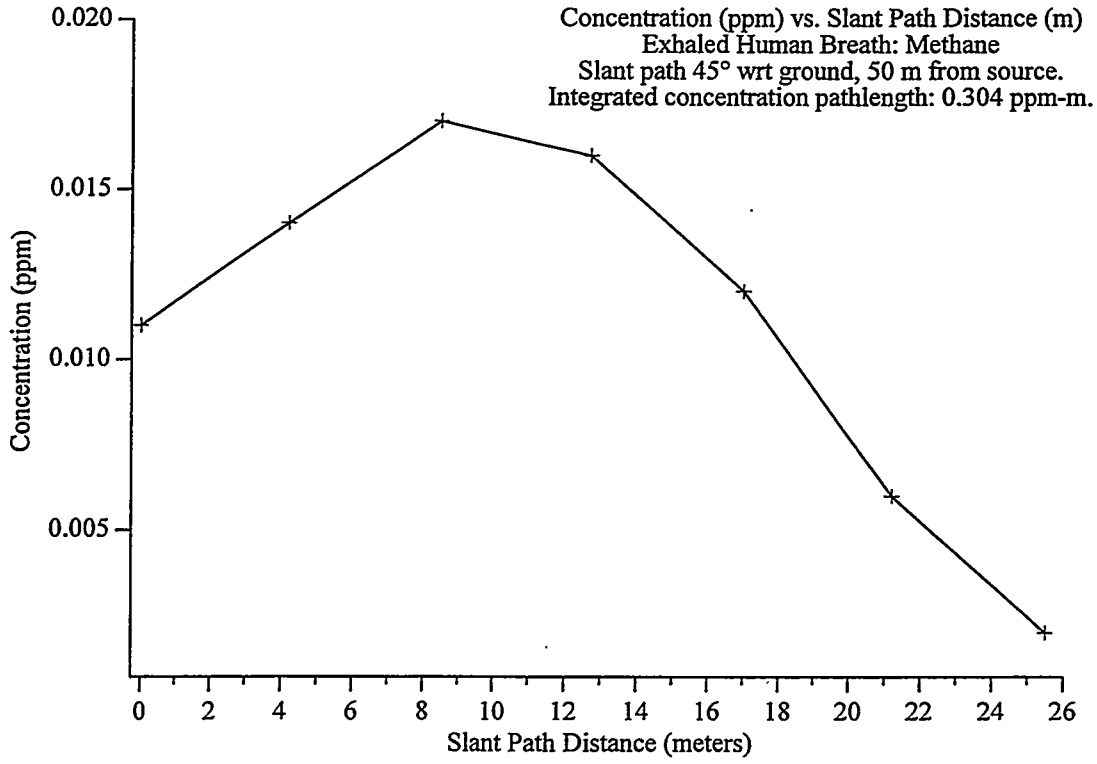
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Human Breath: Methane, 0.0005 g/sec, one vent, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Exhaled Human Breath: Methane
0.0005 g/sec, one hour plume, 9 m receptor height
Concentration (ppm)
0.1
0.01
0.001
0.0001
0
20
40
60
80
100
120
140
160
180
200
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Exhaled Human Breath: Methane
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 0.304 ppm-m.
Concentration (ppm)
0.020
0.015
0.010
0.005
0
2
4
6
8
10
12
14
16
18
20
22
24
26
Slant Path Distance (meters)

CHARM Version 9.3

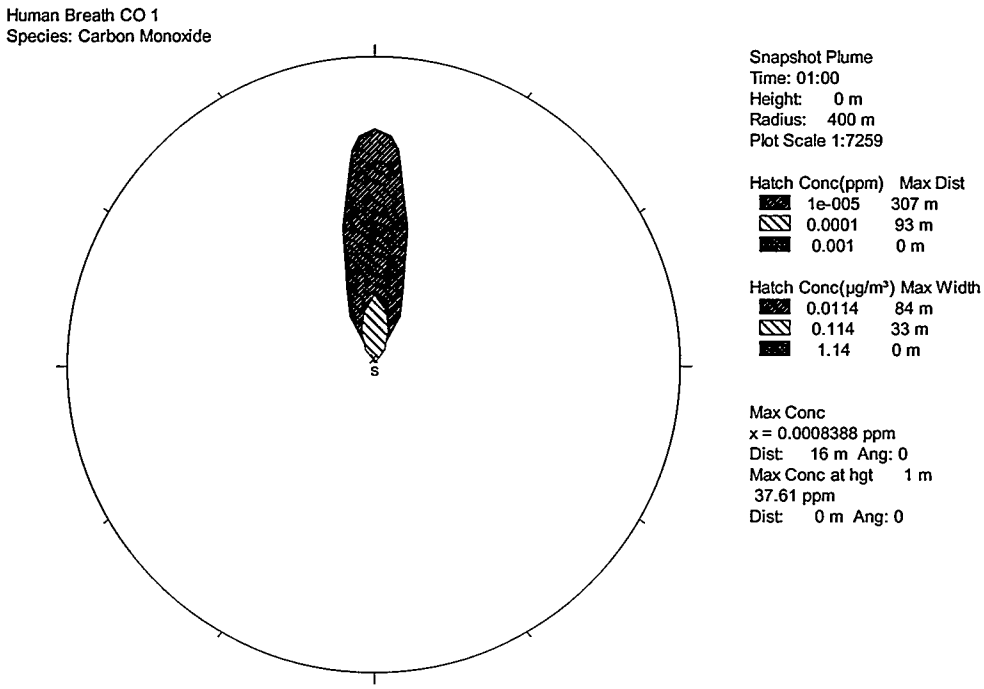
Title:	Human Breath CO
Species:	Carbon Monoxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1e-005, 0.0001, 0.001
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.0001 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

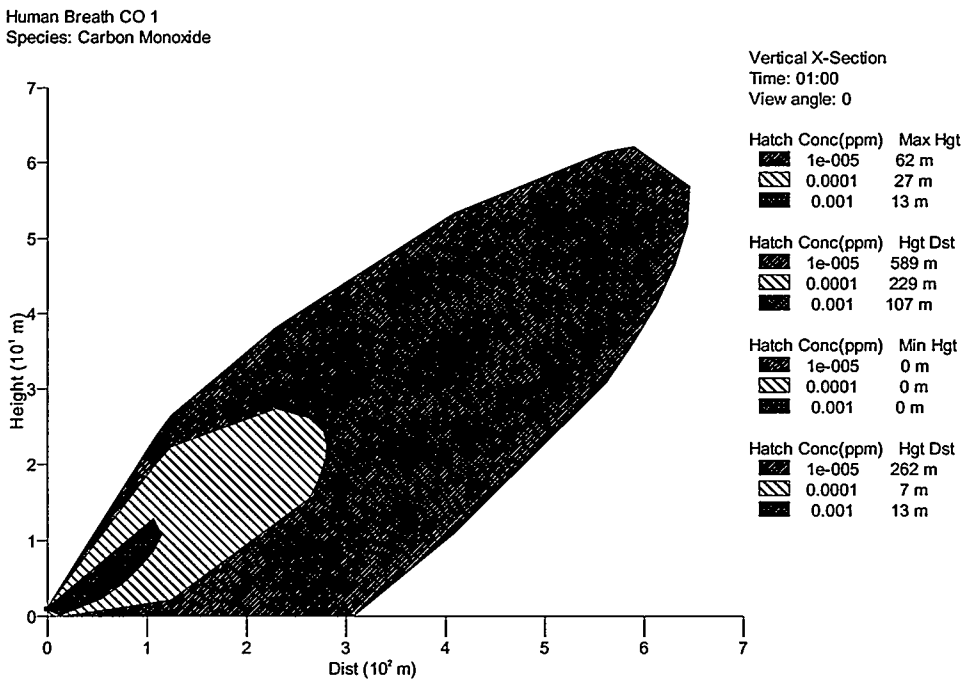
****

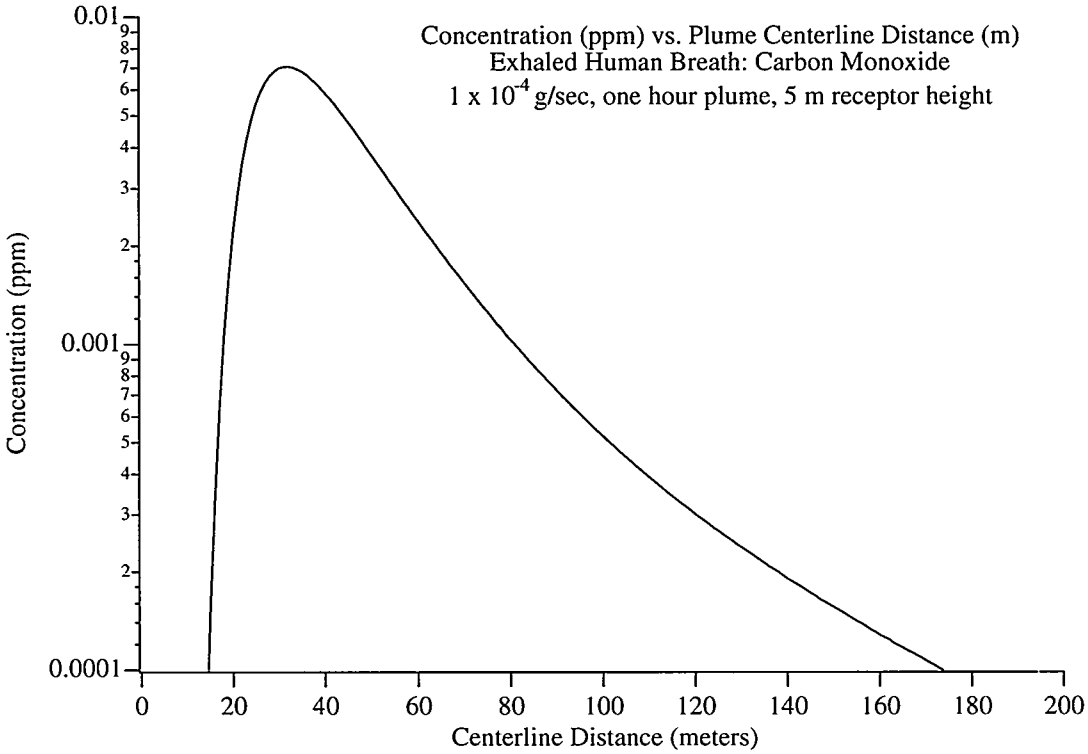
Met Data

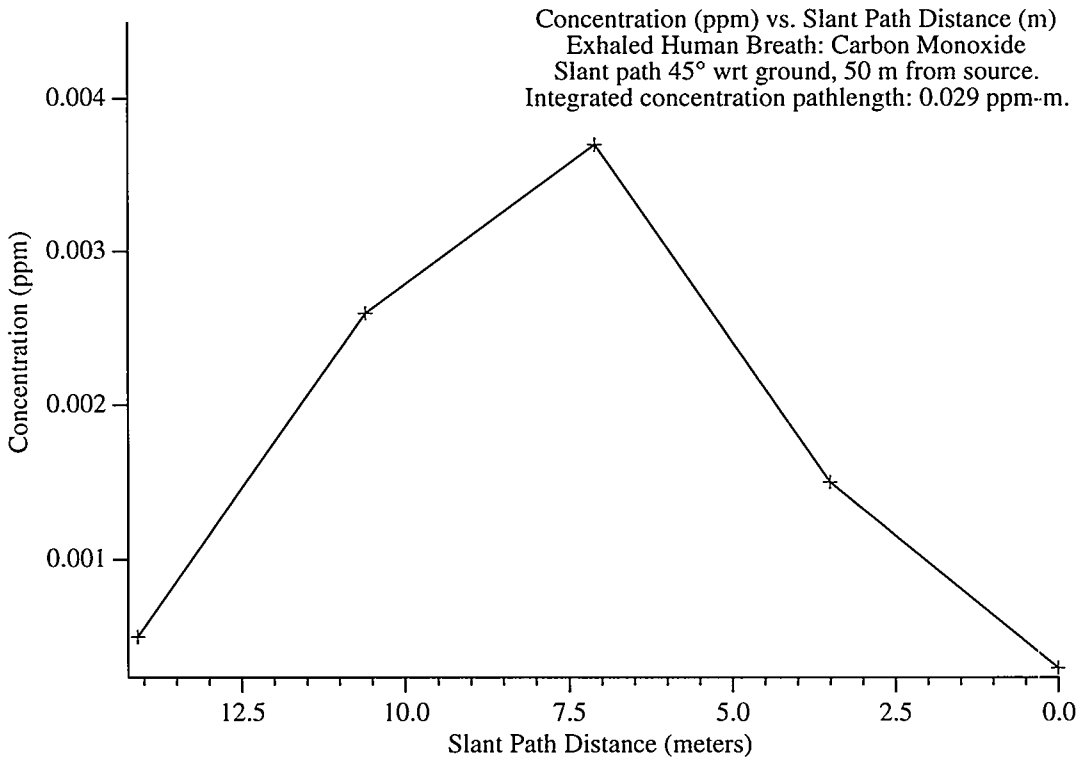
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation;	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Human Breath: Carbon Monoxide, 0.0001 g/sec, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Exhaled Human Breath: Carbon Monoxide
1 x 10^-4 g/sec, one hour plume, 5 m receptor height
Concentration (ppm)
0.01
0.001
0.0001
0
20
40
60
80
100
120
140
160
180
200
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Exhaled Human Breath: Carbon Monoxide
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 0.029 ppm-m.
Concentration (ppm)
0.004
0.003
0.002
0.001
12.5
10.0
7.5
5.0
2.5
0.0
Slant Path Distance (meters)

CHARM Version 9.3

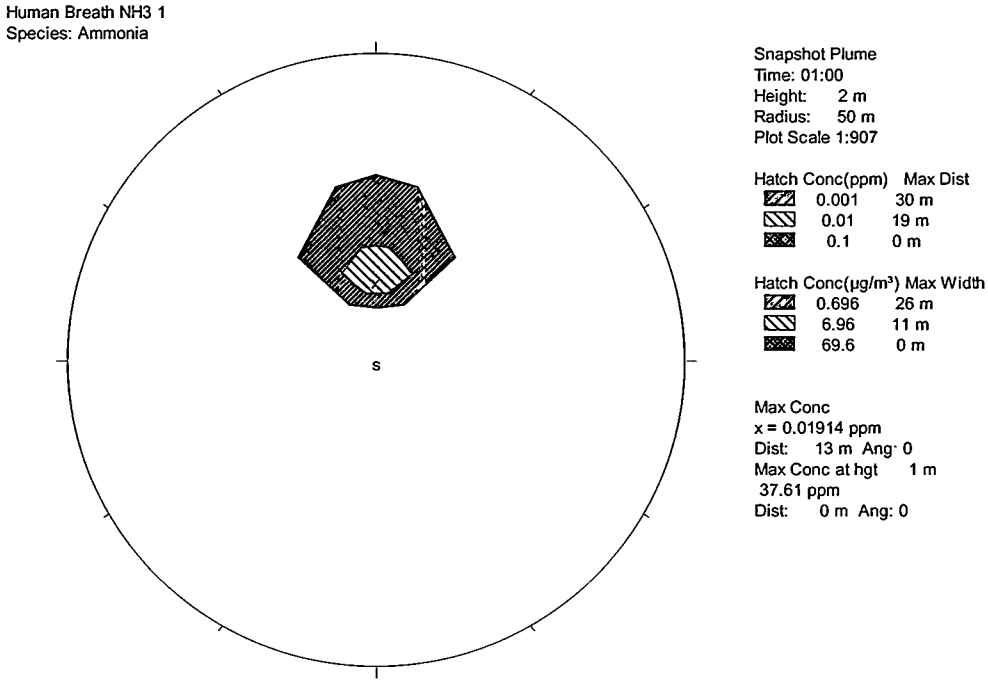
Title:	Human Breath NH3
Species:	Ammonia
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	1e-005 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

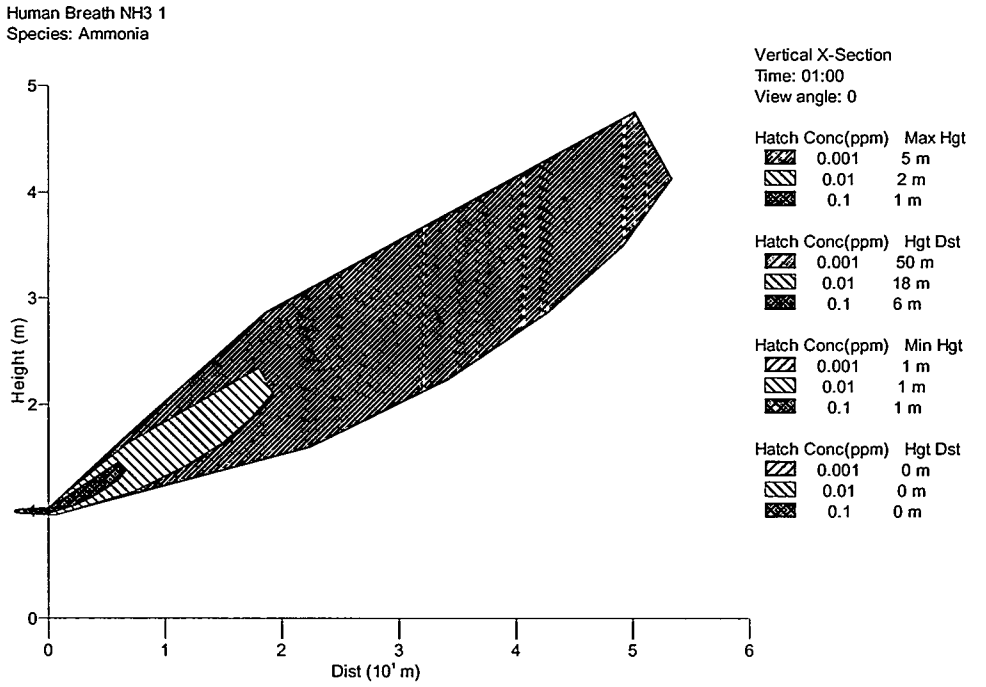
****

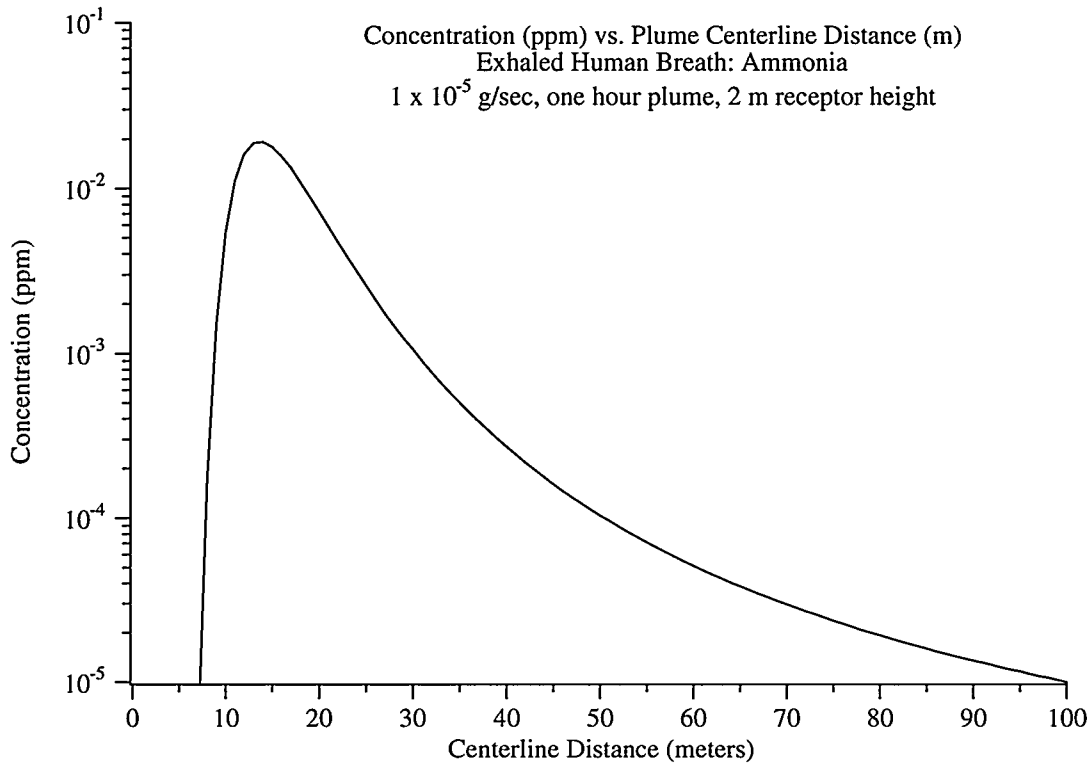
Met Data

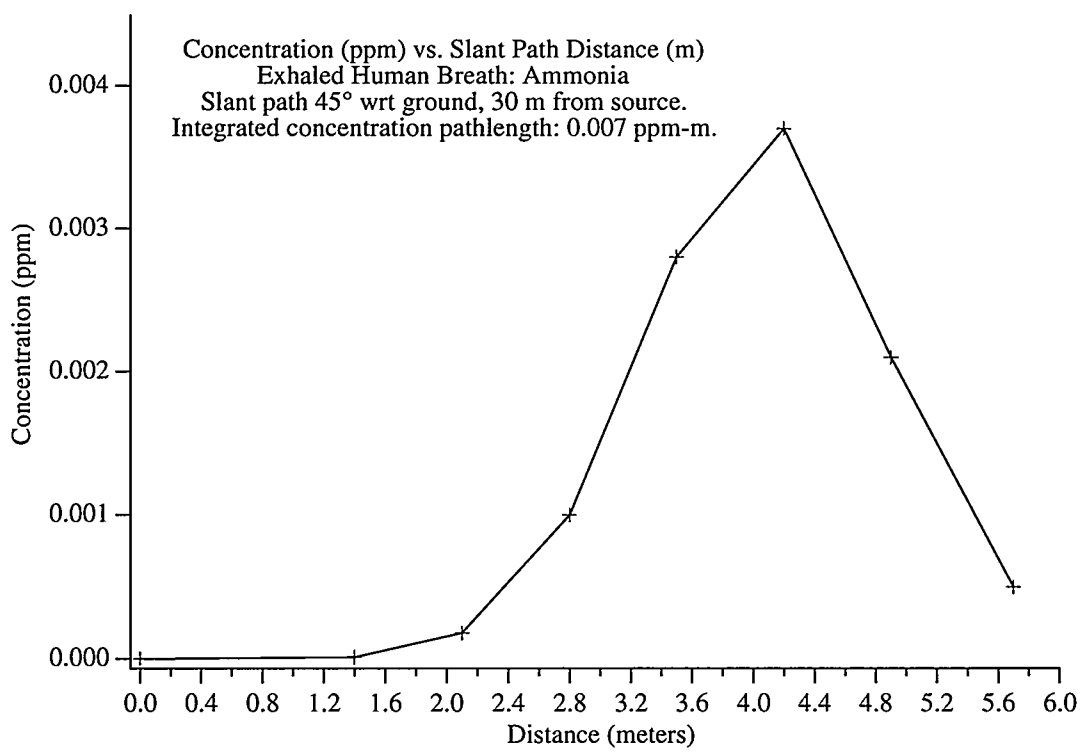
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	10
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/sec

Human Breath: Ammonia, 1e-5 g/sec, one vent, one-hour plume.

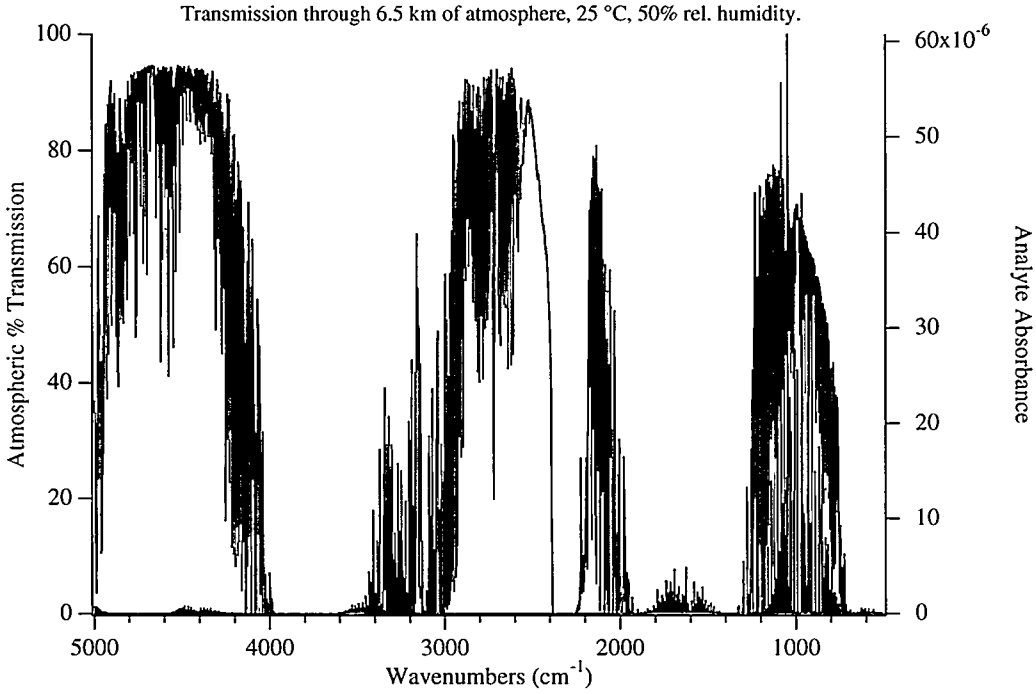




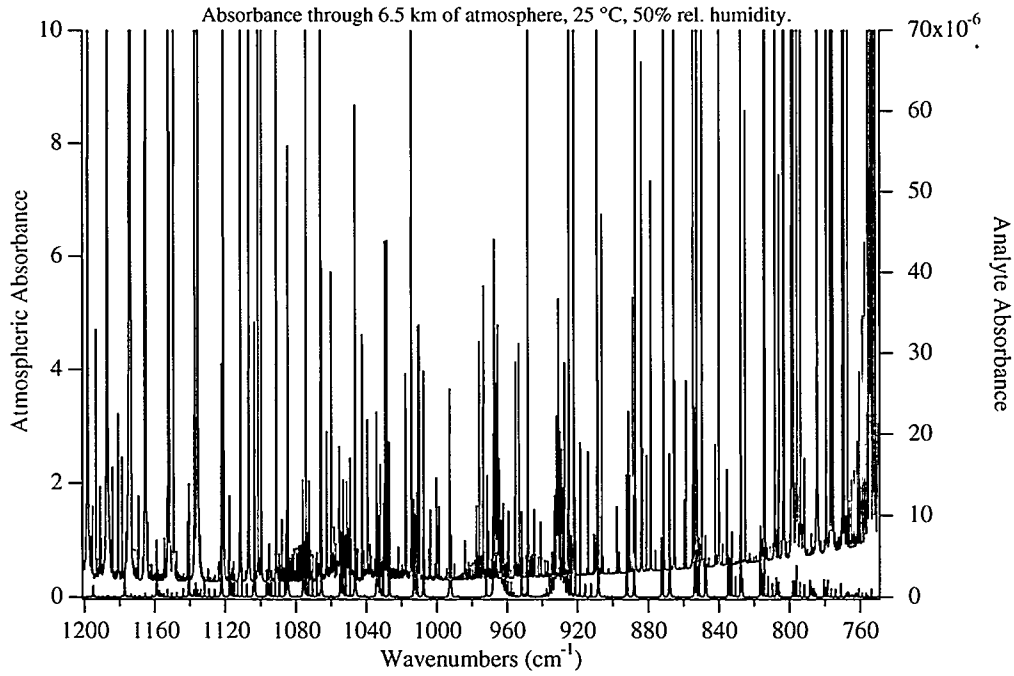

Concentration (ppm) vs. Plume Centerline Distance (m)
Exhaled Human Breath: Ammonia
1 x 10^-5 g/sec, one hour plume, 2 m receptor height
Concentration (ppm)
10^-1
10^-2
10^-3
10^-4
10^-5
0
10
20
30
40
50
60
70
80
90
100
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Exhaled Human Breath: Ammonia
Slant path 45° wrt ground, 30 m from source.
Integrated concentration pathlength: 0.007 ppm-m.
Concentration (ppm)
0.004
0.003
0.002
0.001
0.000
0.0
0.4
0.8
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
Distance (meters)

Ammonia from Exhaled Human Breath
Ammonia absorbance, 25 °C, 0.007 ppm-m, 50 m from vent.



Ammonia from Exhaled Human Breath
Ammonia absorbance, 25 °C, 0.007 ppm-m, 50 m from vent.
Detail of ν_2 band.



CHARM Version 9.3

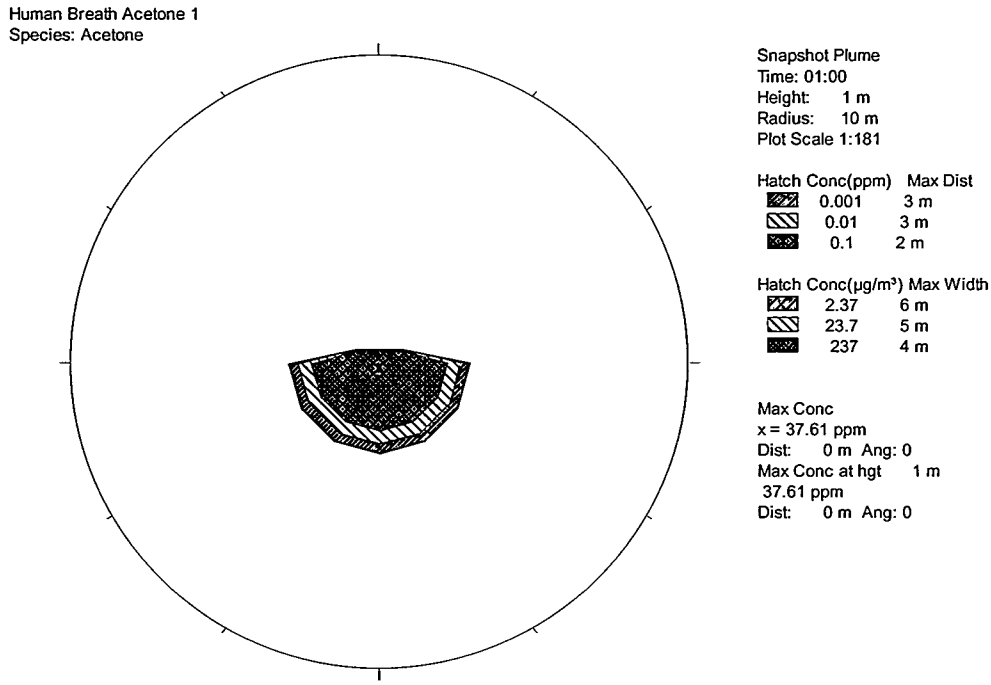
Title:	Human Breath Acetone
Species:	Acetone
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 ft
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	5e-006 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

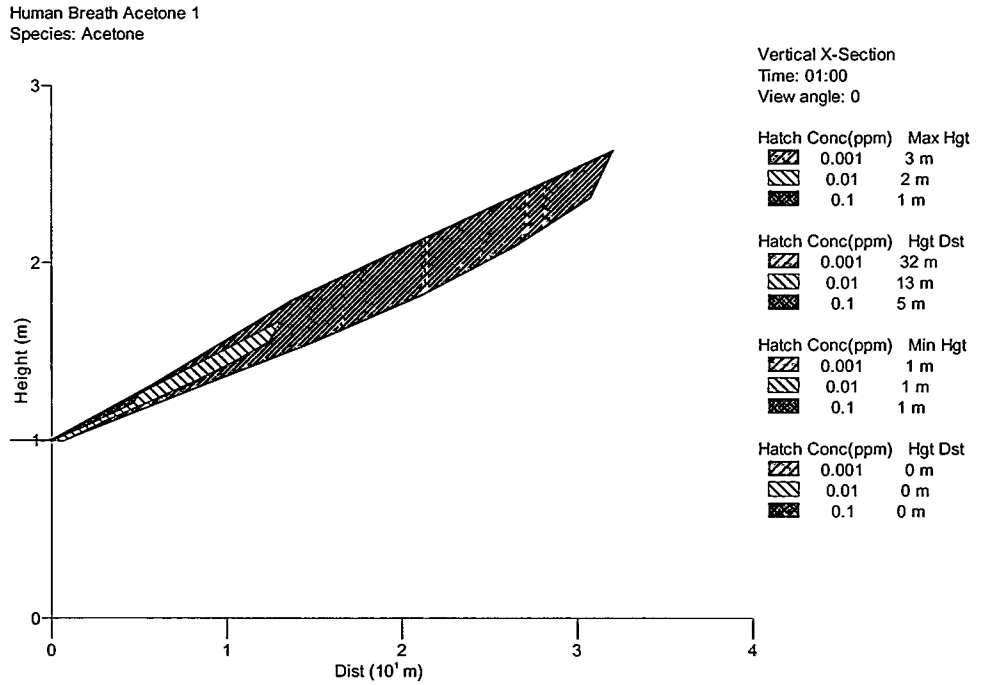
****

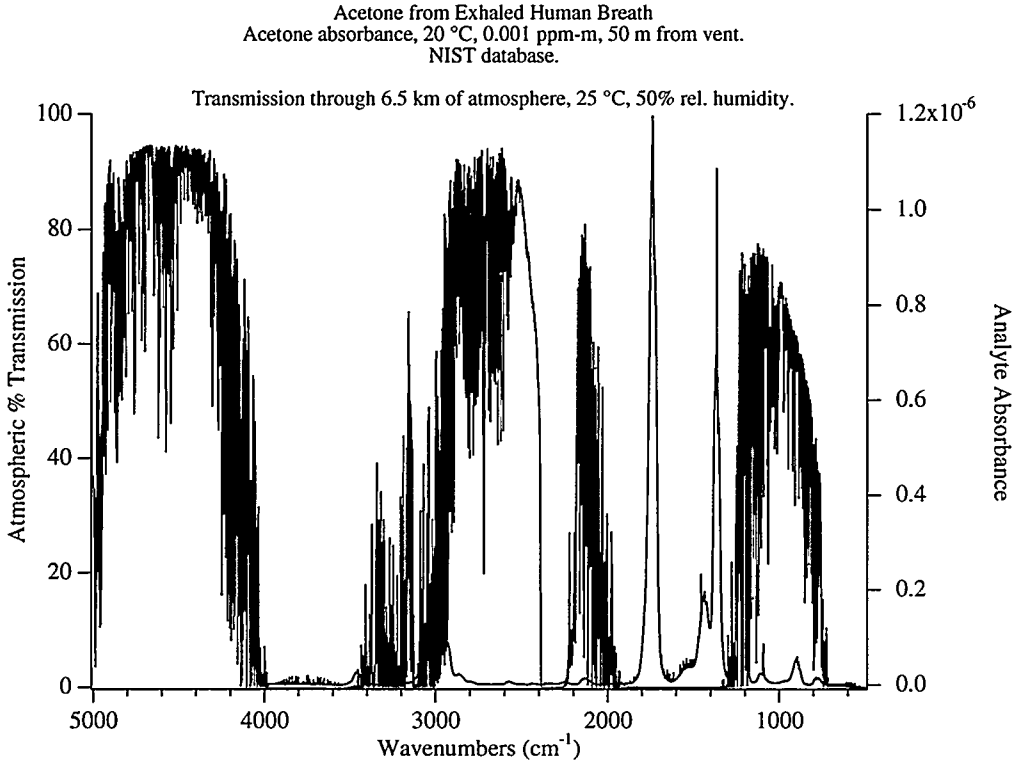
Met Data

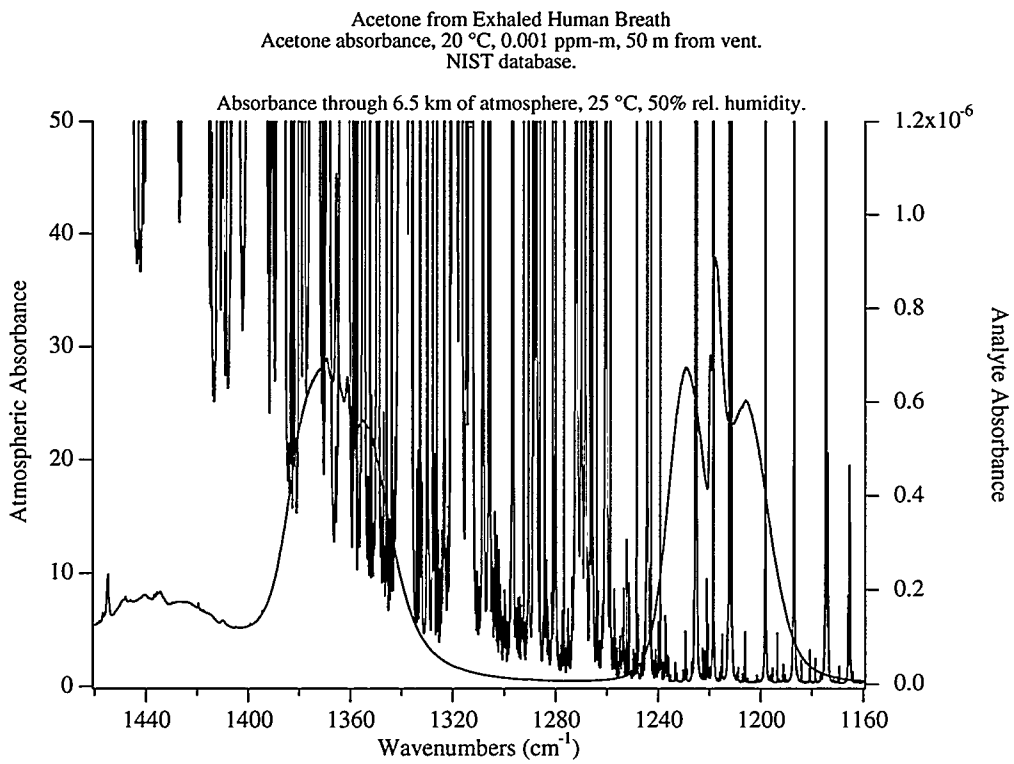
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	10
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/sec

Human Breath: Acetone, 5e-6 g/sec, one vent, one-hour plume.






Acetone from Exhaled Human Breath
Acetone absorbance, 20 °C, 0.001 ppm-m, 50 m from vent.
NIST database.
Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric % Transmission
Analyte Absorbance
Wavenumbers (cm-1)
100
80
60
40
20
0
1.2x10-6
1.0
0.8
0.6
0.4
0.2
0.0
5000
4000
3000
2000
1000


Acetone from Exhaled Human Breath
Acetone absorbance, 20 °C, 0.001 ppm-m, 50 m from vent.
NIST database.
Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric Absorbance
Analyte Absorbance
Wavenumbers (cm-1)
50
40
30
20
10
0
1.2x10-6
1.0
0.8
0.6
0.4
0.2
0.0
1440
1400
1360
1320
1280
1240
1200
1160

CHARM Version 9.3

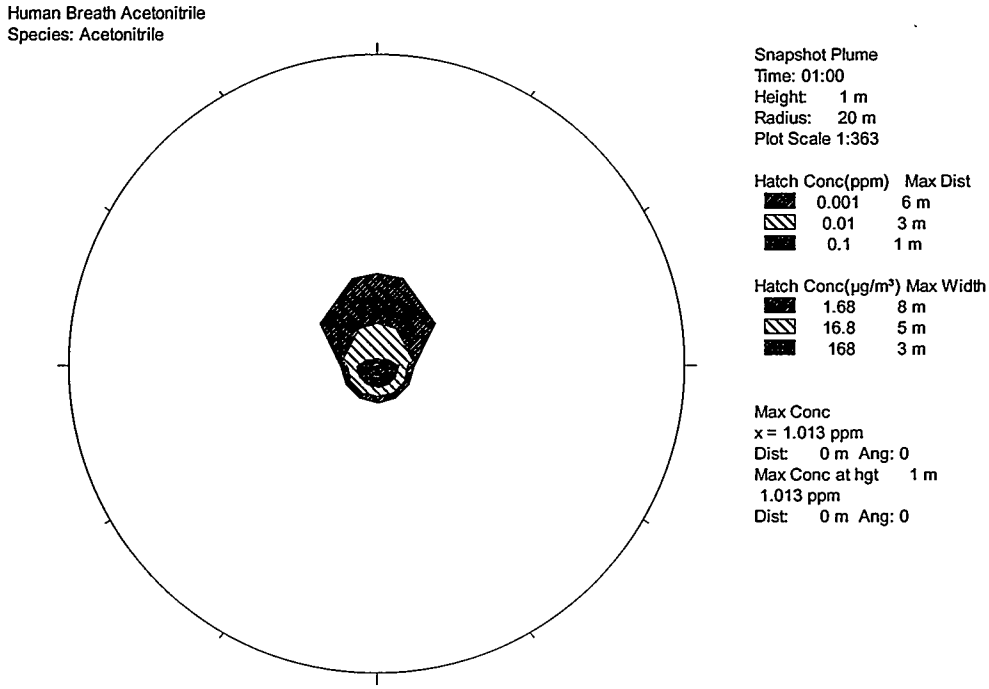
Title:	Human Breath Acetonitrile
Species:	Acetonitrile
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001 , 0.01 , 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	2e-006 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

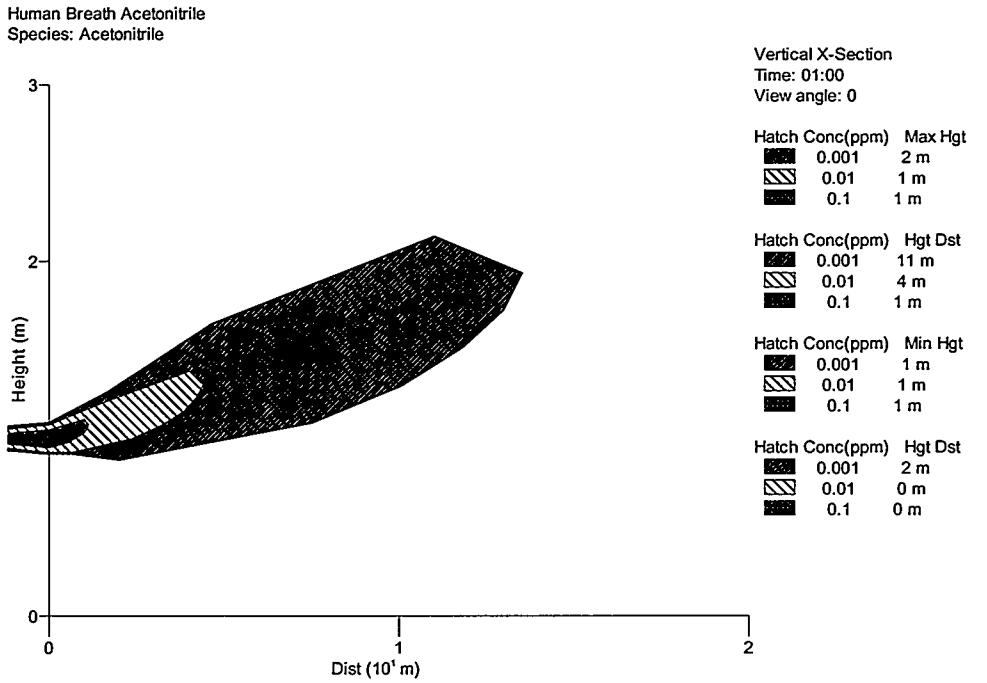
****

Met Data

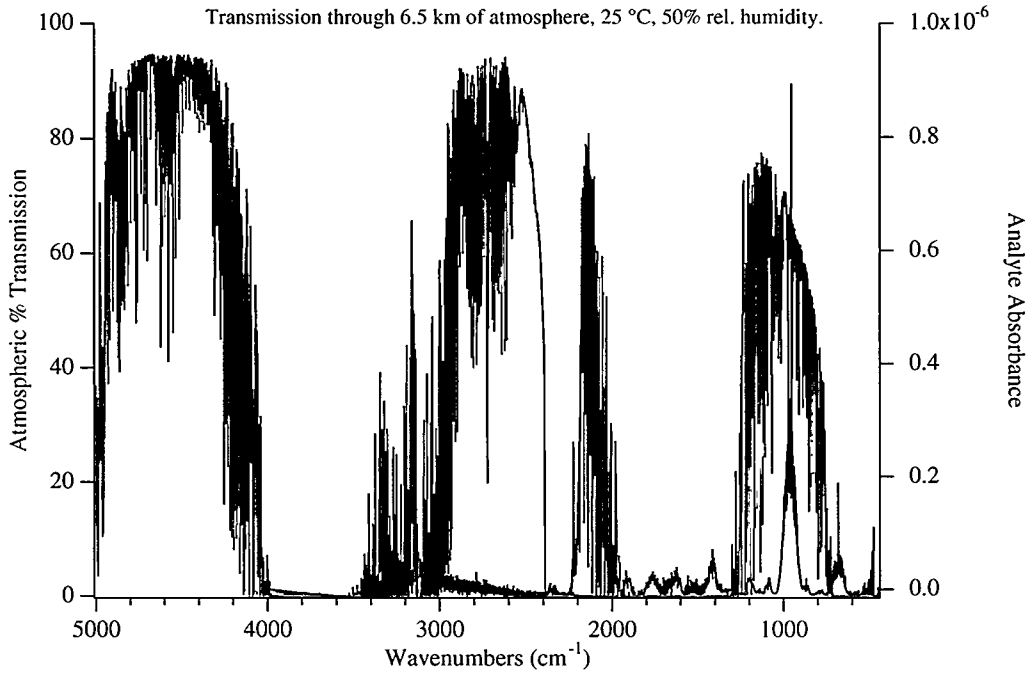
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	10
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/sec

Human Breath: Acetonitrile, 2e-6 g/sec, one vent, one-hour plume.

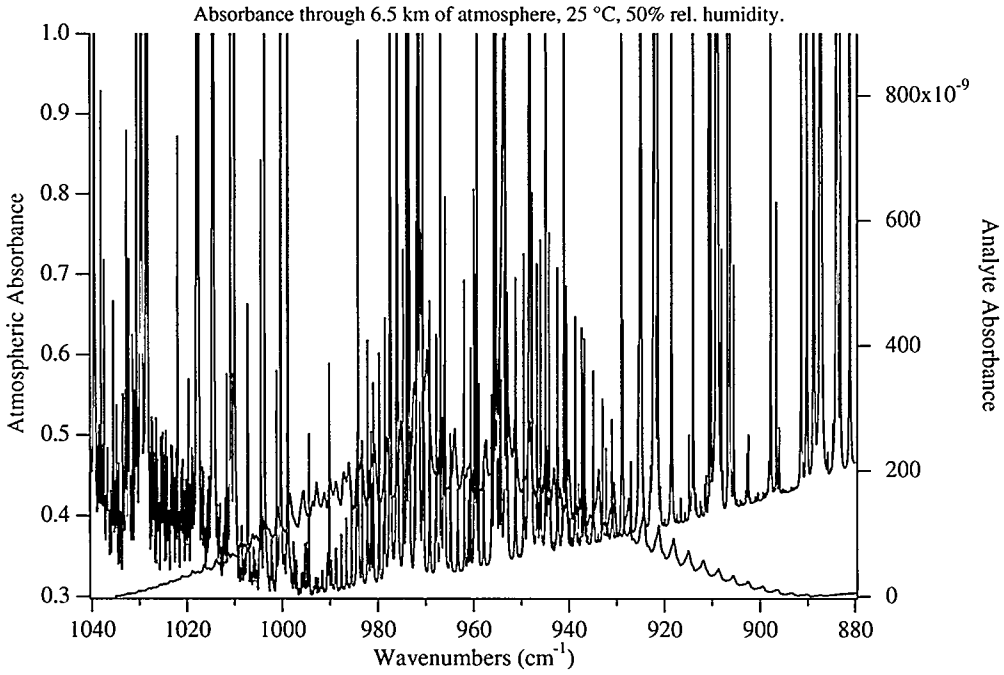




Acetonitrile from Exhaled Human Breath
Acetonitrile absorbance, 20 °C, 0.001 ppm-m, 50 m from vent.
Hanst database.



Acetonitrile from Exhaled Human Breath
Acetonitrile absorbance, 20 °C, 0.001 ppm-m, 50 m from vent.
ν_4 band. Hanst database.



CHARM Version 9.3

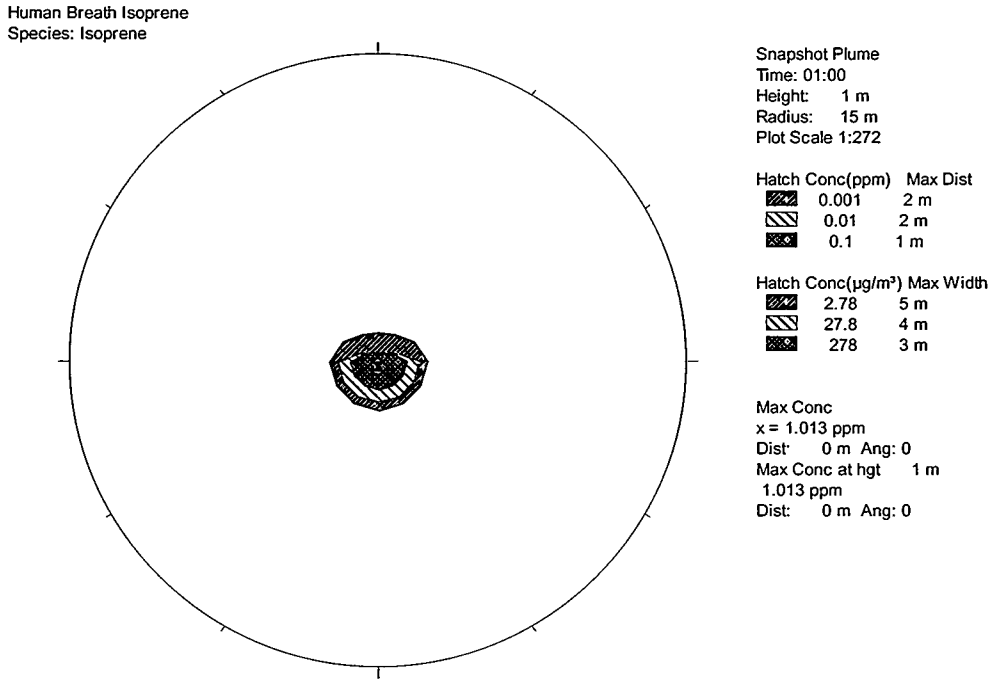
Title:	Human Breath Isoprene
Species:	Isoprene
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	1.5e-006 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	2 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed:	10.62 m/s
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	1

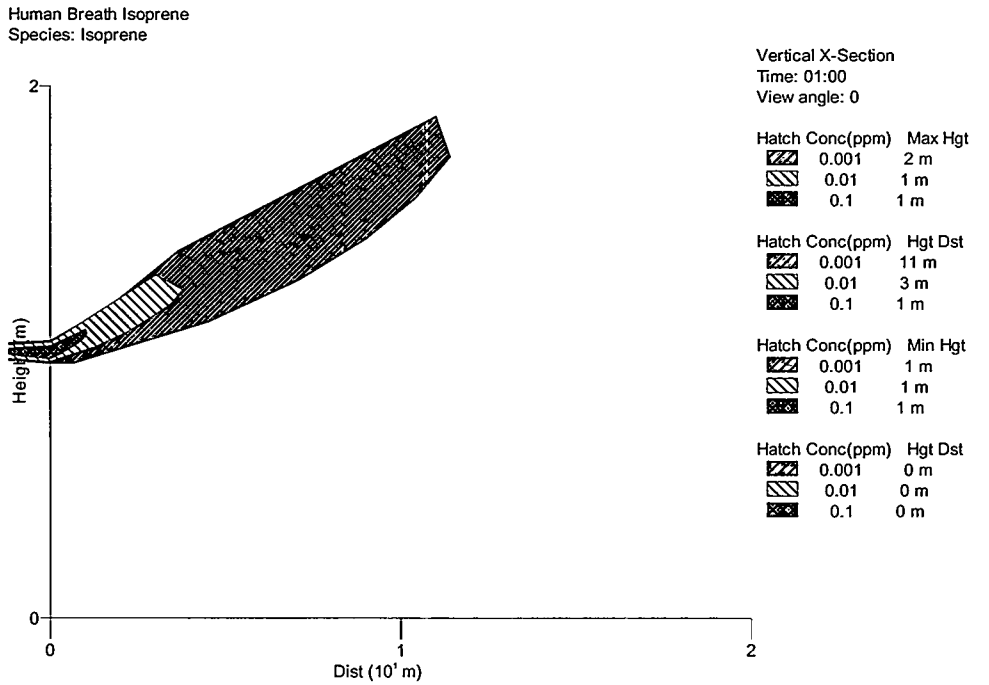
****

Met Data

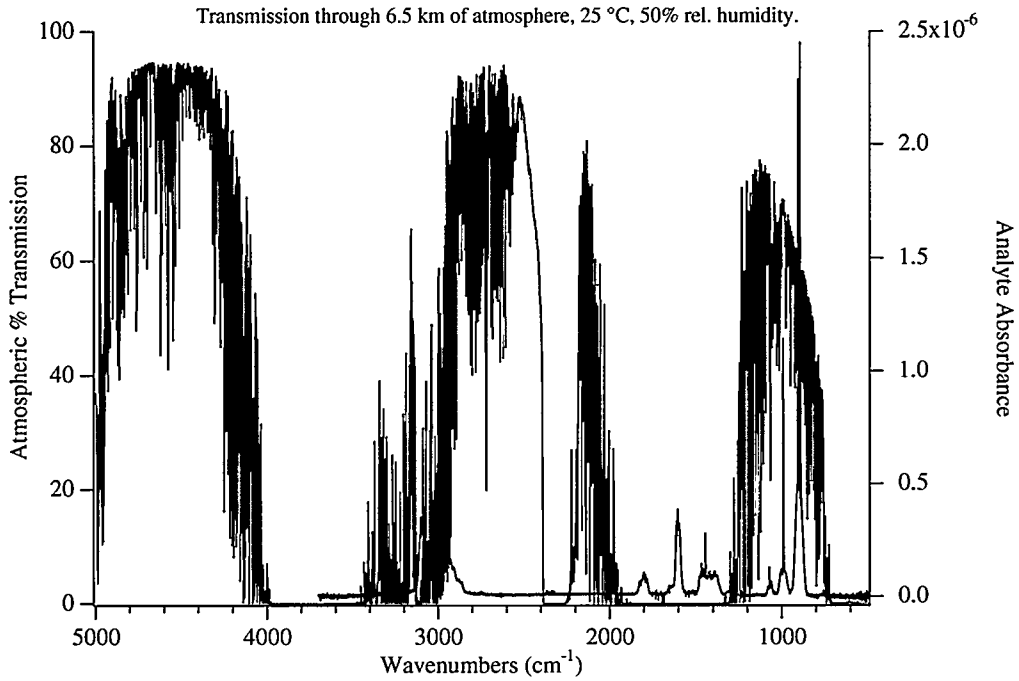
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/sec

Human Breath: Isoprene, 1.5e-6 g/sec, one vent, one-hour plume.

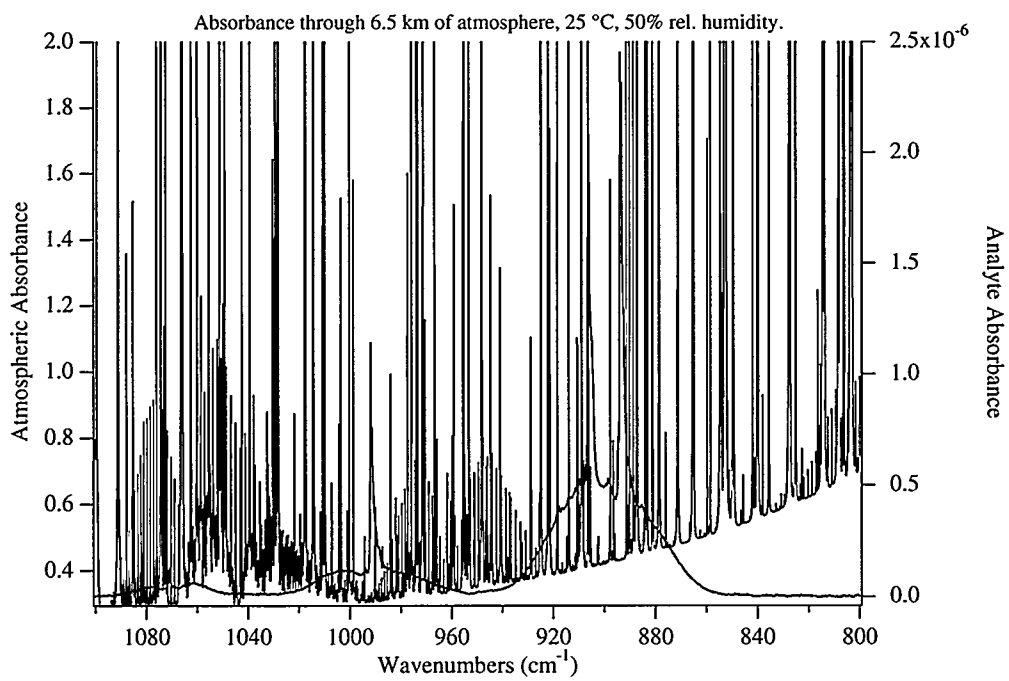




Isoprene from Exhaled Human Breath
Isoprene absorbance, 20 °C, 0.001 ppm-m, 50 m from vent.
Hanst database.



Isoprene from Exhaled Human Breath
Isoprene absorbance, 20 °C, 0.001 ppm-m, 50 m from vent.
Hanst database.



4.2 Cook Stoves

Compound[a,b,c]	Emission Rate (g/sec) for One One-Hour Period[a,b,c]
Carbon dioxide	80
Carbon monoxide	0.7
Formaldehyde	0.008
Acetaldehyde	0.006
Benzaldehyde	0.004
Propionaldehyde	0.002
Crotonaldehyde	0.002
Methane	0.001
Nitrous oxide	0.001

(a) Zhang, J., and K. R. Smith. 1999. "Emissions of Carbonyl Compounds from Various Cookstoves in China." *Environ. Sci. Tech.* **33**:2311-2320.
(b) Smith, K. R., M. A. K. Khalil, R. A. Rasmussen, S. A. Thorneloe, F. Manegdeg, and M. Apte. 1993. "Greenhouse Gases from Biomass and Fossil Fuel Stoves in Developing Countries: A Manila Pilot Study." *Chemosphere* **26**:479-505.
(c) Atmospheric Environment. 1993. "Characterization and Problems of Indoor Pollution Due to Cooking Stove Smoke." *Atmospheric Environment* **27A**:1643-1655.

Scenario: Food is cooked on stoves fueled with liquefied petroleum gas. Ten MJ used per person per day. Emission rate averaged over two one-hour cook periods per day (Zhang and Smith 1999; Smith *et al.* 1993; *Atmospheric Environment* 1993).

CHARM Version 9.3

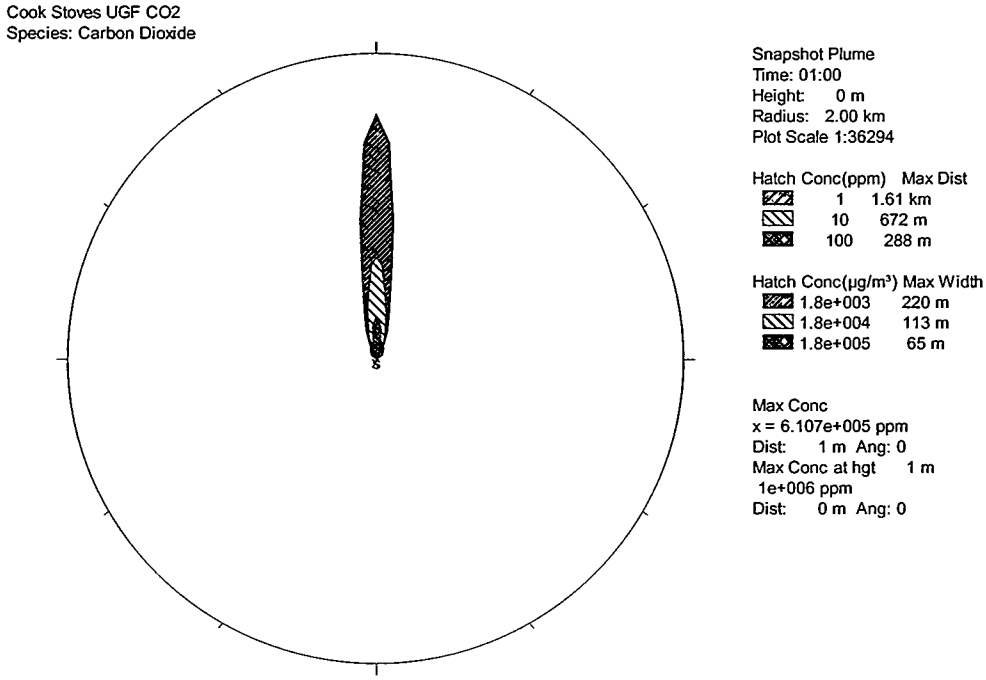
Title:	Cook Stoves CO2
Species:	Carbon Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	80 g/s
Release Duration:	1 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.2455 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

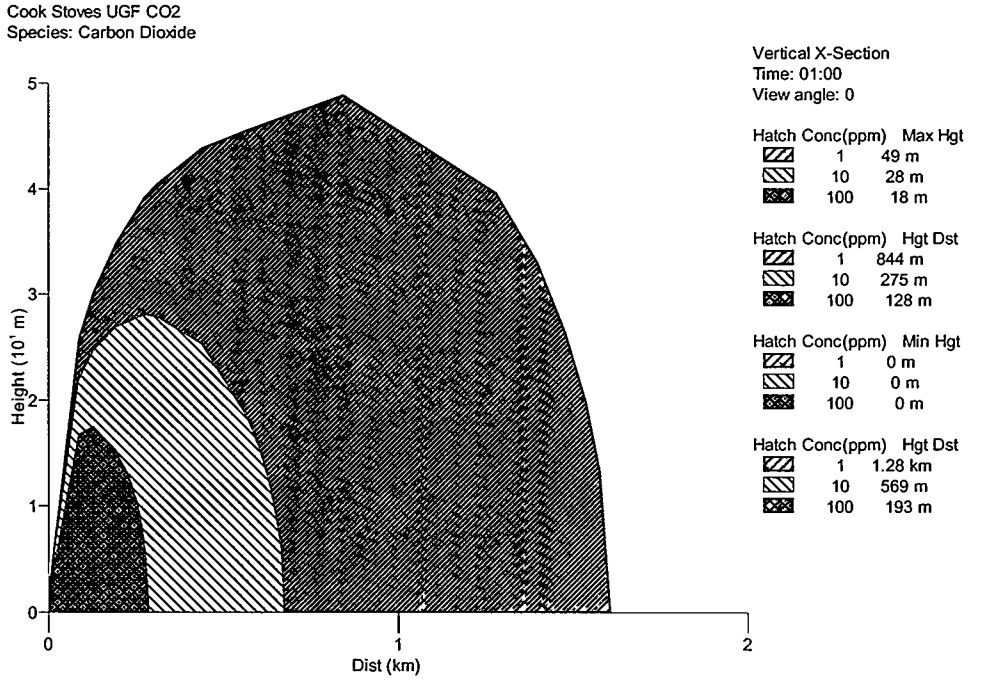
****

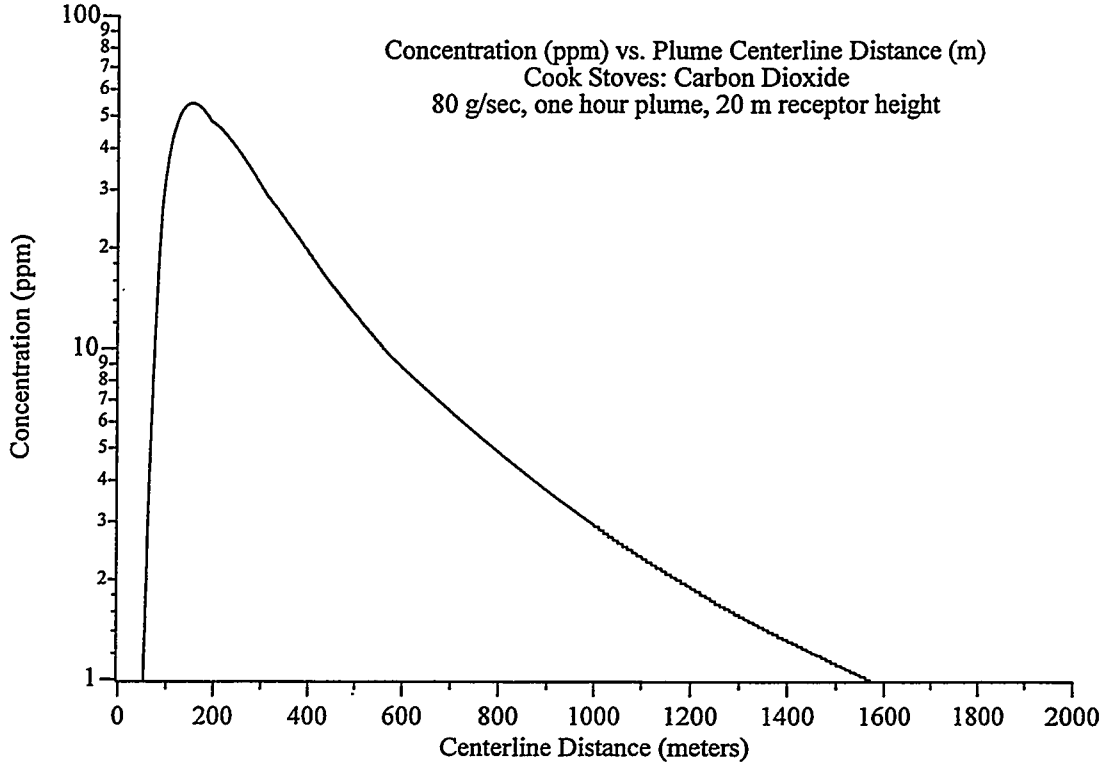
Met Data

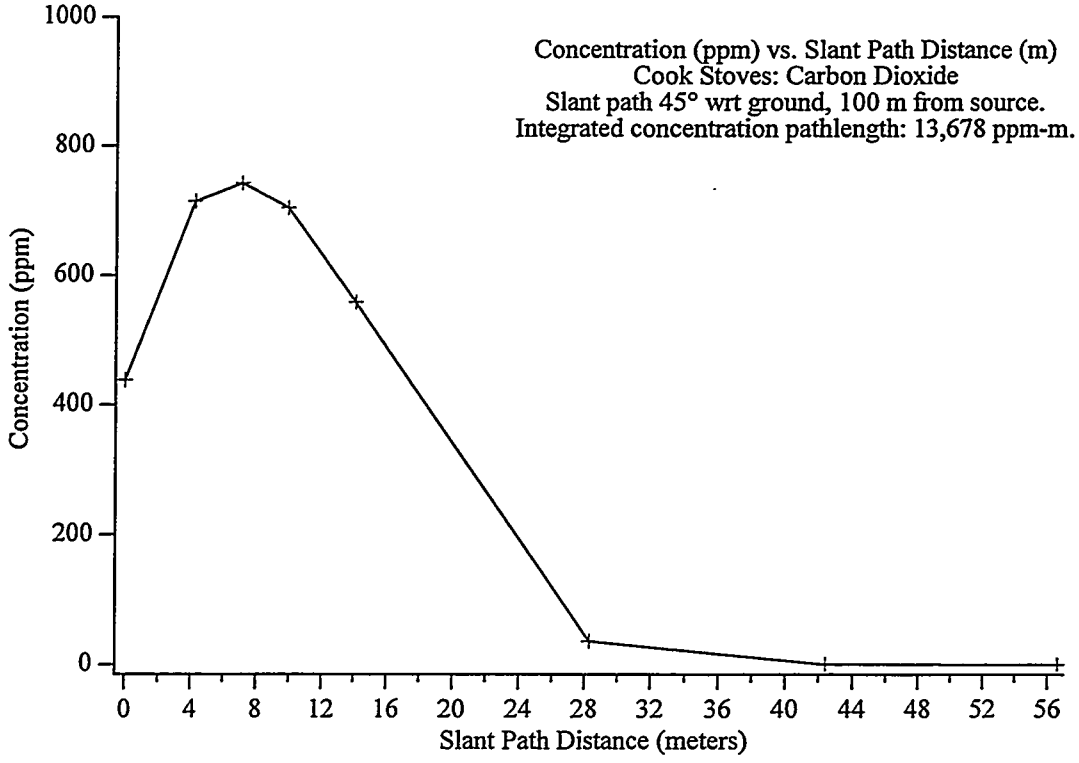
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Cook Stoves: Carbon Dioxide, 80 g/sec, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Cook Stoves: Carbon Dioxide
80 g/sec, one hour plume, 20 m receptor height
Concentration (ppm)
100
10
1
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Cook Stoves: Carbon Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 13,678 ppm-m.
Concentration (ppm)
1000
800
600
400
200
0
0
4
8
12
16
20
24
28
32
36
40
44
48
52
56
Slant Path Distance (meters)

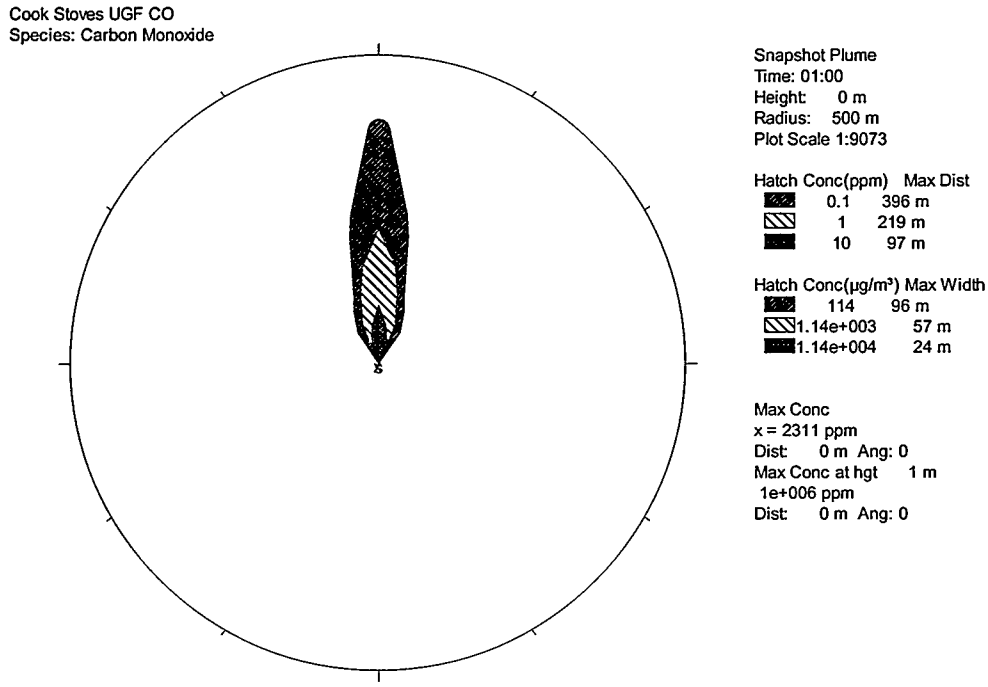
CHARM Version 9.3

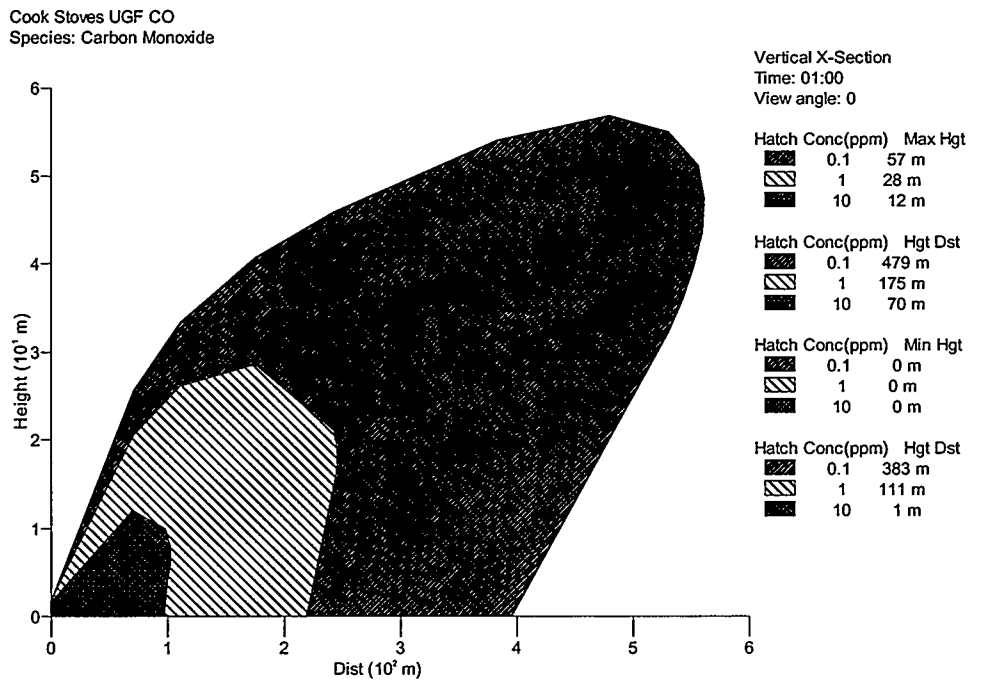
Title:	Cook Stoves CO
Species:	Carbon Monoxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.7 g/s
Release Duration:	1 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.003375 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

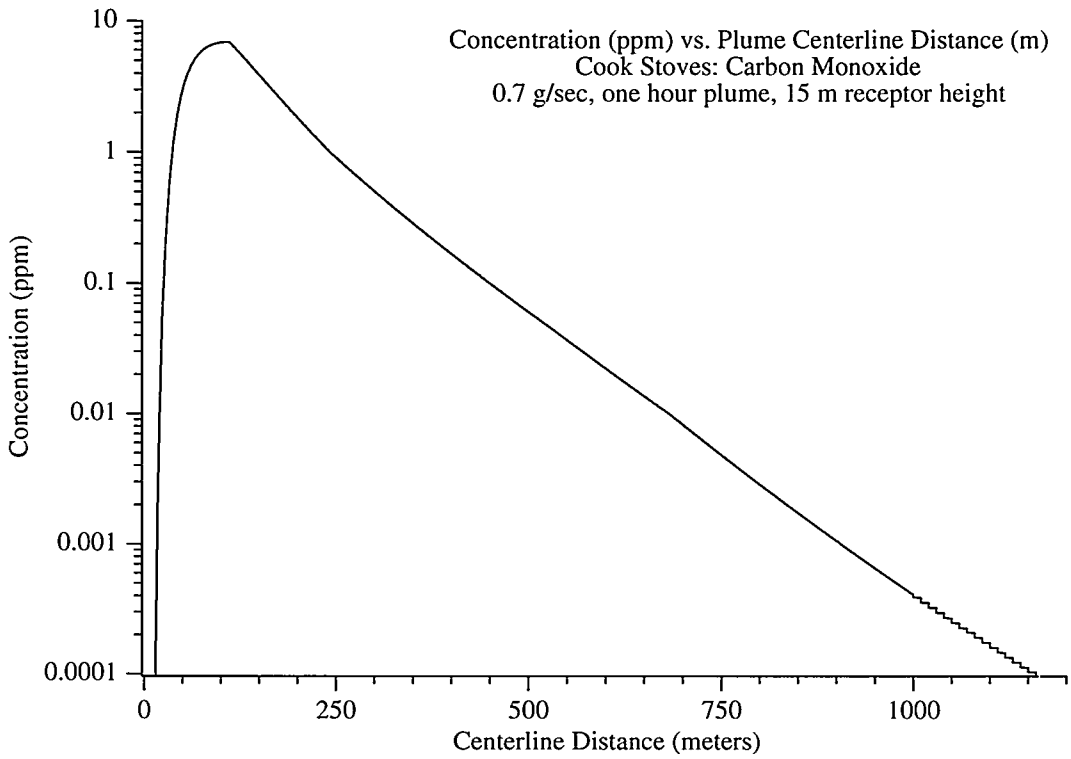
****

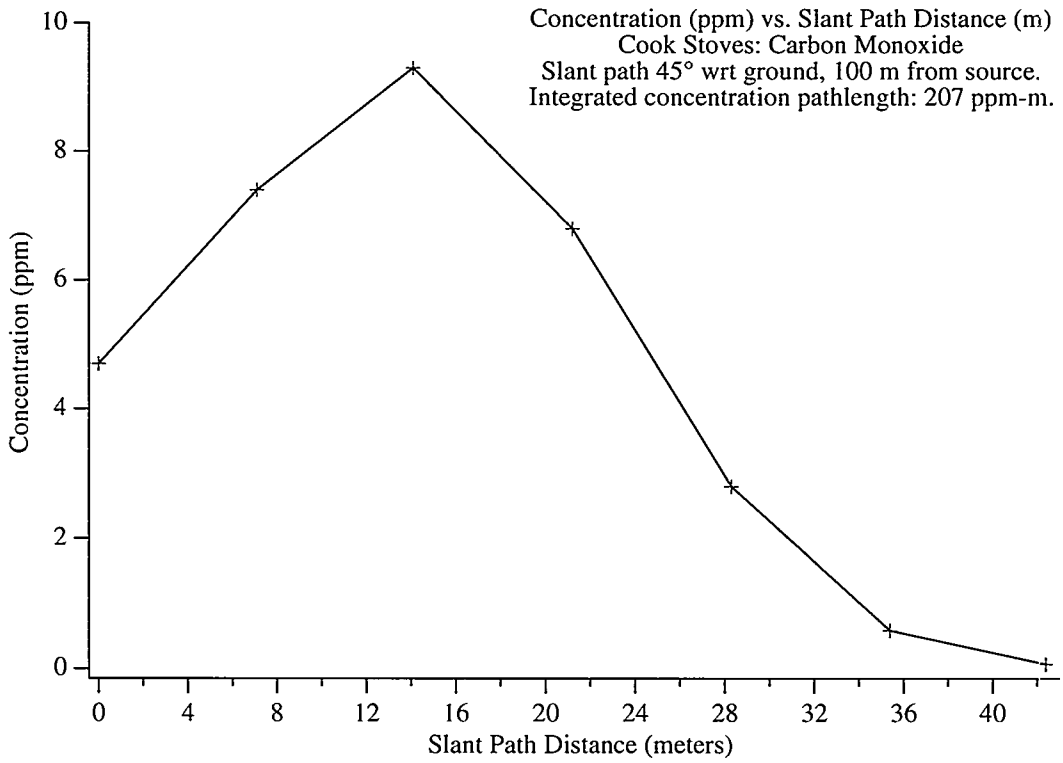
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Cook Stoves: Carbon Monoxide, 0.7 g/sec, one-hour plume.



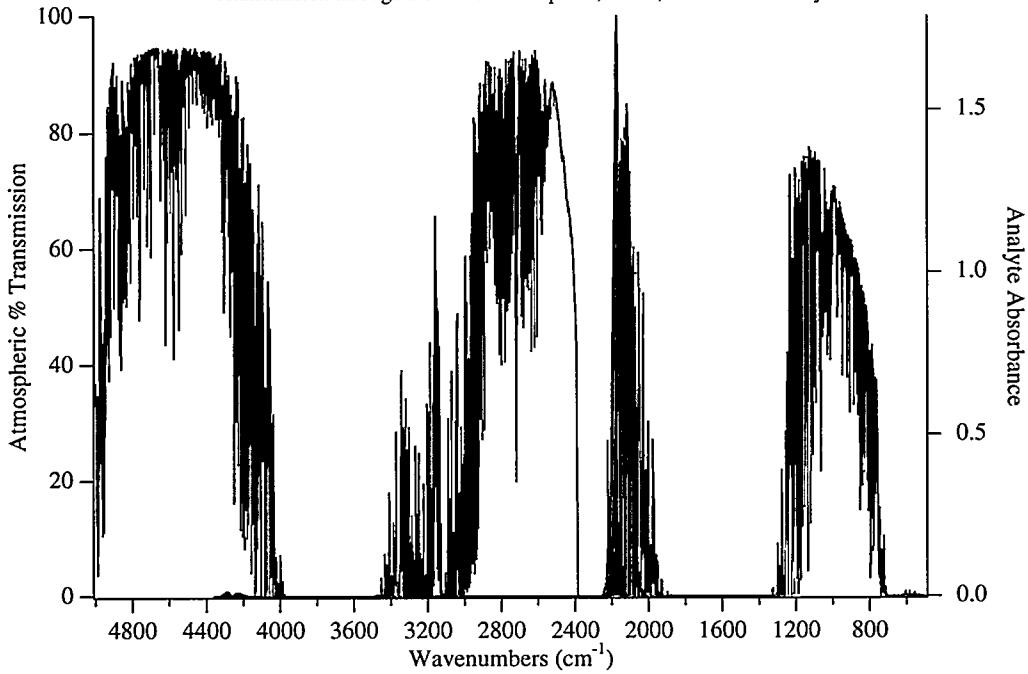



Concentration (ppm) vs. Plume Centerline Distance (m)
Cook Stoves: Carbon Monoxide
0.7 g/sec, one hour plume, 15 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
250
500
750
1000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Cook Stoves: Carbon Monoxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 207 ppm-m.
Concentration (ppm)
10
8
6
4
2
0
0
4
8
12
16
20
24
28
32
36
40
Slant Path Distance (meters)

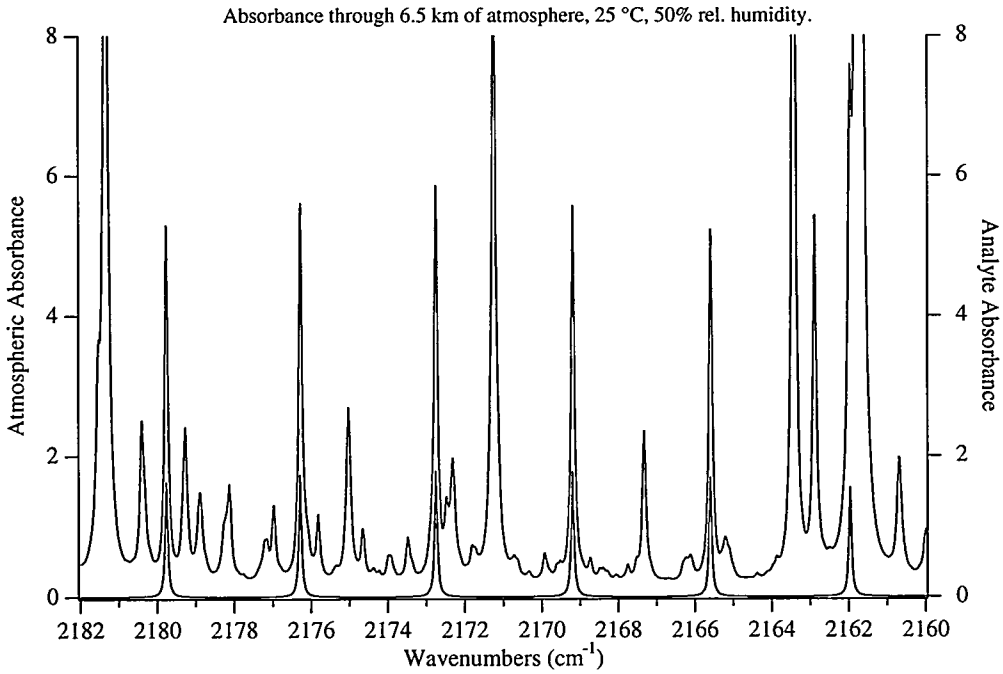
Carbon Monoxide from Cook Stoves
Carbon monoxide absorbance, 25 °C, 207 ppm-m, 100 m from vent.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Carbon Monoxide from Cook Stoves
Carbon monoxide absorbance, 25 °C, 207 ppm-m, 100 m from vent.
Detail of the R-branch of the fundamental band.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



CHARM Version 9.3

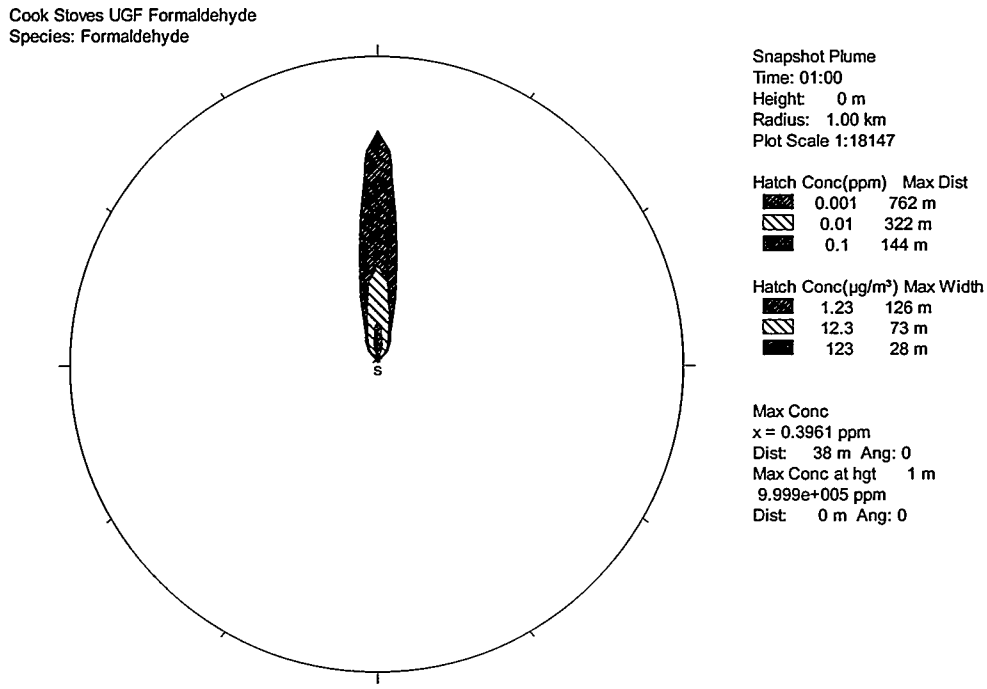
Title:	Cook Stoves Formaldehyde
Species:	Formaldehyde
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.01, 0.1, 1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.008 g/s
Release Duration:	1 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	3.598e-005 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

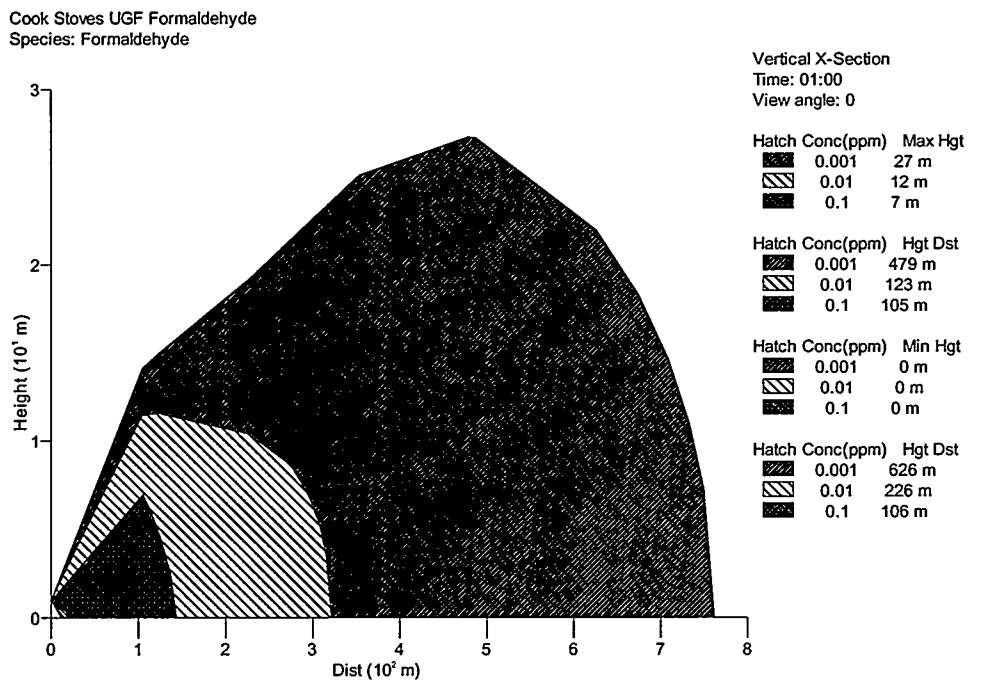
****

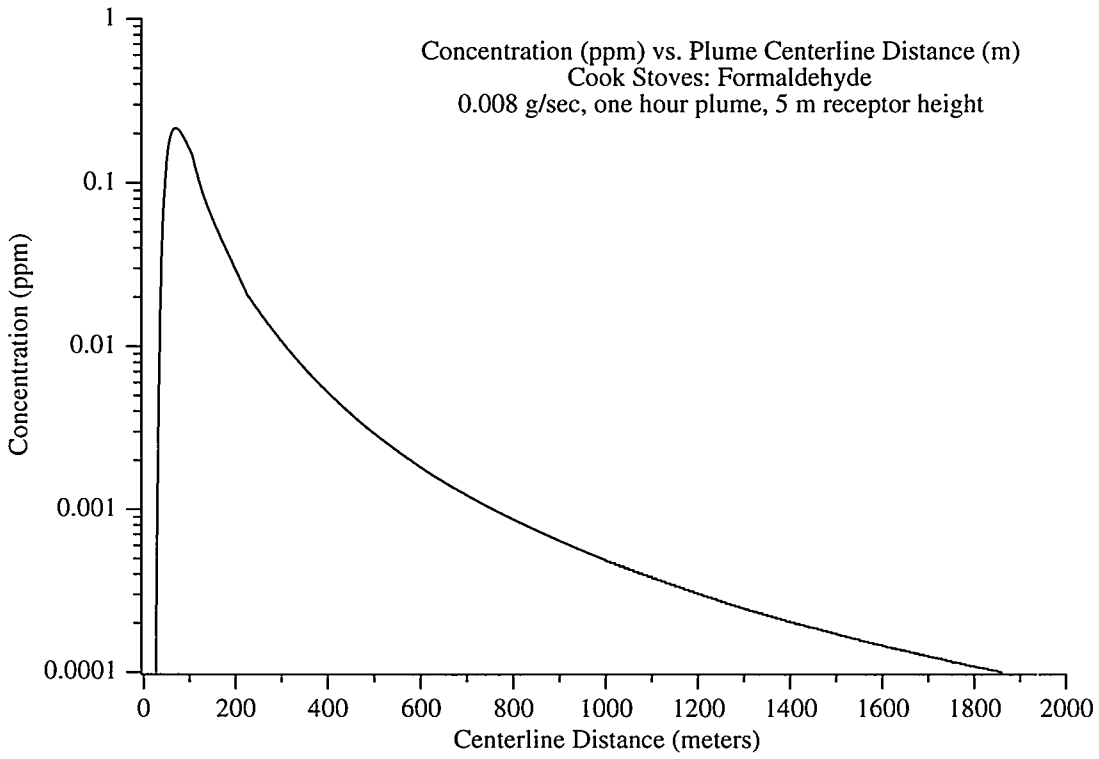
Met Data

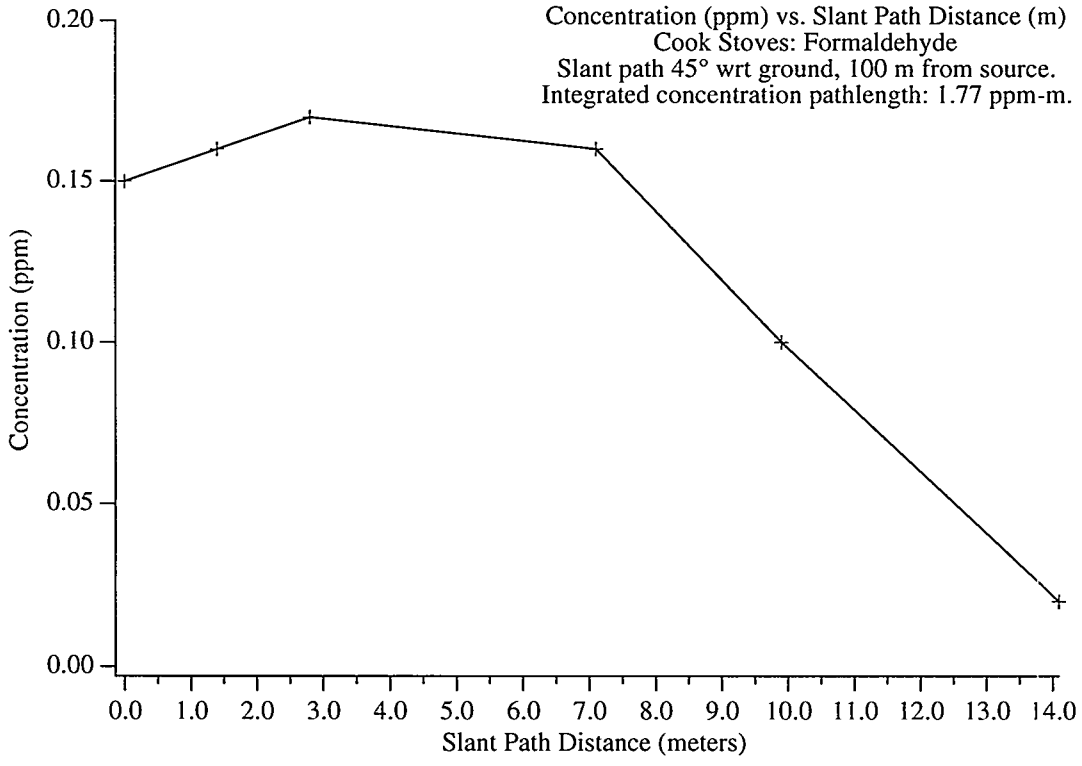
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Cook Stoves: Formaldehyde, 0.008 g/sec, one-hour plume.



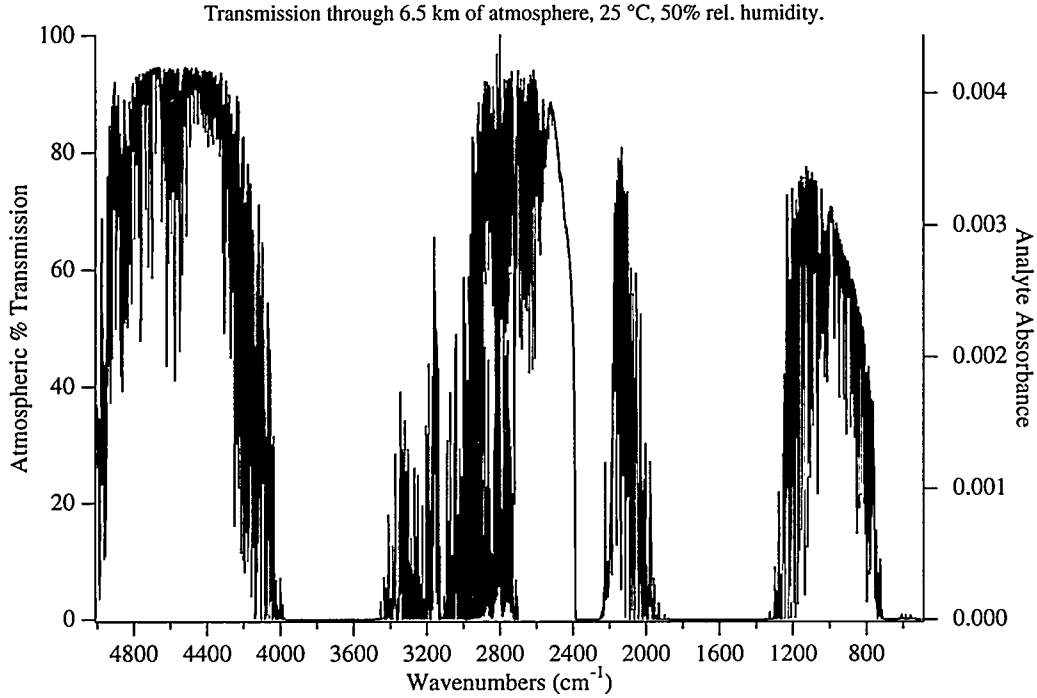



Concentration (ppm) vs. Plume Centerline Distance (m)
Cook Stoves: Formaldehyde
0.008 g/sec, one hour plume, 5 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Cook Stoves: Formaldehyde
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 1.77 ppm-m.
Concentration (ppm)
0.20
0.15
0.10
0.05
0.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
Slant Path Distance (meters)

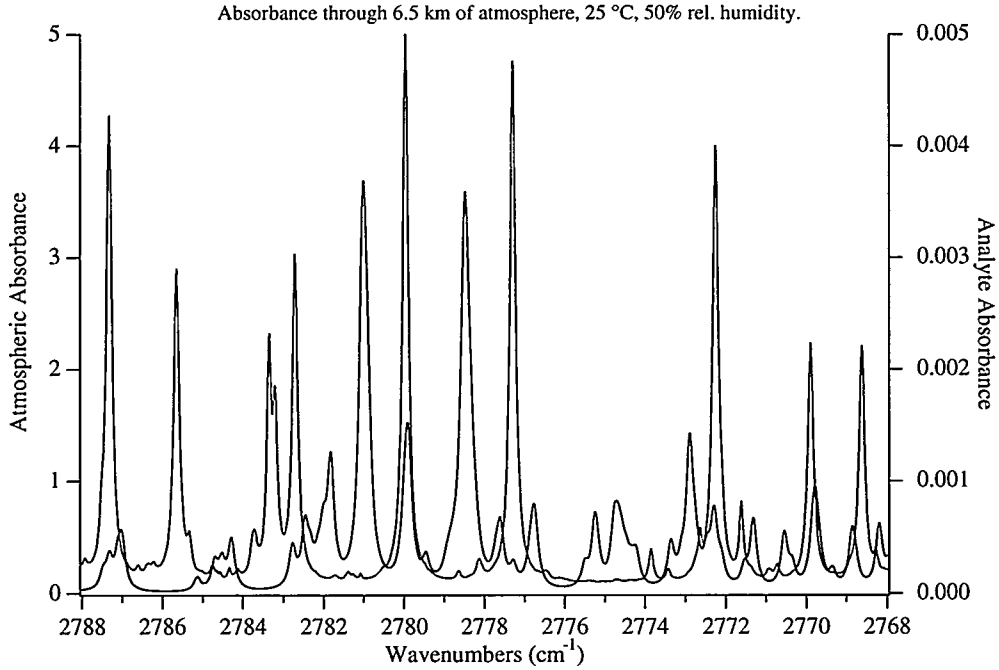
Formaldehyde from Cook Stoves
Formaldehyde absorbance, 25 °C, 1.77 ppm-m, 100 m from fire.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Formaldehyde from Cook Stoves
Formaldehyde absorbance, 25 °C, 1.77 ppm-m, 100 m from vent.
Detail of ν_5 band

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



CHARM Version 9.3

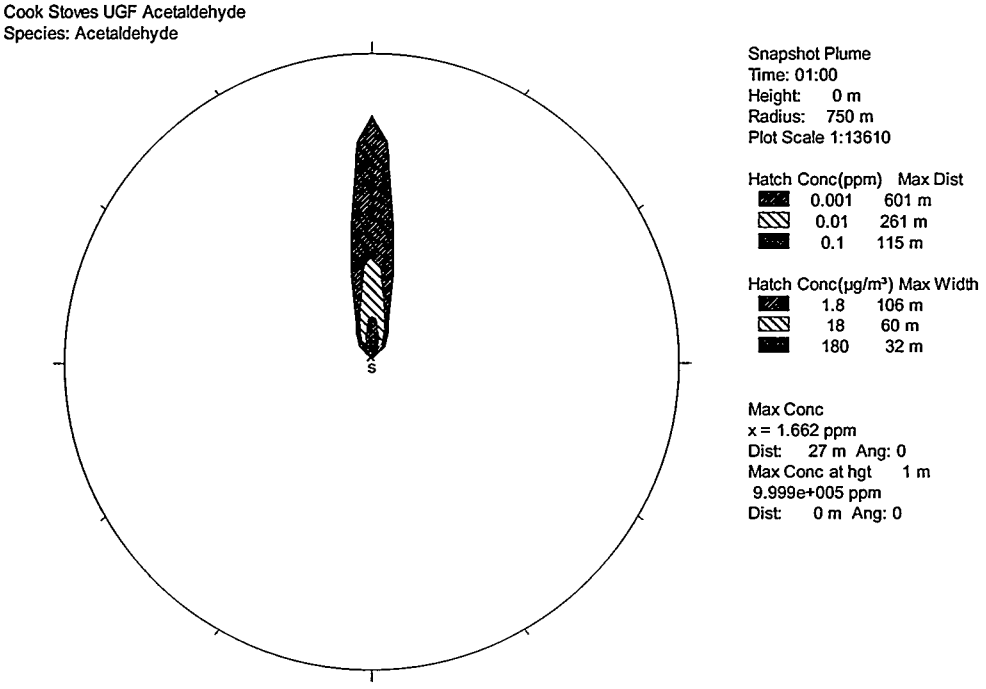
Title:	Cook Stoves Acetaldehyde
Species:	Acetaldehyde
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.006 g/s
Release Duration:	1 hrs
Puff Temperature:	50°C
Puff Diameter:	0.5 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	1.839e-005 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

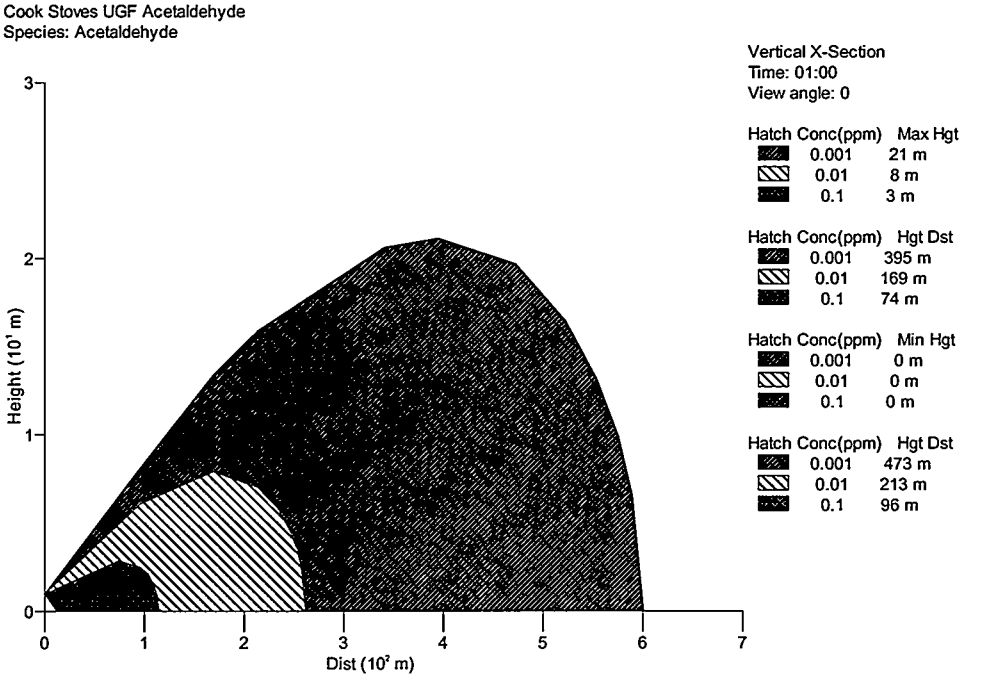
****

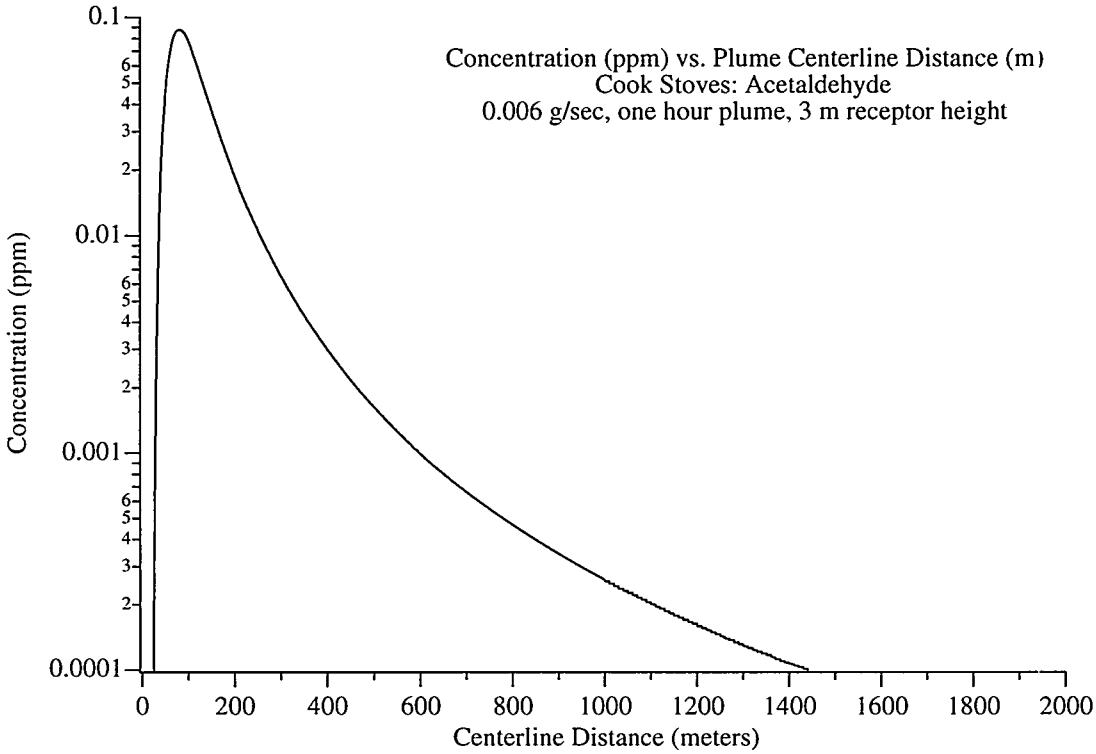
Met Data

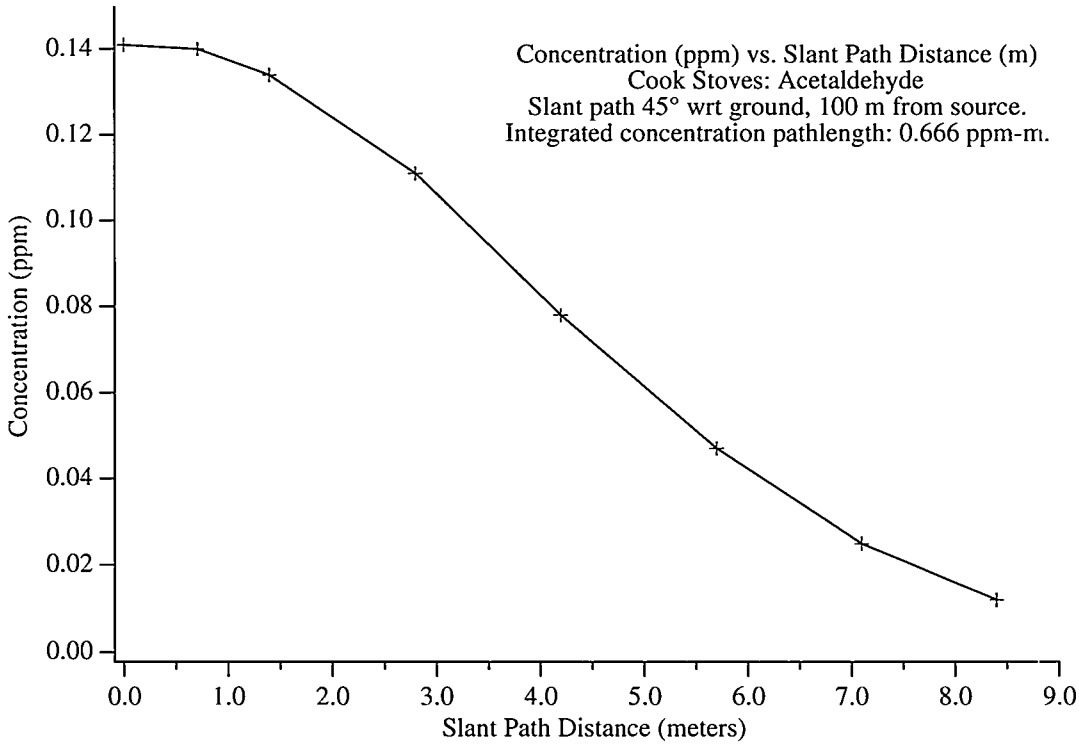
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Cook Stoves: Acetaldehyde, 0.006 g/sec, one-hour plume.

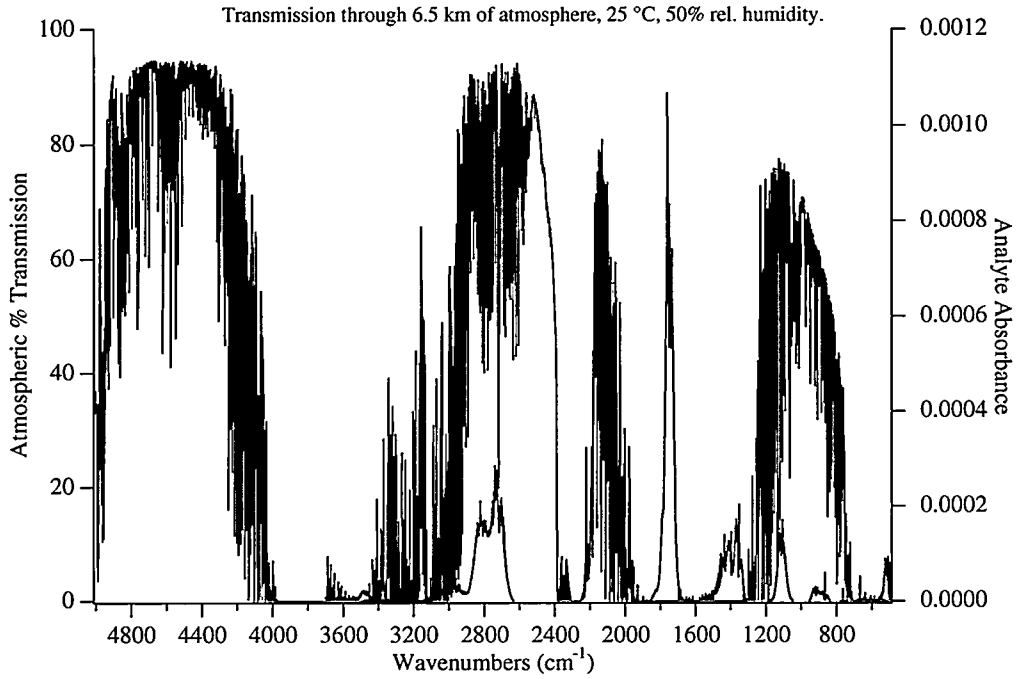




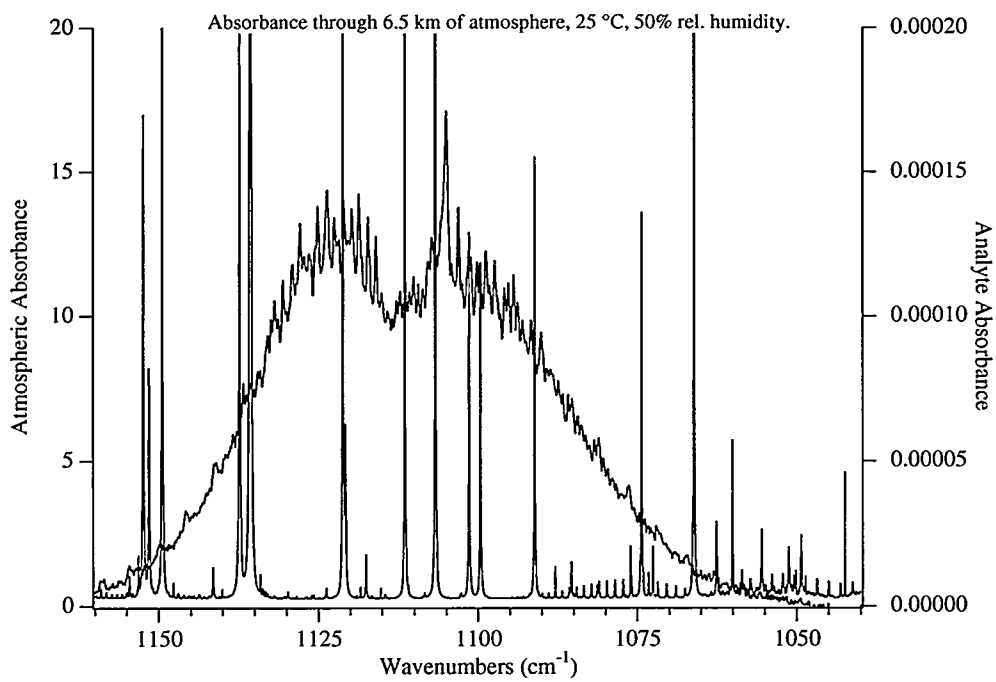

Concentration (ppm) vs. Plume Centerline Distance (m)
Cook Stoves: Acetaldehyde
0.006 g/sec, one hour plume, 3 m receptor height
Concentration (ppm)
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Cook Stoves: Acetaldehyde
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 0.666 ppm-m.
Concentration (ppm)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
Slant Path Distance (meters)

Acetaldehyde from Cook Stoves
Acetaldehyde absorbance, 20 °C, 0.666 ppm-m, 100 m from vent.
Hanst database.

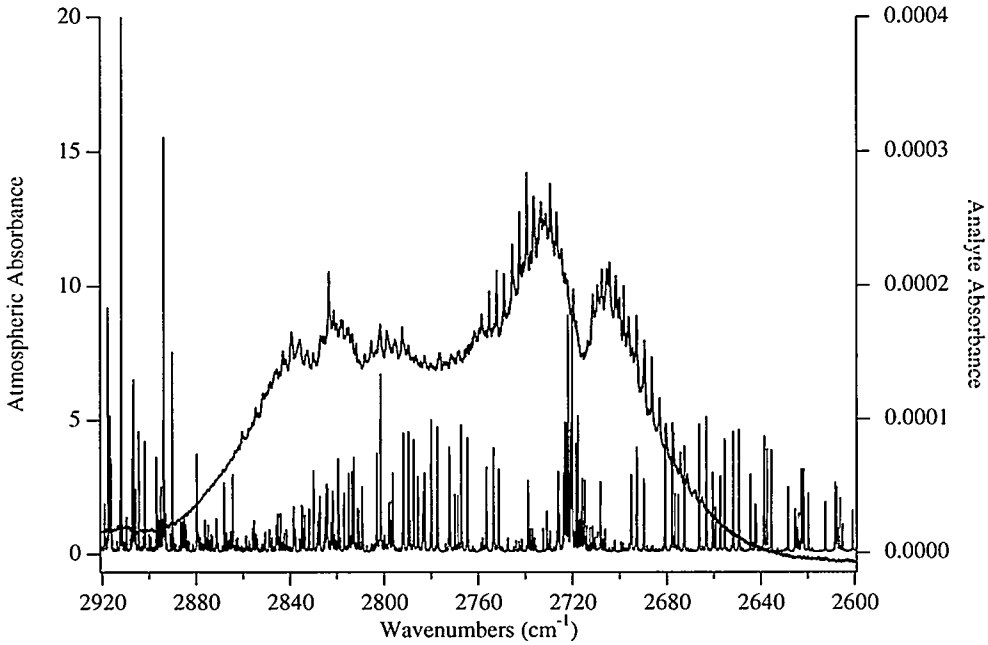


Acetaldehyde from Cook Stoves
Acetaldehyde absorbance, 20 °C, 0.666 ppm-m, 100 m from vent.
ν_8 band, Hanst database.



Acetaldehyde from Cook Stoves
Acetaldehyde absorbance, 20 °C, 0.666 ppm-m, 100 m from vent.
ν_2 and ν_3 region, Hanst database.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



4.3 Septic System

Compound	Emission Rate (g/sec)
Carbon dioxide	0.2
Methane	0.1
Ammonia	0.05
Hydrogen sulfide	8×10^{-4}

Scenario: Anaerobic decomposition of excreta from one-thousand people. Gases released from a vented, 500 m^3 holding tank (White 1970; Mahlie 1964; Kachniarz 1996).

CHARM Version 9.3

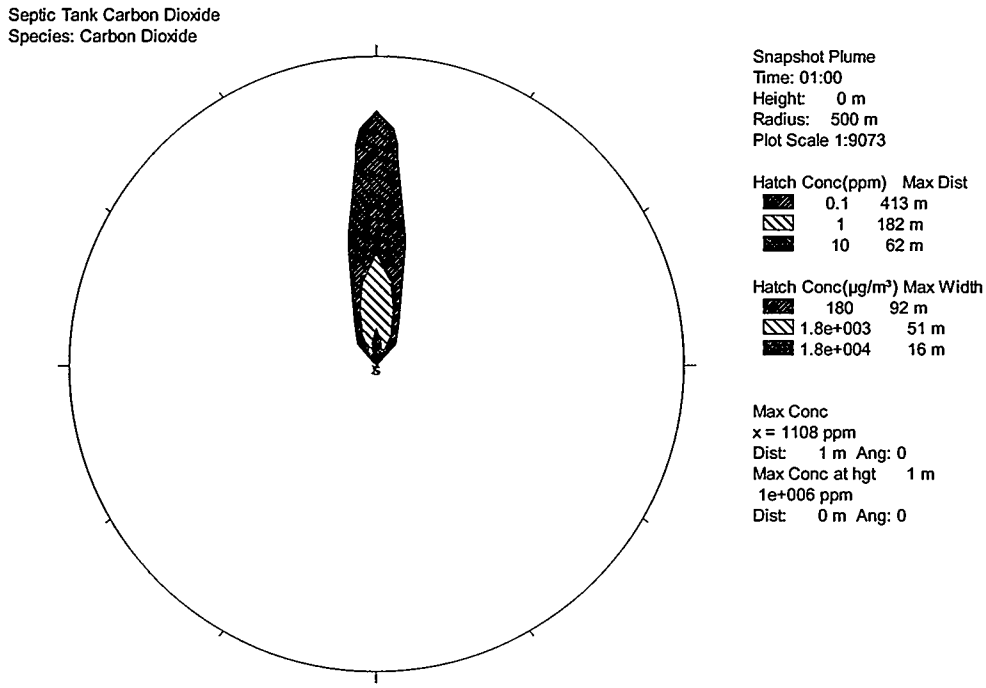
Title:	Septic Tank Carbon Dioxide
Species:	Carbon Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.2 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.002265 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

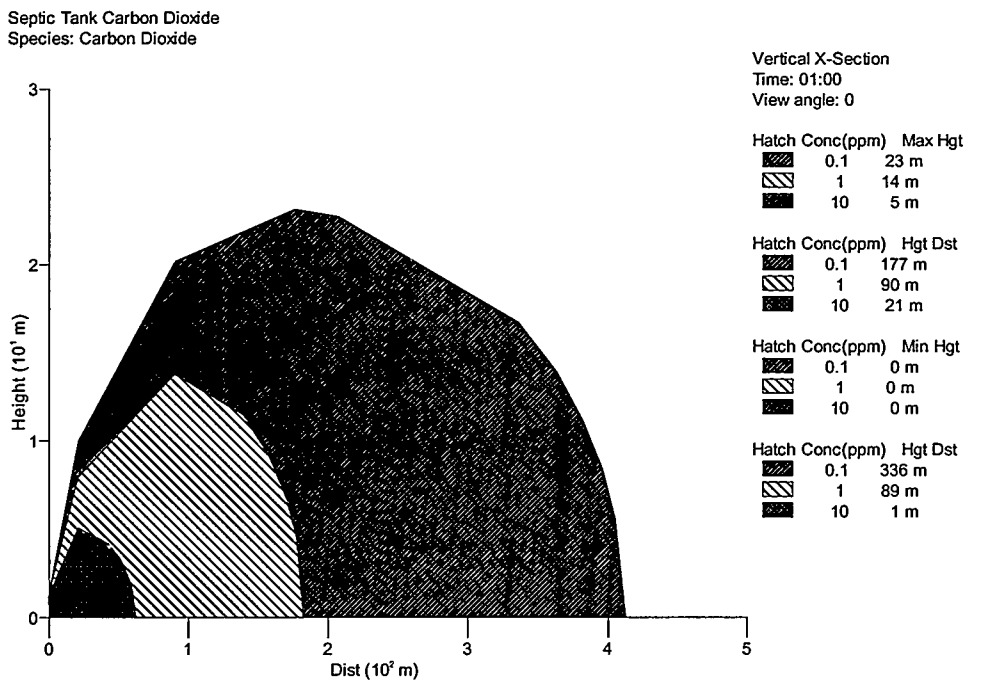
****

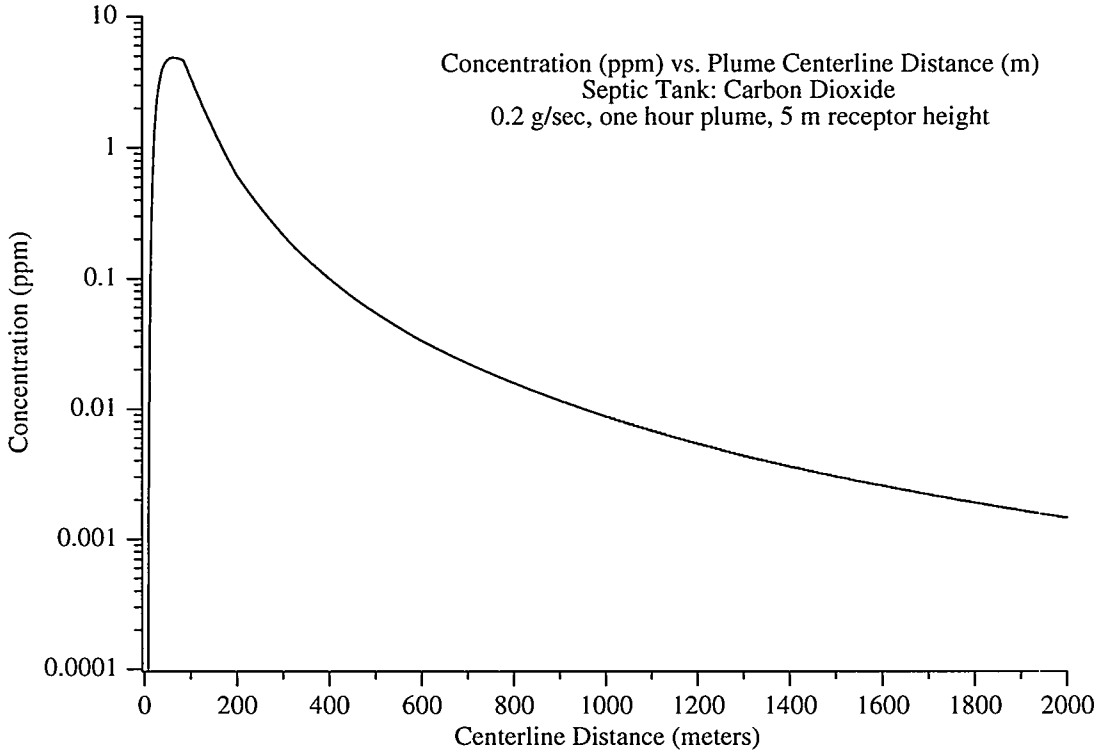
Met Data

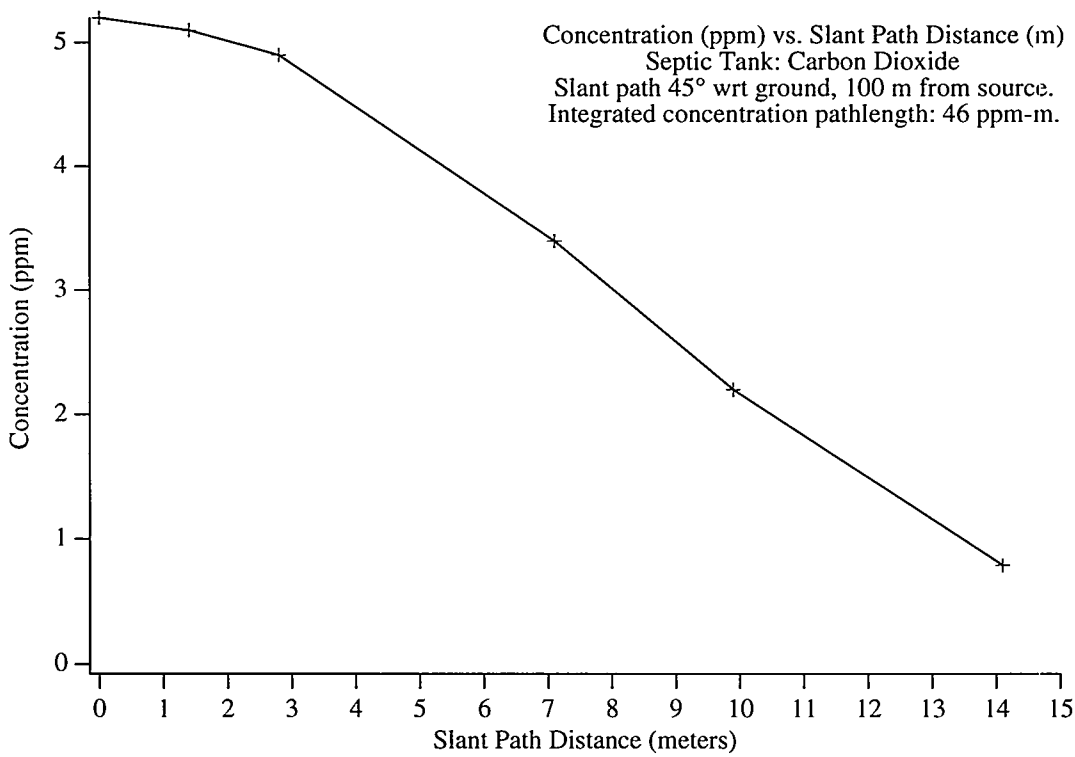
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m²
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Septic Tank: Carbon Dioxide, 0.2 g/sec, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Septic Tank: Carbon Dioxide
0.2 g/sec, one hour plume, 5 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Septic Tank: Carbon Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 46 ppm-m.
Concentration (ppm)
5
4
3
2
1
0
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
Slant Path Distance (meters)

CHARM Version 9.3

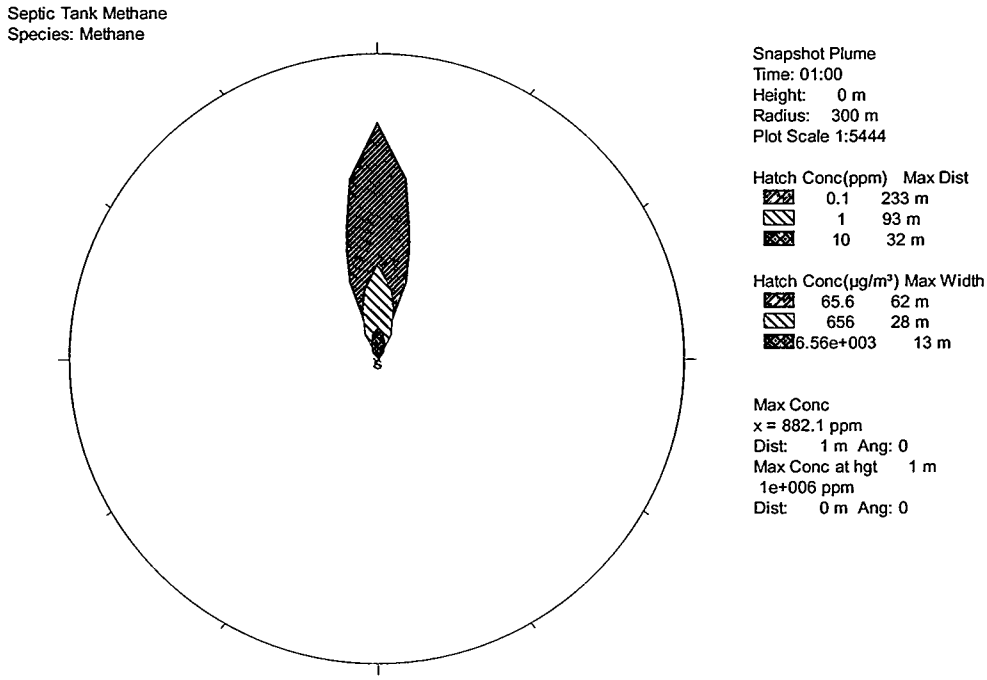
Title:	Septic Tank Methane
Species:	Methane
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.1 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.003107 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

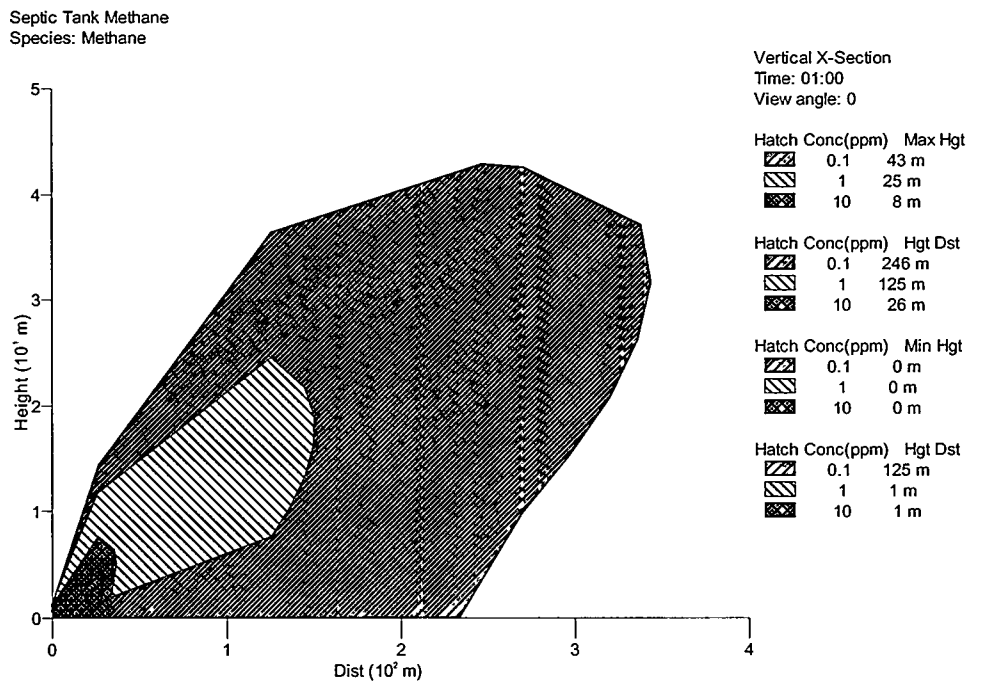
****

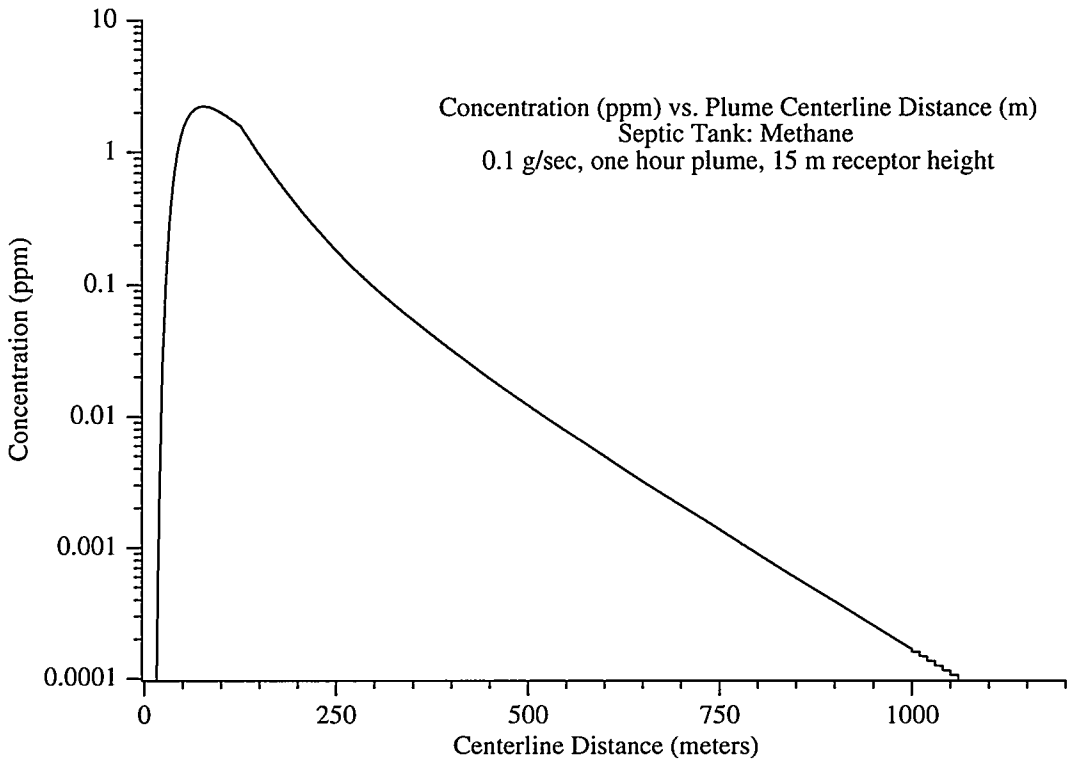
Met Data

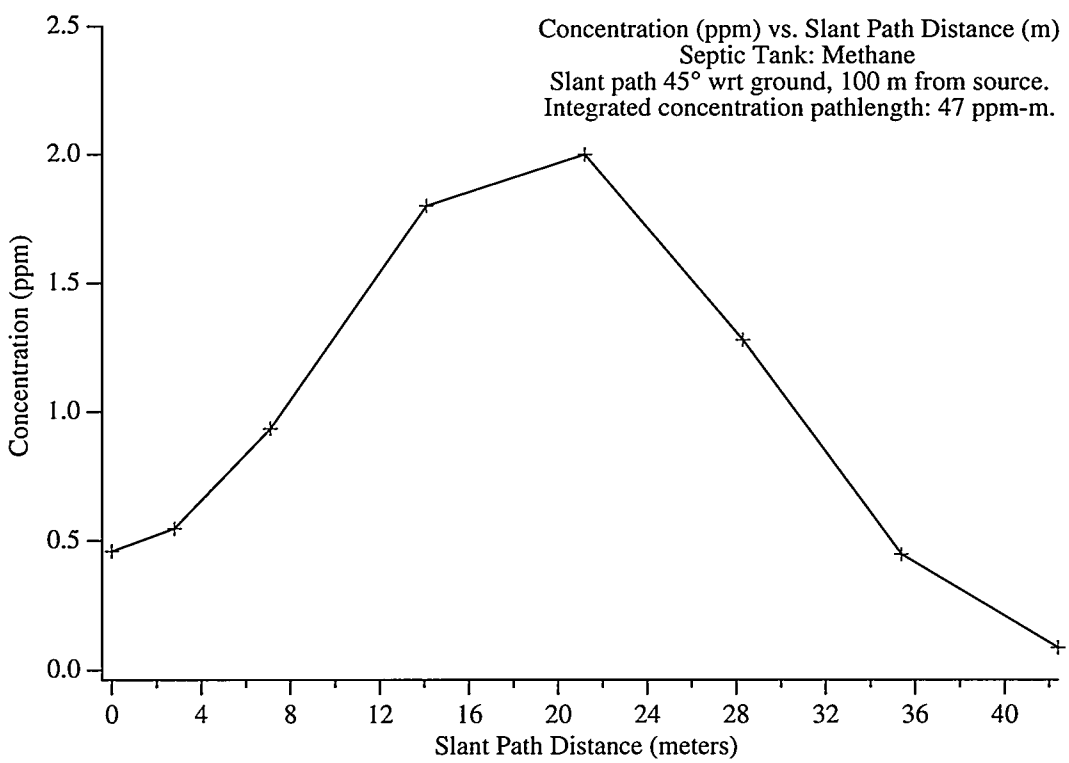
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	
Wind Direction:	180°
Wind Speed:	5 m/s

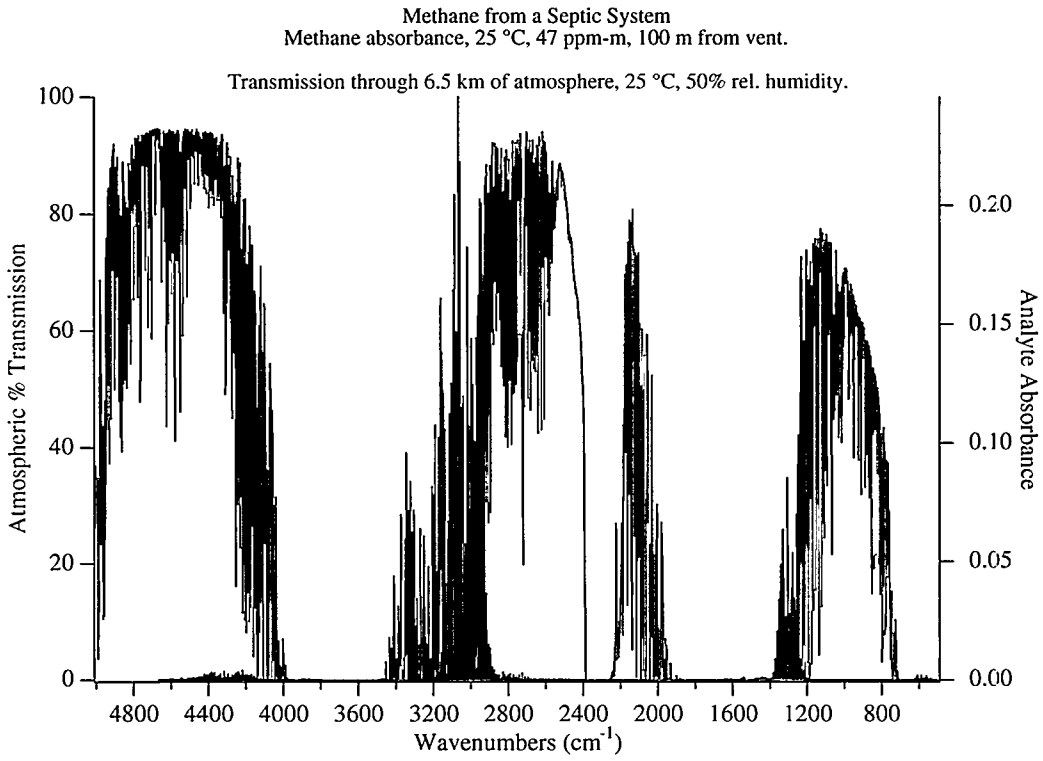
Septic Tank: Methane, 0.1 g/sec, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Septic Tank: Methane
0.1 g/sec, one hour plume, 15 m receptor height
Concentration (ppm)
10
1
0.1
0.01
0.001
0.0001
0
250
500
750
1000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Septic Tank: Methane
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 47 ppm-m.
Concentration (ppm)
2.5
2.0
1.5
1.0
0.5
0.0
0
4
8
12
16
20
24
28
32
36
40
Slant Path Distance (meters)


Methane from a Septic System
Methane absorbance, 25 °C, 47 ppm-m, 100 m from vent.
Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric % Transmission
100
80
60
40
20
0
Analyte Absorbance
0.20
0.15
0.10
0.05
0.00
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
Wavenumbers (cm-1)

CHARM Version 9.3

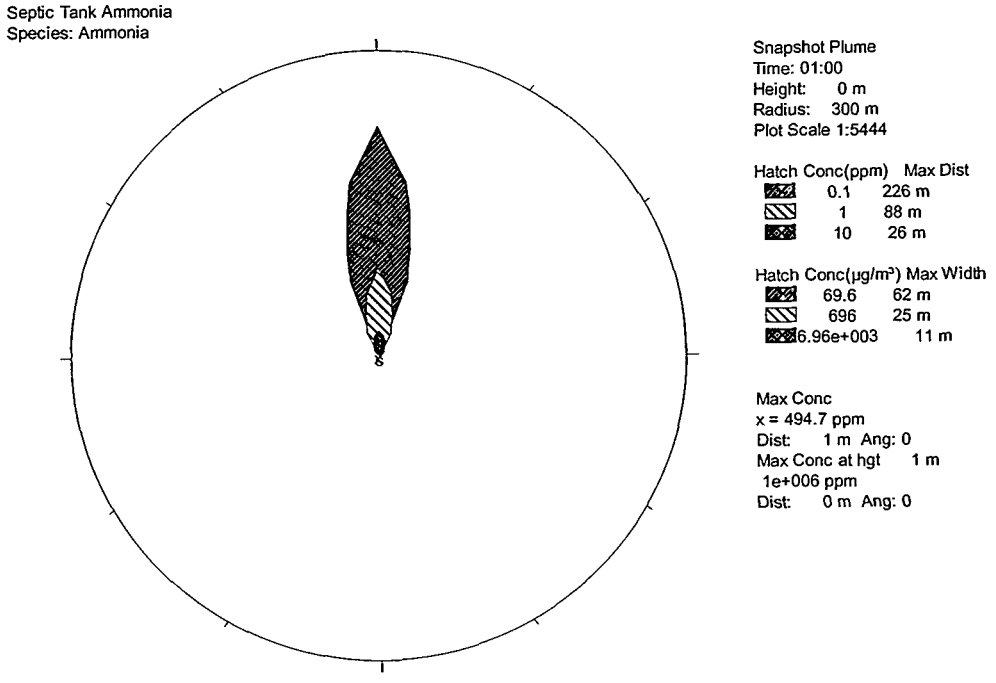
Title:	Septic Tank Ammonia
Species:	Ammonia
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.1, 1, 10
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.05 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.001463 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

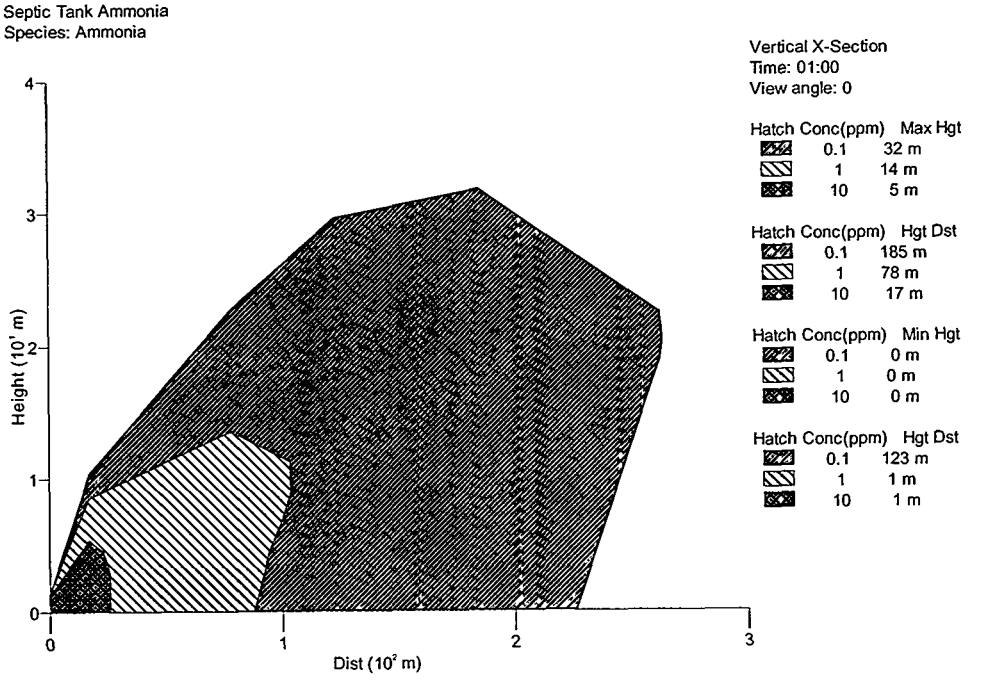
****

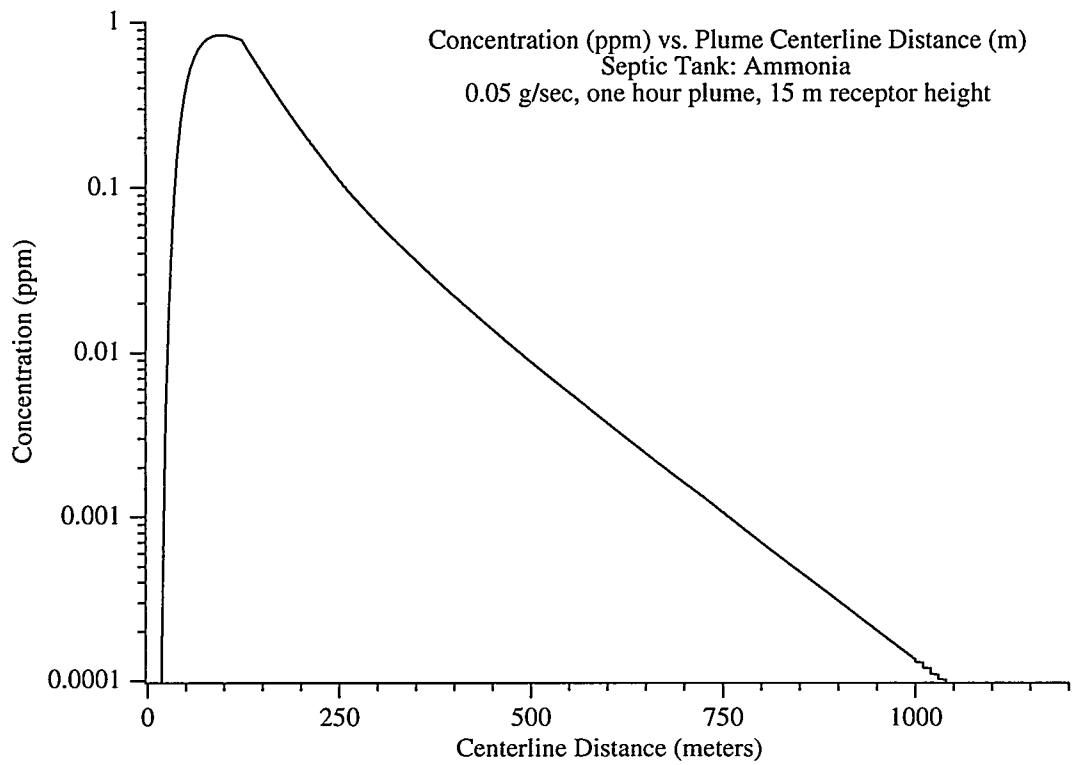
Met Data

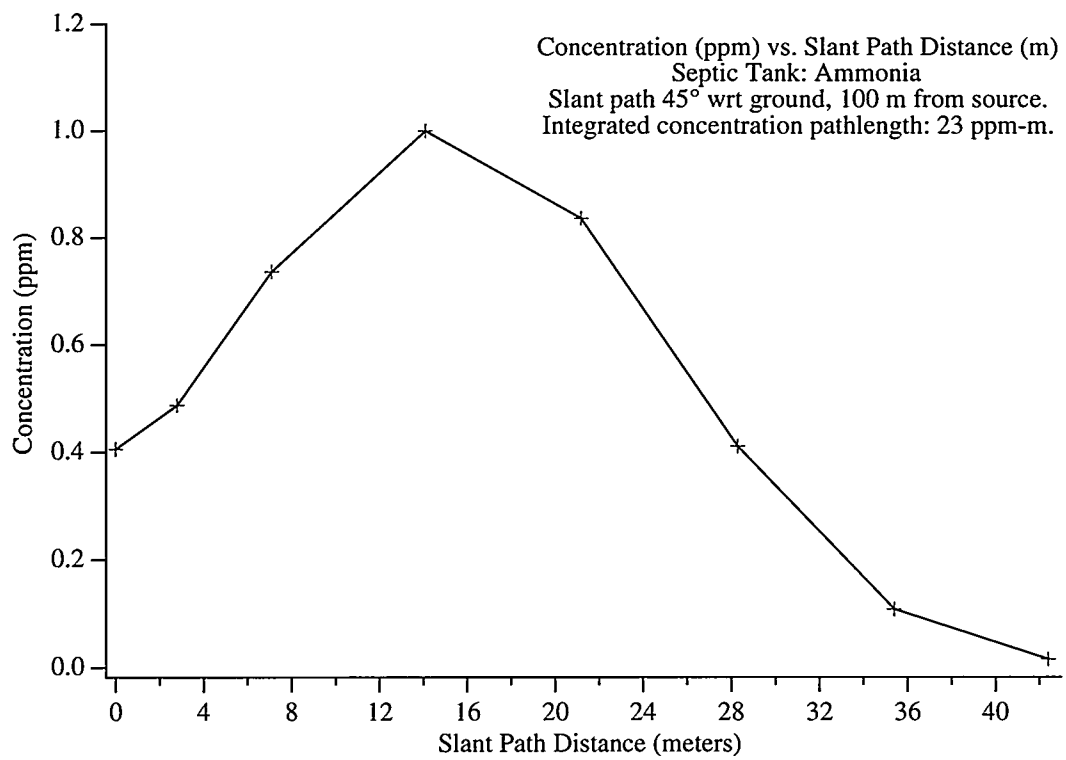
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Winds Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

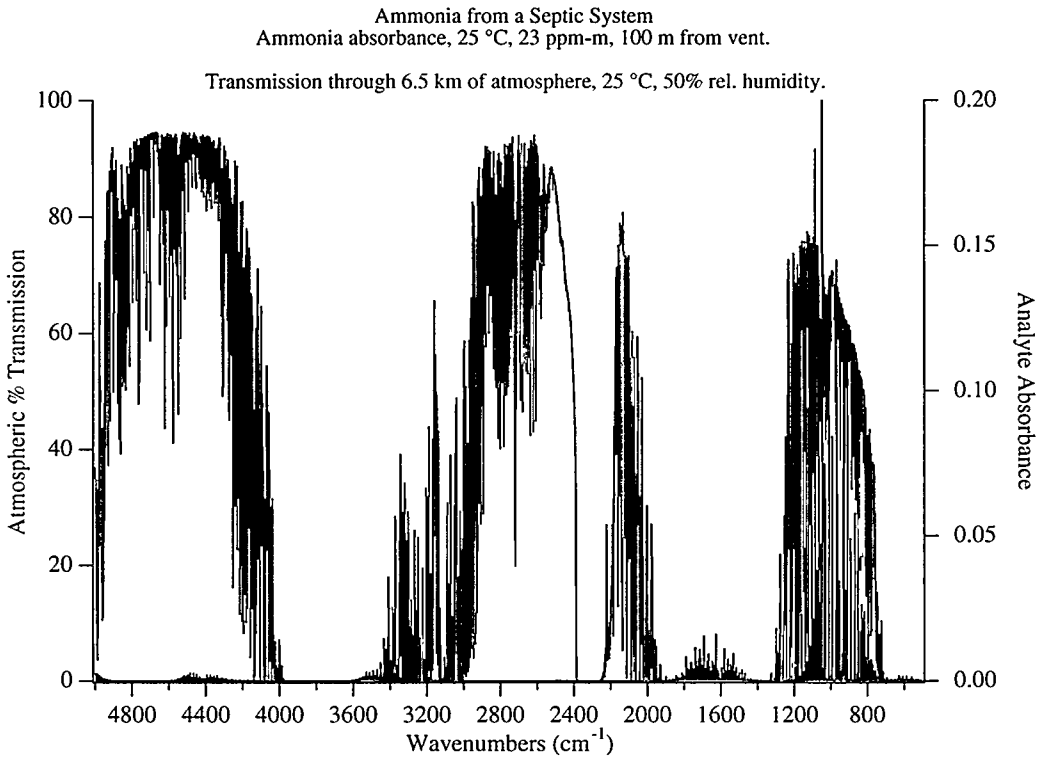
Septic Tank: Ammonia, 0.05 g/sec, one-hour plume.

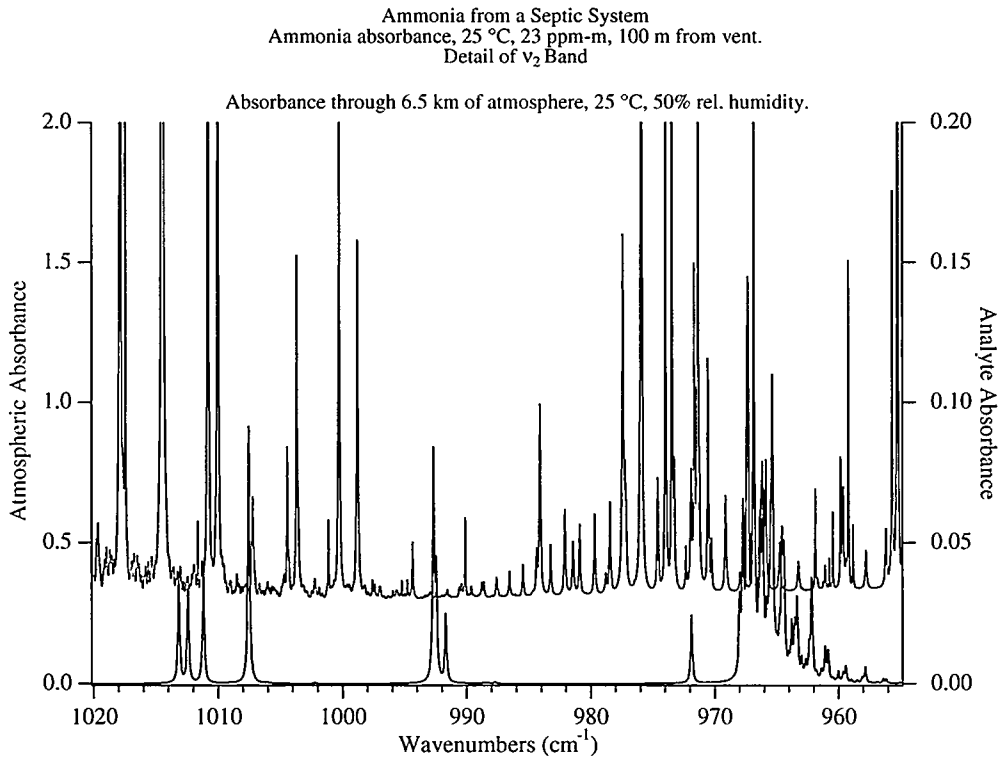





Concentration (ppm) vs. Plume Centerline Distance (m)
Septic Tank: Ammonia
0.05 g/sec, one hour plume, 15 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
250
500
750
1000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Septic Tank: Ammonia
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 23 ppm-m.
Concentration (ppm)
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
4
8
12
16
20
24
28
32
36
40
Slant Path Distance (meters)


Ammonia from a Septic System
Ammonia absorbance, 25 °C, 23 ppm-m, 100 m from vent.
Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric % Transmission
Analyte Absorbance
Wavenumbers (cm-1)
100
80
60
40
20
0
0.20
0.15
0.10
0.05
0.00
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800


Ammonia from a Septic System
Ammonia absorbance, 25 °C, 23 ppm-m, 100 m from vent.
Detail of ν_2 Band
Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.
Atmospheric Absorbance
Analyte Absorbance
Wavenumbers (cm-1)
2.0
1.5
1.0
0.5
0.0
0.20
0.15
0.10
0.05
0.00
1020
1010
1000
990
980
970
960

CHARM Version 9.3

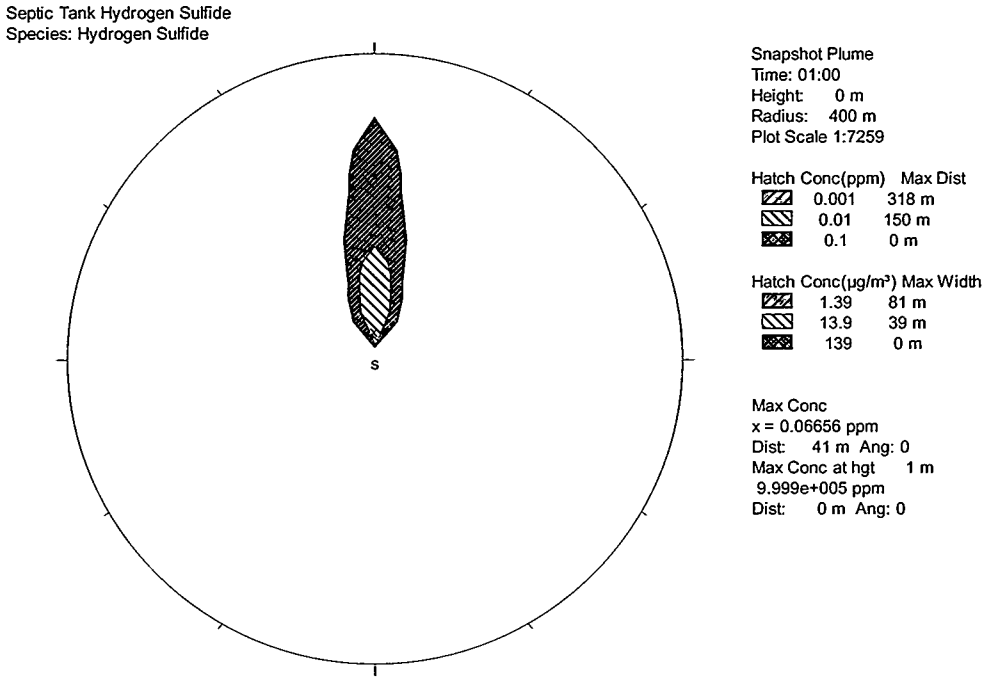
Title:	Septic Tank Hydrogen Sulfide
Species:	Hydrogen Sulfide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.001, 0.01, 0.1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.0008 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	1.17e-005 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

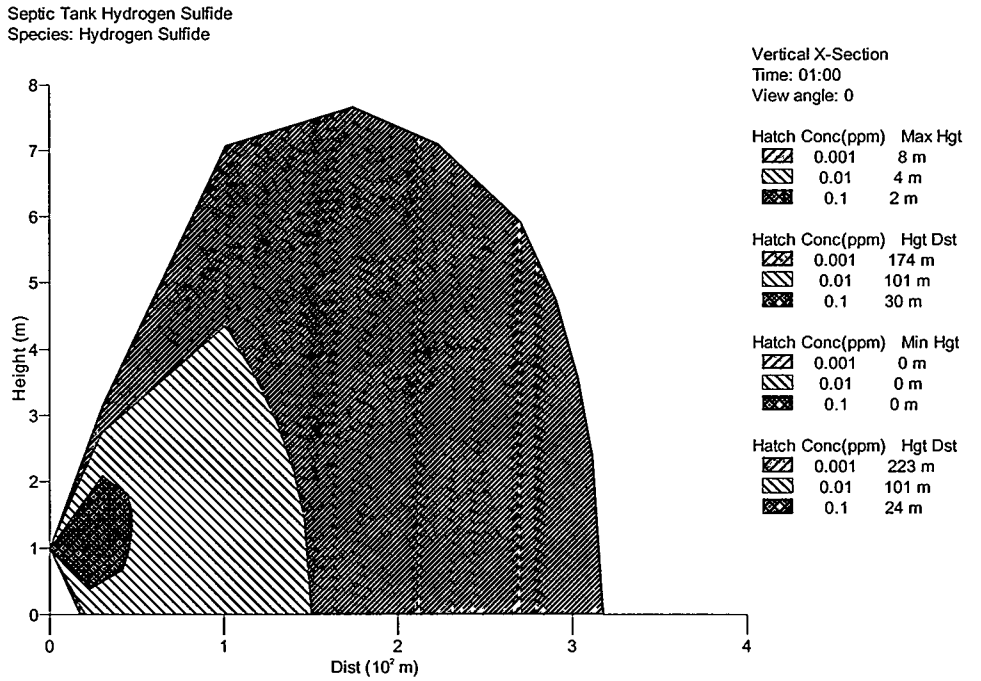
****

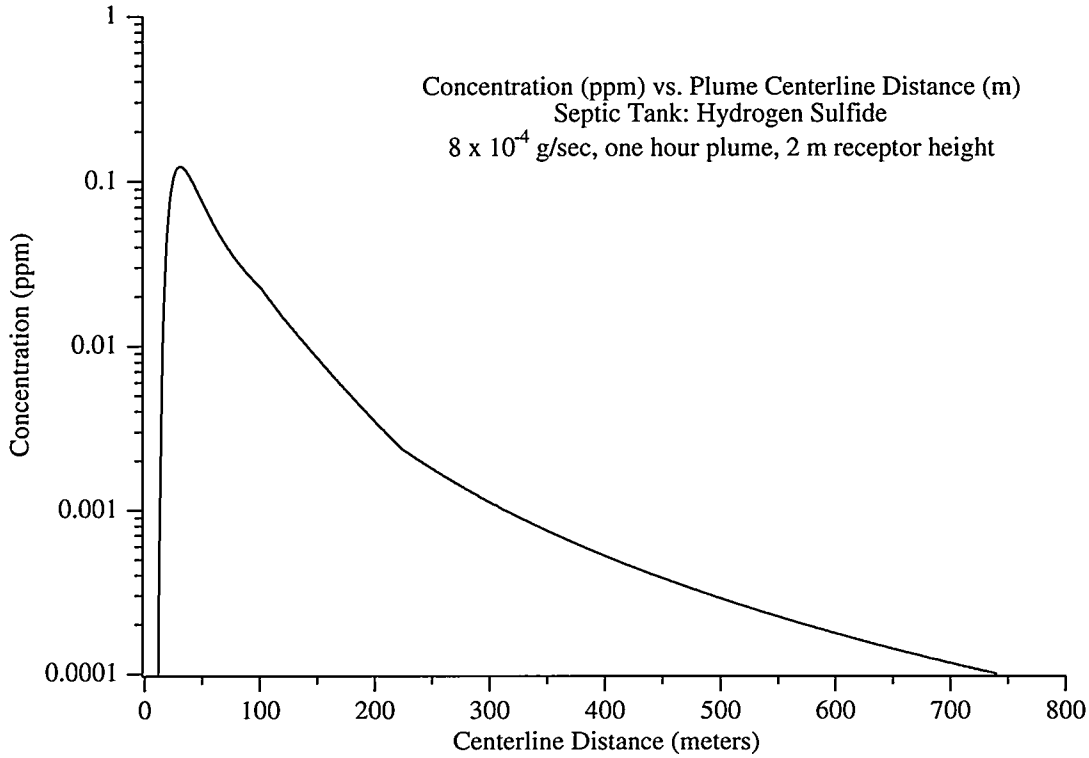
Met Data

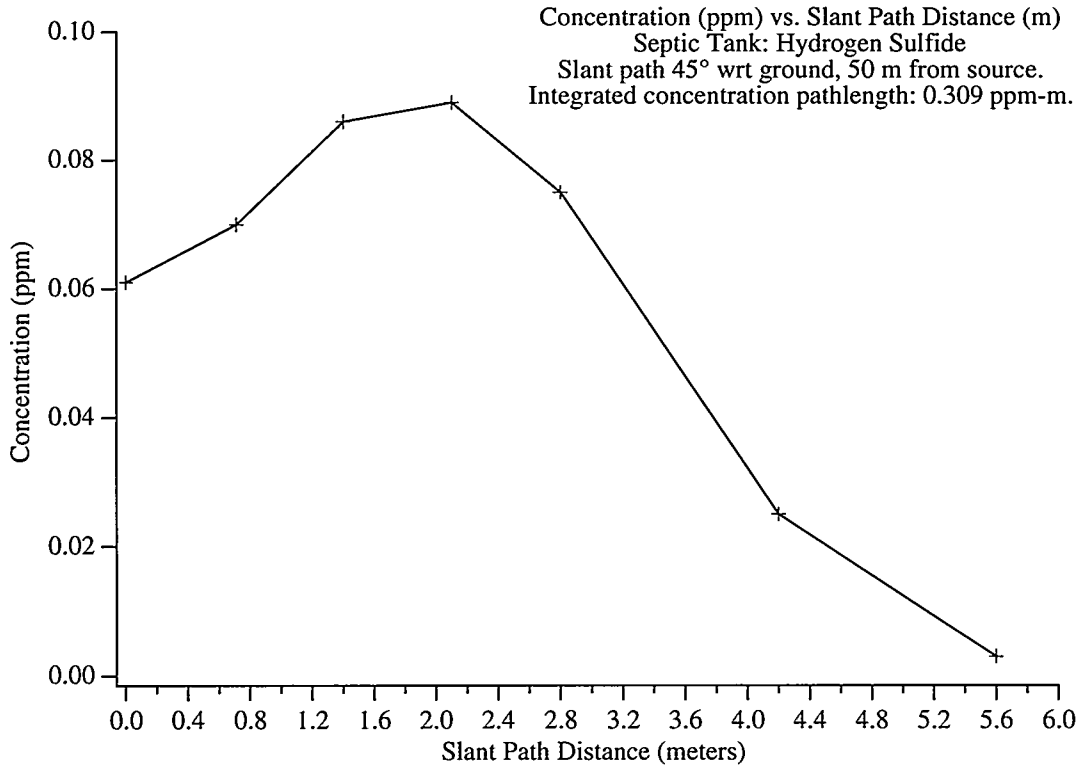
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m²
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	
Wind Direction:	180°
Wind Speed:	5 m/s

Septic Tank: Hydrogen Sulfide, 0.0008 g/sec, one-hour plume,



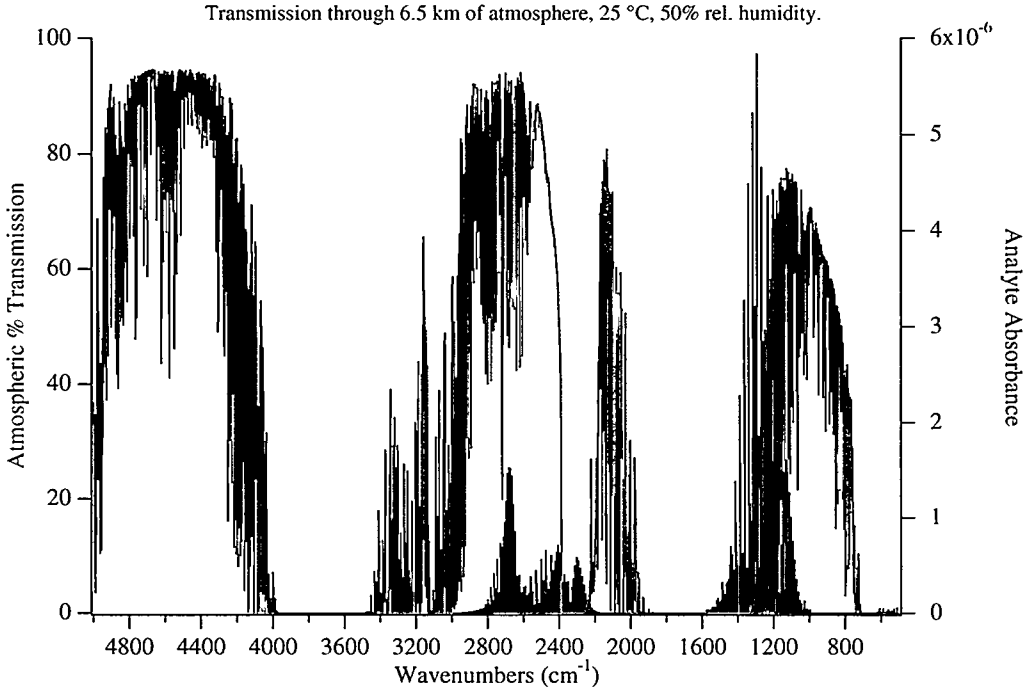



Concentration (ppm) vs. Plume Centerline Distance (m)
Septic Tank: Hydrogen Sulfide
8 x 10^-4 g/sec, one hour plume, 2 m receptor height
Concentration (ppm)
1
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Septic Tank: Hydrogen Sulfide
Slant path 45° wrt ground, 50 m from source.
Integrated concentration pathlength: 0.309 ppm-m.
Concentration (ppm)
0.10
0.08
0.06
0.04
0.02
0.00
0.0
0.4
0.8
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
Slant Path Distance (meters)

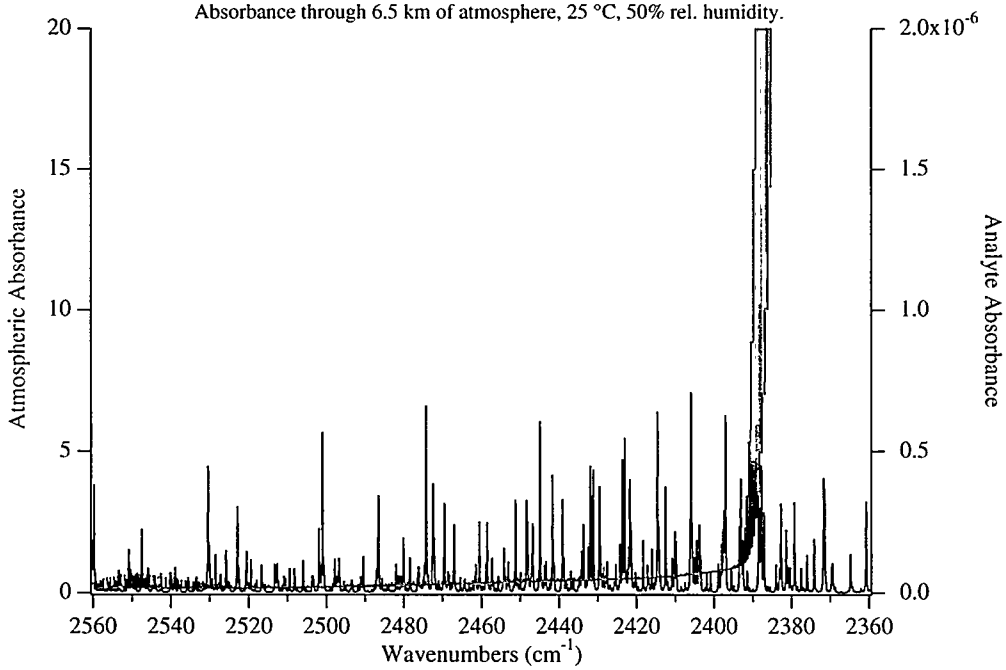
Hydrogen Sulfide from a Septic System
Hydrogen sulfide absorbance, 25 °C, 0.309 ppm-m, 100 m from vent.

Transmission through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



Hydrogen Sulfide from a Septic System
Hydrogen sulfide absorbance, 25 °C, 0.309 ppm-m, 100 m from vent.
Detail of $2\nu_2$ band.

Absorbance through 6.5 km of atmosphere, 25 °C, 50% rel. humidity.



4.4 Landfill

Compound[a]	Emission Rate (g/sec)[a]
Carbon Dioxide	2
Methane	1
Heptane	0.03
Octane	0.02
Hexane	0.01
Nitrogen	0.007
Nonane	0.007
Oxygen	0.002
n-Pentane	0.001
iso-Pentane	0.0007
Propane	0.0003
n-Butane	0.0003
iso-Butane	0.0002
Hydrogen	0.0001
Hydrogen sulfide	0.00006

(a) Hodgson, A. T., K. Garbesi, R. G. Sextro, and J. M. Daisey. 1992. "Soil-Gas Contamination and Entry of Volatile Organic Compounds into a House Near a Landfill." *J. Air Waste Manage. Assoc.* **42**:277-283.

Scenario: This scenario assumes that each person disposes of one kilogram of biomass material (food scraps, paper, cardboard, wood materials, etc.) per day. Methane release rate (liter/kg of biomass waste) from a sanitary municipal was calculated from SECO Fact Sheet No. 16.[a] This number was then used to calculate release rates for other gases listed in Brosseau and Heitz (1994).

(a) "Clean Energy from Texas Landfills," SECO Fact Sheet No. 16, http://www.InfinitePower.com/pdf/fs16.pdf

CHARM Version 9.3

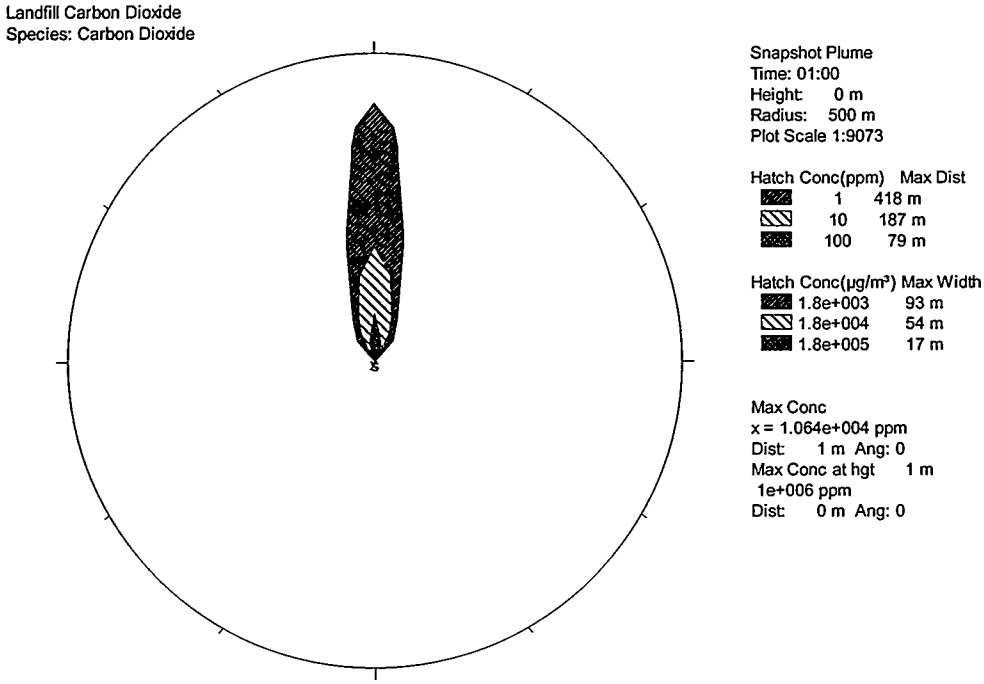
Title:	Landfill Carbon Dioxide
Species:	Carbon Dioxide
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	2 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.02265 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

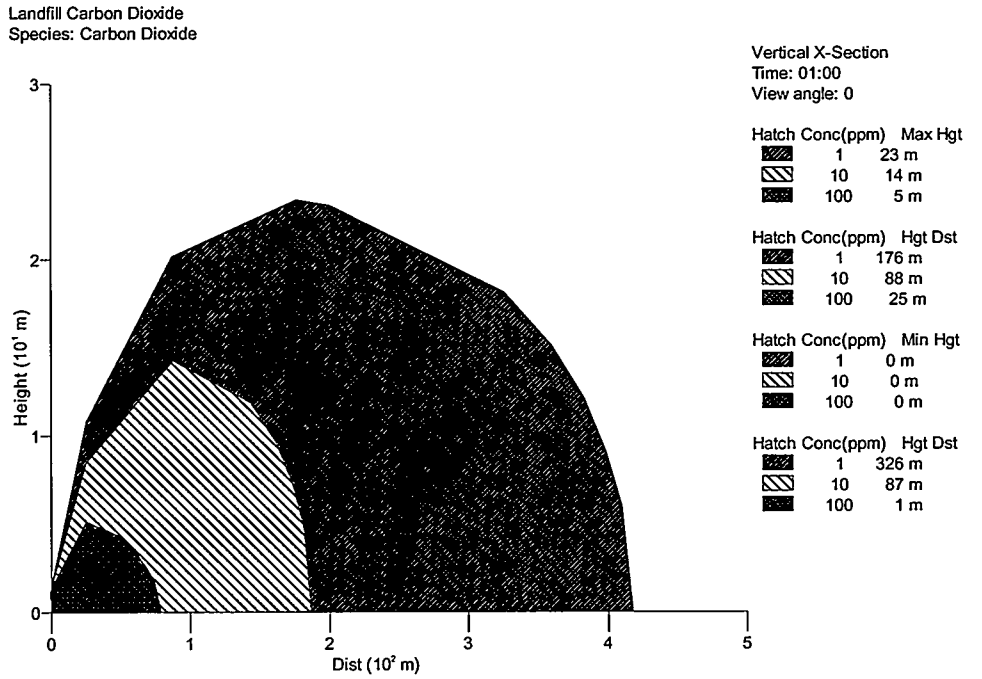
****

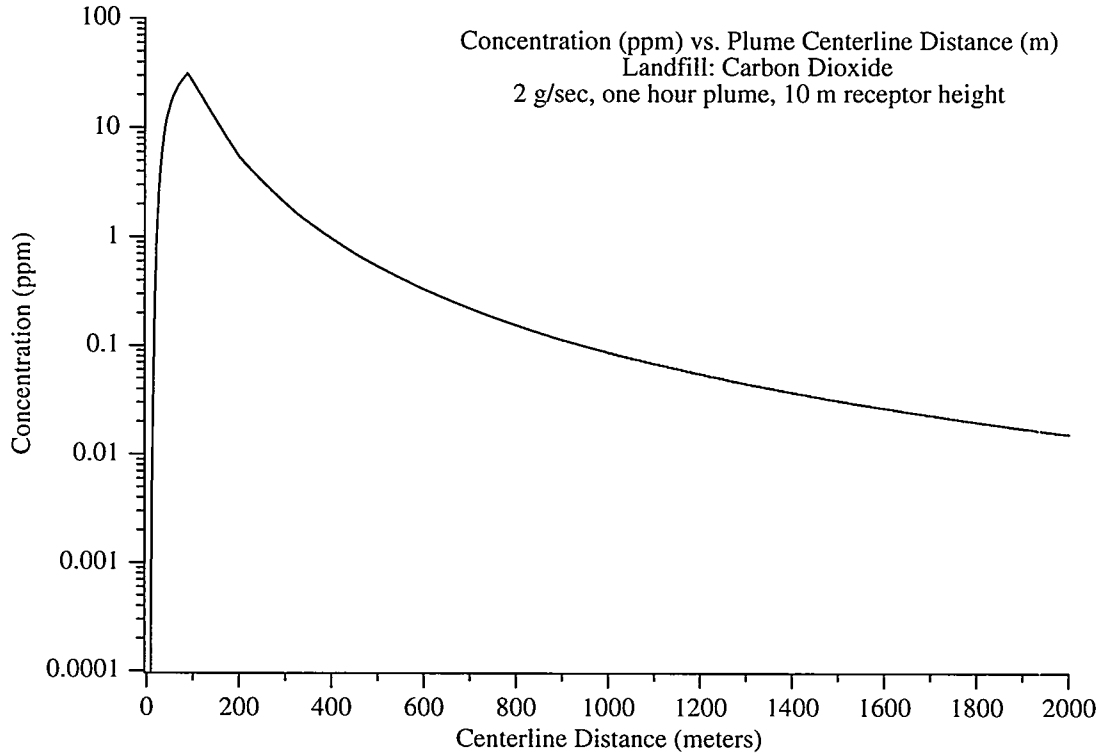
Met Data

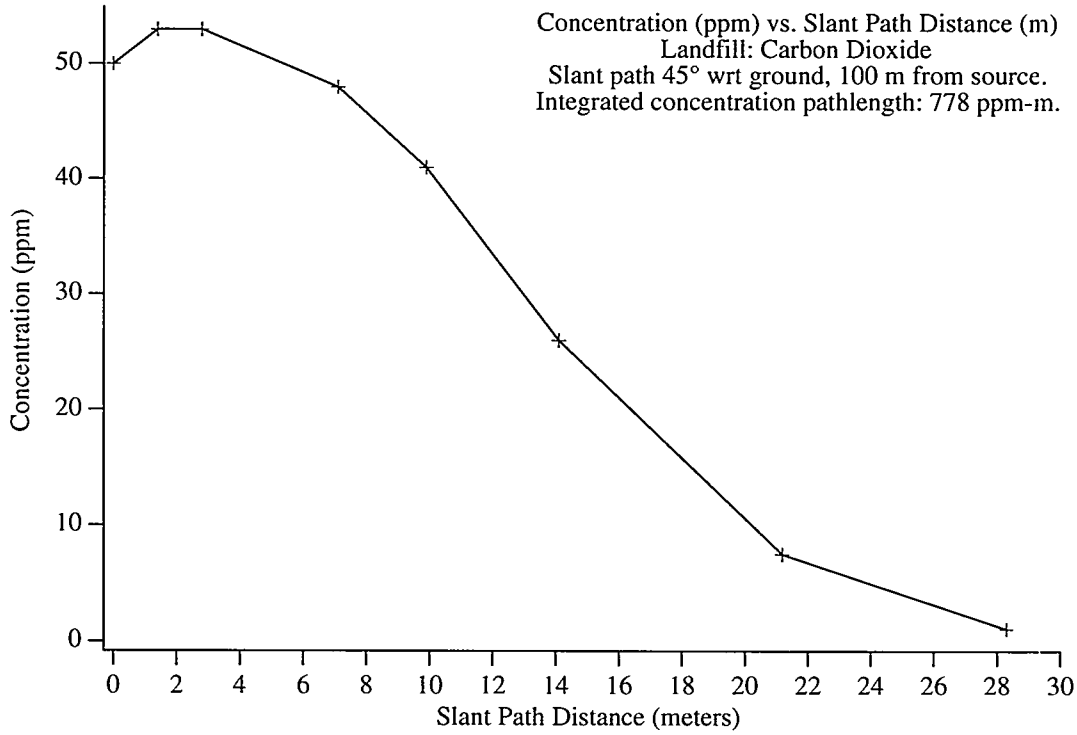
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Winds Time:	00:00
Wind direction:	180°
Wind Speed:	5 m/s

Landfill: Carbon Dioxide, 2 g/sec, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Landfill: Carbon Dioxide
2 g/sec, one hour plume, 10 m receptor height
Concentration (ppm)
100
10
1
0.1
0.01
0.001
0.0001
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Landfill: Carbon Dioxide
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 778 ppm-m.
Concentration (ppm)
50
40
30
20
10
0
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
Slant Path Distance (meters)

CHARM Version 9.3

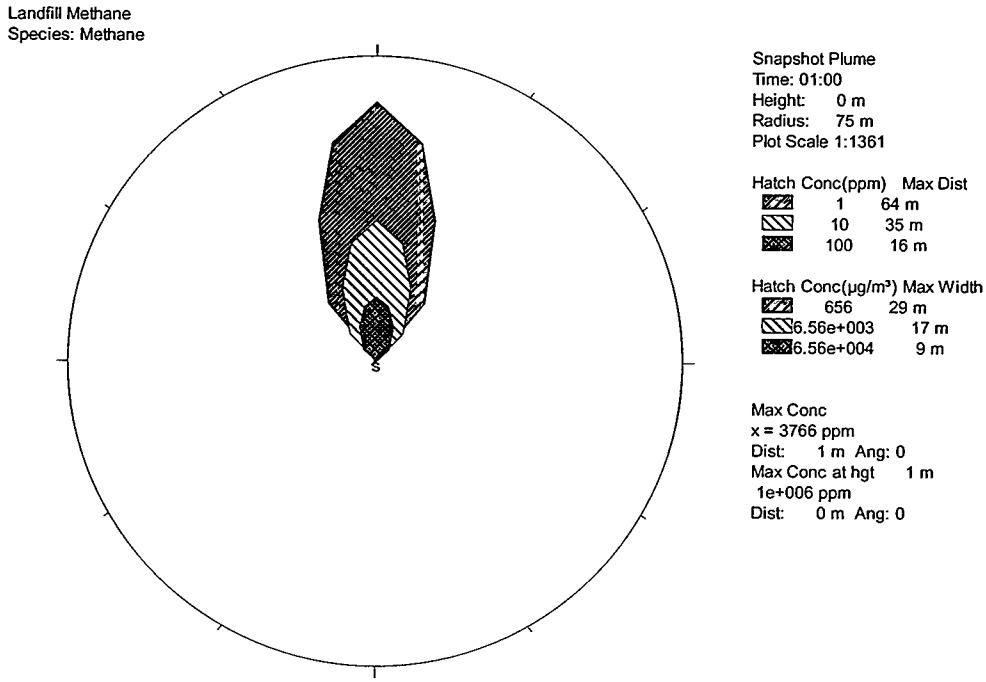
Title:	Landfill Methane
Species:	Methane
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	1, 10, 100
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	1 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	0.03107 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

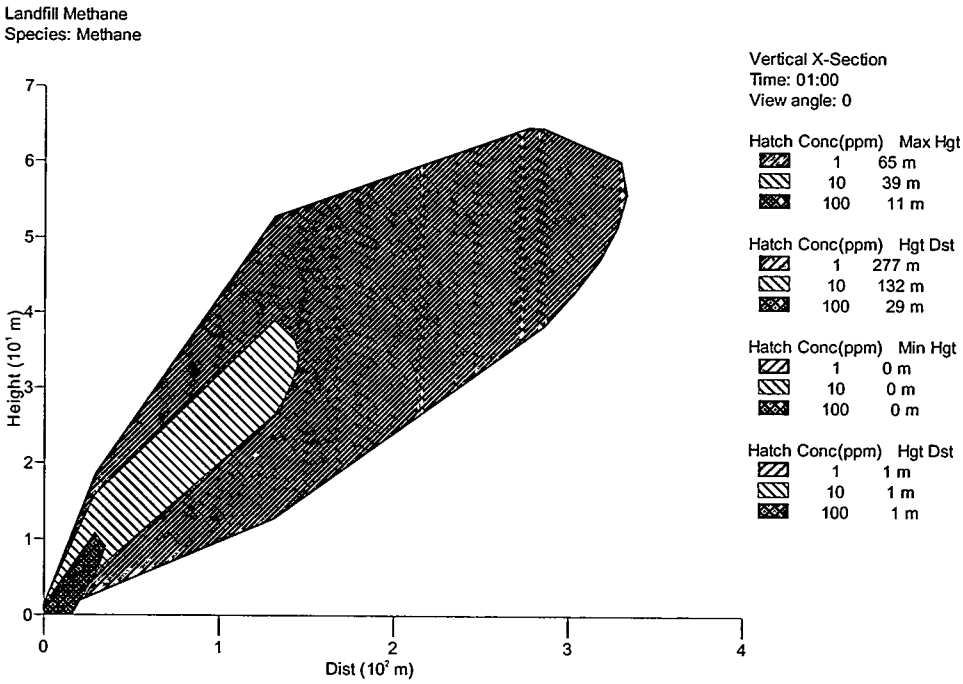
****

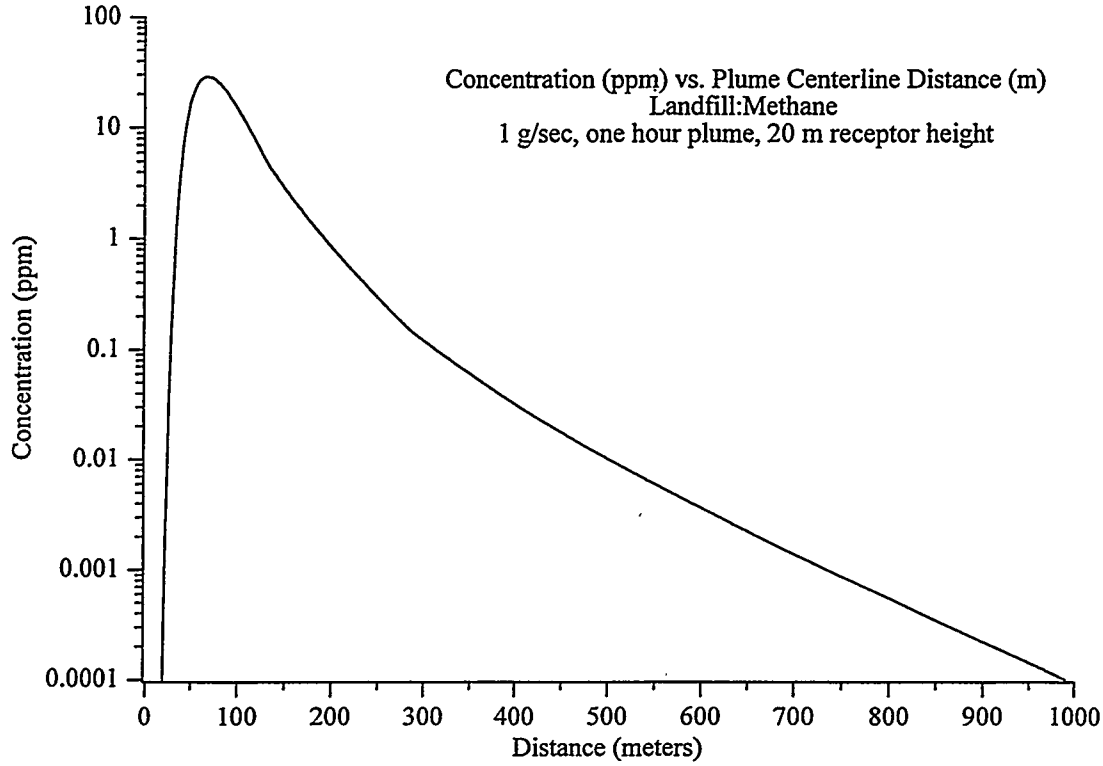
Met Data

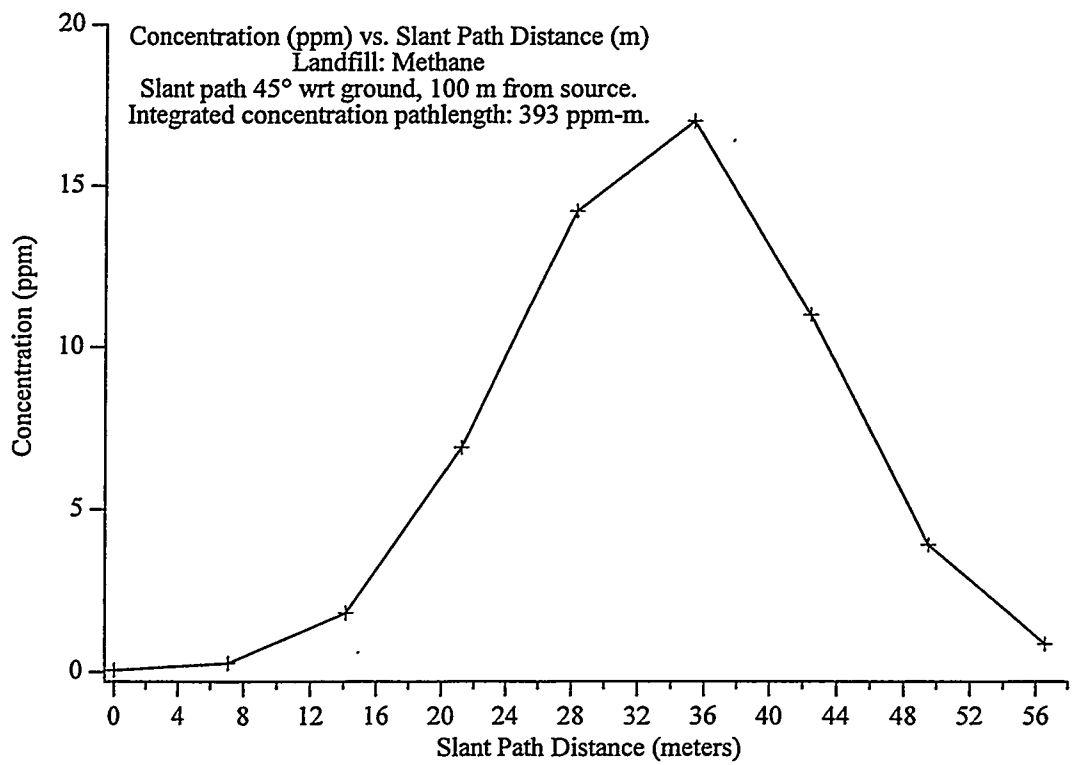
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Landfill: Methane, 1 g/sec, one-hour plume.






Concentration (ppm) vs. Plume Centerline Distance (m)
Landfill:Methane
1 g/sec, one hour plume, 20 m receptor height
Concentration (ppm)
100
10
1
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
900
1000
Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Landfill: Methane
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 393 ppm-m.
Concentration (ppm)
20
15
10
5
0
0
4
8
12
16
20
24
28
32
36
40
44
48
52
56
Slant Path Distance (meters)

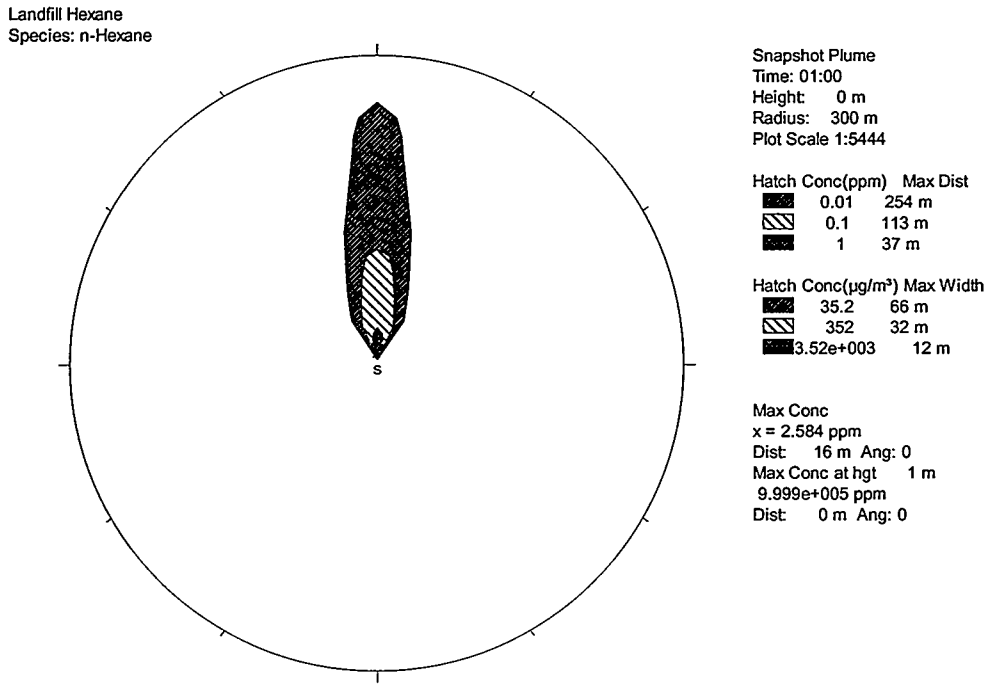
CHARM Version 9.3

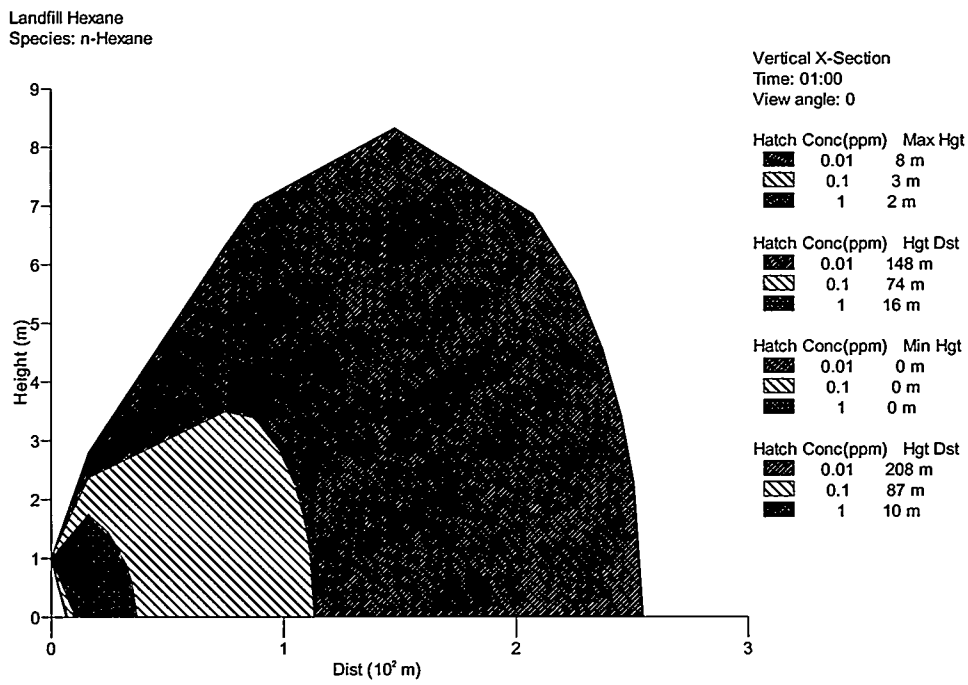
Title:	Landfill Hexane
Species:	n-Hexane
Release Type:	User Specified After-Release Conditions
Emergency Response Output:	Plume
X location:	0 m
Y location:	0 m
Isopleth Concentrations (ppm):	0.01 , 0.1 , 1
Building Height:	0 m
Building Width:	0 m
Source to Building Distance:	0 m
Source to Building Direction:	0°
Release Height Above Ground:	1 m
Continuous Emission Rate is constant	
Initial Emission Rate:	0.01 g/s
Release Duration:	24 hrs
Puff Temperature:	25°C
Puff Diameter:	0.25 m
Puff Depth will be calculated by CHARM	
Puff moving opposite of wind direction	
Horizontal Puff Speed:	0 m/s
Vertical Puff Speed (Calculated):	5.783e-005 m/s
Exit state assumed vapor	
Droplet Mass Fraction:	0
Molar Water Vapor Fraction:	0
Molar Air Fraction:	0

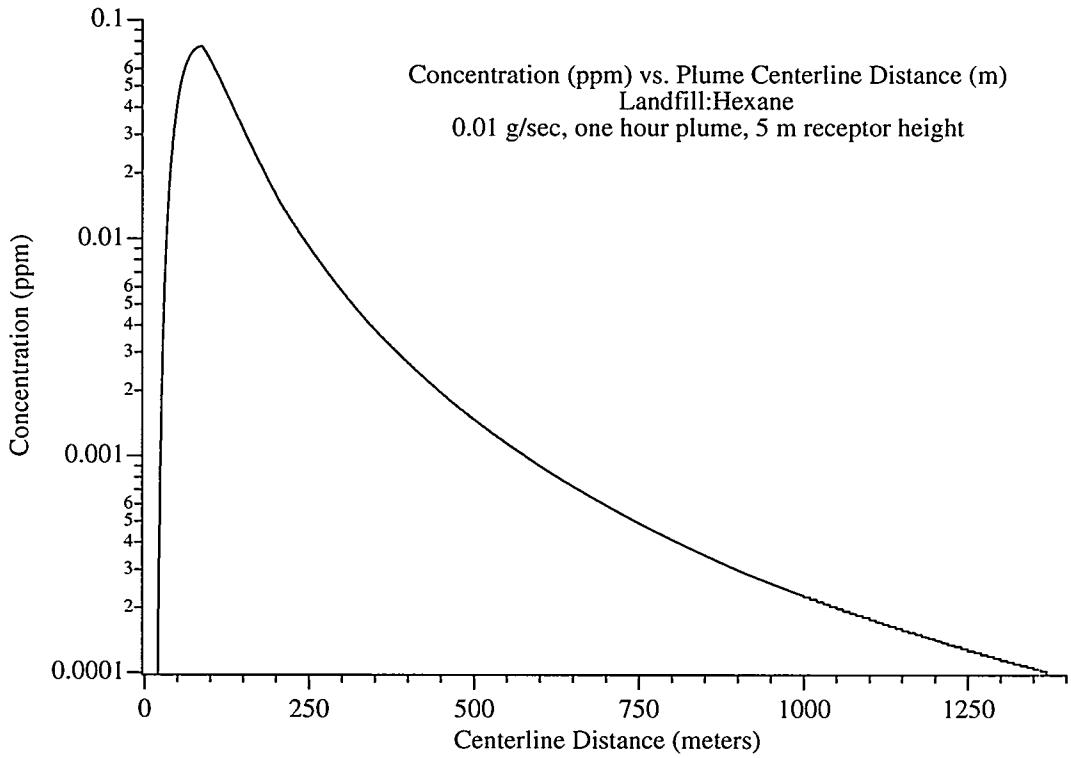
****

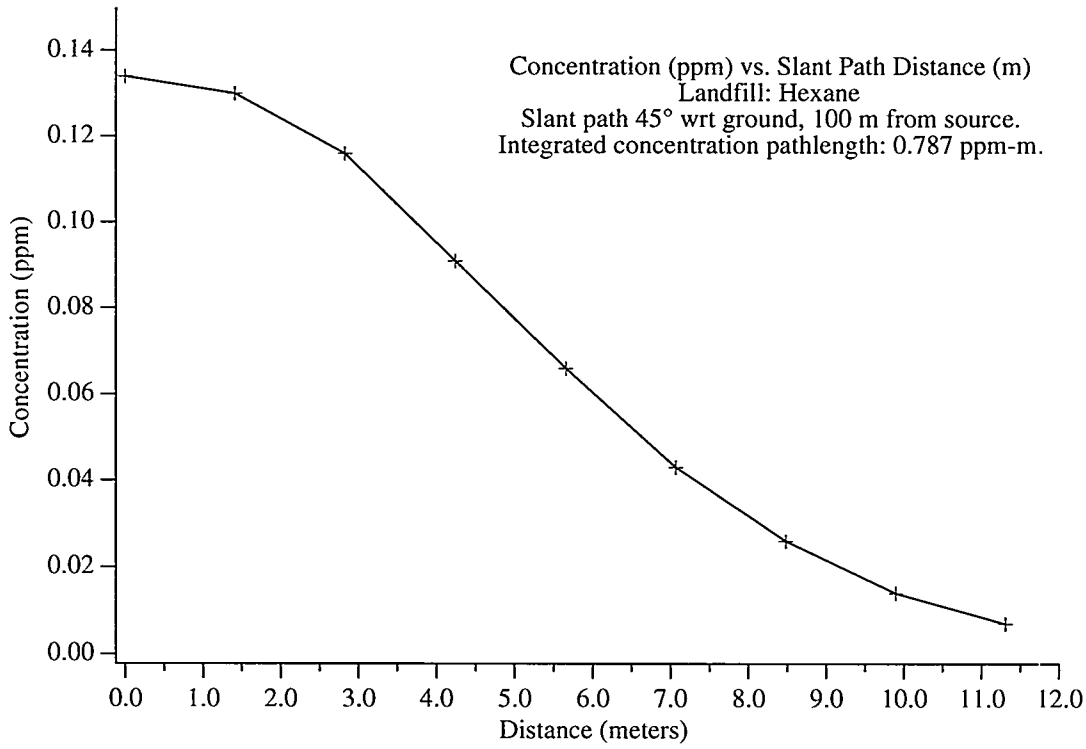
Met Data	
Relative Humidity:	50 %
Ambient Temperature:	25°C
Ambient Pressure:	1 atms
Cloud Cover (tenths):	0
Stability Class:	D (User supplied)
Solar Radiation:	0 kW/m^2
No inversion present	
Surface Roughness:	1 cm
Wind Measurement Altitude:	10 m
Wind Time:	00:00
Wind Direction:	180°
Wind Speed:	5 m/s

Landfill: Hexane, 0.01 g/sec, one-hour plume.

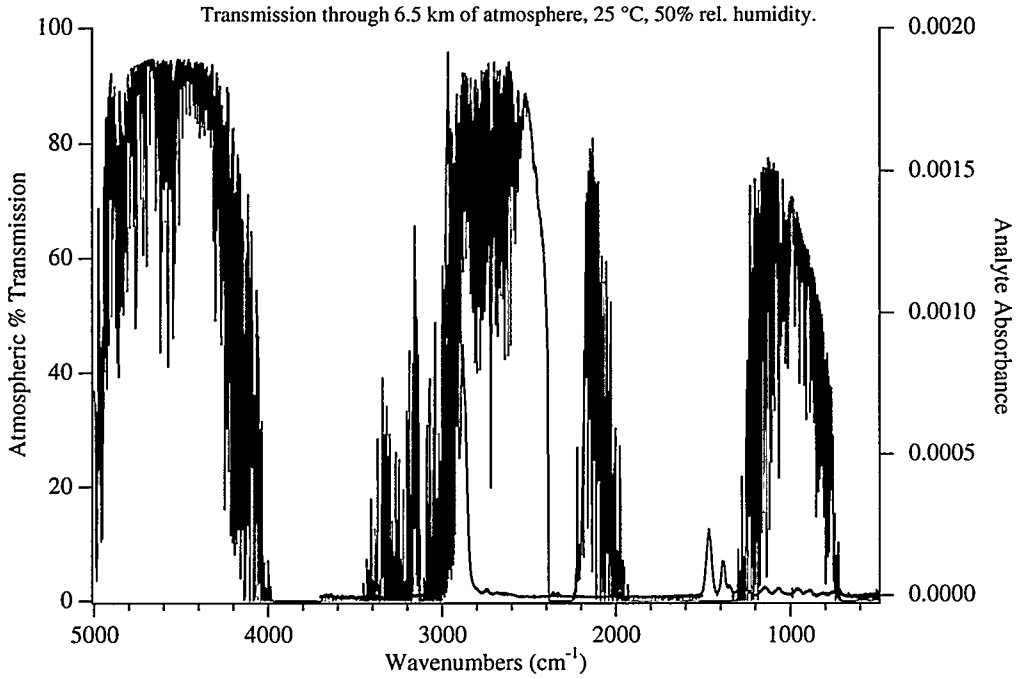




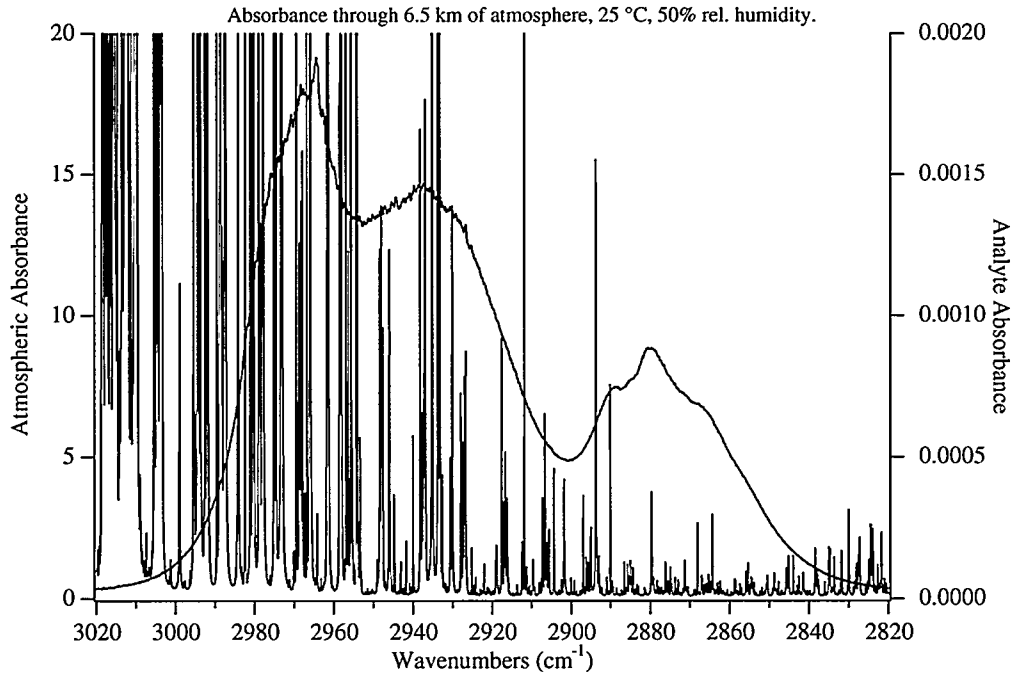

Concentration (ppm) vs. Plume Centerline Distance (m)
Landfill:Hexane
0.01 g/sec, one hour plume, 5 m receptor height
Concentration (ppm)
0.1
0.01
0.001
0.0001
0
250
500
750
1000
1250
Centerline Distance (meters)


Concentration (ppm) vs. Slant Path Distance (m)
Landfill: Hexane
Slant path 45° wrt ground, 100 m from source.
Integrated concentration pathlength: 0.787 ppm-m.
Concentration (ppm)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
Distance (meters)

n-Hexane from Landfill
n-Hexane absorbance, 20 °C, 0.787 ppm-m, 50 m from vent.
Hanst database.



n-Hexane from Landfill
n-Hexane absorbance, 20 °C, 0.787 ppm-m, 50 m from vent.
Hanst database.



5.0 Conclusion

Table 1 summarizes the calculations performed in this study. The table lists the compounds for each scenario with the largest emission rates, the rate or evaporation amount, the distance from the source the concentration-pathlength is calculated, the concentration-pathlength, the Lorentzian and Gaussian linewidth parameters, the frequency of the infrared transition (or group of transitions) that is the best candidate for detection, the absorbance of that transition (log base e), and the absorptance (fractional absorption) of the transition.

As might be expected, those scenarios that have the largest emission rate will be the easiest to detect using infrared laser spectroscopy. These include diesel electric generator exhaust, SCUD missile fueling, burning ammunition, and burning sarin. The most abundant compound in many of the scenarios, carbon dioxide, cannot be observed because it is obscured by the large burden of that compound in the atmosphere. Other common compounds, such as carbon monoxide, can be observed only when their concentration-pathlength in the plume exceeds their atmospheric burden over the laser detection pathlength.

Recent experiments here at PNNL have shown that mixing of hot exhaust with the surrounding air rapidly thermalizes the plume to ambient temperature within a few meters of the vent. The possibility of detecting hot carbon dioxide in diesel exhaust using active remote sensing seems unlikely, unless the distance from the exhaust manifold is short, the gases are above 200°C, and detection is performed at the outlet of the vent.

There is the possibility, however, of using passive remote sensing to detect some of the more abundant diesel exhaust compounds. If the exhaust gases travel a fair distance through ducting underground before being released, the plume may come out colder than the surrounding air during the day; that is, the plume temperature may equilibrate to a ground temperature of 15°C and be released to warm (30°C) or hot (40°C) ambient air. Detecting the radiance contrast between the cold plume and the surrounding air with a broad pass-band sensor should be easy to see. Modeling this passive detection scenario is the subject of another report that is now being prepared.

Detection of the other diesel electric generator exhaust compounds listed in the table using infrared spectroscopy is feasible. The same is true of the nitric acid in the SCUD fueling scenario and perhaps the hydrogen fluoride as well (it is not clear at this point if the HF will volatilize or remain associated in the liquid state in the evaporating pool). The carbon monoxide, nitric oxide, hydrogen cyanide, and formaldehyde in a burning ammunition plume and the hydrogen fluoride in the burning sarin plume should also be easily detected; though again the time available for detecting these plumes will be short—less than one half hour. The burning sarin should leave copious quantities of phosphoric acid on the ground. This might be detectable by infrared reflectance spectroscopy.

Finally, it should be remembered that emission rates given for the scenarios in this report will have to be scaled and the plumes and spectra remodeled when any significant changes are made to the input paramters of the scenarios.

Table 1. Summary of Calculations Performed

Compound	Rate (g/s) or Evap. Amt. (kg)	Detect. Distance from Source (m)	Conc. Path. (ppm-m)	Lorentzian Linewidth FWHM (cm^{-1})	Gaussian Linewidth FWHM (cm^{-1})	Detection Freq. (cm^{-1})	Absorbance	Absorptance
Diesel Electric Generator Exhaust, one hour plume, 50°C spectral simulation temperature								
Carbon dioxide	600 g/s	112	99,800	0.14	0.005	–	–	–
Nitrogen dioxide	6	100	2400	0.14	0.005	2921.46	0.91	0.58
Carbon monoxide	3	100	900	0.08	0.006	2172.76	7.5	1.0
Sulfur dioxide	0.6	100	137	0.2	0.004	1139.66	0.03	0.03
Formaldehyde	0.06	100	11	0.2	0.006	2778.47	0.02	0.02
Acetaldehyde	0.02	100	2.5	–	–	1105.01	0.0006	0.0006
TEL Diesel Exhaust, one hour plume, 25°C spectral simulation temperature								
Carbon dioxide	75 g/s	100	1756	0.14	0.005	–	–	–
Nitrogen dioxide	0.8	100	7.6	0.14	0.005	2921.46	0.003	0.003
Carbon monoxide	0.3	100	5.3	0.08	0.006	2172.76	0.05	0.05
Sulfur dioxide	0.08	100	0.576	0.2	0.004	1139.66	0.0001	0.0001
Formaldehyde	0.008	100	0.39	0.2	0.006	2780.99	0.0008	0.0008
Acetaldehyde	0.003	100	0.251	–	–	1105.01	0.00006	0.00006
Diesel Fuel Storage Evaporation, one hour plume, 25°C spectral simulation temperature								
m-Xylene	0.003 g/s	50	0.2	–	–	767.95	0.0003	0.0003
Toluene	0.002	50	0.15	–	–	1031.91	0.00003	0.00003
Benzene	0.002	50	0.18	–	–	1037.77	0.00005	0.00005
SCUD Missile Fueling, ten-minute plume, 25°C spectral simulation temperature								
Nitric acid	35 kg	100	98	0.2	0.004	878.94	0.36	0.3
Hydrogen fluoride	0.4	100	240	0.1	0.007	4038.96	8.8	1.0
SCUD Missile Fueling, one-hour plume, 25°C spectral simulation temperature								
Nitric acid	35 kg	100	129	0.2	0.004	885.30	0.22	0.2
Hydrogen fluoride	0.4	100	83	0.1	0.007	4038.96	3.0	0.95

Compound	Rate (g/s) or Evap. Amt. (kg)	Detect. Distance from Source (m)	Conc. Path. (ppm-m)	Lorentzian Linewidth FWHM (cm^{-1})	Gaussian Linewidth FWHM (cm^{-1})	Detection Freq. (cm^{-1})	Absorbance	Absorptance
Burning Ammunition, ten-minute plume, 25°C spectral simulation temperature								
Carbon monoxide	23,000 kg	1000	33,700	0.08	0.006	2172.76	290.7	1.0
Nitric oxide	16,000	1000	17,800	0.1	0.006	1903.12	33.5	1.0
Carbon dioxide	11,000	1000	7734	0.14	0.005	–	–	–
Hydrogen cyanide	500	1000	129	0.2	0.006	735.61	0.20	0.18
Formaldehyde	300	3250	1163	0.2	0.006	2797.95	2.92	0.95
Burning Sarin, ten-minute plume, 25°C spectral simulation temperature								
Sarin	909 kg	500	313	–	–	–	–	–
Carbon dioxide	1141	3250	3408	0.14	0.005	–	–	–
Hydrogen fluoride	130	3250	1533	0.1	0.007	4038.96	56.1	1.0
Exhaled Human Breath, one-hour plume, 25°C spectral simulation temperature								
Carbon dioxide	2.25 g/s	50	127	0.14	0.005	–	–	–
Methane	0.0005	50	0.304	0.12	0.008	–	–	–
Carbon monoxide	0.0001	50	0.029	0.08	0.006	–	–	–
Ammonia	1×10^{-5}	50	0.007	0.16	0.007	1046.40	6×10^{-5}	6×10^{-5}
Acetone	5×10^{-6}	50	≅ 0.001	–	–	1365.48	1×10^{-6}	1×10^{-6}
Acetonitrile	2×10^{-6}	50	≅ 0.001	–	–	953.80	9×10^{-7}	9×10^{-7}
Isoprene	2×10^{-6}	50	≅ 0.001	–	–	893.78	2×10^{-6}	2×10^{-6}
Cook Stoves, one-hour plume, 25°C spectral simulation temperature								
Carbon dioxide	80 g/s	100	13,678	0.14	0.005	–	–	–
Carbon monoxide	0.7	100	207	0.08	0.006	2172.76	1.8	0.83
Formaldehyde	0.008	100	1.77	0.2	0.006	2781.00	0.004	0.004
Acetaldehyde	0.006	100	0.666	–	–	1105.01	0.0002	0.0002

Compound	Rate (g/s) or Evap. Amt. (kg)	Detect. Distance from Source (m)	Conc. Path. (ppm-m)	Lorentzian Linewidth FWHM (cm^{-1})	Gaussian Linewidth FWHM (cm^{-1})	Detection Freq. (cm^{-1})	Absorbance	Absorptance
Septic System, one-hour plume, 25°C spectral simulation temperature								
Carbon dioxide	0.2 g/s	100	46	0.14	0.005	–	–	–
Methane	0.1	100	47	0.12	0.008	–	–	–
Ammonia	0.05	100	23	0.16	0.007	992.69	0.084	0.081
Hydrogen sulfide	8×10^{-4}	100	0.309	0.16	0.005	2405.91	7×10^{-7}	7×10^{-7}
Landfill, one-hour plume, 25°C spectral simulation temperature								
Carbon dioxide	2 g/s	100	778	0.14	0.005	–	–	–
Methane	1	100	393	0.12	0.008	–	–	–
Hexane	0.01	100	0.787	–	–	2880.05	0.0009	0.0009

6.0 References

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Appendix A

Fuel Fire

Appendix A

Fuel Fire

Compound	Emission Factor (grams/gram of fuel burned)	Percent of Total Emission
Carbon Dioxide	2.6	63
Water	1.3	31
Carbon Monoxide	0.09	2.2
Smoke	0.13	3.1
PAHs	0.001	0.024
Hydrocarbons (C_2-C_{16})	0.004	0.097
Aldehydes/ketones (C_1-C_{16})	0.0035	0.085
Sulfur dioxide	0.0025	0.061
NOx	0.000012	2.9×10^{-4}

Relative inventory of compounds measured in the plumes of burning fuels from jet fuel to crude oil. Hydrocarbons include straight chain and branched alkanes, benzene, and substituted benzenes (*Am. Ind. Assoc. Hyg J.* 1997).

Appendix B

Human Effluents

Appendix B

Human Effluents

Input[a]		Effluents[a]	
Oxygen	840 kg	Carbon dioxide	1000 kg
Food solids	620	Resp. & persp. water	2280
Water in food	1150	Food prep latent water	36
Food prep water	760	Urine	1500
Drink	1620	Urine flush water	500
Metabolized water	350	Feces water	91
Hand/face wash water	4090	Sweat solids	18
Shower water	2730	Urine solids	59
Urinal flush	490	Feces solids	320
Clothes wash water	12,500	Hygiene water	12,580
Dish wash water	5450	Clothes wash water	12,500
Total	30,600 kg	Total	30,600

(a) *Designing for Human Presence in Space*, Chapter 2, http://augusta.msfc.nasa.gov/ed61/papers/rp1324/chap2.html .

Scenario: The values shown are for one-thousand people per day based on an average metabolic rate of 136.7 W/person/day and a respiration quotient of 0.87. The quotient is the molar ratio of CO_2 generated to O_2 consumed.

Appendix C

Machine Shop

Appendix C

Machine Shop

Compound	Source Term
Degreasing[a]	
Trichloroethane	10^{-2} (g/sec)
Welding[b,c]	
Iron	300 $\mu g/m^3$
Manganese	40 $\mu g/m^3$
Chromium (total)	60 $\mu g/m^3$
Nickel	10 $\mu g/m^3$
Nitrogen dioxide	100 ppb
Ozone	3 ppb
Carbon monoxide	5 ppm
Grinding[b]	
Iron	2000 $\mu g/m^3$
Manganese	50 $\mu g/m^3$
Chromium	1000 $\mu g/m^3$
Nickel	300 $\mu g/m^3$

(a) Berdowski, J. J. M., P. F. J. van der Most, and P. Verhoeve. 1996. "Metal Degreasing," SNAP Code 060201 in *Joint EMEP/CORINAIR Atmospheric Emission Inventory Guidebook*, G. McInnes, ed. EEA Copenhagen.

(b) Karlsen, J. T., T. Torgrimsen, and S. Langard. 1994. "Exposure to Solid Aerosols During Regular MMA Welding and Grinding Operations on Stainless Steel." *Am. Ind. Hyg. Assoc. J.* **55**:1149-1153.

(c) van der Wal, J. F. 1990. "Exposure of Welders to Fumes and Gases in Dutch Industries: Summary of Results." *Ann. Occup. Hyg.* **34**:45-54.

Degreasing scenario: Assumes ten open-top maintenance-degreasing units, room temperature, holding on the order of 10^2 liters.

Welding scenario: This scenario assumes a "large room without local exhaust ventilation" in which workers are performing manual metal arc welding of stainless steel. The literature on this subject does not give details on the number of workers or otherwise quantify the welding operations performed, which makes it difficult to determine an emission rate; however, the concentration values given, represent values averaged over several eight hour periods, so these values represent a static source term.

Grinding scenario: Assumes grinding on stainless steel. Again no values are given to quantify the activity except to say that it is a "large" shop.

Appendix D

Surface Background Concentrations of Common Atmospheric Gases in Parts per Billion

Appendix D

Surface Background Concentrations of Common Atmospheric Gases in Parts per Billion (ppb)[a]

Compound	Remote	Rural/Suburban	Urban/Industrial	Lifetime
Acetaldehyde	0.1 - 1	0.1 - 4	1 - 18	11 hours
Acetone	0 - 1	0.2 - 8	0.2 - 9	30 days
Ammonia	0.05	0.2 - 5		10 days
Benzene	0.008 - 0.2	0.1 - 0.6	0.9 - 26	10 days
1,3-butadiene	0.02 - 0.13	0.03 0.6	0.1 - 6	2 hours
Carbon Dioxide	350,000 surface global average			
Carbon Monoxide	50 - 150	1000	10,000	1 - 4 months
Formaldehyde	0.3 - 2	0.1 - 10	1 - 60	1.5 days
Isoprene		0.005 - 5.5	0.1 - 2	1.7 hours
Methane	1720 surface global average			10 years
Nitric Acid	0.03 - 0.3	0.14 - 0.6	25	
Nitric Oxide	0.002	0.2 - 1	200	
NOx	0.02	0.8 - 1	200	1 - 10 days
Ozone	30 - 40	80 - 150	500	
Pentane	0.007 - 0.19	0.07 - 0.4	0.7 - 67	
Sulfur Dioxide	0.01 - 0.05	1 - 20	300	10 days
1,1,1-trichloroethane	0.16 surface global average			5 years
m-xylene	0.002 - 0.008	0.02 - 0.12	0.3 - 30	7 hours

(a) Finlayson-Pitts, B. J., and J. N. Pitts. 2000. *Chemistry of the Upper and Lower Atmosphere*, Academic Press, San Francisco.

Appendix E

Nominal Detection Limits for FTIR Systems

Appendix E

Nominal Detection Limits for FTIR Systems (ppb)[a]

Species	300 Meter Open Path	100 Meter Cell*	Species	300 Meter Open Path	100 Meter Cell*
Acetaldehyde	20	30	Hydrocarbon Continuum	10	15
Acetic acid	5	7 SL	Hydrogen Chloride	2	4
Acetone	30	10	Hydrogen Cyanide	5	4
Acetonitrile	50	70	Hydrogen Sulfide	300	500
Acetylene	2	2	Isobutane	2	1
Acrolein	5	7	Isobutanol	4	6 SL
Acrylic acid	10	5 SL	Isobutyl Acetate	5	7
Acrylonitrile	6	10	Isobutylene	4	4
Ammonia	2	3 SL	Isoprene	4	5
Benzene	25	3**	Isopropanol	10	10 SL
1,3-Butadiene	2	3	Isopropyl Ether	10	5
Butane	HC		Methanol	4	6 SL
Butanol	15	20 SL	Methylamine	20	20 SL
1-Butene	10	15	Methyl Benzoate	20	30
cis-2-Butene	25	30	Methyl Chloride	60	80
Trans-2-Butene	10	15	Methylene Chloride	5	8
Butyl Acetate	5	7	Methyl Ether	10	15
Carbon Disulfide	dry only	50	Methyl Ethyl Ketone	40	60 SL
Carbon Monoxide	1	4	Methyl Isobutyl Ketone	15	25 SL
Carbon Tetrachloride	2	2	Methyl Mercaptan	40	60
Carbonyl Sulfide	2	3	Methyl Methacrylate	5	5
Chlorobenzene	10	10	2-Methyl Propene	2	4
Chloroethane	10	15	Morphaline	2	3
Chloroform	2	2	Nitric Acid	1	2
m-Cresol	20	15	Nitric Oxide	25	20
o-Cresol	4	8	Nitrogen Dioxide	50	50
p-Cresol	10	15	Nitrous Acid	5	7
Cyclohexane	3	5	Ozone	3	5
1,2-Dibromoethane	5	7	Pentane	HC	
m-Dichlorobenzene	3	5	Phosgene	1	2
o-Dichlorobenzene	3	5	Phosphine	2	3

Species	300 Meter Open Path	100 Meter Cell*		Species	300 Meter Open Path	100 Meter Cell*
p-Dichlorobenzene	2	3		Propane	10	10
1,1-Dichloroethane	10	10		Propanol	20	30 SL
1,2-Dichloroethane	30	40		Propionaldehyde	10	15
1,1-Dichloroehtylene	2	4		Propylene	4	10
Dimethylamine	20	30 SL		Propylene Dichloride	10	15
Dimethyl Disulfide	10	15		Propylene Oxide	10	15
1,4 Dimethyl Piperazine	3	5		Pyridine	20	20
1,4 Dioxane	2	3		Silane	1	1
Ethane	10	10		Styrene	1	2
Etanol	10	10 SL		Sulfur Dioxide	30	30
Ethyl Acetate	4	4		Sulfur Hexafluoride	<1	0.1
Ethylamine	20	10 SL		1,1,1,2-Tetrachloroethane	4	6
Ethylbenzene	20	30**		1,1,2,2-Tetrachloroethane	20	16
Ethylene	1	3		Tetrachloroethylene	2	2
Ethylene Oxide	10	15		Toluene	25	10**
Ethyl Mercaptan	50	70		1,1,1-Trichloroethane	4	10
Formaldehyde	5	8		1,1,2-Trichloroethane	10	15
Formic Acid	2	3 SL		Trichloroethylene	2	3
Furan	3	5		Trimethylamine	10	15 SL
Halocarb-11 (CCl3F)	1	1		1,2,4-Trimethylbenzene	5	7
Halocarb-12 (CCl2F2)	1	1		Vinyl Chloride	4	5
Halocarb-22 (CHClF2)	1	1		m-Xylene	10	10**
Halocarb-113 (CFCl2CF2Cl)	2	2		o-Xylene	20	5**
Hexafluoropropene	1	2		p-Xylene	20	10**

GM = A generalized method for this species only (and normal interferrents).
HC = This species would normally be calculated as part of the hydrocarbon continuum.
* = The cell measurements assume water drying.
** = These species (BETEX compounds) require CO2 scrubbing in addition to drying.
SL = These species suffer "slight loses" going through Permapure dryer.
(a) Table from a technical note by the Industrial Monitoring & Control Corp., Round Rock, Texas, (512) 341-8189, http://www.imacc-instruments.com/compound.html .