

| General Characteristics | | |
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| 1 | Abstract of Model Capabilities | AFTOX is a Gaussian dispersion model that is used by the Air Force to calculate toxic corridors in case of accidental releases. It is limited to non-dense gases. It can directly calculate the evaporation rate from liquid spills. AFTOX treats instantaneous or continuous releases from any elevation, and can calculate the rise of buoyant plumes. It is intended to be consistent with the ADAM model for passive (neutrally buoyant) gas releases. |
| 2 | Sponsor and/or Developing Organization | Phillips Laboratory Directorate of Geophysics Air Force Systems Command Hanscom AFB, MA 01731-5000 |
| 3 | Last Custodian/ Point of Contact | Steven Sambol 30 WS/WES Vandenberg AFB, CA 93437-5000 805-734-8232 |
| 4 | Life-Cycle | AFTOX was developed by the U.S. Air Force in the late 1980s in order to estimate toxic corridors in the case of accidental releases of hazardous chemicals to the atmosphere. AFTOX is intended to be a replacement for the empirical OB/DG model, which was used by the Air Force for similar purposes since the 1960s. |
| 5 | Model Description Summary | AFTOX requires input of gas or liquid release amount (for instantaneous sources) or release rate (for continuous sources). It can calculate the evaporation of liquid spills. If the release is positively buoyant, it can calculate the buoyant plume rise. Dense gas effects are not accounted for. Dispersion calculations are carried out with standard Gaussian formulas. Stability class is treated as a continuous variable. Averaging time is accounted for. Outputs include maps of toxic corridors, estimates of concentration at specific positions, and estimates of the magnitude and location of the maximum concentration occurring a certain time after release. |
| 6 | Application Limitation | The code calculates evaporative emissions from liquid spills, but has no other capabilities for determining source emissions. Dense gases are not accounted for. Batch runs are difficult to make. Outputs are limited to contour plots and simplified tables. |
| 7 | Strengths/ Limitations | Strengths: A strength of AFTOX is that it has undergone extensive testing and troubleshooting. The developer, Bruce Kunkel, has made sure that AFTOX and ADAM (valid for dense gases) approach each other in the limit of passive (non-dense) releases. The meteorological processor/stability class estimator represents the state of the art in boundary layer theory. AFTOX allows 90% confidence bounds to be printed out for toxic corridors and concentrations at a point. Limitations: The major weakness of AFTOX is that it does not treat dense gases, which are frequently encountered in accidental release scenarios. Also, it would help the user if an algorithm were added to calculate the emission rate from pressurized tank or pipe ruptures. AFTOX could be made more useful by modifying the input and output modules so that batch runs could be made and so that more extensive output files could be printed or plotted. |
| 8 | Model References | ! Kunkel, B. A., 1991: AFTOX 4.0 — The Air Force Toxic Chemical Dispersion Model — A User's Guide. PL-TR-91-2119, Environmental Research Papers No. 1083, Phillips Laboratory, Directorate of Geophysics, Air Force Systems Command, Hanscom AFB, MA 01731-5000, 62 pages. ! Kunkel, B.A., 1985: Development of an Atmospheric Diffusion Model for Toxic Chemical Releases. AFGL-TR-85-0338, AFGL/AFSC, USAF, Hanscom AFB, MA 01731-5000. ! Kunkel, B.A., 1988: User's Guide for the Air Force Toxic Chemical Dispersion Model (AFTOX). AFGL-TR-88-0009, AFGL/AFSC, USAF, Hanscom AFB, MA 01731-5000. |
| 9 | Input Data/Parameter Requirements | The user must specify the site and time information, chemical information, release information, ground conditions, atmospheric conditions, and output options in order to make a model run. The chemical database for AFTOX contains properties for roughly 80 chemicals. The specification of the source strength is mandatory for all releases, except for a continuous liquid spill where the evaporation rate can be estimated by the model. By default, AFTOX determines atmospheric stability using Golder's nomogram, based on the surface roughness specified by the user and the Monin-Obukhov length internally calculated by the model. If the standard deviation of wind direction is known and is provided as an input, AFTOX will use it to determine atmospheric stability. (The same procedure is also used in the ADAM model to determine atmospheric stability.) One deficiency with the input structure for AFTOX is that the user cannot save the input data for a case so that it can be rerun later on. |

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| 10 | Output Summary | The output generated by the AFTOX model includes three options: (1) concentration contours on the computer screen for up to three user-defined concentration values, (2) concentration at a specified location and time, and (3) maximum concentration at a specified elevation and time. For option (2), the user must specify the receptor locations one at a time. That is, AFTOX does not automatically generate a distribution (or table) of predicted concentrations with downwind distance. For option (3), AFTOX will calculate the location of the maximum concentration for a given elevation and elapsed time. |
| 11 | Applications | See item 8 above. Also, Hanna et al. (1993) included AFTOX in their comprehensive exercise in which 15 models were evaluated using field data from eight sites (see number 19 below). |
| 12 | User-Friendliness | The AFTOX model has a text-based interactive user interface, where the user is prompted with a series of questions in order to define a scenario. The user needs to further decide an output option (see number 10 above) before the model performs any calculations. Due to the interactive nature of its input structure, AFTOX can be considered as user friendly in that the user seldom needs to consult the user's manual. However, it is a tedious task to obtain predicted concentrations at a series of downwind distances, since, as mentioned in number 10 above, the user can specify receptor locations only one at a time. Furthermore, AFTOX does not allow the user to save the input data for one case for later use for other cases. Therefore, if it is necessary to run the same case again, all information will have to be entered again. |
| 13 | Hardware-Software Interface Constraints/ Requirements | Computer operating system: The AFTOX model runs in the MS-DOS environment. Computer platform: Disk space requirements: A minimum of less than 1 MB. Run execution time (for a typical problem): The model takes only a few seconds to run on a Pentium PC for a typical scenario. Programming language: Both the computational and graphical output portions of the code are written in Zenith BASIC (ZBASIC), which is specific to PCS. Other computer peripheral information: AFTOX cannot be directly ported to other computer platforms. The model does not interface with other codes; however, the ADAM dense gas code has been designed to reduce to AFTOX in the passive gas limit (both models were developed for the U.S. Air Force). |
| 14 | Operational Parameters | Identify whether the code has any error diagnostic messages to assist the user in troubleshooting operational problems: The AFTOX model validates some, but not all, input parameters that the user specifies from the keyboard. The user will be asked to reenter the value for a variable if that value is found to be out of range. The model has no runtime error diagnostics. However, since simple Gaussian-type dispersion algorithms are used, the code is quite robust and rarely encounters numerical difficulties. Set up time for: Requires minimal initial setup. After the model files are copied onto a computer's hard disk, the user simply types "AFTOX" to run the model. |
| 15 | Surety Considerations | All quality assurance documentation: No information provided. Benchmark runs: No information provided. Validation calculations: No information provided. Verification with field experiments that has been performed with respect to this code: AFTOX was included in the comprehensive model evaluation exercise reported by Hanna et al. (1993). Since AFTOX does not treat the dispersion of denser-than-air gases, the model was mainly evaluated using the Prairie Grass and Hanford field experiments where the releases were neutrally buoyant. In general, AFTOX overpredicted the observed concentrations by a small amount (less than a factor of 2). |
| 16 | Runtime Characteristics | The AFTOX model is intended to be run in interactive mode, where the user is prompted with a series of questions during the runtime. However, if the user is very familiar with the input requirements for AFTOX, it is possible to run the model in batch mode using the feature of input-redirection, i.e., redirecting the keyboard input to a file, available in MS-DOS. |

Specific Characteristics

Part A: Source Term Submodel Type

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| A1 | Source Term Algorithm? | <input checked="" type="checkbox"/> YES <input type="checkbox"/> NO |
| A2 | For Chemical Consequence Assessment Models | Liquid spill: <input checked="" type="checkbox"/> pool evaporation <input type="checkbox"/> particulate resuspension Pressurized releases: <input type="checkbox"/> two-phase jets <input type="checkbox"/> flashing <input type="checkbox"/> entrainment <input type="checkbox"/> aerosol formation Solid spills: <input type="checkbox"/> resuspension <input type="checkbox"/> sublimation |

| Part B: Dispersion Submodel Type | | |
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| B1 | Gaussian | <input checked="" type="checkbox"/> Straight-line plume <input type="checkbox"/> Segmented plume <input type="checkbox"/> Statistical plume <input type="checkbox"/> Statistical puff |
| B2 | Similarity | <input checked="" type="checkbox"/> Plume <input checked="" type="checkbox"/> Puff Plume releases are modeled by the direct input of χ/Q_s to the program by the user. Puff releases are modeled by requesting the program to calculate s_y or the user can directly input s_y . |
| Part C: Transport Submodel Type | | |
| C2 | Deterministic | Yes |
| C4 | Frame of Reference | <input checked="" type="checkbox"/> Eulerian <input type="checkbox"/> Lagrangian <input type="checkbox"/> Hybrid <input type="checkbox"/> Eulerian-Lagrangian |
| Part D: Fire Submodel Type (Not Applicable) | | |
| Part E: Energetic Events Submodel Type (Not Applicable) | | |
| Part F: Health Consequence Submodel Type | | |
| F1 | For Chemical Consequence Assessment Models | Health effects: <input type="checkbox"/> fatalities <input type="checkbox"/> cancers <input type="checkbox"/> latent cancers <input type="checkbox"/> symptom onset Health criteria <input type="checkbox"/> IDLH <input type="checkbox"/> STEL <input type="checkbox"/> TLV <input type="checkbox"/> TWA <input type="checkbox"/> ERPG <input type="checkbox"/> TEEL <input type="checkbox"/> AEGL <input type="checkbox"/> WHO Zones with flammable limits: <input type="checkbox"/> UFL <input type="checkbox"/> LFL Blast overpressure regions: Fire radiant energy zones: Risk qualification: Concentration: <input checked="" type="checkbox"/> single value <input type="checkbox"/> time-history <input type="checkbox"/> integrated dose Probits: Probits are used to compute the probability of a particular health consequence (e.g., fatality). Expressed as chemical specific probability units computed with a logarithmic probit equation. Other: 90% confidence intervals are generated for toxic corridors and concentrations. |
| Part G: Effects and Countermeasures Submodel Type (No Information Provided.) | | |
| Part H: Physical Features of Model | | |
| H2 | Release Elevation | <input checked="" type="checkbox"/> ground <input checked="" type="checkbox"/> roof |
| H4 | Horizontal Plume Meander | s_y increases as averaging time increases according to a power-law approximation |
| H7 | Cloud Buoyancy | <input type="checkbox"/> neutral [passive] <input type="checkbox"/> dense [negative] <input type="checkbox"/> plume rise [positive] |
| Part I: Model Input Requirements | | |
| I1 | Radio(chemical) and Weapon Release Parameters | Release rate: <input type="checkbox"/> Continuous <input type="checkbox"/> Time dependent <input type="checkbox"/> Instantaneous Release container characteristics: <input checked="" type="checkbox"/> vapor temperature <input type="checkbox"/> tank diameter <input type="checkbox"/> tank height <input type="checkbox"/> tank temperature <input type="checkbox"/> tank pressure <input type="checkbox"/> nozzle diameter <input type="checkbox"/> pipe length Jet release: <input type="checkbox"/> initial size <input type="checkbox"/> shape <input type="checkbox"/> concentration profile at end of jet affected zone Release dimensions: <input type="checkbox"/> point <input type="checkbox"/> line <input checked="" type="checkbox"/> area Release elevation: <input checked="" type="checkbox"/> ground <input checked="" type="checkbox"/> roof <input checked="" type="checkbox"/> stack |

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| I2 | Meteorological Parameters | <p>Wind speed and wind direction: <input checked="" type="checkbox"/> single point <input type="checkbox"/> single tower/multiple point <input type="checkbox"/> multiple towers</p> <p>Temperature: <input checked="" type="checkbox"/> single point <input type="checkbox"/> single tower/multiple point <input type="checkbox"/> multiple towers</p> <p>Dew point temperature: <input type="checkbox"/> single point <input type="checkbox"/> single tower/multiple point <input type="checkbox"/> multiple towers</p> <p>Precipitation: <input type="checkbox"/> single point <input type="checkbox"/> single tower/multiple point <input type="checkbox"/> multiple towers</p> <p>Turbulence typing parameters: <input type="checkbox"/> temperature difference <input checked="" type="checkbox"/> sigma theta <input type="checkbox"/> sigma phi <input type="checkbox"/> Monin-Obukhov length <input type="checkbox"/> roughness length <input type="checkbox"/> cloud cover <input type="checkbox"/> incoming solar radiation <input type="checkbox"/> user-specified</p> <p>Four dimensional meteorological fields from prognostic model:</p> |
| Part J: Model Output Capabilities | | |
| J1 | Hazard Zone | Yes |
| J2 | Graphic Contours and Resolution | The area of a hazard zone is calculated and displayed on the computer screen. |
| J3 | Concentration Versus Time Plots | Yes |
| J4 | Tabular at Fixed Downwind Locations | Yes |
| Part K: Model Usage Considerations (No Information Provided.) | | |