

USER'S MANUAL

for

USAF TOXIC CHEMICAL DISPERSION MODEL - AFTOX

VERSION 4.1

Mr Bruce Kunkel, PL/GPA  
Capt Cliff Dungey, HQ AWS/XTX

4 Jan 93

Table of Contents

1. Basic program information
2. File structure
  - 2.1 Ancillary files
  - 2.2 Data files
  - 2.3 Printer files
3. Setting up AFTOX
4. Running AFTOX
  - 4.1 General
  - 4.2 Printing and storing data
  - 4.3 Station data
  - 4.4 Date and time
  - 4.5 Type of release
  - 4.6 Chemical data
  - 4.7 Meteorological data
  - 4.8 Roughness length at spill site
  - 4.9 Source information
  - 4.10 Worst cast scenario
  - 4.11 Continuous buoyant plume release
  - 4.12 Concentration averaging time
  - 4.13 Elapsed time since start of spill
  - 4.14 Types of output
  - 4.15 Exposure limits
  - 4.16 Confidence limits
5. Special considerations

1. Basic program information

The USAF Toxic Chemical Dispersion Model (AFTOX) is a

dispersion model that will determine toxic chemical concentrations and give the user the option of calculating a toxic corridor (hazard distances), the concentration at a specific location, or the maximum concentration and its location. AFTOX will handle instantaneous or continuous, gas or liquid releases (non-buoyant) from either ground or elevated sources. The program contains an additional option for continuous, heated (buoyant) plumes from stacks. AFTOX Version 4.1 is designed to run on a Zenith Z-248 microcomputer and the Zenith Z-180 series laptop microcomputers, running the Microsoft MS-DOS(TM) 3 (or later) operating system. Version 4.1 may operate on other true IBM-PC compatibles using EGA or CGA video and MS-DOS(TM) 3, such as the Zenith Z-150 series. Version 4.1 will not run on the Zenith Z-100 microcomputers, which are not true IBM compatibles.

Use of AFTOX for Air Weather Service (AWS) units is governed by AFR 355-1.

## 2. File Structure

The AFTOX program contains five component program files, three printer files, and six data files. Of the data files, four are for input data and two for output. Three ancillary files are used for editing the data in three of the input data files. CHAIN statements are used to connect the various program files. A list of the files is shown in Table 1.

Table 1. List of files in AFTOX

---

PROGRAM FILES	
AFTOX.EXE	Introduction
DSP1.EXE	defines chemical properties and the meteorological conditions
DSP2.EXE	Defines source conditions (that is, emission rate, spill duration, and spill area)
DSPHP.EXE	Defines source conditions for buoyant plume from a stack
DSP3.EXE	Computes 1) the hazard area, 2) the maximum concentration, and 3) the concentration at a given point and time
DATA FILES	
SD.DAT	Station data

CH.DAT            Chemical name and data, and toxic limits  
EVAP.DAT        Chemical data for Vossler evaporation model  
AFT.DAT        File for storing all input and output data  
                 when printer is off  
CONCXY.DAT     File for storing x, y positions of  
                 concentration  
                 contour  
DEVICE.DAT     Contains information on computer and screen  
                 type

#### ANCILLARY FILES

SETUP.EXE       Establishes computer and screen type  
SDFIL.EXE       Edits station data file (SD.DAT)  
CHFIL.EXE       Edits chemical data file (CH.DAT)

#### PRINTER FILES

PSCMX80.COM    Configures system for EPSON-type printer  
PSCOI.COM      Configures system for OKIDATA-type printer  
PSCMPI.COM     Configures system for old Zenith printers

---

## 2.1 Ancillary files

### SETUP.EXE

Before running AFTOX for the first time, SETUP.EXE should be run to establish the type of computer and screen. When running SETUP.EXE, a screen as shown in Figure 1 will appear. Enter the appropriate code for the computer and monitor types. The appropriate information will be stored in DEVICE.DAT.

---

## A F T O X

### AIR FORCE TOXIC CHEMICAL DISPERSION MODEL

#### SET UP FOR GRAPHICS PROGRAM

Enter code for type of graphics card/monitor.

E = EGA/VGA    C = CGA      N = Other or no graphics ? E

Enter code for monitor type

C = COLOR    M = MONOCHROME    ? C

---

Figure 1. Screen display for SETUP routine.

SDFIL.EXE

The SDFIL.EXE file is used to set up the station data file, SD.DAT. SDFIL allows one to view, delete, add, and edit data in SD.DAT. The file may contain one or more stations.

To run SDFIL, type SDFIL and press <ENTER>. The computer will display a screen with several options as shown in Figure 2. Choose the appropriate option and proceed as instructed.

---

1--display or print station data  
2--set up new SD.DAT file  
3--edit data  
4--add station  
5--delete station  
6--quit

-----  
Choose one of the above

---

Figure 2. List of options in SDFIL.

The following is a list of data required for each station stored in SD.DAT.

Station name  
1-Metric 2-English Units  
Standard Deviation of Wind Direction (Y/N)  
Standard Deviation Averaging Time (min)  
Latitude (deg)  
Longitude (deg)  
Surface Roughness (cm)  
Height of Wind Measurement (m or ft)  
Time Difference (Greenwich-local standard)  
Station Elevation (m or ft)

Stations that are located reasonably close to each other (<50 km) do not have to be listed separately because the latitude, longitude, and elevation are not highly sensitive parameters.

However, if the stations have a different surface roughness or wind measurement height then they must be listed separately.

The units refer to the meteorological and distance parameters. The user will have the option of entering either metric or English units for the spill rate or quantity.

As a guide for inputting the proper surface roughness, a table, as shown below, is automatically displayed on the screen. The surface roughness need not be restricted to one of the values shown in Figure 3, but it is recommended that the value fall between 0.5 and 100 cm.

---

TERRAIN DESCRIPTION	SURFACE ROUGHNESS (cm)
SNOW, NO VEGETATION, MUD FLATS, NO OBSTACLES	0.5
RUNWAY, OPEN FLAT TERRAIN, GRASS, FEW ISOLATED OBSTACLES	3
LOW CROPS, OCCASIONAL LARGE OBSTACLES	10
HIGH CROPS, SCATTERED OBSTACLES	25
PARKLAND, BUSHES, NUMEROUS OBSTACLES	50
REGULAR LARGE OBSTACLE COVERAGE (SUBURB, FOREST)	100

---

Figure 3. Roughness length as a function of terrain type.

#### CHFIL.EXE

The CHFIL.EXE file is used to view, make changes, deletions or additions to the chemical data file, CH.DAT. The current CH.DAT file contains 130 chemicals. The chemicals are listed in alphabetical order.

To run CHFIL, type CHFIL and press <ENTER>. The computer will display a screen with several options as shown in Figure 4. Choose the appropriate option and proceed as instructed.

---

```
1--display or print data
2--edit exposure limits for specific chemical
3--edit data for specific chemical
4--add chemical
5--delete chemical
6--quit
-----
Choose one of the above
```

---

Figure 4. List of options in CHFIL.

In viewing the chemical data, several options exist: 1) data may be displayed on the screen or sent to the printer; 2) either the chemical numbers and names or all the chemical data may be displayed or printed; and 3) chemical data for a particular chemical or for all the chemicals may be displayed or printed.

The exposure limits are used only as a guide for the user. The user must input the exposure limits when running AFTOX, but may default to the STEL values. The base bioenvironmental engineers can assist if you have any questions.

When editing the chemical data under option 3, the user must re-enter all the data for a particular chemical, even though he may be changing only one value. The old data is displayed on the screen to make it easy for the user to re-enter the data. One word of caution--the names hydrazine, monomethylhydrazine (MMH), dimethylhydrazine (UDMH), and nitrogen tetroxide must be spelled correctly because the model must recognize the name, and not the number, in order for it to use the Vossler evaporation model.

The data for each chemical consist of the following:

- Chemical number
- Chemical name
- Time weighed average (TWA) exposure limits (ppm and mg/m<sup>3</sup>)
- Short term exposure limits (STEL) (ppm and mg/m<sup>3</sup>)
- Molecular weight
- Boiling temperature (K)
- Critical temperature (K)
- Critical pressure (atm)
- Critical volume (cm<sup>3</sup>/g-mole)
- Vapor pressure constants (3)
- Liquid density constants (2)
- Molecular diffusivity constants (2)

If the chemical is a gas at all expected ambient temperatures, then only information up through the boiling temperature is needed.

If the chemical is a liquid, vapor pressure information must be in the chemical file. The exception is for the four chemicals, hydrazine, monomethylhydrazine (MMH), dimethylhydrazine (UDMH), and nitrogen tetroxide, that use the Vossler evaporation model (1989). The chemical data required for the Vossler model, including the

vapor pressure data, are included in EVAP.DAT. All other chemicals use either the Shell's SPILLS evaporation model (Fleischer, 1980) or the Clewell model (1983).

The vapor pressure may be defined in one of three ways: 1) by the Antoine equation, in which case three constants are required, 2) by the Frost-Kalkwarf equation in which two constants are required, or 3) by directly inputting the vapor pressure in atm. The model determines which method to use by the number of constants in the file. To use the Frost-Kalkwarf equation, the critical temperature and critical pressure must be known.

The liquid density is required for all chemicals in the liquid state, including those using the Vossler evaporation model. The liquid density is defined in one of two ways: 1) by the Guggenheim equation, in which case two constants are required, or 2) by directly inputting the liquid density in g/cm<sup>3</sup>. As with the vapor pressure, the model determines which method of defining the liquid density by the number of constants. The Guggenheim equation requires both the critical temperature and critical volume. If no density is entered, the model will assume a density of 1 g/cm<sup>3</sup>.

The molecular diffusivity constants are the effective diameter of the molecule, (A), and the energy of molecular interaction, (J). The diffusivity is required for the Shell evaporation model. If either of these two constants is not available, the model defaults to the Clewell evaporation model.

## 2.2 Data files

There are six data files, three of which have been discussed in Section 2.1. The remaining three are EVAP.DAT, CONCXY.DAT, and AFT.DAT. The latter will be described in Section 4.2.

### EVAP.DAT

EVAP.DAT is the chemical data file for the Vossler evaporation model. The chemicals listed in this file are hydrazine, monomethylhydrazine (MMH), dimethylhydrazine (UDMH), and nitrogen tetroxide. The chemical data include the following:

- Molecular weight
- Boiling temperature
- Freezing temperature
- Molecular diffusion volume

Constants and applicable temperature ranges for:

- Vapor viscosity
- Vapor heat capacity
- Vapor thermal conductivity
- Heat of vaporization
- Saturation vapor pressure
- Liquid thermal conductivity

Data may be changed using an edit program. However, if a new chemical is added to the file, the code in DSP2.BAS must be changed so that the new chemical will be recognized.

#### CONCXY.DAT

CONCXY.DAT is an output data file containing information on the X, Y coordinates of up to three requested concentrations. Data stored in the file include the concentration of interest, either mg/m<sup>3</sup> or ppm, the time since release for an instantaneous or finite continuous release, and the contour half width for various distances downwind in either m or ft. The half width has 20 m resolution. The actual half width will be within 20 m but always less than the calculated.

### 2.3 Printer files

Three print files accompany the AFTOX program. They are used to configure your computer to your printer so you can make a hardcopy of the graphics output from AFTOX. Most of the newer computers can use the GRAPHICS.COM file in your DOS directory, but if this doesn't work, try one of these:

- PSCMX80.COM for printers that emulate EPSON printers
- PSCOKI.COM for printers that emulate OKIDATA printers
- PSCMPI.COM for older Zenith printers (most are obsolete).

All you have to do is place the proper command somewhere in your AUTOEXEC.BAT file and the configuration is done automatically everytime you turn on your computer.

### 3. Setting up AFTOX

AFTOX may be run directly from the diskette, but if your computer has a hard disk it is recommended that the program be transferred to the hard disk. Create a directory on your hard disk where you would like the program to reside (e.g., C:>MD AFTOX4). Then copy the files from the diskette to the hard disk (e.g., A:>COPY \*.\* C:>AFTOX4).



To tailor the program to your particular computer, run SETUP.EXE. Specify whether your machine is VGA/EGA, CGA, or no graphics. If your machine has Hercules graphics, you will have to choose no graphics. Also, specify whether your monitor is color or monochrome. Once SETUP has been run, there will be no need to run it again unless you transfer the program to a different type of computer.

Information on your location must be stored in the station data file, SD.DAT, by running SDFIL.EXE. Once you input the station data into SD.DAT, there will be no need to run SDFIL.EXE again unless you change your location.

You are now ready to run AFTOX.

## 4. Running AFTOX

### 4.1 General

AFTOX is a very user friendly program. Simply proceed through the program, answering the questions as you go along. Default values are frequently given <in brackets>. If you wish to go with the default value, simply press <ENTER>. The program has the unique feature of being able to back up by entering <999> <ENTER>, thus eliminating the need to start over if you accidentally entered the wrong data. The exception is that you can not back up into the previous file (e.g., you can not back up from DSP2 into DSP1).

### 4.2 Printing and storing data

Type AFTOX at the DOS prompt and press <ENTER>. This will start the program execution. If you are using a printer, and wish the plume plot to be sent to the printer, you must load the appropriate PSC utility program before you start AFTOX. If you haven't, the program will remind you, and you will have to start over. If the printer is off, then the input and output data are stored in AFT.DAT for viewing or printing out at a later time. Each time AFTOX is run, the data in AFT.DAT is erased. If you wish to save the data in AFT.DAT, the file can be saved by renaming the file (e.g., C:>AFTOX4:ren aft.dat spill#1.dat).

### 4.3 Station data

If there is more than one station in the station data file

(SD.DAT), you will be asked to enter the appropriate station. The data stored in SD.DAT has been discussed in Section 2.1.

#### 4.4 Date and time

The computer date and time are displayed. If the spill is for a different date or time, a new date and time may be entered. The program converts the date to a Julian date which it uses in conjunction with the time, latitude and longitude to determine the solar elevation, and subsequently, the solar insolation and surface heat flux.

#### 4.5 Type of release

AFTOX handles five types of releases:

- Continuous gas
- Continuous liquid
- Instantaneous gas
- Instantaneous liquid
- Continuous buoyant stack

The user has a choice of a continuous, instantaneous, or buoyant release. An instantaneous release is defined as occurring over a 15 sec period. A continuous release is any release occurring over a period greater than 15 sec. For the continuous and instantaneous releases, the model determines whether it is a gas or liquid, based on whether the air temperature is above or below the boiling point of the chemical.

#### 4.6 Chemical data

A list of 130 chemicals is displayed on the screen. This list is shown in Appendix A. The user enters the appropriate number. If the chemical of interest is not listed, the user may press <ENTER> at the end of the list of chemicals. He will then be asked the name of the chemical and its molecular weight. If the molecular weight is entered, the model asks for the vapor pressure in mm Hg. If the vapor pressure is known, the model uses Clewell's formula for determining the evaporation rate. If either the molecular weight or vapor pressure is not known, the model assumes the worst case; that is, the evaporation rate is equal to the spill rate. Also, if the molecular weight is not entered, the concentrations must be in mg/m<sup>3</sup> since conversion to ppm is not possible without knowing the molecular weight.

For a buoyant plume release, the model bypasses the chemical list and data file and asks only for the molecular weight. Again, if the molecular weight is not known, concentrations must be in mg/m<sup>3</sup>.

#### 4.7 Meteorological data

The meteorological data consist of the following:

- Air temperature
- Wind direction
- Wind speed
- Standard deviation of wind direction and time over which it is determined (optional)
- Cloud amount
- Predominant cloud category
- Ground condition - dry, wet, snow covered (daytime only)
- Inversion base height

The air temperature is a necessary input parameter but does not have a large influence on the results. If a temperature reading is not available, a reasonable guess would be sufficient.

Calm winds are not allowed. If a zero wind speed is entered, the model will adjust the speed to either 0.5 m/sec or 1 kt, depending on which units the user chooses. The model converts the wind speed measurement, whose height is specified in the station file SD.DAT, to a 10-m height wind speed. The 10-m wind speed is used in all of the calculations, and therefore the user should be aware that the plume may move downwind at a faster rate than the measured wind speed would indicate.

If the standard deviation of wind direction is normally available, it is so indicated in SD.DAT along with the time over which it is determined. If the standard deviation is not available at the time that the model is being run, simply press <ENTER> and the model will default to using the wind speed and solar conditions for computing stability and the corridor width.

The cloud amount is entered in eighths. There are three cloud categories to choose from - high, middle, and low. If there are two cloud layers present, the operators should use the layer with the larger cloud amount. If there are two layers with equal cloud amount, the operator should choose the lower cloud layer. The cloud type is not a factor at night.

There are three ground types to choose from - wet, dry, snow covered. If in doubt as to whether the ground is wet or dry, the user should choose wet, which will result in a more conservative hazard distance. If the air temperature is 20C (68F) or greater, the model assumes no snow cover.

If the base of an inversion is below 500 m (2000 ft), the height of its base is entered. Inversion heights greater than 500 m (2000 ft) may be entered but will have no effect on the plume. If the base of the inversion is below 50 m (164 ft), the model assumes no inversion but does assume a stability parameter of 6. When there is an inversion, the model assumes that the pollutants are trapped below its base. In the rare case that the release is above the inversion, the pollutants remain above the inversion.

#### 4.8 Roughness length at spill site

For a non-buoyant release, the surface roughness length at the spill site must be entered. For a buoyant plume, it is assumed that the elevated plume is minimally affected by the surface roughness, which is set at 3 cm. The user has the option to call up the table of roughness lengths (Figure 3) for different types of terrain. When uncertain as to the appropriate roughness length for the spill site, the user should choose a lower value, which will produce longer hazard distances. Input roughness lengths below 0.5 cm or greater than 100 cm are set at 0.5 or 100 cm, respectively.

#### 4.9 Source information

The source information required varies depending on the type of spill - continuous, instantaneous, gas, or liquid.

##### Continuous Gas Release

For a continuous gas release, the following information is required:

Height of leak above ground (m, ft)  
Emission rate through rupture (kg/min, lb/min)  
Total time of release (min)

The emission rate is assumed constant for the total time of the spill. If the duration of the release is finite then the total amount released is displayed.

### Continuous liquid release

For a continuous liquid release, the following information is required:

Spill rate through rupture (kg/min, m<sup>3</sup>/min,  
lb/min, gal/min)  
Total time of spill (min)  
Spill area (m<sup>2</sup>, ft<sup>2</sup>) - otherwise default value is used  
Pool temperature - for those chemicals using the Clewell  
evaporation model (default = air temperature)

The height of the leak is not entered since it is assumed that the liquid spills to the ground. The default spill area is based on the volume spilled and the assumption of a 1-cm deep pool. For an ongoing continuous spill, the volume spilled is based on a 10-min spill. The default spill area is displayed but if the user has information on the size of the spill area, he may over-ride the default value. Based on the input data and the chemical properties, the model computes the evaporation (emission) rate into the atmosphere and the total evaporation (release) time for a finite continuous release.

### Instantaneous gas release

For an instantaneous gas release, the following information is required:

Release height (m, ft)  
Amount released (kg, lb)

The model assumes a cylindrical volume source in which the height is equal to the radius. The initial volume of the spill is a function of the amount released.

### Instantaneous liquid release

For an instantaneous liquid release, the following information is required:

Amount spilled (kg, m<sup>3</sup>, lb, gal)  
Spill area (m<sup>2</sup>, ft<sup>2</sup>) - otherwise default value is used  
Pool temperature - for those chemicals using the Clewell  
evaporation model (default = air temperature)

The default spill area is based on the volume spilled and the

assumption of a 1-cm deep pool. Based on the input data and the chemical properties, the model computes the emission rate into the atmosphere and the total time of release.

#### 4.10 Worst case scenario

When the initial spill alert is sounded, quite often very little source information is available. In this case, AFTOX 4.1 has the option of computing a worst case scenario. The toxic corridor length calculation is based on Air Force Regulation 355-1/AWSSUP1, Attachment 1, dated 24 September 1990.

This regulation states that the corridor length is equal to the current wind speed in knots x 6,000. This represents the distance in feet that the plume will travel in one hour.

The corridor width is a function of the wind speed, or standard deviation of wind direction if available. The computation of the width is based on the magnitude of the wind speed. The exception is that there is no width adjustment for the duration of the spill since the duration may be unknown.

Having computed the worst case scenario, the user can then proceed and enter the source information when it becomes available without re-entering the meteorological information. However, if you need to change the name of the chemical or the source type (continuous, instantaneous), then you must start over.

#### 4.11 Continuous buoyant plume release

For a continuous buoyant plume release from a stack, the following information is required:

- Molecular weight (if available)
- Emission rate (kg/min or lbs/min)
- Elapsed time of emissions (min)
- Stack height (m or ft)
- Gas stack temperature (C or F)
- Volume flow rate (m<sup>3</sup>/min or ft<sup>3</sup>/min)

With these data, the model calculates the equilibrium plume height and the downwind distance at which the plume reaches the equilibrium height. If the equilibrium plume height is higher than the inversion, the plume height is adjusted down to the inversion height. If the stack height is higher than the inversion the program terminates because the input meteorological

conditions most likely do not apply above the inversion. If molecular weight is not available, concentrations will be in mg/m<sup>3</sup>.

#### 4.12 Concentration averaging time

The user must specify the concentration averaging time. For continuous releases, the default value is 15 min, which corresponds to the short term exposure limit (STEL) which is defined as a 15 minute time-weighted average exposure. For releases of less than 15 min duration, the default averaging time is equal to the release time. For instantaneous gas releases, the averaging time is 1 min. The user can not enter averaging times less than 1 min. Also, the averaging time cannot be greater than the release time since changes in the concentrations during the averaging period are not taken into account. The averaging time affects the dispersion coefficients such that the longer the averaging time the greater the dispersion coefficients, thus resulting in shorter and wider plumes. The averaging time and dispersion coefficients are related by the 1/5 power law.

#### 4.13 Elapsed time since start of spill

For instantaneous and finite continuous releases, the user must specify the elapsed time since the start of the spill. For an ongoing continuous release, the model defaults to a sufficiently large elapsed time to assure a steady state condition (maximum hazard distance). For an instantaneous liquid release or a finite continuous release, the default elapsed time is equal to the release time. Except for short duration spills (a few minutes), the default time would normally give the greatest hazard distance. For instantaneous gas releases, the default elapsed time is arbitrarily set at 10 min. For small releases, the plume may dispersed within 10 min, in which case the user may wish to enter a shorter elapsed time.

#### 4.14 Types of output

The user can specify one of three types of output.

1. Toxic corridor plot
2. Concentration at specified location and time
3. Maximum concentration at given height and time

The one exception is when the no graphics option is chosen in SETUP, the corridor plot is replaced with a printout of the hazard

distance for a given concentration(s).

#### Toxic corridor plot

If the user chooses not to use the default concentration, he may specify up to three contours in any order. The concentrations can be specified in either mg/m<sup>3</sup> or ppm. The exception is if the molecular weight is not known, then the concentration is in mg/m<sup>3</sup>. The default concentration is the short term exposure limit (STEL) in ppm, if available, otherwise the time weighted average (TWA) exposure limit. If neither is available then the user must enter one or more concentrations. The user must also input the height of interest or choose the default height of 2 m (6 ft).

AFTOX computes the Y position of the concentration of interest for increasing values of X. X varies in increments of 100 to 400 m depending how rapidly Y is varying in the X direction. For slowly varying Y, X increments approach 400 m. The model starts the Y computation at 100 m from the source. However, if the centerline concentration at 100 m is less than the specified concentration of interest, calculations start at 10 m and progress outward in 10 m increments. Plumes < 10 m in length will not be plotted. The model first computes the concentration at the centerline and then moves outward in the Y direction in 20 m increments when X>100 m, and 2 m increments when X<100 m. The point at which the computed concentration is less than the concentration of interest defines the Y position. The X, Y positions are stored in CONCX.Y.DAT.

The model first computes the appropriate scale by calculating centerline concentrations for the specified time and height. The concentration contours are then plotted on the screen as computations are taking place. The contours are plotted in order of increasing concentrations no matter in what order they are entered. These contours represent average distances, which means that 50 percent of the time the actual distance may be greater than shown and 50 percent of the time may be less than shown. The 90 percent hazard area for the lowest concentration is outlined on the contour plot and represents the area within which the plume is confined 90 percent of the time. This 90 percent area represents the toxic corridor.

The plume plot represents the position and size of a plume at the specified time after the start of the release. Depending on the time after release, this may not be the maximum distance that the plume will extend downwind, especially if it is an



instantaneous release. The 90 percent hazard area, however, represents the area at the time when the plume reaches its maximum distance downwind. It may or may not be at the specified time after release. For more discussion on the confidence limits, the reader should refer to Section 3.3.15 in Kunkel (1991).

Once the contour plot is completed, the user may proceed to make any of the changes listed below, obtain a printer plot, run another case, or terminate the program.

1. time and meteorological conditions
2. source conditions
3. concentration averaging time
4. elapsed time since start of spill
5. concentration contours
6. height of interest
7. scale
8. option
9. no change

#### Concentration at a specified location and time

If this option is chosen, the user must enter the downwind and crosswind distances, the height, and the time after start of the release. The model then computes the concentration for that particular point and time. The user may then change the location and/or time, choose another option, run another case, or terminate the program.

#### Maximum concentration at a specified height and time

This option will give the user the maximum concentration and its location for a specified height and time. The user enters the height of interest and the time from start of release. If it is a continuous spill that is still taking place and the specified height is the release height, the maximum concentration will be at the source. In this case, AFTOX computes the concentration at 30 m from the source. If the specified height is different than the release height, or if the time after start of release is greater than the duration of the release, the maximum concentration will most likely occur at a distance greater than 30 m from the source. The location of the maximum concentration is determined within an accuracy of +/-5 m along the X axis, and of course would be located on the centerline of the plume at the specified height. When completed, the user may change the height and/or time, choose another option, run another case, or terminate the program.

#### 4.15 Exposure concentrations

If exposure concentrations have been established for the chemical of interest, AFTOX lets the user choose from two default concentrations. In general, they represent a short- (15 min) and long-term (8 hours) exposure limit.

In some instances, several government organizations have established or recommended exposure limits for particular chemicals. When available, AFTOX uses evacuation concentrations which are intended for the general public rather than employees in an occupational environment. Evacuation concentrations are generally higher than occupational concentrations. This is one reason AFTOX forecasts longer toxic corridors than other toxic dispersion programs.

If your unit is responsible for calculating toxic corridors at your base, your operating instructions should include contacting the bioenvironmental engineers. You know the weather observation and the forecast, but they know the chemicals. They should be in the loop, especially when the chemical is not contained in the AFTOX chemical list.

#### 4.16 Confidence limits

The model predicts the mean hazard distance. However, operationally, one would like to be at least 90 percent confident that the actual hazard distance will not exceed the predicted distance. The model's concentration contour plot also shows the 90 percent confidence level hazard area, or toxic corridor. The evaluation study described in Kunkel (1988) concluded that the predicted hazard distance must be multiplied by 2.1 to be 90 percent certain that the actual will not exceed the predicted distance. Earlier versions of AFTOX showed the 90 percent hazard area only for continuous releases. In AFTOX 4.1, the 90 percent hazard area is shown for all spills even though the 2.1 factor was derived from continuous release data. It should be pointed out that in deriving the 90 percent hazard area, it is assumed that the input data is correct. Errors in the input data, such as the wind speed and source strength will enlarge this area. Zettlemoyer (1990) examined the effect that data input uncertainties have on the concentration uncertainties using a Monte Carlo simulation technique. He look at wind speed, emission rate, spill height, and the horizontal and vertical dispersion coefficients. He concluded that errors in the wind speed had

greater effect on the concentration uncertainty than the other parameters. The greatest uncertainties occurred within one kilometer of the source.

The method used to determine the width of the hazard area for the 90 percent confidence level remains similar to the method used by the Air Weather Service (see Kahler, et al., 1980). If the measured wind is less than 1.8 m/sec, (<3.5 kt), the hazard area is a circle of radius equal to 2.1 times the predicted hazard distance. If the standard deviation of wind direction (SD) is known and the wind speed is greater than 1.8 m/sec, then the toxic corridor width (W) is equal to:

$$W = 6 SD$$

The measured SD is adjusted by the one-fifth power law to the time duration of the spill, up to a maximum of one hour. If the width is calculated to be less than 30 degrees, it is set at 30 degrees.

If SD is not known, then the following rules apply:

1) For neutral or stable conditions, that is, a stability parameter of 3.5 or greater, the width is equal to 90 degrees for measured winds of 1.8 to 5.15 m/sec (3.5 to 10 kt). For winds greater than 5.15 m/sec (10 kt), the width is equal to 45 degrees.

2) For unstable conditions, the width is a function of the stability parameter (STB) as shown in the following equation.

$$W = 165 - 30 STB$$

The width will vary from 60 degrees for neutral conditions to 150 degrees for very unstable conditions.

## 5. Special Considerations

a. Time input must be in local standard time (LST). If local time changes to Daylight Savings Time, then time input should remain in LST.

b. Calm winds are not allowed because of the mathematics of the program. If a zero wind speed is entered, the model assumes 1 knot (0.5 m/s).

c. If the user is uncertain about roughness length, the user

should choose a lower number, which gives a more conservative answer (i.e., larger corridors and higher concentrations).

d. If two or more cloud layers are present, user should use the layer with the largest cloud amount. If layers are equal amounts, use the lowest layer.

e. If the user is unsure whether the ground is wet or dry, the user should use wet. Choosing the wet option will give a more conservative answer.

f. If chemical molecular weight or vapor pressure is not known, the model sets the evaporation rate equal to spill rate. This is a worst case scenario.

g. If molecular weight is not known, concentration contours must be in  $\text{mg m}^{-3}$ .

h. Concentration averaging time must be greater than or equal to 1 minute, but less than 60 minutes, and less than the release time.

i. When computing concentration at a specified location, downwind distance must be greater than or equal to 30 m (approximately 100 ft).

j. If stack height is above inversion height, then program terminates because surface input conditions most likely do not apply above the inversion.

## REFERENCES

Clewell, H.J. (1983) A Simple Formula for Estimating Source Strengths from Spills of Toxic Liquids, ESL-TR-83-03.

Fleischer, M.T. (1980) SPILLS - An Evaporation/Air Dispersion Model for Chemical Spills on Land, Shell Development Company, PB 83109470.

Kahler, J.P., Curry, R.G., and Kandler, R.A. (1980) Calculating Toxic Corridors, AWS/TR-80/003, ADA101267.

Kunkel B.A. (1988) User's Guide for the Air Force Toxic Chemical Dispersion Model (AFTOX), AFGL-TR-88-0009, ADA199096.

Kunkel B.A. (1991) AFTOX 4.0 - The Air Force Toxic Chemical Dispersion Model - A User's Guide, PL-TR-91-2119.

Vossler, T.L. (1989) Comparison of Steady State Evaporation Models for Toxic Chemical Spills: Development of a New Evaporation Model, GL-TR-89-0319, ADA221752.

Zettlemoyer, M.D. (1990) An Attempt to Estimate Measurement Uncertainty in the Air Force Toxic Chemical Dispersion (AFTOX) Model, Master of Science Thesis, The Florida State University.

#### Appendix A

- |                                     |                                       |
|-------------------------------------|---------------------------------------|
| 1. ACETALDEHYDE                     | 67. FORMALDEHYDE (56%)                |
| 2. ACETONE                          | 68. FREON 12                          |
| 3. ACETONITRILE                     | 69. HYDRAZINE                         |
| 4. ACROLEIN                         | 70. HYDRAZINE (54%)                   |
| 5. ACRYLIC ACID                     | 71. HYDRAZINE (70%)                   |
| 6. AEROZINE-50                      | 72. MONOMETHYLHYDRAZINE (MMH)         |
| 7. ALLYL ALCOHOL                    | 73. DIMETHYLHYDRAZINE (UDMH)          |
| 8. ALLYL CHLORIDE                   | 74. HYDROGEN CHLORIDE                 |
| 9. AMMONIA                          | 75. HYDROGEN CYANIDE                  |
| 10. AMMONIA (29%)                   | 76. HYDROGEN FLUORIDE                 |
| 11. ANILINE                         | 77. HYDROGEN SULFIDE                  |
| 12. BENZENE                         | 78. ISOAMYLENE (2-METHYL-2-BUTENE)    |
| 13. BENZYL CHLORIDE                 | 79. ISOBUTANE (2-METHYLPROPANE)       |
| 14. BROMINE PENTAFLUORIDE           | 80. ISOBUTYRALDEHYDE                  |
| 15. BROMOFORM                       | 81. ISOPRENE (2-METHYL-1,3-BUTADIENE) |
| 16. BROMOMETHANE                    | 82. ISOPROPANOL (2-PROPANOL)          |
| 17. BUTADIENE (1,3)                 | 83. ISOPROPYL ETHER                   |
| 18. BUTANE                          | 84. JP-4                              |
| 19. BUTYL ALCOHOL (n)               | 85. JP-9                              |
| 20. BUTYL ALCOHOL (sec) (BUTANOL-2) | 86. JP-10                             |
| 21. BUTYL ALCOHOL (t)               | 87. MESITYL OXIDE                     |
| 22. BUTYLENE                        | 88. METHANE                           |
| 23. BUTYRALDEHYDE                   | 89. METHANOL                          |
| 24. CARBON DISULFIDE                | 90. METHYLENE CHLORIDE                |
| 25. CARBON MONOXIDE                 | 91. METHYL ETHYL KETONE               |
| 26. CARBON TETRACHLORIDE            | 92. METHYL IODIDE                     |
| 27. CHLORINE                        | 93. METHYL ISOBUTYL KETONE            |
| 28. CHLORINE PENTAFLUORIDE          | 94. METHYL METHACRYLATE               |
| 29. CHLORINE TRIFLUORIDE            | 95. NITRIC ACID (PURE)                |
| 30. CHLOROENZENE                    |                                       |
| 31. CHLOROETHANE                    |                                       |

- |                                       |                                     |
|---------------------------------------|-------------------------------------|
| 32. CHLOROFORM                        | 96. FUMING NITRIC ACID<br>(IRFNA)   |
| 33. CHLOROMETHANE                     | 97. NITROBENZENE                    |
| 34. CRESOL (-o)                       | 98. NITROGEN DIOXIDE                |
| 35. CRESOL (-m)                       | 99. NITROGEN TETROXIDE              |
| 36. CRESOL (-p)                       | 100. NITROGEN TRIFLUORIDE           |
| 37. CUMENE (ISOPROPYL BENZENE)        | 101. NITROPROPANE                   |
| 38. CYCLOHEXANE                       | 102. OXYGEN DIFLUORIDE              |
| 39. DIALLYL AMINE                     | 103. PERCHLORYL FLUORIDE            |
| 40. DIBUTYL PHTHALATE                 | 104. PENTABORANE                    |
| 41. DICHLOROBENZENE (1 2) (-o)        | 105. PERCHLORYL FLUORIDE            |
| 42. DICHLOROBENZENE (1 3) (-m)        | 106. PHENOL                         |
| 43. DICHLOROBENZENE (1 4) (-p)        | 107. PHOSGENE                       |
| 44. DICHLORODIMETHYLSILANE            | 108. PROPANE                        |
| 45. DICHLOROETHYLENE (1 2)<br>(cip)   | 109. PROPIONALDEHYDE                |
| 46. DICHLOROETHYLENE (1 2)<br>(trans) | 110. PROPYLENE                      |
| 47. DICHLOROPROPANE (1 2)             | 111. PROPYLENE OXIDE                |
| 48. DIETHANOL AMINE                   | 112. PYRIDINE                       |
| 49. DIMETHYLANILINE (n n)             | 113. STYRENE                        |
| 50. DIMETHYL PHTHALATE                | 114. SULFUR DIOXIDE                 |
| 51. DIOXANE (1 4)                     | 115. TETRACHLOROETHANE<br>(1 1 2 2) |
| 52. DI-t-BUTYLETHYL DIAMINE           | 116. TETRACHLOROETHYLENE            |
| 53. EPICHLOROHYDRIN                   | 117. TITANIUM TETRACHLORIDE         |
| 54. ETHANOL                           | 118. TOLUENE                        |
| 55. ETHYL ACRYLATE                    | 119. TOLUIDINE (-o)                 |
| 56. ETHYL BENZENE                     | 120. TRICHLOROETHANE (1 1 1)        |
| 57. ETHYL CHLORIDE                    | 121. TRICHLOROETHANE (1 1 2)        |
| 58. ETHYL HEXANOL (2)                 | 122. TRICHLOROETHYLENE              |
| 59. ETHYLENE                          | 123. TRICHLOROTRIFLUOROETHANE       |
| 60. ETHYLENE DIBROMIDE                | 124. TRIMETHYLBENZENE (1 3 5)       |
| 61. ETHYLENE DICHLORIDE               | 125. VINYL ACETATE                  |
| 62. ETHYLENE GLYCOL                   | 126. VINYL CHLORIDE                 |
| 63. ETHYLENE OXIDE                    | 127. VINYLIDENE CHLORIDE            |
| 64. FLUORINE                          | 128. XYLENE (-o)                    |
| 65. FORMALDEHYDE (PURE)               | 129. XYLENE (-m)                    |
| 66. FORMALDEHYDE (37%)                | 130. XYLENE (-p)                    |