

Environmental Research Papers, No.1083

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| REPORT DOCUMENTATION PAGE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                             |                                                            | Form Approved<br>OMB No. 0704-0188                                            |                                                                        |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------|------------------------------------------------------------|-------------------------------------------------------------------------------|------------------------------------------------------------------------|
| Public reporting for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.                                                                                                                                                                                                                                                                        |                                                             |                                                            |                                                                               |                                                                        |
| 1. AGENCY USE ONLY (Leave blank)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                             | 2. REPORT DATE<br>8 May 1991                               |                                                                               | 3. REPORT TYPE AND DATES COVERED<br>Scientific Interim Apr 89 - Apr 91 |
| 4. TITLE AND SUBTITLE<br>AFTOX 4.0 - The Air Force Toxic Chemical Dispersion Model - A User's Guide                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                             |                                                            | 5. FUNDING NUMBERS<br>PE - 62101F<br>PR - 6670<br>TA - 14<br>WU - 09          |                                                                        |
| 6. AUTHOR(S)<br>Bruce A. Kunkel                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                             |                                                            |                                                                               |                                                                        |
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)<br>Phillips Laboratory (LYA)<br>Hanscom AFB<br>Massachusetts 01731-5000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                             |                                                            | 8. PERFORMING ORGANIZATION<br>REPORT NUMBER<br>PL-TR-91-2119<br>ERP, No. 1083 |                                                                        |
| 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                             |                                                            | 10. SPONSORING/MONITORING<br>AGENCY REPORT NUMBER                             |                                                                        |
| 11. SUPPLEMENTARY NOTES                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                             |                                                            |                                                                               |                                                                        |
| 12a. DISTRIBUTION/AVAILABILITY STATEMENT<br>Approved for Public Release; Distribution Unlimited                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                             |                                                            | 12b. DISTRIBUTION CODE                                                        |                                                                        |
| 13. ABSTRACT (Maximum 200 words)<br>The accidental release of toxic chemicals into the atmosphere is an ongoing concern, not only for the Air Force, but for any group working with hazardous materials. To evaluate the extent of the hazard area resulting from the atmospheric dispersion of the toxic vapors, the computer model AFTOX, was developed and approved for use by the Air Weather Service in 1988. AFTOX is a Gaussian puff dispersion model for uniform terrain and wind conditions. It will handle continuous or instantaneous releases, liquid or gas, elevated or surface releases from a point or area source. AFTOX 4.0 represents an upgraded version based on comments from the users after operating the model for two years in the field. The changes make the program more user-friendly and improve it technically. This report includes a complete technical description and instructions on the use of the model. Example runs are provided in the Appendix. |                                                             |                                                            |                                                                               |                                                                        |
| 14. SUBJECT TERMS<br>Toxic chemical, Chemical hazard, Atmospheric dispersion, Dispersion                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                             |                                                            | 15. NUMBER OF PAGES<br>62                                                     |                                                                        |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                             |                                                            | 16. PRICE CODE                                                                |                                                                        |
| 17. SECURITY CLASSIFICATION<br>OF REPORT<br>UNCLASSIFIED                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 18. SECURITY CLASSIFICATION<br>OF THIS PAGE<br>UNCLASSIFIED | 19. SECURITY CLASSIFICATION<br>OF ABSTRACT<br>UNCLASSIFIED | 20. LIMITATION OF ABSTRACT<br>SAR                                             |                                                                        |

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| Accession For |                                           |
| NTIS          | CRA&I <input checked="" type="checkbox"/> |
| DTIC          | FA8 <input type="checkbox"/>              |
| Unpublished   | <input type="checkbox"/>                  |
| Justification |                                           |
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# **AFTOX 4.0 - The Air Force Toxic Chemical Dispersion Model - A User's Guide**

## **1. INTRODUCTION**

The AFTOX model is an interactive Gaussian puff/plume dispersion model designed to run on a desk top computer. The program, written in GW-BASIC language, is user-oriented and written in a conversational mode to allow its operation with only a minimum knowledge of the computer or the model. The model is designed to handle continuous and instantaneous, liquid and gas, surface and elevated releases from a point or area source. The model will 1) plot concentration contours and toxic corridor, 2) compute concentration at a specified point and time, and 3) compute maximum concentration at a given elevation and time. It contains a library of 129 chemicals but may be run for other chemicals as well. The model also predicts the dispersion of a continuous buoyant plume from a stack.

The model has many unique features, including the computation of a continuous stability parameter, the inclusion of the concentration averaging time and surface roughness, the ability to print now or save/print later, the ability to correct input data without restarting, easy access to the chemical data file for adding, deleting and changing data, and a plot of the plume and 90 percent hazard area with automatic scaling.

The AFTOX model was developed as a result of a need by the U.S. Air Force to update its toxic corridor prediction capability. The Air Force had been using the Ocean Breeze/Dry Gulch model, which was an empirical model derived in the mid-sixties from two sets of diffusion

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Received for Publication 29 April 1991

experiments: Ocean Breeze, conducted at Cape Canaveral, Florida and Dry Gulch, conducted at Vandenberg AFB, California.

The requirements for the new model were: 1) that it be able to run on a microcomputer, 2) that it be very user-friendly, 3) that the input data be limited to data that would normally be available to the operator, and 4) that the computation time be kept to a minimum.

To meet these criteria, it was decided that a Gaussian puff dispersion model would be most appropriate. As a result, AFTOX was developed and evaluated against 243 diffusion tests from the Prairie Grass,<sup>1,2,3</sup> Ocean Breeze and Dry Gulch,<sup>4,5</sup> and Green Glow<sup>6</sup> experiments. In 1988, the model was officially endorsed by the Air Weather Service, and is now used extensively throughout the Air Force.

AFTOX 4.0 is an updated version of the original model.<sup>7</sup> Many of the changes made to the original version were a result of suggestions made by the users. Many of these changes are designed to reduce the chances of input error and to provide more default values. The most significant technical changes are 1) an expansion of the chemical data base from 76 to 129 chemicals; 2) the inclusion of the more universal Antoine equation for computing the saturated vapor pressure, thus making it possible to include more chemicals in the data base; 3) a new evaporation model for the hypergols and nitrogen tetroxide; 4) a slight adjustment in the vertical dispersion coefficients to bring them more in line with the Pasquill-Gifford<sup>8</sup> dispersion coefficients; and 5) the inclusion of the 90 percent hazard area for all spills and not just for continuous releases as in the original version.

Section 2 of this report presents a technical description of the model. This section is similar to the same section in the previous user's guide,<sup>7</sup> but with some important differences. The entire technical discussion is repeated here for completeness. Section 3 is a user's guide to the operation of the model.

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<sup>1</sup> Barad, M.L., Ed. (1958) *Project Prairie Grass, A Field Program in Diffusion*, Vol. I, AFCRC-TR-58-235(I), AD 152572.

<sup>2</sup> Barad, M.L., Ed. (1958) *Project Prairie Grass, A Field Program in Diffusion*, Vol. II, AFCRC-TR-58-235(II), AD 152573.

<sup>3</sup> Haugen, D.A., Ed. (1959) *Project Prairie Grass, A Field Program in Diffusion*, Vol. III, AFCRC-TR-58-235(III), AD 217076.

<sup>4</sup> Haugen, D.A. and Fuquay, J.J., Eds. (1963) *The Ocean Breeze and Dry Gulch Diffusion Programs*, Vol. 1, AFCRL-63-791(I), AD 428436.

<sup>5</sup> Haugen, D.A. and Taylor, J.H., Eds. (1963) *The Ocean Breeze and Dry Gulch Diffusion Programs*, Vol. 2, AFCRL-63-791(II), AD 427687.

<sup>6</sup> Barad, M.L. and Fuquay, J.J., Eds. (1962) *The Green Glow Diffusion Program*, Vol. I & II, AFCRL-62-25(I & II).

<sup>7</sup> Kunkel, B.A. (1988) *User's Guide for the Air Force Toxic Chemical Dispersion Model (AFTOX)*, AFGL-TR-88-0009, ADA 199096.

<sup>8</sup> Turner, D.B. (1970) *Workbook of Atmospheric Dispersion Estimates*, Public Health Service Publication No. 999-AP-26 (PB 191 482), U.S. Dept. of Health, Education and Welfare.

## 2. THEORY

### 2.1 Basic Diffusion Equations

The Gaussian puff model uses an equation to describe the dispersion of a puff with time. The equation assumes that the material is conserved during transport and diffusion, that is, there is no decay or deposition. It further assumes that the distribution of concentration within the puff is Gaussian.

The Gaussian puff equation can be written

$$G(x, y, z, t - t') = \frac{Q(t')}{2\pi^{3/2}\sigma_x\sigma_y\sigma_z} \cdot \exp\left[-\frac{1}{2}\left(\frac{x - u(t - t')}{\sigma_x}\right)^2\right] \cdot \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \cdot \left\{ \exp\left[-\frac{1}{2}\left(\frac{z - H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z + H}{\sigma_z}\right)^2\right] \right\} \quad (1)$$

where  $G$  is the concentration in the puff at a given point  $(x, y, z)$  and time  $(t - t')$ .  $Q$  is the total mass in the puff. The diffusion parameters,  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$  are the standard deviation of the material concentration in the  $x$ ,  $y$ , and  $z$  directions. It is assumed that  $\sigma_x = \sigma_y$ , thus producing a circular horizontal puff cross-section. The variable  $t$  represents the total elapsed time since the spill, and the  $t'$  is the time of emission of the puff. Thus,  $(t - t')$  is the travel time or elapsed time since the puff emission;  $u$  is the wind speed at 10 m; and  $H$  is the height of the source.

When there is an inversion, Eq. (1) is modified by adding the following expression to the last two terms in Eq. (1)

$$\sum \left\{ \exp\left[-\frac{1}{2}\left(\frac{z - H - 2NL}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z + H - 2NL}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z - H + 2NL}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z + H + 2NL}{\sigma_z}\right)^2\right] \right\} \quad (2)$$

where  $L$  is the mixing layer height and  $N$  is the number of iterations. The computer program considers the series converged when the above expression has a value less than 0.01 for a given  $N$ . If there is no inversion, the expression is ignored in the program.

When the series requires a large number of iterations to converge (>200) the program assumes a uniformly distributed plume between the earth's surface and the inversion height. If this is the case, then the concentration at a given point and time in the puff is described by the expression:

$$G(x, y, z, t - t') = \frac{Q(t')}{2 \pi \sigma_x \sigma_y L} \cdot \exp \left\{ -\frac{1}{2} \left[ \frac{x - u(t - t')}{\sigma_x} \right]^2 \right\} \cdot \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \quad (3)$$

The concentration at a point in space at a given time depends on the number of nearby puffs, their size, and the amount of material in each puff. The sum effect of all these puffs is given by summing over all emission times:

$$G(x, y, z, t) = \sum_{t'=0}^{\infty} G(x, y, z, t - t') \quad (4)$$

For an instantaneous gas release there is only one emission time and one puff. Therefore, a summation is not necessary. However, for a continuous spill, or a spill of finite duration, the summation is performed over puffs whose centers are located within four standard deviations of the puff concentrations upwind and downwind from the location of interest. It is assumed that concentrations from puffs further than four standard deviations contribute little to the concentration at the specified location.

In a spill of finite duration, the model assumes 20 puffs/min. out to 300 m from the source, 4 puffs/min. from 300 m to 3 km and then 3 puffs/min. beyond 3 km for winds less than or equal to 4 m/sec. For winds greater than 4 m/sec, the number of puffs per minute (N) is equal to

$$N = \text{INT} (N_1 u/4), \quad (5)$$

where  $N_1$  is 20, 4, or 3 depending on the distance from the source. The reason for increasing the frequency of puffs is that higher winds cause greater distances between puffs, thus reducing the number of overlapping puffs. By increasing the frequency of puffs according to Eq. (5), approximately the same number of overlapping puffs is retained no matter how strong the wind.

Under steady-state, non-inversion conditions, keeping track of the individual puffs is not necessary. A simple Gaussian plume model will suffice. In this situation, the model uses the following Gaussian plume equation in place of Eq. (1):

$$C = \frac{Q}{2 \pi \sigma_x \sigma_y u} \cdot \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \cdot \left\{ \exp \left[ -\frac{1}{2} \left( \frac{z-H}{\sigma_z} \right)^2 \right] + \exp \left[ -\frac{1}{2} \left( \frac{z+H}{\sigma_z} \right)^2 \right] \right\}. \quad (6)$$

## 2.2 Atmospheric Stability

The atmospheric stability and the distance from the source affect the dispersion parameters ( $\sigma_y$ ,  $\sigma_z$ ). In diffusion modeling, the atmospheric stability is often defined by the Pasquill stability categories, which range from category A for a very unstable atmosphere to F for a very stable atmosphere. In AFTOX, a continuous stability parameter ranging from 0.5 to 6 is used in place of the discrete stability categories. This prevents sharp changes in the hazard distance when going from one stability category to another; this can happen with a slight change in wind speed, solar angle, or cloud cover. The relationship between Pasquill stability category and the continuous stability parameter is shown in Table 1.

Table 1. Relation Between the Pasquill Stability Categories, SC, and the Continuous Stability Parameter, SP

| SC | A   | B   | C   | D   | E   | F   |
|----|-----|-----|-----|-----|-----|-----|
| SP | 0-1 | 1-2 | 2-3 | 3-4 | 4-5 | 5-6 |

AFTOX employs one of two methods to define the stability parameter: (1) uses the wind speed and solar insolation, or (2) uses the standard deviation of the wind direction to define the stability parameter. In the first method, the stability is determined using Golder's nomogram<sup>9</sup> where the Monin-Obukhov length (L) and surface roughness are related to the Pasquill stability categories. Since L is not measured, it must be calculated, and because L is a function of the friction velocity ( $u_*$ ) and sensible heat flux (H), these latter two parameters must also be calculated. In the second method, the stability is determined using the Modified Sigma Theta (MST) approach introduced by Mitchell and Timbre<sup>10</sup> and presented in more detail in a later report by Mitchell.<sup>11</sup>

<sup>9</sup> Golder, D. (1972) Relations between stability parameters in the surface layer, *Boundary Layer Met.* 3:46-58.

<sup>10</sup> Mitchell, A.E., Jr. and Timbre, K. (1979) Atmospheric stability class from horizontal wind fluctuation, paper 79-29.2, Air Pollution Control Association Annual Meeting, Cincinnati, OH.

<sup>11</sup> Mitchell, A.E., Jr. (1982) A comparison of short-term dispersion estimates resulting from various atmospheric stability classification methods, *Atmos. Environ.* 16:765-773.

### 2.2.1 CALCULATING $u_*$ AND $L$

To determine  $u_*$  and hence  $L$ , an iterative procedure similar to that described by Koo et al<sup>12</sup> is applied to the surface layer wind profile equations below, as summarized by Ragland and Dennis,<sup>13</sup> for neutral, unstable, and stable conditions.

$$\text{Neutral: } \frac{ku}{u_*} = \ln \frac{Z}{Z_o}; \quad (7a)$$

$$\text{Unstable: } \frac{ku}{u_*} = 2 \left( \tan^{-1} x - \tan^{-1} x_o \right) + \ln \frac{x-1}{x_o+1} - \ln \frac{x+1}{x_o+1}; \quad (7b)$$

where  $x = (1-15Z/L)^{1/4}$  and  $x_o = (1-15Z_o/L)^{1/4}$ , and

$$\text{Stable: } \frac{ku}{u_*} = \ln \frac{Z}{Z_o} + 5.2 \alpha, \quad (7c)$$

where  $u$  is the measured wind speed,  $u_*$  is the friction velocity,  $k$  is the von Karman constant,  $Z$  is the anemometer height,  $Z_o$  is the roughness length at the wind measurement site,  $L$  is the Monin-Obukhov length, and  $\alpha = Z/L$  when  $Z < L$  and  $\alpha = 1$  when  $Z > L$ .

The Monin-Obukhov length  $L$  is defined as

$$L = \frac{\rho C_p T u_*^3}{kgH}, \quad (8)$$

where  $\rho$  is the ambient air density,  $C_p$  is the specific heat of air,  $T$  is the air temperature,  $k$  is the von Karman constant,  $g$  is the gravitational constant, and  $H$  is the sensible heat flux. Equation (8) may be rewritten

<sup>12</sup> Koo, E., Chang, W.L., and Lee, B.Y. (1984) An alternative stability classification scheme for air quality modeling. Fourth Joint Conference on Applications of Air Pollution Meteorology, Portland, OR, 95-98.

<sup>13</sup> Ragland, K.W. and Dennis, B.L. (1975) Point source atmospheric diffusion model with variable wind and diffusivity profiles, *Atmos. Environ.*, 9:175-189.

$$L = - \frac{pu_s^3}{0.0112H}, \quad (9)$$

where  $L$  is in  $\text{m}$ ,  $p$  is the atmospheric pressure in  $\text{mb}$ ,  $u_s$  is in  $\text{m sec}^{-1}$  and  $H$  is in  $\text{W m}^{-2}$ . The method used to compute the heat flux is described in Section 2.2.2.

To start the iteration, an estimate of  $u_s$  is required. That estimate is calculated from Eq. (10):

$$u_s = \frac{1}{12} \left( u + \frac{0.8H}{H + 1000} \right) \quad (10)$$

where the wind speed at 10 m ( $u$ ) is estimated from the measured wind ( $u_z$ ) using the power law with an exponent of 0.2:

$$u = u_z \left( \frac{10}{z} \right)^{0.2}. \quad (11)$$

The iteration continues until successive values of  $u_s/u$  differ by less than 0.001.  $L$  is then calculated from this value of  $u_s$ . Once  $u_s$  is derived, the wind speed at 10 m is determined and used in the Gaussian puff equation [Eq. (1)] or plume equation [Eq.(6)].

## 2.2.2 CALCULATING SENSIBLE HEAT FLUX

The sensible heat flux ( $H$ ) is needed for calculating the Monin-Obukhov length and for determining the appropriate wind profile equation. A positive heat flux greater than  $1 \text{ W m}^{-2}$  is unstable [Eq. (7b)], while a negative heat flux less than  $-1 \text{ W m}^{-2}$  is stable [Eq. (7c)]. A heat flux between 1 and  $-1 \text{ W m}^{-2}$  is neutral [Eq. (7a)]. The heat flux is also used to determine an initial estimate of  $u_s$ . The sensible heat flux is calculated for daytime conditions using a method described by Holtslag and Van Ulden.<sup>14</sup>

The incoming solar radiation at ground level (SR) is very much a function of the solar elevation angle ( $\phi$ ). Under clear skies, it can be determined from the empirical formula:

$$SR_o = a_1 \sin \phi + a_2. \quad (12)$$

<sup>14</sup> Holtslag, A.A.M. and Van Ulden, A.P. (1983) A simple scheme for daytime estimates of the surface fluxes from routine weather data, *J. Climate Appl. Meteorol.*, **22**:517-529.

The turbidity coefficients,  $a_1$  and  $a_2$ , describe the average atmospheric attenuation of  $K_0$  by water vapor and dust for a given site. These coefficients will vary from one location to another and from one time period to another because of the variation in the turbidity of the atmosphere. In this model,  $a_1 = 990 \text{ W m}^{-2}$  and  $a_2 = -30 \text{ W m}^{-2}$  were used since they represent a reasonable average of coefficients determined at various locations. The method of determining the solar elevation angle ( $\phi$ ) is described in Section 2.2.3.

The presence of clouds reduces the incoming solar radiation. Kasten & Czeplak<sup>15</sup> proposed the following:

$$SR = SR_0 (1 + b_1 N^{b_2}), \quad (13)$$

where  $N$  is the fraction of the sky covered with clouds and  $b_1$  and  $b_2$  are empirical coefficients. From ten years of observation at Hamburg, Kasten and Czeplak obtained  $b_1 = -0.75$  and  $b_2 = 3.4$  on the average. Using these coefficients implies that the solar radiation reaching the ground under overcast conditions is 25 percent of that reaching the ground under clear skies. Kasten and Czeplak also show that the transmittances (TR) of cirrus, altus, cumulus, stratus, and nimbostratus are 0.61, 0.27, 0.25, 0.18, and 0.16, respectively. Therefore, to take into account the type of cloud, Eq. (13) has been modified to read:

$$SR = SR_0 (1 - (1 - TR) N^{b_2}). \quad (14)$$

In the model, the cloud types have been condensed into three groups representing high, medium, and low clouds. The cloud groups and their transmittances are shown in Table 2.

Table 2. Transmittances for High, Medium and Low Clouds

|        |                |      |
|--------|----------------|------|
| HIGH   | Cl, Cc, Cs     | 0.61 |
| MEDIUM | Ac, As, Sc, Cu | 0.26 |
| LOW    | St, Ns, Fog    | 0.17 |

To determine the net radiation, the following equation from Holtslag and Van Ulden is used:

<sup>15</sup> Kasten, F. and Czeplak, G. (1980) Solar and terrestrial radiation dependent on the amount and type of cloud. *Solar Energy*, **24**:177-189.

$$Q = \frac{(1-r)SR + C_1 T^6 - \sigma T^4 + C_2 N}{1 + C_3} \quad (15)$$

where  $r$  is the albedo of the surface, equal to 0.25, except when there is a snow cover, when it is set at 0.75.  $T$  is the air temperature in Kelvin,  $\sigma$  is the Stefan-Boltzmann constant, equal to  $5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ , and the empirical constants  $C_1$  and  $C_2$  are equal to  $5.31 \times 10^{-13} \text{ W m}^{-2} \text{ K}^{-6}$  and  $60 \text{ W m}^{-2}$ , respectively. The surface heating coefficient  $C_3$  varies from 0.12 for a wet surface to 0.38 for dry, bare soil. In the model,  $C_3$  is equal to 0.12 for a wet surface and 0.25 for a dry surface.

The surface energy budget relates the net radiation  $Q$  to the various heat fluxes at the earth's surface

$$H + \lambda E + G = Q, \quad (16)$$

where  $H$  is the sensible heat flux,  $\lambda E$  the latent heat flux, and  $G$  the soil heat flux which is set equal to 0.1  $Q$ . For snow-covered surfaces,  $G$  is set to 0 to reflect the poor conductivity of snow.

DeBruin and Holtslag<sup>16</sup> present a simplified parameterization for the sensible heat flux ( $H$ ) and latent heat flux ( $E$ )

$$H = \frac{1 - \alpha + \gamma/s}{1 + \gamma/s} (Q - G) - \beta' \gamma, \quad (17)$$

$$E = \frac{\alpha}{1 + \gamma/s} (Q - G) + \beta' \gamma. \quad (18)$$

Here  $s = q_s / T$ , where  $q_s$  is the saturation specific humidity,  $\gamma = C_p / \lambda$  where  $C_p$  is the specific heat of air at constant pressure and  $\lambda$  the latent heat of water vaporization, and  $\alpha$  and  $\beta'$  are empirical parameters. Holtslag and Van Ulden present  $\gamma/s$  values as a function of temperature for a standard pressure of 1000 mb. A regression line can be fitted to the data such that

$$\gamma/s = 119.56 - 0.7843T + 1.2887 \times 10^{-3} T^2, \quad (19)$$

<sup>16</sup> DeBruin, H.A.R. and Holtslag, A.A.M. (1982) A simple parameterization of the surface fluxes of sensible and latent heat during daytime compared with the Penman-Monteith concept, *J. Appl. Meteorol.*, 21:1610-1621.

where T is the air temperature in Kelvin.

From Holtslag and Van Ulden,<sup>14</sup> the surface moisture parameter  $\alpha$  is set at 1.0 for wet conditions and 0.45 for dry conditions. The parameter  $\beta'$  is set at  $20 \text{ W m}^{-2}$ .

For nighttime, the sensible heat flux is related to the total cloud cover (N) by Smith's<sup>17</sup> formula:

$$H = -40 (1 - N) \quad (20)$$

where H is in  $\text{W m}^{-2}$ .

### 2.2.3 CALCULATING SOLAR ELEVATION ANGLE

The solar elevation angle for a given time and location may be calculated by a method described by Woolf.<sup>18</sup> The following relation is used to determine the solar elevation angle,  $\phi$ :

$$\sin \phi = \sin LA \sin D + \cos LA \cos D \cos H \quad (21)$$

where LA is the station latitude, D the solar declination angle, and H the solar hour angle.

The solar declination angle is a sinusoidal function of time with maximum and minimum angles occurring during summer and winter, respectively. There is, however, a slight asymmetry, due to the ellipticity of the earth's orbit, which is accounted for in the following expression for calculating the declination:

$$\sin D = \sin 23.4438 \sin \sigma, \quad (22)$$

where

$$\begin{aligned} \sigma (\text{deg}) = & a + 279.9348 + 1.914827 \sin a - 0.079525 \cos a \\ & + 0.019938 \sin 2a - 0.001620 \cos 2a. \end{aligned} \quad (23)$$

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<sup>17</sup> Smith, F.B. (1972) A scheme for estimating the vertical dispersion of a plume from a source near ground level, *Proceedings of the Third Meeting of the Expert Panel on Air Pollution Modeling*, NATO committee on the Challenges of Modern Society, Paris, France.

<sup>18</sup> Woolf, H.M. (1980) *On the Computation of Solar Elevation Angles and the Determination of Sunrise and Sunset Times*, National Meteorological Center, Environmental Sciences Services Administration, Hillcrest Heights, MO.

The angular fraction of a year ( $a$ ) for a particular date is given by

$$a = 360 (JO - 1) / 365.242, \quad (24)$$

where JO is the Julian date.

The solar hour angle ( $H$ ), a measure of the longitudinal distance to the sun from the point for which the calculation is made, is given by

$$H(\text{deg}) = 15(ZO - M) - LO \quad (25)$$

where ZO (hour) is the Greenwich mean time (GMT) of the calculation, M (hour) the time of meridian passage, or true solar noon, and LO (deg) the station longitude, positive being west of Greenwich. M is derived from

$$M = 12 + 0.12357 \sin a - 0.004289 \cos a + 0.153809 \sin 2a + 0.06078 \cos 2a. \quad (26)$$

## 2.2.4 CALCULATING THE STABILITY PARAMETER

### Method 1

Based on data collected at five sites, Golder<sup>9</sup> developed a nomogram relating the Monin-Obukhov length ( $L$ ) and surface roughness ( $Z_o$ ) to the Pasquill stability categories. This nomogram is shown as Figure 1. To use this nomogram in the model, it was necessary to find a mathematical relationship between  $L$ ,  $Z_o$ , and the stability parameter (SP). The following formulation gives a good approximation of SP for a given  $L$  and  $Z_o$ , where  $Z_o$  is the surface roughness at the wind measurement site.

$$SP = A + B \log_{10}(100 Z_o) \quad (27)$$

where

$$A = 3.5 + 21.67/L$$

$$B = 0.48 \text{ when } |1/L| > 0.015$$

$$B = 43.63 |1/L|^{1.08} \text{ when } |1/L| < 0.015$$

$B = -B$  when  $1/L < 0$   
where  $Z_0$  and  $L$  are in m.

To stay within the bounds of the chart,  $Z_0$  is restricted to the 0.1 to 40 cm range in the model. Values of SP are allowed to vary from 0.5 to 6.0. Extrapolating below 0.5 is not very reliable, and using 0.5 as a minimum value is a conservative approach.

When the stability parameter is equal to 6, which occurs at nighttime under light wind conditions, the model assumes that horizontal meandering occurs. When concentration averaging times are greater than 1 min, the model assumes a stability parameter for horizontal diffusion of 3.5, or a neutral condition. Mean concentrations taken over averaging times of 1 min or less are considered to be unaffected by the rather large oscillation period of the meandering wind. Since meandering does not affect the vertical diffusion, the stability parameter for the vertical diffusion remains at 6.

If the inversion height is less than 50 m above the ground during either daytime or nighttime, the stability parameter for the vertical diffusion is set at 6.0. At night, when meandering may be occurring, the stability parameter for horizontal diffusion is set at 3.5 when the concentration averaging time is  $> 1$  min.

## Method 2

If the standard deviation of the horizontal wind direction ( $\sigma_\theta$ ) is known, then the stability parameter can be calculated using the Modified Sigma Theta (MST) approach of Mitchell.<sup>11</sup> In this method, the stability category relationship outlined in the NRC Regulatory Guide 1.23<sup>19</sup> is used. However, for nighttime when the  $\sigma_\theta$  is greater than 12.5 degrees, Mitchell assumes that the large  $\sigma_\theta$  is due to meandering and not to instability. Since meandering does not affect the vertical diffusion, an adjustment is made in the stability classes for the vertical diffusion. The MST method is summarized in Table 3.

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<sup>19</sup> USNRC (1972) *Onsite Meteorological Programs Regulatory Guide 1.23*, U.S. Nuclear Regulatory Commission.

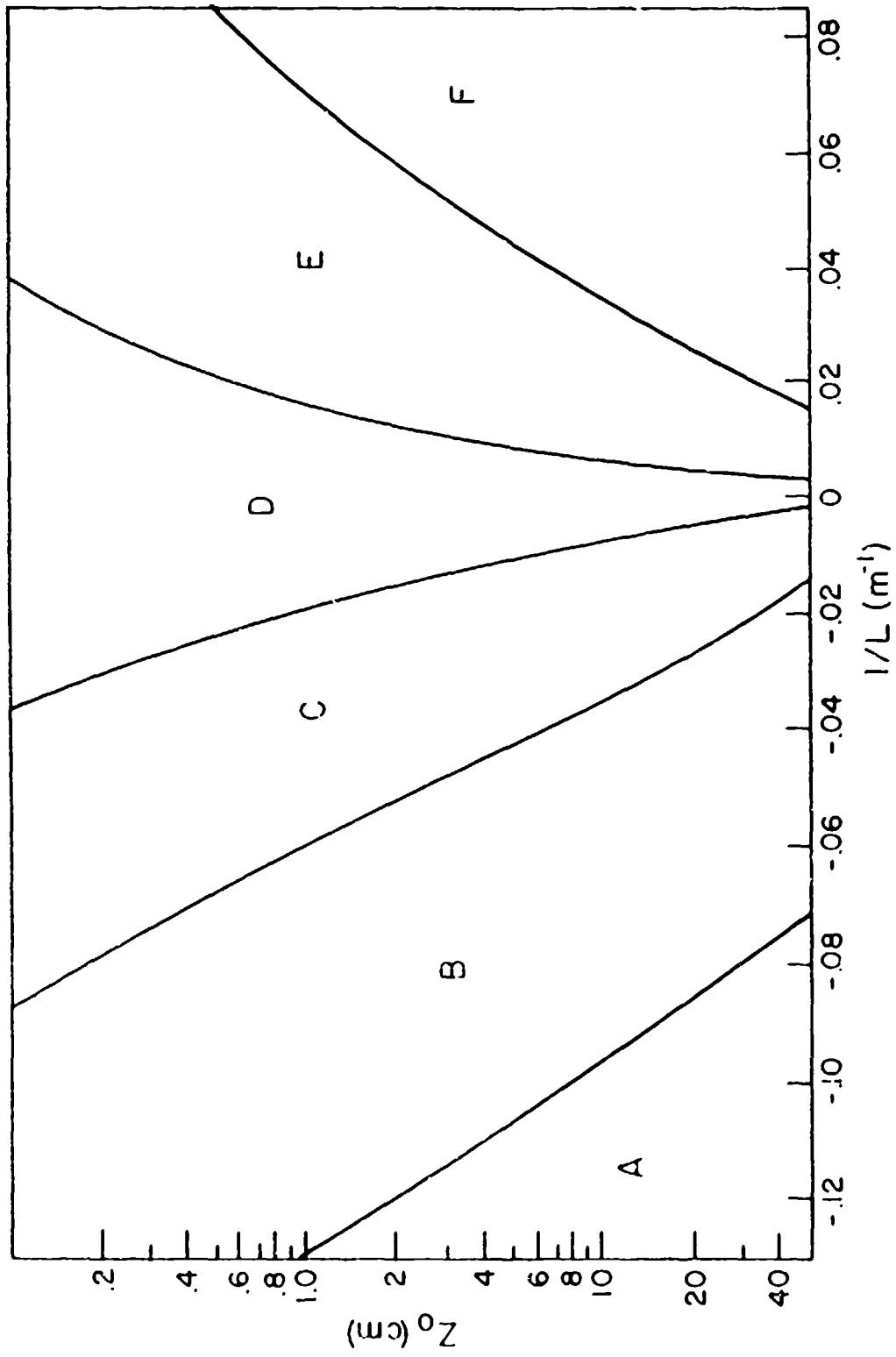


Figure 1.  $1/L$  as a Function of Pasquill Stability Classes and Surface Roughness ( $z_0$ ).

Table 3. Modified Sigma Theta (MST) Method to Determine Atmospheric Stability Class (from Mitchell<sup>11</sup>)

| $\sigma_\theta$<br>(Degrees)  | Daytime<br>Stability<br>Class <sup>2</sup> | Wind Speed<br>(m s <sup>-1</sup> ) | Nighttime <sup>1</sup><br>Stability<br>Class <sup>3</sup> |
|-------------------------------|--------------------------------------------|------------------------------------|-----------------------------------------------------------|
| $\sigma_\theta > 22.5$        | A                                          | $u < 2.4$                          | G                                                         |
|                               |                                            | $2.4 < u < 2.9$                    | F                                                         |
|                               |                                            | $2.9 < u < 3.6$                    | E                                                         |
|                               |                                            | $3.6 < u$                          | D                                                         |
| $22.5 > \sigma_\theta > 17.5$ | B                                          | $u < 2.4$                          | F                                                         |
|                               |                                            | $2.4 < u < 3.0$                    | E                                                         |
|                               |                                            | $3.0 < u$                          | D                                                         |
| $17.5 > \sigma_\theta > 12.5$ | C                                          | $u < 2.4$                          | E                                                         |
|                               |                                            | $2.4 < u$                          | D                                                         |
| $12.5 > \sigma_\theta > 7.5$  | D                                          | all windspeeds                     | D                                                         |
| $7.5 > \sigma_\theta > 3.8$   | E                                          | all windspeeds                     | E                                                         |
| $3.8 > \sigma_\theta > 2.1$   | F                                          | all windspeeds                     | F                                                         |
| $2.1 > \sigma_\theta$         | G                                          | all windspeeds                     | G                                                         |

<sup>1</sup> Nighttime is defined as the period from 1 hour before sunset to 1 hour after sunrise.

<sup>2</sup> More applicable to describing horizontal dispersion parameter  $\sigma_y$  at night.

<sup>3</sup> More applicable to describing vertical dispersion parameter  $\sigma_z$  at night.

As in Method 1, when the concentration averaging periods are 1 min or less, the concentrations are less affected by the rather large oscillation period of the meandering wind. Therefore, the stability parameter for the horizontal diffusion is set equal to the more stable stability parameter for vertical diffusion.

The  $\sigma_\theta$  values in Table 3 are for a 10 m level and a 60-min time period. Therefore, the measured  $\sigma_\theta$ , if for a height other than 10 m and a time period other than 1 hour, must be adjusted to a 10 m height and a 60-min time period. This is first done by adjusting the  $\sigma_\theta$  to the 10 m height through the relationship

$$(\sigma_\theta)_{10} = \sigma_\theta (10/Z)^{-0.2}, \quad (28)$$

and then adjusting the 10 m  $\sigma_\theta$  to the 60-min time period using

$$(\sigma_\theta)_{60} = (\sigma_\theta)_{10} (60/t)^{0.2}, \quad (29)$$

where Z is the wind measurement height and t is the time period over which  $\sigma_\theta$  is measured.

In AFTOX, the following equation, derived from the information in Table 3, is used to determine the stability parameter (SP) for all cases except for the stability parameter for vertical dispersion at night when  $\sigma_\theta < 12.5^\circ$ :

$$SP = 6.46 - 0.341 \sigma_\theta + 0.0045 \sigma_\theta^2, \quad (30)$$

where  $\sigma_\theta$  is now the corrected  $\sigma_\theta$  for a 10 m height and 60-min time period.

Table 4 shows how the model determines the stability parameters for vertical diffusion for nighttime when  $\sigma_\theta > 12.5$  degrees.

Table 4. The Nighttime Stability Parameter for Vertical Dispersion as a Function of  $\sigma_\theta$  and Wind Speed

| $\sigma_\theta$<br>(Degrees)  | Wind Speed<br>(m sec <sup>-1</sup> ) | Vertical Stability<br>Parameter (SP) |
|-------------------------------|--------------------------------------|--------------------------------------|
| $\sigma_\theta > 22.5$        | $u > 4.1$                            | SP = 3.5                             |
|                               | $2.4 < u < 4.1$                      | SP = 14.4/u                          |
| $22.5 > \sigma_\theta > 17.5$ | $u < 2.4$                            | SP = 6.0                             |
|                               | $u > 3.4$                            | SP = 3.5                             |
|                               | $2.0 < u < 3.4$                      | SP = 12/u                            |
|                               | $u < 2.0$                            | SP = 6.0                             |
| $17.5 > \sigma_\theta$        | $u > 2.7$                            | SP = 3.5                             |
|                               | $1.9 < u < 2.7$                      | SP = 9.6/u                           |
|                               | $u < 1.9$                            | SP = 5.0                             |

The AFTOX model makes three exceptions to the MST method:

1) During the daytime, no matter how small the  $\sigma_\theta$ s are, the model does not allow, as in Method 1, the stability parameters to exceed 3.5 (D stability class). In other words, only unstable or neutral conditions exist during the daytime.

2) Any time, day or night, that the height of the inversion base is less than 50 meters above the ground, the stability parameter for the vertical diffusion is adjusted to 6.0.

3) As in Method 1, during meandering wind or low inversion conditions, the stability parameter for the horizontal diffusion is set equal to the more stable stability parameter for vertical diffusion for concentration averaging periods of 1 min or less.

### 2.3 Dispersion Parameters

The Pasquill-Gifford (P-G) dispersion parameters<sup>8</sup> ( $\sigma_y$ ,  $\sigma_z$ ) are used in the dispersion model. These values were derived from the Prairie Grass experiments<sup>1,2,3</sup> and therefore are appropriate for a surface roughness of 3 cm, and are based on 10-min. concentration averages. The  $\sigma_y$  and  $\sigma_z$  parameters are adjusted for other surface roughnesses at the spill site ( $ZZ_0$ ) and concentration averaging times ( $t_c$ ). A schematic showing the steps taken in the model to arrive at the appropriate dispersion parameters is presented in Figure 2.

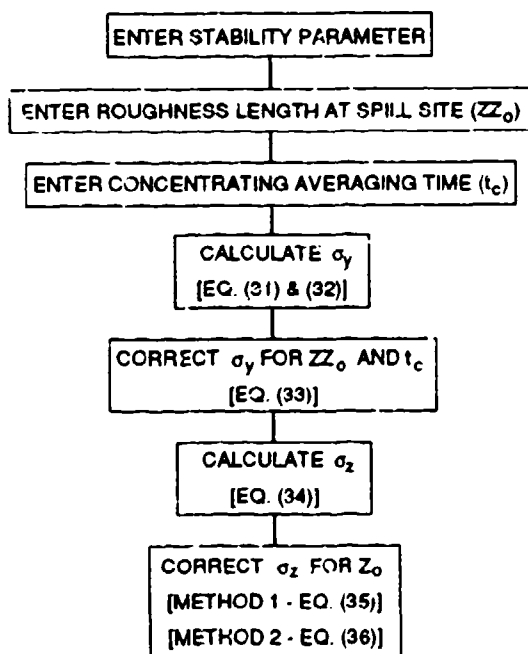


Figure 2. Procedure for Computing  $\sigma_y$  and  $\sigma_z$

#### 2.3.1 HORIZONTAL DISPERSION PARAMETER ( $\sigma_y$ )

The (P-G) horizontal dispersion parameter for different stabilities and for any distance ( $x$ ) can be approximated by using a power law curve

$$\sigma_y = a x^b \quad (31)$$

where a and b are given in Table 5 (from Hansen<sup>20</sup>) for the different stability categories and parameters. These values apply when  $\sigma_y$  and x are in meters.

Table 5. Coefficients and Exponents for the Horizontal Dispersion Parameter

| Stab. Category(SC)  | A    | B    | C    | D     | E     | F     |
|---------------------|------|------|------|-------|-------|-------|
| Stab. Parameter(SP) | 0.5  | 1.5  | 2.5  | 3.5   | 4.5   | 5.5   |
| a                   | 0.40 | 0.32 | 0.22 | 0.143 | 0.102 | 0.076 |
| b                   | 0.9  | 0.9  | 0.9  | 0.9   | 0.9   | 0.9   |

The relationship between the coefficient a and the stability parameter (SP) can be approximated by the formula:

$$a = 0.479 - 0.1232 \text{ SP} + 0.00904 \text{ SP}^2. \quad (32)$$

Since Eq. (31) gives  $\sigma_y$  for a surface roughness of 3 cm and a concentration averaging time of 10 min, the  $\sigma_y$  must be corrected for other surface roughnesses at the spill site ( $ZZ_0$ ) and pollutant concentration averaging time ( $t_c$ ). The following relationship is used in the model to arrive at the corrected horizontal dispersion parameter,  $(\sigma_y)_c$ :

$$(\sigma_y)_c = \sigma_y (ZZ_0/3)^{0.2} (t_c/10)^{0.2}. \quad (33)$$

### 2.3.2 VERTICAL DISPERSION PARAMETER ( $\sigma_z$ )

The vertical dispersion parameter,  $\sigma_z$ , for a roughness length of 3 cm can be determined using the power law

$$\sigma_z = c x^d, \quad (34)$$

where x and  $\sigma_z$  are in meters and c and d are given in Table 6. The constants c and d were derived by fitting power law curves to the Pasquill  $\sigma_z$  curves.

<sup>20</sup> Hansen, F.V. (1979) *Engineering Estimates for the Calculation of Atmospheric Dispersion Coefficients*, Internal Report, U.S. Army Atmospheric Science Laboratory, White Sands Missile Range, NM.

TABLE 6. Coefficients and Exponents for the Vertical Dispersion Parameter

| Stab. Category(SC)  | A                      | B      | C      | D      | E      | G      |
|---------------------|------------------------|--------|--------|--------|--------|--------|
| Stab. Parameter(SP) | 0.5                    | 1.5    | 2.5    | 3.5    | 4.5    | 5.5    |
| x(m)<               | 745                    | 745    | 2000   | 1100   | 1400   | 1400   |
| c                   | 0.0414                 | 0.1036 | 0.1173 | 0.0975 | 0.1050 | 0.0617 |
| d                   | 1.3155                 | 1.0026 | 0.9112 | 0.8414 | 0.7692 | 0.7884 |
| x(m)>               | 745                    | 745    | 2000   | 1100   | 1400   | 1400   |
| c                   | $1.928 \times 10^{-4}$ | 0.0534 | 0.4422 | 0.6097 | 0.8788 | 0.9990 |
| d                   | 2.1234                 | 1.1029 | 0.7382 | 0.5808 | 0.4771 | 0.4771 |

The  $\sigma_z$  for the derived stability parameter is determined by linearly interpolating between the  $\sigma_z$ s for the stability parameter in Table 6 just above and below the derived stability parameter. This approach was taken because a reasonable line of best fit could not be found for c.

Through the numerical solution of the two-dimensional equation of diffusion, F.B. Smith<sup>17</sup> derived correction factor curves for  $\sigma_z$  for different roughness lengths. Quite often, a simple empirical approximation to Smith's results is used,

$$(\sigma_z)_c = \sigma_z (ZZ_o/3)^{0.2}. \quad (35)$$

When using  $\sigma_\theta$  to determine the stability parameter (Method 2),  $\sigma_z$  needs to be corrected only if the surface roughness at the spill site ( $ZZ_o$ ) is different than the surface roughness at the wind measurement site ( $Z_o$ ). The corrected vertical dispersion parameter,  $(\sigma_z)_c$  is

$$(\sigma_z)_c = \sigma_z (ZZ_o/Z_o)^{0.2}. \quad (36)$$

Correction of  $\sigma_z$  for the concentration averaging time is not needed for either method since large eddies are much less likely to occur in the vertical direction than in the horizontal. In the model, Eqs (33), (35) and (36) apply for values of  $ZZ_o$  between 0.5 and 100 cm. The accuracy of these equations is questionable beyond these limits.

## 2.4 Evaporation

During a liquid release, it is assumed that a liquid pool will be formed on the ground after the chemical exits the original container. AFTOX 4.0 contains three evaporation models. The model that is used depends on the available chemical data. The three models are 1) the Vossler steady-state energy balance model;<sup>21</sup> 2) the Shell Oil Company's evaporation model used in their SPILLS model;<sup>22</sup> and 3) the Clewell evaporation model.<sup>23</sup> For a more detailed description of these models, the reader should refer to the above references.

### 2.4.1 VOSSLER EVAPORATION MODEL

This model is a steady-state model in which the pool temperature is adjusted based on the net energy input into the pool from all possible sources. The pool temperature is used to determine the evaporation rate. These sources of energy include solar radiation ( $Q_{sol}$ ), long wave radiation emitted by the pool ( $Q_{pol}$ ) and the atmosphere ( $Q_{atm}$ ), convective heat transfer from the atmosphere ( $Q_{he}$ ), heat conducted from the ground ( $Q_{grd}$ ), and heat loss due to evaporation ( $Q_{ev}$ ). The steady-state temperature is the temperature at which the sum of all sources of heat (energy) transported into the pool exactly balances the heat transfer out of the pool; that is, the sum of energy terms described above is zero. The steady-state energy balance is expressed as:

$$Q_{sol} + Q_{atm} + Q_{pol} + Q_{he} + Q_{ev} + Q_{grd} = Q_{total} \quad (37)$$

where  $Q_{total} = 0$  at steady state. Many of these energy terms can be expressed as a function of the pool surface temperature. The equation is solved iteratively for the pool temperature, which is then used to calculate evaporation rate. The evaporation rate is proportional to the mass transfer coefficient at the liquid pool-atmosphere interface and the vapor pressure of the chemical, both of which are functions of the pool surface temperature.

This model requires a great deal of chemical data as can be seen in Section 3.1.2. In the model, these data are stored in a separate file called EVAP.DAT. Currently, only four chemicals are stored in this file. They include nitrogen tetroxide, hydrazine, monomethylhydrazine (MMH), and unsymmetrical dimethylhydrazine (UDMH).

<sup>21</sup> 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.

<sup>22</sup> Fleischer, M.T. (1980) *SPILLS: An Evaporation/Air Dispersion Model for Chemical Spills on Land*, Shell Development Company, PB 83109470.

<sup>23</sup> Clewell, H.J. (1983) *A Simple Formula for Estimating Source Strengths from Spills of Toxic Liquids*, ESL-T-83-03.

## 2.4.2 SHELL EVAPORATION MODEL

In the Shell model, the evaporation rate is primarily a function of the forced convection over the liquid pool due to the wind. It is assumed that there is no heat transfer due to evaporative cooling or radiation, and that the pool temperature is the same as the air temperature. The evaporation rate ( $\dot{Q}$ ) is equal to:

$$\dot{Q} = (\text{Sh } D/L) L^2 \rho_v, \quad (38)$$

where Sh is the Sherwood number, D is the molecular diffusion coefficient,  $\rho_v$  is the vapor density, and L is the pool width. For turbulent flows ( $\text{Re} > 320000$ ), the Sherwood number is equal to:

$$\text{Sh} = 0.037 \text{Sc}^{1/3} [\text{Re}^{0.8} - 15200]. \quad (39)$$

For laminar flows ( $\text{Re} < 320000$ ), the Sherwood number is

$$\text{Sh} = 0.664 \text{Sc}^{1/3} \text{Re}^{1/2}, \quad (40)$$

where Sc is the Schmidt number and Re is the Reynolds number. The Schmidt number is given by  $\nu/D$ , and the Reynolds number by  $uL/\nu$ , where  $\nu$  is the kinematic viscosity of air in  $\text{m}^2/\text{sec}$ , and  $u$  is the wind speed at 10 m above ground level in  $\text{m}/\text{sec}$ .

The molecular diffusion coefficient, D, is equal to:

$$D = cT^{3/2} \frac{[(M_A + M_B)/M_A M_B]^{1/2}}{P \sigma_{AB}^2 \Omega_D}, \quad (41)$$

where the binary diffusivity (D) is in  $\text{cm}^2/\text{sec}$ , T is the temperature in Kelvin,  $M_A$  and  $M_B$  are molecular weights of the chemical and of air, P is the pressure in atmospheres,  $\sigma_{AB}$  is the hard core diameter of the binary pair, and  $\Omega_D$  is the collision integral for diffusion.

The collision integral  $\Omega_D$  is calculated from the expression

$$\Omega_D = A_1 (T^*)^{-B_1} + A_2 \exp(-B_2 T^*), \quad (42)$$

where the  $A_i$  and  $B_i$  are constants obtained by curve fitting calculated values of  $\Omega_D$  versus  $T^*$ .  $T^*$  is the temperature reduced by the potential well depth  $\epsilon_{AB}$ .  $T^*$  may be expressed

$$T^* = T/\epsilon_{AB}. \quad (43)$$

where

$$\epsilon_{AB} = (\epsilon_A \epsilon_B)^{1/2}, \quad (44)$$

where  $\epsilon_B$  for air is = 78.6. The AFTOX chemical data file for the chemical includes  $\epsilon_A$  which is approximately equal to 1.15 times the boiling point of the chemical.

The constants in Eq. (42) used in the model are given in Table 7.

Table 7. The A and B Constants Used in Eq. (42) in AFTOX

|   | i = 1   | j = 1   | j = 2   | j = 3   |
|---|---------|---------|---------|---------|
| A | 0.06036 | 0.193   | 1.03587 | 1.76474 |
| B | 0.1561  | 0.47635 | 1.52996 | 3.89411 |

In Eq. (41)  $\sigma_{AB}$  is equal to

$$\sigma_{AB} = 0.5 (\sigma_A + \sigma_B), \quad (45)$$

where  $\sigma_A$  is the effective diameter of the gas molecule and  $\sigma_B$  is the effective diameter of the air molecule (set at 3.711 in the model).  $\sigma_A$  is included in the AFTOX chemical data file.

The constant c in Eq. (41) is taken to be

$$10^3 c = 2.17 - 0.5[(M_A + M_B)/M_A M_B]^{1/2}. \quad (46)$$

The molecular weight of air,  $M_B$ , is set at 28.966.

### 2.4.3 CLEWELL EVAPORATION MODEL

For those chemicals for which only the molecular weight and vapor pressure are known, the Clewell evaporation model is used. This model is a crude approximation to the Ille and Springer model,<sup>24</sup> which is similar to the Vossler model. The model is represented by a single formula:

$$Q = 0.08 u^{3/4} A F_t Z, \quad (47)$$

where  $Q$  is the evaporation rate in kg/hr,  $u$  is the wind speed in m/sec,  $A$  is the spill area in  $m^2$ ,  $F_t$  is a pool temperature factor, and  $Z$  is a volatility factor. The pool temperature factor is equal to:

$$F_t = 1 + 4.3 \times 10^{-3} T_p^2 \text{ for } T_p > 0^\circ\text{C}, \text{ or } = 1 \text{ for } T_p < 0^\circ\text{C}, \quad (48)$$

where  $T_p$  is the pool temperature in  $^\circ\text{C}$ . An estimate of the pool temperature must be made. In general, under sunny conditions the pool temperature may be several degrees warmer than the air temperature, and for highly volatile chemicals it may be several degrees cooler than the air temperature.

The volatility factor ( $Z$ ) is the ratio of the vapor pressure ( $VP$ ) and molecular weight ( $MW$ ) of the chemical to that of hydrazine, or

$$Z = (VP \text{ MW}) / (VP_H \text{ MW}_H) . \quad (49)$$

In the model, the molecular weight for hydrazine is set at 32.045 and vapor pressure for hydrazine is set at .02113 atm.

### 2.5 Saturated Vapor Pressure

All three methods of determining evaporation rates require the saturated vapor pressure ( $VP$ ). Depending on the available chemical data, one of two formulae is used to compute the

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<sup>24</sup> Ille, G. and Springer, C. (1978) *The Evaporation and Dispersion of Hydrazine Propellants from Ground Spills*, CEEDO-TR-83-30, ADA 059407.

vapor pressure. They are the Antoine equation and the Frost-Kalkwarf equation. The Antoine equation is:

$$VP = A_r - B_r / (T_p + C_r), \quad (50)$$

where  $A_r$ ,  $B_r$ , and  $C_r$  are empirical constants, and are included in the AFTOX chemical data file.

The Frost-Kalkwarf equation is:

$$\ln P_r = A_r(1 - 1/T_r) - B_r \ln T_r + D_r(P_r/T_r - 1), \quad (51)$$

where  $P_r$  is the reduced vapor pressure  $VP/P_c$ ,  $T_r$  is the reduced temperature,  $T_p/T_c$ , and where  $P_c$  and  $T_c$  are the critical pressure and temperature, respectively, and are included in the chemical data file.  $D_r$  is equal to 27/64, and  $A_r$  and  $B_r$  are empirical constants included in the chemical data file.

The vapor pressure is then equal to:

$$VP = P_r P_c. \quad (52)$$

Either equation is used for determining the vapor pressure for the Shell evaporation model. Since the Shell model assumes that the pool temperature is equal to the air temperature,  $T_p$  is the air temperature. The Vossler model uses an expanded version of the Antoine equation. The Clewell model uses a constant vapor pressure that is either stored in the chemical data file or entered by the user when running the model for a chemical not in the chemical data file.

## 2.6 Liquid Density

When the source strength of a liquid release is given in volume per unit time for a continuous spill or volume for an instantaneous spill, the liquid density must be known to convert the source strength to mass.

The liquid density can be calculated from the Guggenheim equation

$$\rho_L = MW [1 + a(1 - T_r)^{1/3} + b(1 - T_r)] / V_c, \quad (53)$$

where a and b are empirical constants that are included in the chemical data file. When the constants are not available, a liquid density value may be included in the file in place of the "a" constant. If no values are available, the model assumes a liquid density of 1 g/cm<sup>3</sup>. V<sub>c</sub> is the critical volume and is included in the chemical data file.

## 2.7 Continuous Buoyant Plumes

The buoyant plume routine considers a steady state emission from a single stack over a finite or infinite time period. The final centerline rise height and the distance downwind at which the plume reaches that height are calculated using the widely accepted Briggs plume rise formulas.<sup>25</sup>

The initial buoyancy flux (F) is defined by

$$F = (g/\pi) V (T_p - T)/T_p \quad (54)$$

where g is the acceleration of gravity (m/sec<sup>2</sup>), T<sub>p</sub> is the temperature of the plume (°K), T the ambient temperature (°K), and V the plume volume flux (m<sup>3</sup>/sec).

For a buoyant bent-over plume in unstable or neutral conditions, the height of the centerline of the plume is given by

$$Z = 1.6 F^{1/3} X^{2/3}/u \quad (55)$$

where Z and X are in km and u is wind speed in m/sec.

The plume reaches its equilibrium height at a distance (X') downstream defined as the point at which atmospheric turbulence dominates the entrainment. In the model this distance is defined as follows:

For F > 55

$$X' = 119 F^{0.4} \quad (56a)$$

<sup>25</sup> Briggs, G.A. (1975) Plume Rise Predictions, Lectures on Air Pollution and Environmental Impact Analyses, Workshop Proceedings, Boston, MA Sept. 27 - Oct. 3, 1975, pp. 59-111, American Meteorological Society, Boston, MA.

For  $F < 55$

$$X' = 49 F^{0.625}. \quad (56b)$$

For a buoyant, bent-over plume in stable air, the final plume centerline height is given by

$$Z = 2.6 \left( \frac{F_{-}}{US} \right)^{1/3}. \quad (57)$$

For a buoyant, vertical plume with a wind of 1 m/sec or less, the final centerline height is given by

$$Z = 5.0 F^{1/4} s^{-3/8}, \quad (58)$$

where  $s$  is a stability parameter equal to:

$$s = g/T \, DT/DZ, \quad (59)$$

and where  $DT/DZ$  is the potential temperature lapse rate, which in the model is set equal to  $0.02^{\circ}/m$  for slightly stable and  $0.035^{\circ}/m$  for more stable conditions.

The distance downwind where the plume reaches the equilibrium height is defined as:

$$X' = \pi u/s^{1/2}. \quad (60)$$

Unlike the unstable and neutral case, this distance is not required for computing the equilibrium height, but is calculated and printed out for information purposes only.

The source effective emission height,  $H$ , is equal to the sum of the equilibrium height,  $Z$ , and the stack height,  $H_s$ :

$$H = H_s + Z. \quad (61)$$

If H is higher than the inversion height, then H is set equal to the inversion height. In other words, we assume that the buoyant plume does not penetrate the inversion. This is a conservative approach when calculating concentration levels near the ground. In calculating the distribution of pollutant concentrations, the model assumes that the pollutants are released at the source effective emission height and not at the stack height.

### **3. AFTOX COMPUTER PROGRAM OPERATION**

This section provides the program structure and execution instructions for the AFTOX computer program. The code is written in the GW-BASIC programming language.

#### **3.1 File Structure**

The AFTOX program contains five component program files and six data files, four 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 8.

Table 8. List of files in AFTOX

|                        |            |                                                                                                               |
|------------------------|------------|---------------------------------------------------------------------------------------------------------------|
| <b>PROGRAM FILES</b>   |            |                                                                                                               |
|                        | 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 |
| <b>DATA FILES</b>      |            |                                                                                                               |
|                        | 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                                                              |
| <b>ANCILLARY FILES</b> |            |                                                                                                               |
|                        | SETUP.EXE  | Establishes computer and screen type                                                                          |
|                        | SDFIL.EXE  | Edits station data file (SD.DAT)                                                                              |
|                        | CHFIL.EXE  | Edits chemical data file (CH.DAT)                                                                             |

### 3.1.1 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 3 will appear. Enter the appropriate code for the computer and monitor types. The appropriate information will be stored in DEVICE.DAT.

## AFTOX

### 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 3. 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 4. 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 4. 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 different surface roughnesses or wind measurement heights 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, shown below, is automatically displayed on the screen. The surface roughness need not be restricted to one of the values shown in Figure 5, 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 BUILDINGS          | 0.5                    |
| RUNWAY, OPEN FLAT TERRAIN, GRASS, FEW SMALL BUILDINGS | 3                      |
| LOW CROPS, OCCASIONAL LARGE BUILDINGS                 | 10                     |
| HIGH CROPS, SCATTERED BUILDINGS                       | 25                     |
| PARKLAND, BUSHES, NUMEROUS BUILDINGS                  | 50                     |
| REGULAR LARGE OBSTACLE COVERAGE (SUBURB, FOREST)      | 100                    |

Figure 5. 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 129 chemicals. A list of the chemicals is given in the Appendix. The chemicals are listed in alphabetical order, except for the U.S. Air Force's CH.DAT file in which the first ten chemicals listed are chemicals most frequently used by the Air Force.

To run CHFIL, type CHFIL and press <ENTER>. The computer will display a screen with several options as shown in Figure 6. 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 6. 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.

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 exactly 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 weighted 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 constant (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. The chemical data required for the Vossler model, including the vapor pressure data, are included in EVAP.DAT.

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. If the Frost-Kalkwarf equation is to be used, 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.

### 3.1.2 DATA FILES

There are six data files, three of which have been discussed in Section 3.1.1. The remaining three are EVAP.DAT, CONCCY.DAT, and AFT.DAT.

## 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:

- Molecular weight
- Boiling temperature
- Freezing temperature
- Molecular diffusion volume
- Constants and applicable temperature ranges for:
  - Vapo. 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  $\text{mg}/\text{m}^3$  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.

### 3.2 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 (for example, C:\>md AFTOX). Then copy the files from the diskette to the hard disk (for example, A:\copy.\* C:\>AFTOX).

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.

### **3.3 Running AFTOX**

#### **3.3.1 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 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 (for example, you can not back up from DSP2 into DSP1).

#### **3.3.2 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 (for example, C:>AFTOX:ren aft.dat spill#1.dat).

#### **3.3.3 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 3.1.1.

#### **3.3.4 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.

### 3.3.5 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. If the type of release is unknown, the user should choose an instantaneous release for a conservative corridor.

### 3.3.6 CHEMICAL DATA

A list of 129 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  $\text{mg}/\text{m}^3$  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  $\text{mg}/\text{m}^3$ .

### 3.3.7 METEOROLOGICAL DATA

The meteorological data consist of:

- 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 20°C (68°F) 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 where the release is above the inversion, the pollutants remain above the inversion.

### 3.3.8 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 5) 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.

### 3.3.9 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. The model assumes that the spill area remains constant with time.

### **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.

### **3.3.10 WORST CASE SCENARIO**

When the initial spill alert is sounded, quite often very little source information is available. In this case, AFTOX 4.0 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 described in Section 3.3.15. 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

### 3.3.11 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>.

### 3.3.12 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-min. 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 as described in Section 2.2.4.

### 3.3.13 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.

### 3.3.14 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. Then 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  $\text{mg}/\text{m}^3$  or ppm. The exception is that when the molecular weight is not known the concentration is in  $\text{mg}/\text{m}^3$ . 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 on 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.

meaning 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. Examples of the toxic corridor plots are given in Appendix B.

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. Run 3 in Appendix B is an example of the maximum distance occurring after the specified time after release. For more discussion on the confidence limits, the reader should refer to Section 3.3.15.

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

#### 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 a +/-5 m accuracy

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.

### 3.3.15 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<sup>7</sup> 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 4.0, 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. If errors in the input data were to be taken into account, the toxic corridor would be considerably longer. Zettlemoyer<sup>26</sup> examined the effect that data input uncertainties have on the concentration uncertainties using a Monte Carlo simulation technique. He looked 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<sup>27</sup>). 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 ( $\sigma_\theta$ ) is known and the wind speed is greater than 1.8 m/sec, then the toxic corridor width (W) is equal to:

$$W = 6 \sigma_\theta. \quad (62)$$

The measured  $\sigma_\theta$  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  $\sigma_\theta$  is not known, then the following rules apply:

---

<sup>26</sup> 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.

<sup>27</sup> Kahler, J.P., Curry, R.G., and Kandler, R.A. (1980) *Calculating Toxic Corridors*, AWS/TR-80/003, AD A101267.

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 equivalent to that derived from the  $\sigma_0$  for the different stabilities shown in Table 3. Equation (63) shows the relationship between the width (W) and the stability parameter (STB).

$$W = 165 - 30 \text{ STB.} \quad (63)$$

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

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## **Appendix A**

### **Chemical Data Base**

|    |                                     |    |                                   |
|----|-------------------------------------|----|-----------------------------------|
| 1  | Aerazine-50                         | 44 | m-Cresol                          |
| 2  | Hydrazine                           | 45 | p-Cresol                          |
| 3  | Hydrazine (54%)                     | 46 | Cumene (Isopropyl Benzene)        |
| 4  | Hydrazine (70%)                     | 47 | Cyclohexane                       |
| 5  | Monomethylhydrazine (MMH)           | 48 | D-D Soil Fumigant                 |
| 6  | Dimethylhydrazine (UDMH)            | 49 | Diallyl Amine                     |
| 7  | JP-9                                | 50 | Dibutyl Phthalate                 |
| 8  | JP-10                               | 51 | o-Dichlorobenzene                 |
| 9  | Fuming Nitric Acid (IRFNA)          | 52 | m-Dichlorobenzene                 |
| 10 | Nitrogen Tetroxide                  | 53 | p-Dichlorobenzene                 |
| 11 | Acetaldehyde                        | 54 | Dichlorodimethylsilane            |
| 12 | Acetone                             | 55 | 1 2 Dichloroethylene (cis)        |
| 13 | Acetonitrile                        | 56 | 1 2-Dichloroethylene (trans)      |
| 14 | Acrolein (2-propenal)               | 57 | 1 2-Dichloropropane               |
| 15 | Acrylic Acid                        | 58 | Diethanol Amine                   |
| 16 | Allyl Alcohol (2-propene-1-ol)      | 59 | Dimethyl Phthalate                |
| 17 | Allyl Chloride (3-Chloro-1-Propene) | 60 | 1 4-Dioxane                       |
| 18 | Ammonia                             | 61 | Di-t-Butylethyl Diamine           |
| 19 | Ammonia (29%)                       | 62 | Epichlorohydrin                   |
| 20 | Aniline                             | 63 | Ethanol                           |
| 21 | Benzene                             | 64 | Ethyl Acrylate                    |
| 22 | Benzoyl Chloride                    | 65 | Ethyl Benzene                     |
| 23 | Bromine Pentafluoride               | 66 | Ethylene                          |
| 24 | Bromoform                           | 67 | Ethyl Chloride                    |
| 25 | Bromomethane                        | 68 | Ethylene Dibromide                |
| 26 | 1 3-Butadiene                       | 69 | Ethylene Dichloride               |
| 27 | Butane                              | 70 | Ethylene Glycol                   |
| 28 | n-Butyl Alcohol (1-Butanol)         | 71 | Ethylene Oxide                    |
| 29 | sec-Butyl Alcohol (2-Butanol)       | 72 | 2-Ethyl Hexanol                   |
| 30 | t-Butyl Alcohol                     | 73 | Fluorine                          |
| 31 | Butylene                            | 74 | Formaldehyde (Pure)               |
| 32 | Butyraldehyde                       | 75 | Formaldehyde (37%)                |
| 33 | Carbon Disulfide                    | 76 | Formaldehyde (56%)                |
| 34 | Carbon Monoxide                     | 77 | Freon 12                          |
| 35 | Carbon Tetrachloride                | 78 | Hydrogen Chloride                 |
| 36 | Chlorine                            | 79 | Hydrogen Cyanide                  |
| 37 | Chlorine Pentafluoride              | 80 | Hydrogen Fluoride                 |
| 38 | Chlorine Trifluoride                | 81 | Hydrogen Sulfide                  |
| 39 | Chlorobenzene                       | 82 | Isoamylene (2-Methyl-2-Butene)    |
| 40 | Chloroethane                        | 83 | Isobutane (2-Methylpropane)       |
| 41 | Chloroform                          | 84 | Isobutyraldehyde                  |
| 42 | Chloromethane                       | 85 | Isoprene (2-Methyl-1 3-Butadiene) |
| 43 | o-Cresol                            | 86 | Isopropanol (2-Propanol)          |

- 87 Isopropyl Ether
- 88 Mesityl Oxide
- 89 Methane
- 90 Methanol
- 91 Methyl Iodide
- 92 Methylene Chloride
- 93 Methylethyl Ketone
- 94 Methyl Isobutyl Ketone
- 95 Methyl Methacrylate
- 96 Nitric Acid (Pure)
- 97 Nitrobenzene
- 98 Nitrogen Dioxide
- 99 Nitrogen Trifluoride
- 100 Nitropropane
- 101 N N-Dimethylaniline
- 102 Oxygen Difluoride
- 103 Perchloryl Fluoride
- 104 Pentaborane
- 105 Phenol
- 106 Phosgene
- 107 Propane
- 108 Propionaldehyde
- 109 Propylene
- 110 Propylene Oxide
- 111 Pyridine
- 112 Styrene
- 113 Sulfur Dioxide
- 114 1 1 2 2-Tetrachloroethane
- 115 Tetrachloroethylene
- 116 Titanium Tetrachloride
- 117 Toluene
- 118 o-Toluidine
- 119 1 1 1-Trichloroethane
- 120 1 1 2-Trichloroethane
- 121 Trichloroethylene
- 122 Trichlorotrifluoroethane
- 123 1 2 4-Trimethylbenzene
- 124 Vinyl Acetate
- 125 Vinyl Chloride
- 126 Vinylidene Chloride
- 127 o-Xylene
- 128 m-Xylene
- 129 p-Xylene

## **Appendix B**

### **Example Model Runs**

USAF Toxic Chemical Dispersion Model  
AFTOX

Hanscom AFB MA

Date: 02-26-1991

Time: 1028 LST

Continuous release

Hydrogen Chloride

Time Weighted Average (TWA) is not available

Short Term Exposure Limit (STEL) is 3 ppm (5 MG M-3)

Temperature = 20 C

Wind direction = 240

Wind speed = 4 M/S

Sun elevation angle is 34 degrees

Cloud cover is 5 eighths

Cloud type is high (Ci, Cc, Cs)

Ground is wet

The inversion height is 300 M

Atmospheric stability parameter is 3.14

Spill site roughness length is 10 cm

This is a gas release

Spill is at ground level

Emission rate is 100 KG/min

Elapsed time of spill is 60 min

Total amount spilled is 6000 KG

Concentration averaging time is 15 min

Elapsed time since start of spill is 60 min

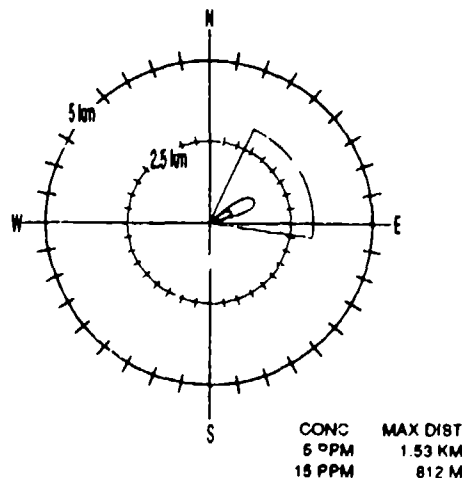
Height of interest is 2 M

-----  
At 60 min, the maximum distance for 5 PPM is 1.53 KM

Maximum toxic corridor length = 3.24 KM at 60 min

Direction & width 60 +/- 35 deg

At 60 min, the maximum distance for 15 PPM is 812 M  
-----



USAF Toxic Chemical Dispersion Model  
AFTOX

Hanscom AFB MA

Date: 02-26-1991

Time: 1110 LST

Continuous release

Aerazine-50

Short Term Exposure Limit (STEL) is .48 PPM (1.15 MG M-3)

Time Weighted Average (TWA) is .06 PPM (.14 MG M-3)

Temperature = 50 F

Wind direction = 240

Wind speed = 8 knots

Sun elevation angle is 37 degrees

Cloud cover is 2 eighths

Cloud type is high (Ci, Cc, Cs)

Ground is dry

There is no inversion

Atmospheric stability parameter is 2.59

Spill site roughness length is 50 cm

This is a liquid release

Spill is 100 gal/min

Chemical is still leaking

Area of spill is 4000 sq ft

Evaporation rate is 44.76 lbs/min

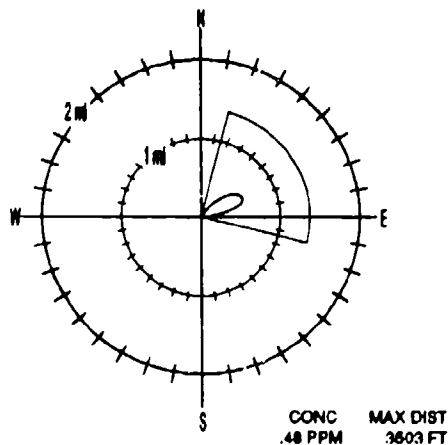
Concentration averaging time is 15 min

Height of interest is 6 ft

-----  
The maximum distance for .48 PPM is 3504 ft

Maximum toxic corridor length = 1.39 mi

Direction & width 60 +/- 43 deg  
-----



USAF Toxic Chemical Dispersion Model  
AFTOX

Hanscom AFB MA

Date: 02-26-1991

Time: 1244 LST

Instantaneous release

Nitrogen Tetroxide

Short Term Exposure Limit (STEL) is 2 PPM

Time Weighted Average (TWA) is .25 PPM

Temperature = 75 F

Wind direction = 300

Wind speed = 7 knots

Sun elevation angle is 37 degrees

Cloud cover is 0 eighths

Ground is wet

There is no inversion

Atmospheric stability parameter is 3.07

Spill site roughness length is 10 cm

This is a gas release

Spill is at ground level

Total amount released is 1000 lbs

Concentration averaging time is 1 min

Elapsed time since start of spill is 10 min

Height of interest is 6 ft

-----  
The maximum concentration is 7.81 PPM (14.67 MG M-3)

It occurs at x = 2609 M (8560 ft)

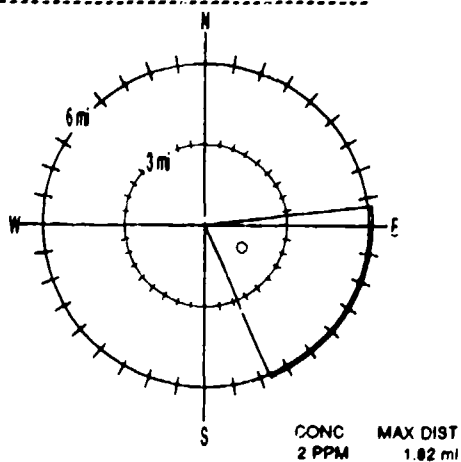
Elapsed time since start of spill is 10 min

Height of Interest is 6 ft

-----  
At 10 min, the maximum distance for 2 PPM is 1.82 mi

Maximum toxic corridor length = 6.18 mi at 18 min

Direction & Width 120 +/- 36 deg



**USAF Toxic Chemical Dispersion Model  
AFTOX**

**Vandenberg AFB**

**Date: 02-26-1991**

**Time: 1305 LST**

**Instantaneous release**

**Dimethylhydrazine (UDMH)**

**Short Term Exposure Limit (STEL) is .48 PPM (1.15 MG M-3)**

**Time Weighted Average (TWA) is .06 PPM (.14 MG M-3)**

**Temperature = 68 F**

**Wind direction = 270**

**Wind speed = 108 knots**

**Standard deviation of wind direction = 15 deg**

**Standard deviation averaging time = 15 min**

**Sun elevation angle is 44 degrees**

**Cloud cover is 0 eighths**

**Ground is dry**

**There is no inversion**

**Atmospheric stability parameter is 1.46**

**Spill site roughness length is 100 cm**

**This is a liquid release**

**Total amount spilled is 1000 M3**

**Area of spill is 10000 sq ft**

**Evaporation rate is 56.64 KG/min**

**The chemical will evaporate in 13970.2 min**

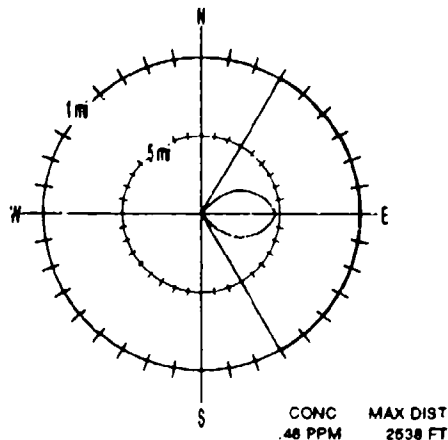
**Concentration averaging time is 15 min**

**Height of interest is 6 ft**

-----  
**The maximum distance for .48 PPM is 2539 ft**

**Maximum toxic corridor length = 1 mi**

**Direction & width 90 +/- 39 deg**  
-----



# USAF Toxic Chemical Dispersion Model

## AFTOX

Hanscom AFB MA

Date: 02-26-1991

Time: 1313 LST

Continuous buoyant plume

Temperature = 20 C

Wind direction = 280

Wind speed = 6 M/S

Sun elevation angle is 36 degrees

Cloud cover is 0 eighths

Ground is wet

The inversion height is 500 M

Atmospheric stability parameter is 3.38

Emission rate (KG/min) = 50

Effluent is still being emitted.

Stack height above ground (M) = 50

Gas stack temp (C) = 200

Volume flow rate (M3/min) = 5000

Effective plume height (M) = 132 at distance (M) = 747

Concentration averaging time is 15 min

Height of interest is 2 M

-----  
The maximum distance for .2 MG/M3 is 11.05 KM

Maximum toxic corridor length = 23.2 KM

Direction & width 100 +/- 31 deg  
-----

