

## SUMMARY DESCRIPTIONS OF ALTERNATIVE AIR QUALITY MODELS

### Introduction and Availability

We have provided a list of compendia for *preferred/recommended* refined air dispersion models in Appendix A of the *Guideline on Air Quality Models* (Appendix W of 40 CFR Part 51), hereafter, *Guideline*. Alternatively, in **this** document is a compendium of refined air quality models justified for use on a case-by-case basis for individual regulatory applications. For each model, information is provided on availability, approximate cost (where applicable), regulatory use, data input, output format and options, simulation of atmospheric physics and accuracy. The models are listed by name in alphabetical order. The list may, at our discretion, be changed at any time. To the extent practicable, this process will be “vetted” on this website whereby we will post a notice of candidate models to be purged and entertain objections. If it comes to our attention that a model’s developer is no longer “findable” per information provided in the *Availability* section, we may remove the summary description from the list. It is the model developer’s responsibility to keep us informed of changes to availability status. Otherwise, we will to a reasonable extent revise summary descriptions at the behest of a model’s developer. Additions and updates by model developers are welcome. We ask, however, that these be provided to the Webmaster in WordPerfect® format, adhering to the structure used for the model summary descriptions.

There are three separate conditions under which these models will normally be approved for use by a reviewing authority:

1. A demonstration can be made that the model produces concentration estimates equivalent to the estimates obtained using a preferred model (e.g., the maximum or high, second-high concentration is within 2% of the estimate using the comparable *preferred* model);
2. A statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the model appearing in this list performs better for the application than a comparable model in Appendix A; and
3. There is no preferred model for the specific application but a refined model is needed to satisfy regulatory requirements.

Any one of these three separate conditions may warrant use of these models. See subsection 3.2, Use of Alternative Models, of the *Guideline* for additional details.

Addition of a model to this list does not imply that the model has necessarily been subject to any formal performance review. Some of these models have been subject to a performance evaluation by comparison with observed air quality data. Where possible, several of the models contained herein have been subjected to rigorous evaluation exercises, including (1) statistical performance measures recommended by the American Meteorological Society and (2) peer scientific reviews.

Codes and documentation for some models listed in this appendix are available from EPA’s Support Center for Regulatory Air Models (SCRAM) website at [www.epa.gov/scram001](http://www.epa.gov/scram001). Documentation is also available from the National Technical Information Service (NTIS), U.S. Department of Commerce, Springfield, VA 22161; phone: (800) 553-6847. Where possible, accession numbers are provided.

## **Alternative models for use with case-by-case justification**

Atmospheric Dispersion Modeling System (ADMS)

Comprehensive Air Quality Model with Extensions (CAMx)

Dense Gas Dispersion Model (DEGADIS)

HGSYSTEM

HOTMAC / RAPTAD

HYROAD

Open Burn/Open Detonation Dispersion Model (OBODM)

Panache

Plume Visibility Model (PLUVUE II)

Second-order Closure Integrated PUFF Model (SCIPUFF)

Shoreline Dispersion Model (SDM)

SLAB

## Atmospheric Dispersion Modeling System (ADMS)

### *Reference*

ADMS 3 User Guide, Version 3.2. July 2004, Cambridge Environmental Research Consultants. Available for download: <http://www.cerc.co.uk/software/publications.htm>

Carruthers, D.J., R.J. Holroyd, J.C.R.Hunt., W.-S. Weng, A.G. Robins, D.D. Apsley, D.J. Thompson and F.B. Smith, 1994. UK-ADMS: A new approach to modelling dispersion in the earth's atmospheric boundary layer. *Journal of Wind Engineering and Industrial Aerodynamics*, 52: 139-153. Elsevier Science B.V.

### *Availability*

The model code is available on diskette or CD from Cambridge Environmental Research Consultants (CERC), 3 King's Parade, Cambridge, CB2 1SJ. UK. Tel: 00 44 1223 357773, Fax: 00 44 1223 357492; e-mail: [ADMS@cerc.co.uk](mailto:ADMS@cerc.co.uk)

### *Abstract*

ADMS is an advanced model for calculating concentrations of pollutants emitted both continuously from point, line, volume and area sources, or discretely from point sources. The model includes algorithms which take account of the following: effects of main site building; complex terrain; wet deposition, gravitational settling and dry deposition; short term fluctuations in concentration; chemical reactions; radioactive decay and  $\gamma$ -dose; plume rise as a function of distance; jets and directional releases; averaging time ranging from very short to annual; condensed plume visibility; meteorological preprocessor.

#### *a. Recommendations for Regulatory Use*

The model can be used for the following regulatory purposes:

- multiple buoyant or passive industrial emissions
- urban or rural areas
- flat or complex terrain
- transport distances less than 50km
- short term (seconds) to annual averaging times

#### *b. Input Requirements*

Source data: location, emission rate, physical stack height, stack gas exit velocity, stack inside diameter, and stack gas temperature. Operational inputs include source elevation, building dimensions, particle size distribution with corresponding settling velocities, and surface reflection coefficients.

Meteorological data: hourly surface observations for input into the meteorological preprocessor and/or boundary layer parameters (boundary layer height, Monin-Obukhov length, surface heat flux, etc).

### *c. Output*

Concentration for specified averaging times at receptor points or on an output grid: averages of concentration over a specified period and percentiles of these averages. Short and long term averages of wet, dry and total deposition and radioactive activity. Number of exceedences of specified standard by ensemble mean concentration and by concentration calculated taking account of short term fluctuations. Output for short term fluctuations, percentiles, PDF, toxic dose.

Advanced graphical output: line plotting of centreline variables and link to a contour plotting package.

### *d. Type of Model*

The model is an advanced Gaussian type model using a Gaussian distribution for the concentration except for the case of the vertical distribution in unstable conditions when a skewed Gaussian is employed (Carruthers *et al.*, 1991). Plume spread is calculated using local boundary layer variables.

### *e. Pollutants Types*

May be used to model primary pollutants and continuous releases of toxic and hazardous waste products. Settling and wet and dry deposition are treated. Radioactive decay is calculated.

### *f. Source Receptor Relationship*

Up to 50 receptors may be specified in addition to an output grid with regular or variable spacing (up to 2048 gridded points).

### *g. Plume Behavior*

ADMS uses a Lagrangian plume rise model, a buildings effect model based on a two plume approach, using wake averaged flow values to calculate plume spread (Robins *et al.*, 1997) and a complex terrain module based on the linearised airflow model FLOWSTAR (Carruthers *et al.*, 1988).

### *h. Horizontal Winds*

A steady state wind is assumed for each hour; this varies in the vertical according to specified boundary layer profiles and in the horizontal plane when the boundary or complex terrain algorithm is employed.

### *i. Vertical Wind Speed*

Vertical wind speed is zero except when the buildings or complex terrain algorithms are employed.

### *j. Horizontal Dispersion*

Horizontal dispersion parameters are locally (at mean plume height) derived from the calculated horizontal components of turbulence.

#### *k. Vertical Dispersion*

Vertical dispersion parameters are locally derived from the calculated vertical component of turbulence and the buoyancy frequency.

#### *l. Chemical Transformation*

A generic reaction set is employed to calculate the interaction of NO, NO<sub>2</sub>, and O<sub>3</sub> (McHugh *et al.*, 1997).

#### *m. Physical Removal*

Dry deposition effects for particles are treated using a resistance formulation in which the deposition velocity is the sum of the resistances to pollutant transfer within the surface layer of the atmosphere, across the laminar sublayer and onto the surface, plus a gravitational settling term. For gases the surface layer resistance is calculated as a function of the nature of the gas: reactive, unreactive or inert. Wet deposition is calculated making use of a specified washout coefficient which may be rainfall rate dependent.

#### *n. Evaluation Studies*

Carruthers, D.J., C.A. McHugh, A.G. Robins, B.M. Davies, D.J. Thomson and M.R. Montgomery, 1994. The UK Atmospheric Dispersion Modelling System: Comparisons with data from Kincaid, Lillestrøm and Copenhagen. *Proceedings of the Workshop Intercomparison of Advanced Practical Short-Range Atmospheric Dispersion Models*, 1993. Manno, Switzerland. C. Cuvelier, Ed.

Carruthers D.J., H.A. Edmunds, K.L. Ellis, C.A. McHugh, B.M. Davies and D.J. Thomson, 1995. The Atmospheric Dispersion Modelling System (ADMS): comparisons with data from the Kincaid experiment. *Workshop on Operational Short-range Atmospheric Dispersion Models for Environmental Impact Assessment in Europe*, Mol, Nov. 1994. *Int. J. Environment and Pollution*, **5**(4-6): 111-000.

Carruthers, D.J., H.A. Edmunds, M. Bennett, P.T. Woods, M.J.T. Milton, R. Robinson, B.Y. Underwood and C.J. Franklyn, 1995. Validation of the UK-ADMS Dispersion Model and Assessment of its Performance Relative to R-91 and ISC using Archived LIDAR Data. Study commissioned by Her Majesty's Inspectorate of Pollution. DoE/HMIP/RR/95/022

Carruthers, D.J., H.A. Edmunds, M. Bennett, P.T. Woods, M.J.T. Milton, R. Robinson, B.Y. Underwood and C.J. Franklyn, 1997. Validation of the ADMS Dispersion Model and Assessment of its Performance Relative to R-91 and ISC using Archived LIDAR Data. *Int. J. Environment and Pollution*, Vol 8, Nos. 3-6.

Carruthers, D.J., S. Dyster and C.A. McHugh, 1998. Contrasting Methods for Validating ADMS using the Indianapolis Data set. *Proc. 5<sup>th</sup> Int. Conf. on Harmonisation Within Dispersion Modelling for Regulatory Purposes*. pp. 104-110

Carruthers, D.J., H.A. Edmunds, A.E. Lester, C.A. McHugh and R.J. Singles, 1998. Use and Validation of ADMS-Urban in Contrasting Urban and Industrial Locations. *Proc. 5<sup>th</sup> Int. Conf. on Harmonisation Within Dispersion Modelling for Regulatory Purposes*. pp. 360-367

Carruthers, D.J., A.M. McKeown, D.J. Hall and S. Porter, 1999. Validation of ADMS against Wind Tunnel Data of Dispersion from Chemical Warehouse Fires. *Atmos. Env.*, **33**: 1937 - 1953.

*o. Literature Cited*

Carruthers, D.J., J.C.R. Hunt and W.-S. Weng, 1988. A computational model of stratified turbulent airflow over hills - FLOWSTAR I. *Proceedings of Envirosoft*. In: Computer Techniques in Environmental Studies. P. Zanetti (Ed.), pp. 481-492. Springer-Verlag.

Carruthers, D.J., R.J. Holroyd, J.C.R. Hunt, W.-S. Weng, A.G. Robins, D.D. Apsley, F.B. Smith, D.J. Thomson and B. Hudson, 1991. UK Atmospheric Dispersion Modelling System. *Proceedings of the 19th NATO/CCMS International Technical Meeting on Air Pollution Modelling and its Application*. September 1991, Crete, Greece. Han van Dop and George Kallos, Eds. Plenum Publishing Corporation, New York.

McHugh, C.A., D.J. Carruthers and H.A. Edmunds, 1997. ADMS and ADMS-Urban *Workshop on Operational Short-range Atmospheric Dispersion Models for Environmental Impact Assessment in Europe*, Mol, Nov. 1994. *Int. J. Environment and Pollution*, 8(306): 437-440.

Robins, A.G., D.J. Carruthers and C.A. McHugh, 1997. The ADMS Building Effects Module. *Int. J. Environment and Pollution*, Vol 8, Nos. 3-6.

## Comprehensive Air Quality Model with Extensions (CAMx)

### *Reference*

ENVIRON, 1998. User's Guide to the Comprehensive Air Quality Model with Extensions (CAMx) Version 2.00. ENVIRON International Corporation, 101 Rowland Way, Suite 220, Novato, California 94945-5010.

### *Availability*

The model source code, user's guide, test problem, and documentation on example applications are publicly available from the CAMx website at [www.camx.com](http://www.camx.com) or from ENVIRON International Corporation, 101 Rowland Way, Novato, CA 94945 (415/899-0700) at no cost.

### *Abstract*

CAMx is a multi-scale, three dimensional photochemical grid model. The model contains two-way grid nesting, subgrid-scale Plume-in-Grid (PiG), fast accurate chemistry solver, a chemical mechanism compiler, generalized coordinate system to accommodate multiple map projections, and options for using more accurate solvers for transport and diffusion. CAMx unique attributes include an ozone source apportionment capability whereby the contributions of emissions from geographic source regions and different source categories to ozone concentrations can be calculated within a single simulation. The model incorporates two options for condensed photochemical kinetics mechanisms: the Carbon Bond Version IV (CB-IV) mechanism and the 1997 version of the mechanism from the State Air Pollution Research Center (SAPRC97). The CAMx is designed for computing hourly ozone (O<sub>3</sub>) concentrations at the regional, mesoscale, and urban scales for periods ranging from a day up to months. CAMx also incorporates a capability to compute primary and secondary particulate matter (PM) concentrations. For O<sub>3</sub> calculations, emissions of oxides of nitrogen (NO<sub>x</sub>), volatile organic compounds (VOC), and carbon monoxide (CO) are required. The simulation of PM requires emissions of sulfur oxides (SO<sub>x</sub>), ammonia (NH<sub>3</sub>), and primary PM species in addition to those needed for O<sub>3</sub>. The model treats VOC emissions as either their CB-IV or SAPRC97 surrogates. CAMx can also be run in a "nonreactive mode" to predict carbon monoxide (CO) and other inert or semi-inert species concentrations.

#### *a. Recommendations for Regulatory Use*

CAMx is appropriate for simulating hourly ozone, CO, and PM concentrations from the urban-scale to regional-scale; the hourly concentration estimates can be used to generate mean ozone, CO, and PM concentrations at longer than hourly time-scales, including 8-hour, daily, monthly, seasonal, and annual.

CAMx has many options, such as the CB-IV (Gery *et al.*, 1989) with enhanced isoprene chemistry (Carter, 1990) or SAPRC97 (Carter 1990;1996) chemical mechanisms, three optional advection solvers (Smolarkiewicz, 1983, Bott, 1989, or the Piecewise Parabolic Method, PPM), grid resolution (< 1km to > 100km), map projections (e.g., Lat/Long, UTM, Lambert Conformal Projection, Polar Stereographic Projection), cloud inputs, PiG configuration, but no specific recommendations can be made at this time on all options. The reviewing agency should be

consulted on selection of options to be used in regulatory applications.

#### *b. Input Requirements*

Source data for ozone modeling include gridded, hourly emissions of CB-IV or SAPRC97 speciated VOC, CO, NO, and NO<sub>2</sub> for low-level and elevated sources along with stack coordinates, stack height, stack diameter, exit velocity, and exit temperature for elevated sources. For PM modeling, hourly emissions from low-level and elevated sources include those necessary for ozone modeling, along with SO<sub>x</sub>, NH<sub>3</sub>, and primary PM, which can be optionally resolved by size (e.g., PM-2.5 and PM-10) and composition (e.g., elemental carbon, organic carbon, and crustal). For CO modeling, only CO emissions for surface and elevated sources need be specified.

Meteorological data needed are hourly, gridded, three-dimensional horizontal winds, temperature, pressure, vertical turbulent exchange coefficients, and optionally either total opaque cloud cover or cloud cover fraction, depth, and liquid water content. Additional hourly, gridded two-dimensional inputs for rainfall rate (optional), land use cover fractions, total ozone column, albedo, and turbidity are also needed.

Air quality data needed include concentration of all species at the beginning of the simulation for each grid cell (initial concentrations) and hourly concentrations of each pollutant at each level along the lateral boundaries and top boundary of the modeling region (boundary conditions).

Additional input data needed include the chemical reaction rates file and simulation control file which describes the number and definitions of any nested-grids and the definitions of the model options. If the source apportionment option is specified, then additional inputs are required on the type of source apportionment, the geographic regions for which source attribution will be calculated, and separate emissions files for each source category for which separate ozone apportionment will be calculated.

#### *c. Output*

Output includes three-dimensional gridded hourly (or other user--specified averaging period) average and instantaneous concentrations. Information on mass fluxes for all species and all grids are also output along with job summary and diagnostic information.

#### *d. Type of Model*

CAMx is a numerical multi-scale three dimensional, photochemical and particulate matter grid model.

#### *e. Pollutant Types*

CAMx may be used to model ozone (O<sub>3</sub>) formation from oxides of nitrogen (NO<sub>x</sub>) and volatile organic compound (VOC) emissions. Optionally, CAMx may also be used to simulate PM-2.5 and PM-10 and PM components (e.g., sulfate, nitrate, ammonium, secondary organic carbon, and primary elemental carbon, organic carbon, and crustal). It can also be used to model

carbon monoxide (CO).

#### *f. Source-Receptor Relationship*

Low-level area and point source emissions are specified within each surface grid cell. Emissions from major point sources are placed within cells aloft in accordance with calculated effective plume heights; emissions from point sources may be optionally simulated using the subgrid-scale PiG algorithm. An optional ozone source apportionment algorithm allows for the calculation of the ozone contributions due to user-specified source regions and source categories.

Hourly average concentrations of each pollutant are calculated for all grid cells at the surface and optionally at each vertical level.

#### *g. Plume Behavior*

Plume rise is calculated for major point sources using relationships in the TUPOS Gaussian model (Turner *et al.*, 1986). For user-specific point sources, the early plume dynamics and plume-scale chemistry is calculated using a subgrid-scale Plume-in-Grid (PiG) algorithm; when the plume size is commensurate with the grid cell size the PiG algorithm releases the plume mass to the grid model for further computation.

#### *h. Horizontal Winds*

Hourly, gridded, three-dimensional horizontal (U and V) winds are required (see *Input Requirements*).

#### *i. Vertical Wind Speed*

Calculated at each vertical grid cell interface from the compressible mass continuity relationship using the input gridded horizontal wind field (assumes conservation of local density).

#### *j. Horizontal Dispersion*

Hourly, gridded three-dimensional horizontal eddy diffusivities are calculated internally in the model based on the deformation of the wind field (Smagorinsky, 1963).

#### *k. Vertical Dispersion*

Hourly, gridded, three-dimensional vertical eddy diffusivities are provided as input to the model and are usually based on output from a prognostic meteorological model.

#### *l. Chemical Transformation*

CAMx employs two options for photochemistry: Version IV of the Carbon Bond Mechanism with updated isoprene chemistry (CB-IV); and the 1997 chemical mechanism developed at the State Air Pollution Research Center (SAPRC97).

#### *m. Physical Removal*

Dry deposition of pollutants are calculated using the resistance approach algorithm developed by Wesely (1989). Grid cell dependent surface roughness and surface resistance is calculated based the fractional coverage of the input land use categories. Wet scavenging is calculated based on hourly rainfall rate in each grid column using a species-dependent Henry's Law solubility.

*n. Evaluation Studies*

Sonoma Technology, Inc., 1997. Peer Review of ENVIRON's Ozone Source Apportionment Technology and the CAMx Air Quality Model, Final Report STI996203-1732-FR. Prepared for the Division of Air Pollution Control Ohio Environmental Protection Agency.

Sonoma Technology, Inc., 1997. Comparison of CAMx and UAM-V Model Performance for Two Ozone Episodes in the Eastern United States, Final Report STI-996203-1733-FR. Prepared for the Division of Air Pollution Control Ohio Environmental Protection Agency.

Reynolds, S. and P. Roth, 1997. Peer Review of the CAMx Ozone Source Apportionment Technology. Report from the EPA Source Attribution Workshop, July 16-18, 1997 RTP, NC. U.S. Environmental Protection Agency, Research Triangle Park, North Carolina.

TNRCC, 1998. Comparative Evaluation of CAMx and UAM for the Houston/Beaumont COAST Domain. Letter from James W. Thomas P.E. Texas Natural Resources Conservation Commission to Thomas Diggs EPA Region 6 dated April 13, 1998.

McNally, D.E. and T.W. Tesche, 1997a. "Modeled Effects of Indiana Point Source NOx Emissions Reductions on Local and Regional 1-hr and 8-hr Ground Level Ozone Concentrations in 1995 and 2007 Using Two OTAG Oxidant Episodes", prepared for the Indiana Electric Utility Air Workgroup, prepared by Alpine Geophysics, LLC, Golden, CO.

McNally, D.E. and T.W. Tesche, 1997b. "Comparative Evaluation of the CAMx and UAM-V Models Over the Northeastern U.S. Using the July 1995 OTAG Episode and the NARSTO-NE Intensive Field Study Data", prepared for the Virginia Department of Environmental Quality, prepared by Alpine Geophysics, LLC, Golden, CO.

McNally, D.E. *et al.*, 1998. "Photochemical Modeling Analysis of the Effects of Electric Utility NOx Emissions Reductions in Eastern Missouri on 1-Hr and 8-Hr Ozone Concentrations", prepared for the Missouri Electric Utility Environmental Committee, prepared by Alpine Geophysics, LLC, Boulder, CO.

Tesche, T.W. and D.E. McNally, 1998. "Cincinnati-Hamilton Ozone Attainment Demonstration Study: Volume 7: Model Evaluation and Assessment of Model Reliability for Attainment Demonstration", prepared for the Ohio Environmental Protection Agency, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W. *et al.*, 1998a, "Photochemical Modeling Analysis of the Effects of VOC and NOx Emissions Reductions on 1-hr and 8-hr Ozone Concentrations in Kentucky", prepared

for Louisville Gas and Electric Co., prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W. *et al.*, 1998b, “Photochemical Modeling Analysis of the Effects of VOC and NO<sub>x</sub> Emissions Reductions in the Kansas City Nonattainment Area on 1-hr and 8-hr Ozone Concentrations”, prepared for Kansas City Gas and Electric Co., prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W. *et al.*, 1998c, “Photochemical Modeling Analysis of the Subregional Effects of the EPA Section 110 SIP Call Within and Downwind of the State of Virginia”, prepared for Allied Signal, Inc., prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W. *et al.*, 1998d, “Analysis of the Effects of VOC and NO<sub>x</sub> Emissions Reductions in the Eastern United States on Peak 1-hr and 8-hr Ozone Concentrations”, prepared for the Midwest Ozone Group, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Morris R.E., G. Yarwood, G.M. Wilson and K. Lee. 1997. “Comparison of the CAMx Ozone Source Apportionment Results with Targeted Geographic Region UAM-V Emissions Reduction Sensitivity Scenarios” Prepared for Division of Air Pollution Control Ohio Environmental Protection Agency. Environ International Corporation, Novato, California, September.

Lehmann, E., 1998. “The Predictive Performance of The Photochemical Grid Models UAM-V and CAMx for The Northeast Corridor”. Presented at the Air & Waste Management Association 91st Annual Meeting & Exhibition, San Diego, California, June 14-18, 1998.

Morris, R.E., G.M. Wilson, E. Tai and J. Hower, 1998. Assessment of the Contribution of Industrial and Other Source Sectors to Ozone Exceedances in the Eastern United States, Final Report. Prepared for Division of Air Pollution Control Ohio Environmental Protection Agency, prepared by ENVIRON International Corporation, Novato, California, June, 1998.

Yocke, M.A. *et al.*, 1996. Future-Year Boundary Conditions for Urban Airshed Modeling for the State of Texas, Final Report. Prepared for Texas Natural Resource Conservation Commission, prepared by ENVIRON International Corporation, Novato, California, Sonoma Technology, Inc., Santa Rosa, California, and ASTER\*/MRC, Fort Collins, Colorado, August, 1996.

#### *o. Literature Cited*

Bott, A., 1989. A Positive Definite Advection Scheme Obtained by Nonlinear Renormalization of the Advective Fluxes. *Mon. Wea. Rev.*, **117**: 1006-1015.

Carter, W.P., 1990. A Detailed Mechanism for the Gas-Phase Atmospheric Reactions of Organic Compounds. *Atmos. Environ.*, **24A**, 481-518.

Carter, W.P., 1996. Condensed Atmospheric Photooxidation Mechanisms for Isoprene. *Atmos. Environ.*, **30**: 4275-4290.

Smagorinsky, J., 1963. General Circulation Experiments with the Primitive Equations: I. The Basic Experiment. *Mon. Wea. Rev.*, **91**, 99-164.

Smolarkiewicz, P.K., 1983. A Simple Positive Definite Advection Scheme with Small Implicit Diffusion. *Mon. Wea. Rev.*, **111**: 479-486.

Turner D.B., T. Chico and J.A. Catalano, 1986. TUPOS - A Multiple Source Gaussian Dispersion Algorithm Using On-Site Turbulence Data. EPA Publication No. EPA-600/8-86/010. U.S. Environmental Protection Agency, Research Triangle Park, North Carolina.

Wesely, M.L., 1989. Parameterization of Surface Resistances to Gaseous Dry Deposition in Regional-Scale Numerical Models. *Atmos. Environ.*, **23**, 1293-1304.

## Dense Gas Dispersion Model (DEGADIS)

### *Reference*

Environmental Protection Agency, 1989. User's Guide for the DEGADIS 2.1 - Dense Gas Dispersion Model. EPA Publication No. EPA-450/4-89-019. U.S. Environmental Protection Agency, Research Triangle Park, NC 27711. (NTIS No. PB 90-213893)

### *Availability*

The model code is only available on the SCRAM Internet website (see [Introduction and Availability](#)).

### *Abstract*

DEGADIS 2.1 is a mathematical dispersion model that can be used to model the transport of toxic chemical releases into the atmosphere. Its range of applicability includes continuous, instantaneous, finite duration, and time-variant releases; negatively-buoyant and neutrally-buoyant releases; ground-level, low-momentum area releases; ground-level or elevated upwardly-directed stack releases of gases or aerosols. The model simulates only one set of meteorological conditions, and therefore should not be considered applicable over time periods much longer than 1 or 2 hours. The simulations are carried out over flat, level, unobstructed terrain for which the characteristic surface roughness is not a significant fraction of the depth of the dispersion layer. The model does not characterize the density of aerosol-type releases; rather, the user must assess that independently prior to the simulation.

#### *a. Recommendations for Regulatory Use*

DEGADIS can be used as a refined modeling approach to estimate short-term ambient concentrations (1-hour or less averaging times) and the expected area of exposure to concentrations above specified threshold values for toxic chemical releases. The model is especially useful in situations where density effects are suspected to be important and where screening estimates of ambient concentrations are above levels of concern.

#### *b. Input Requirements*

Data may be input directly from an external input file or via keyboard using an interactive program module. The model is not set up to accept real-time meteorological data or convert units of input values. Chemical property data must be input by the user. Such data for a few selected species are available within the model. Additional data may be added to this data base by the user.

Source data requirements are: emission rate and release duration; emission chemical and physical properties (molecular weight, density vs. concentration profile in the case of aerosol releases, and contaminant heat capacity in the case of a nonisothermal gas release; stack parameters (i.e., diameter, elevation above ground level, temperature at release point).

Meteorological data requirements are: wind speed at designated height above ground, ambient temperature and pressure, surface roughness, relative humidity, and ground surface

temperature (which in most cases can be adequately approximated by the ambient temperature).

Receptor data requirements are: averaging time of interest, above-ground height of receptors, and maximum distance between receptors (since the model computes downwind receptor distances to optimize model performance, this parameter is used only for nominal control of the output listing, and is of secondary importance). No indoor concentrations are calculated by the model.

### *c. Output*

Printed output includes in tabular form:

- Listing of model input data;
- Plume centerline elevation, mole fraction, concentration, density, and temperature at each downwind distance;
- $\sigma_y$  and  $\sigma_z$  values at each downwind distance;
- Off-centerline distances to 2 specified concentration values at a specified receptor height at each downwind distance (these values can be used to draw concentration isopleths after model execution);
- Concentration vs. time histories for finite-duration releases (if specified by user).

The output print file is automatically saved and must be sent to the appropriate printer by the user after program execution.

No graphical output is generated by the current version of this program.

### *d. Type of Model*

DEGADIS estimates plume rise and dispersion for vertically-upward jet releases using mass and momentum balances with air entrainment based on laboratory and field-scale data. These balances assume Gaussian similarity profiles for velocity, density, and concentration within the jet. Ground-level denser-than-air phenomena is treated using a power law concentration distribution profile in the vertical and a hybrid top hat-Gaussian concentration distribution profile in the horizontal. A power law specification is used for the vertical wind profile. Ground-level cloud slumping phenomena and air entrainment are based on laboratory measurements and field-scale observations.

### *e. Pollutant Types*

Neutrally- or negatively-buoyant gases and aerosols. Pollutants are assumed to be non-reactive and non-depositing.

### *f. Source-Receptor Relationships*

Only one source can be modeled at a time.

There is no limitation to the number of receptors; the downwind receptor distances are internally-calculated by the model. The DEGADIS calculation is carried out until the plume centerline concentration is 50% below the lowest concentration level specified by the user.

The model contains no modules for source calculations or release characterization.

#### *g. Plume Behavior*

Jet/plume trajectory is estimated from mass and momentum balance equations. Surrounding terrain is assumed to be flat, and stack tip downwash, building wake effects, and fumigation are not treated.

#### *h. Horizontal Winds*

Constant logarithmic velocity profile which accounts for stability and surface roughness is used.

The wind speed profile exponent is determined from a least squares fit of the logarithmic profile from ground level to the wind speed reference height. Calm winds can be simulated for ground-level low-momentum releases.

Along-wind dispersion of transient releases is treated using the methods of Colenbrander (1980) and Beals (1971).

#### *i. Vertical Wind Speed*

Not treated.

#### *j. Horizontal Dispersion*

When the plume centerline is above ground level, horizontal dispersion coefficients are based upon Turner (1969) and Slade (1968) with adjustments made for averaging time and plume density.

When the plume centerline is at ground level, horizontal dispersion also accounts for entrainment due to gravity currents as parameterized from laboratory experiments.

#### *k. Vertical Dispersion*

When the plume centerline is above ground level, vertical dispersion coefficients are based upon Turner (1969) and Slade (1968). Perfect ground reflection is applied.

In the ground-level dense-gas regime, vertical dispersion is also based upon results from laboratory experiments in density-stratified fluids.

#### *l. Chemical Transformation*

Not specifically treated.

*m. Physical Removal*

Not treated.

*n. Evaluation Studies*

Spicer, T.O. and J.A. Havens, 1986. Development of Vapor Dispersion Models for Nonneutrally Buoyant Gas Mixtures - Analysis of USAF/N<sub>2</sub>O<sub>4</sub> Test Data. USAF Engineering and Services Laboratory, Final Report ESL-TR-86-24.

Spicer, T.O. and J.A. Havens, 1988. Development of Vapor Dispersion Models for Nonneutrally Buoyant Gas Mixtures - Analysis of TFI/NH<sub>3</sub> Test Data. USAF Engineering and Services Laboratory, Final Report.

*o. Literature Cited*

Beals, G.A., 1971. A Guide to Local Dispersion of Air Pollutants. Air Weather Service Technical Report #214 (April 1971).

Colenbrander, G.W., 1980. A Mathematical Model for the Transient Behavior of Dense Vapor Clouds, 3rd. International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Basel, Switzerland.

Slade, D.H., 1968. Meteorology and Atomic Energy, U.S. Atomic Energy Commission, 445 pp. (NTIS No. TID-24190)

Turner, D.B., 1969. Workbook of Atmospheric Dispersion Estimates. PHS Publication No. 999-AP-26. U.S. Environmental Protection Agency, Research Triangle Park, NC.

## HGSYSTEM: Dispersion Models for Ideal Gases and Hydrogen Fluoride

### *Reference*

Post, L. (ed.), 1994. HGSYSTEM 3.0 Technical Reference Manual. Shell Research Limited, Thornton Research Centre, Chester, United Kingdom. (TNER 94.059)

Post, L., 1994. HGSYSTEM 3.0 User's Manual. Shell Research Limited, Thornton Research Centre, Chester, United Kingdom. (TNER 94.059)

### *Availability*

The PC-DOS version of the HGSYSTEM software (HGSYSTEM: Version 3.0, Programs for modeling the dispersion of ideal gas and hydrogen fluoride releases, executable programs and source code can be installed from diskettes. These diskettes and all documentation are available as a package from API [(202) 682-8340] or from NTIS as PB 96-501960 (see Introduction and Availability).

### Technical Contacts

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### *Abstract*

HGSYSTEM is a PC-based software package consisting of mathematical models for estimating of one or more consecutive phases between spillage and near-field and far-field dispersion of a pollutant. The pollutant can be either a two-phase, multi-compound mixture of non-reactive compounds or hydrogen fluoride (HF) with chemical reactions. The individual models are:

#### Database program:

DATAPROP                      Generates physical properties used in other HGSYSTEM models

#### Source term models:

SPILL	Transient liquid release from a pressurized vessel
HFSPILL	SPILL version specifically for HF
LPOOL	Evaporating multi-compound liquid pool model

#### Near-field dispersion models:

AEROPLUME	High-momentum jet dispersion model
HFPLUME	AEROPLUME version specifically for HF
HEGABOX	Dispersion of instantaneous heavy gas releases

#### Far-field dispersion models:

HEGADAS(S,T)	Heavy gas dispersion (steady-state and transient version)
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PGPLUME                      Passive Gaussian dispersion

Utility programs:

HFFLASH	Flashing of HF from pressurized vessel
POSTHS/POSTHT	Post-processing of HEGADAS(S,T) results
PROFILE	Post-processor for concentration contours of airborne plumes
GET2COL	Utility for data retrieval

The models assume flat, unobstructed terrain. HGSYSTEM can be used to model steady-state, finite-duration, instantaneous and time dependent releases, depending on the individual model used. The models can be run consecutively, with relevant data being passed on from one model to the next using link files. The models can be run in batch mode or using an iterative utility program.

*a. Recommendations for Regulatory Use*

HGSYSTEM can be used as a refined model to estimate short-term ambient concentrations. For toxic chemical releases (non-reactive chemicals or hydrogen fluoride; 1-hour or less averaging times) the expected area of exposure to concentrations above specified threshold values can be determined. For flammable non-reactive gases it can be used to determine the area in which the cloud may ignite.

*b. Input Requirements*

HFSPILL input data: reservoir data (temperature, pressure, volume, HF mass, mass-fraction water), pipe-exit diameter and ambient pressure.

EVAP input data: spill rate, liquid properties, and evaporation rate (boiling pool) or ambient data (non-boiling pool).

HFPLUME and PLUME input data: reservoir characteristics, pollutant parameters, pipe/release data, ambient conditions, surface roughness and stability class.

HEGADAS input data: ambient conditions, pollutant parameters, pool data or data at transition point, surface roughness, stability class and averaging time.

PGPLUME input data: link data provided by HFPLUME and the averaging time.

*c. Output*

The HGSYSTEM models contain three post-processor programs which can be used to extract modeling results for graphical display by external software packages. GET2COL can be used to extract data from the model output files. HSPOST can be used to develop isopleths, extract any 2 parameters for plotting and correct for finite release duration. HTPOST can be used to produce time history plots.

HFSPILL output data: reservoir mass, spill rate, and other reservoir variables as a function of time. For HF liquid, HFSPILL generates link data to HFPLUME for the initial phase

of choked liquid flow (flashing jet), and link data to EVAP for the subsequent phase of unchoked liquid flow (evaporating liquid pool).

EVAP output data: pool dimensions, pool evaporation rate, pool mass and other pool variables for steady state conditions or as a function of time. EVAP generates link data to the dispersion model HEGADAS (pool dimensions and pool evaporation rate).

HFPLUME and PLUME output data: plume variables (concentration, width, centroid height, temperature, velocity, etc.) as a function of downwind distance.

HEGADAS output data: concentration variables and temperature as a function of downwind distance and (for transient case) time.

PGPLUME output data: concentration as a function of downwind distance, cross-wind distance and height.

#### *d. Type of Model*

HGSYSTEM is made up of four types of dispersion models. HFPLUME and PLUME simulate the near-field dispersion and PGPLUME simulates the passive-gas dispersion downwind of a transition point. HEGADAS simulates the ground-level heavy-gas dispersion.

#### *e. Pollutant Types*

HGSYSTEM may be used to model non-reactive chemicals or hydrogen fluoride.

#### *f. Source-Receptor Relationships*

HGSYSTEM estimates the expected area of exposure to concentrations above user-specified threshold values. By imposing conservation of mass, momentum and energy the concentration, density, speed and temperature are evaluated as a function of downwind distance.

#### *g. Plume Behavior*

HFPLUME and PLUME: (1) are steady-state models assuming a top-hat profile with cross-section averaged plume variables; and (2) the momentum equation is taken into account for horizontal ambient shear, gravity, ground collision, gravity-slumping pressure forces and ground-surface drag.

HEGADAS: assumes the heavy cloud to move with the ambient wind speed, and adopts a power-law fit of the ambient wind speed for the velocity profile.

PGPLUME: simulates the passive-gas dispersion downwind of a transition point from HFPLUME or PLUME for steady-state and finite duration releases.

#### *h. Horizontal Winds*

A power law fit of the ambient wind speed is used.

*i. Vertical Wind Speed*

Not treated.

*j. Horizontal Dispersion*

HFPLUME and PLUME: Plume dilution is caused by air entrainment resulting from high plume speeds, trailing vortices in wake of falling plume (before touchdown), ambient turbulence and density stratification. Plume dispersion is assumed to be steady and momentum-dominated, and effects of downwind diffusion and wind meander (averaging time) are not taken into account.

HEGADAS: This model adopts a concentration similarity profile expressed in terms of an unknown center-line ground-level concentration and unknown vertical/cross-wind dispersion parameters. These quantities are determined from a number of basic equations describing gas-mass conservation, air entrainment (empirical law describing vertical top-entrainment in terms of global Richardson number), cross-wind gravity spreading (initial gravity spreading followed by gravity-current collapse) and cross-wind diffusion (Briggs formula).

PGPLUME: This model assumes a Gaussian concentration profile in which the cross-wind and vertical dispersion coefficients are determined by empirical expressions. All unknown parameters in this profile are determined by imposing appropriate matching criteria at the transition point.

*k. Vertical Dispersion*

See description above.

*l. Chemical Transformation*

Not treated.

*m. Physical Removal*

Not treated.

*n. Evaluation Studies*

PLUME has been validated against field data for releases of liquified propane, and wind tunnel data for buoyant and vertically-released dense plumes. HFPLUME and PLUME have been validated against field data for releases of HF (Goldfish experiments) and propane releases. In addition, the plume rise algorithms have been tested against Hoot, Meroney, and Peterka, Ooms and Petersen databases. HEGADAS has been validated against steady and transient releases of liquid propane and LNG over water (Maplin Sands field data), steady and finite-duration pressurized releases of HF (Goldfish experiments; linked with HFPLUME), instantaneous release of Freon (Thorney Island field data; linked with the box model HEGABOX) and wind tunnel data for steady, isothermal dispersion.

Validation studies are contained in the following references.

McFarlane, K., Prothero, A., Puttock, J.S., Roberts, P.T. and H.W.M. Witlox, 1990. Development and validation of atmospheric dispersion models for ideal gases and hydrogen fluoride, Part I: Technical Reference Manual. Report TNER.90.015. Thornton Research Centre, Shell Research, Chester, England. [EGG 1067-1151] (NTIS No. DE 93-000953)

Witlox, H.W.M., McFarlane, K., Rees, F.J. and J.S. Puttock, 1990. Development and validation of atmospheric dispersion models for ideal gases and hydrogen fluoride, Part II: HGSYSTEM Program User's Manual. Report TNER.90.016. Thornton Research Centre, Shell Research, Chester, England. [EGG 1067-1152] (NTIS No. DE 93-000954)

## HOTMAC/RAPTAD

### *Reference*

Mellor, G.L. and T. Yamada, 1974. A Hierarchy of Turbulence Closure Models for Planetary Boundary Layers. *Journal of Atmospheric Sciences*, 31: 1791-1806.

Mellor, G.L. and T. Yamada, 1982. Development of a Turbulence Closure Model for Geophysical Fluid Problems. *Rev. Geophys. Space Phys.*, 20: 851-875.

Yamada, T., 2000. Lagrangian Dispersion Model for Nonneutrally Buoyant Plumes. *J. Appl. Meteor.*, 39: 427-436.

Yamada, T. and S. Bunker, 1988. Development of a Nested Grid, Second Moment Turbulence Closure Model and Application to the 1982 ASCOT Brush Creek Data Simulation. *J. of Appl. Meteor.*, 27: 562-578.

Yamada, T., 2004. Merging CFD and Atmospheric Modeling Capabilities to Simulate Airflows and Dispersion in Urban Areas. *Comput. Fluid Dyn. J.*, 13(2): S8: 1-13.

### *Availability*

For a cost to be negotiated with the model developer, a CD containing the HOTMAC<sup>®</sup>/RAPTAD<sup>®</sup> computer codes including pre- and post-processors and user manuals, installation, training, and support are available from YSA Corporation, 13 Heiwa, Santa Fe, NM 87506; Phone: (505) 989-7351; Fax: (505) 989-7965.

website: [www.ysasoft.com](http://www.ysasoft.com)

e-mail: [Inquiry@ysasoft.com](mailto:Inquiry@ysasoft.com);

### *Abstract*

HOTMAC/RAPTAD is a comprehensive multi-scale modeling and visualization system for predicting air flows and dispersion of airborne materials in the assessments of air quality issues and **environmental impact studies**. The system includes a mesoscale meteorological code, a transport and diffusion code, a visualization code, and extensive Graphical User Interfaces (GUIs). This system is unique because the diffusion code uses time dependent, three-dimensional winds and turbulence distributions that are forecasted by a mesoscale weather prediction model. The modeling system is applicable from building scale (~ a few centimeters) to mesoscale (~ a few kilometers). Consequently the predicted concentration distributions are more accurate than those predicted by traditional models when surface conditions are heterogeneous. In general, the modeled concentration distributions are non-Gaussian because winds and turbulence distributions change considerably in time and space around urban areas and buildings, and in complex terrain and coastal regions.

The models were originally developed by using super computers. However, recent advancement of computer hardware has made it possible to run complex three-dimensional meteorological models on desktop workstations and PCs. The present versions of the programs are running on workstations and PCs. GUIs are available on Sun Microsystems<sup>®</sup>, Silicon Graphics<sup>®</sup> workstations, and PCs with RedHat Linux<sup>®</sup> 7.3 and Windows<sup>®</sup>. The modeling system

can also run on a laptop workstations and PCs, which makes it possible to run the programs in the field or away from the office.

HOTMAC<sup>®</sup>, Higher Order Turbulence Model for Atmospheric Circulation, is a mesoscale weather prediction model that forecasts wind, temperature, humidity, and atmospheric turbulence distributions around urban areas and buildings having complex surface features. HOTMAC<sup>®</sup> has options to include non-hydrostatic pressure computation, nested grids, land-use distributions, cloud, fog, and precipitation physics. HOTMAC<sup>®</sup> can interface with tower, rawinsonde, and large-scale weather models using a four-dimensional data assimilation method. RAPTAD<sup>®</sup>, Random Puff Transport and Diffusion, is a Lagrangian random puff model that is used to forecast transport and diffusion of airborne materials around urban areas and buildings, and over complex terrain and coastal regions. Concentrations are computed by summing the concentration of each puff at the receptor location. The random puff method is equivalent to the random particle method with a Gaussian kernel for particle distribution. The advantage of the puff method is the accuracy and speed of computation. The particle method requires the release of a large number of particles, which could be computationally expensive. The puff method requires the release of a much less number of puffs, typically 1/10 to 1/100 of the number of particles required by the particle method.

The averaging time for concentration estimates is variable from 5 minutes to 15 minutes for each receptor. In addition to the concentration computation at the receptor sites, RAPTAD<sup>®</sup> computes and graphically displays hourly concentration contours at the ground level. RAPTAD<sup>®</sup> is applicable to point and area sources.

The meteorological data produced from HOTMAC<sup>®</sup> are used as input to RAPTAD<sup>®</sup>. RAPTAD<sup>®</sup> can forecast concentration distributions for neutrally buoyant gas, buoyant gas and denser-than-air gas. The models are significantly advanced in both their model physics and in their operational procedures. GUIs are provided to help the user prepare input files, run programs, and display the modeled results graphically in three dimensions.

#### *a. Recommendation for Regulatory Use*

There are no specific recommendations at the present time. The HOTMAC<sup>®</sup> / RAPTAD<sup>®</sup> modeling system may be used on a case-by-case basis.

#### *b. Input Requirements*

Meteorological Data: The modeling system is significantly different from the majority of regulatory models in terms of how meteorological data are provided and used in concentration simulations. Regulatory models use the wind data, which are obtained directly from measurements or analyzed, by using a simple constraint such as a mass conservation equation. Thus, the accuracy of the computation will depend significantly on the quantity and quality of the wind data. This approach is acceptable as long as the study area is flat and the simulation period is short. As the regulations become more stringent and more realistic surface conditions are required, a significantly large volume of meteorological data is required which could become very expensive.

An alternative approach is to augment the measurements with predicted values from a mesoscale meteorological model. This is the approach we have taken here. This approach has

several advantages over the conventional method. First, concentration computations use the model forecast wind while the conventional method extrapolates the observed winds. Extrapolation of wind data over complex terrain and for an extended period of time quickly loses its accuracy. Secondly, the number of stations for upper air soundings is typically limited from none to at most a few stations in the study area. The corresponding number in a mesoscale model is the number of grid points in the horizontal plane which is typically 50 X 50. Consequently, concentration distributions using model forecasted winds would be much more accurate than those obtained by using winds, which were extrapolated from the limited number of measurements.

HOTMAC<sup>®</sup> requires meteorological data for initialization and to provide boundary conditions if the boundary conditions change significantly with time. The minimum amount of data required to run HOTMAC<sup>®</sup> is wind and potential temperature profiles at a single station. HOTMAC<sup>®</sup> forecasts wind and turbulence distributions in the boundary layer through a set of model equations for solar radiation, heat energy balance at the ground, conservation of momentum, conservation of internal energy, and conservation of mass.

Terrain Data: HOTMAC<sup>®</sup> and RAPTAD<sup>®</sup> use the digitized terrain data from the U.S. Geological Survey and the Defense Mapping Agency. Extraction of terrain data is greatly simplified by using YSA's GUI software called Topo. The user specifies the latitudes and longitudes of the southwest and north east corner points of the study area. Then, Topo extracts the digitized elevation data within the area specified and converts from the latitudes and longitudes to the UTM (Universal Transverse Mercator) coordinates for up to three nested grids.

Emission Data: Emission data requirements are emission rate, stack height, stack diameter, stack location, stack gas exit velocity, and stack buoyancy.

Receptor Data: Receptor data requirements are names, location coordinates, and desired averaging time for concentration estimates, which is variable from 5 to 15 minutes.

### *c. Output*

HOTMAC<sup>®</sup> outputs include hourly winds, temperatures, and turbulence variables at every grid point. Ancillary codes graphically display vertical profiles of wind, temperature, and turbulence variables at selected locations and wind vector distributions at specified heights above the ground. These codes also produce graphic files of wind direction projected on vertical cross sections.

RAPTAD<sup>®</sup> outputs include hourly values of surface concentration, time variations of mean and standard deviation of concentrations at selected locations, and coordinates of puff center locations. Ancillary codes produce color contour plots of surface concentration, time variations of mean concentrations and ratios of standard deviation to mean value at selected locations, and concentration distributions in the vertical cross sections. The averaging time of concentration at a receptor location is variable from 5 to 15 minutes. Color contour plots of surface concentration can be animated on the monitor to review time variations of high concentration areas.

### *d. Type of Model*

HOTMAC<sup>®</sup> is a 3-dimensional Eulerian model for weather forecasting, and RAPTAD is a 3-dimensional Lagrangian random puff model for pollutant transport and diffusion.

*e. Pollutant types*

RAPTAD<sup>®</sup> may be used to model any inert pollutants, including dense and buoyant gases.

*f. Source-Receptor Relationship*

Up to 50 point or area sources are specified and up to 50 sampling locations are selected. Source and receptor heights are specified by the user.

*g. Plume Behavior*

Neutrally buoyant plumes are transported by mean and turbulence winds that are modeled by HOTMAC. Non-neutrally buoyant plume equations are based on Van Dop (1992). In general, plumes are non-Gaussian.

*h. Horizontal Winds*

RAPTAD<sup>®</sup> uses wind speed, wind direction, and turbulence on a gridded array that is supplied hourly by HOTMAC<sup>®</sup>. Stability effect and mixed layer height are incorporated through the intensity of turbulence, which is a function of stability. HOTMAC<sup>®</sup> predicts turbulence intensity by solving a turbulence kinetic energy equation and a length scale equation. RAPTAD<sup>®</sup> interpolates winds and turbulence at puff center locations every 1 second from the values on a gridded array.

*i. Vertical Wind Speed*

RAPTAD<sup>®</sup> uses vertical winds on a gridded array that are supplied hourly by HOTMAC<sup>®</sup>. HOTMAC<sup>®</sup> computes vertical wind either by solving an equation of motion for the vertical wind or a mass conservation equation. RAPTAD<sup>®</sup> interpolates vertical winds at puff center locations every 1 second from the values on a gridded array.

*j. Horizontal Dispersion*

Horizontal dispersion is based on the standard deviations of horizontal winds that are computed by HOTMAC<sup>®</sup>.

*k. Vertical Dispersion*

Vertical dispersion is based on the standard deviations of vertical winds that are computed by HOTMAC<sup>®</sup>.

*l. Chemical Transformation*

HOTMAC<sup>®</sup> can provide meteorological inputs to other models that handle chemical reactions, e.g., UAM.

*m. Physical Removal*

Not treated.

*n. Evaluation Studies*

Koracin, D. and J. Frye, 2000. A method of evaluating atmospheric models using tracer measurements. *J. Appl. Meteor.*, 39: 201-221.

Yamada, T., 2000. Numerical Simulations of Airflows and Tracer Transport in the Southwestern United States. *J. of Appl. Meteor.*, 39: 399-411.

Yamada, T., S. Bunker and M. Moss, 1992. A Numerical Simulation of Atmospheric Transport and Diffusion over Coastal Complex Terrain. *J. Appl. Meteor.*, 31: 565-578.

Yamada, T. and T. Henmi, 1994. HOTMAC: Model Performance Evaluation by Using Project WIND Phase I and II Data. *Mesoscale Modeling of the Atmosphere*, American Meteorological Society, Monograph 47, pp. 123-135.

## **Hybrid Roadway Intersection Model (HYROAD)**

### *Reference*

Carr, E.L., R.G. Johnson, R.G. Ireson, 2002., User Guide to HYROAD - The Hybrid Roadway Intersection Model, SYSAPP-02-073d, 101 Lucas Valley Road, San Rafael, CA.

Carr, E.L., R.G. Johnson, R.G. Ireson, 2002., HYROAD Model Formulation, SYSAPP-02-074d, 101 Lucas Valley Road, San Rafael, CA.

### *Abstract*

Understanding the concentration distribution at a roadway intersection requires knowledge of the interrelationship between the traffic environment, vehicle emissions, and the effects of meteorology and traffic on dispersion. The HYROAD modeling system integrates these three historically individual modules. The traffic module is based on the TRAF-NETSIM model, and is used as the core module for generating the traffic information needed by the emission and dispersion modules. Internal code modifications track vehicle speed and acceleration distributions by signal phase and 10-meter roadway segment for use in both emissions calculations and calculation of induced flows and turbulence. Emission factors from current emission factor models (MOBILE5 or MOBILE6) are used as inputs, but speed distributions from the traffic module are used in a regression analysis for each time period to calculate composite emission factors whose underlying speed distribution best fits current conditions. Spatial and temporal distribution of emissions is based on the vehicle operation simulations rather than being uniformly distributed. A Lagrangian (trajectory-based) puff formulation is used along with a gridded non-uniform wind and stability field derived from traffic module outputs, to describe near-roadway dispersion characteristics.

HYROAD is designed to predict hourly concentrations of carbon monoxide (CO) from vehicle emissions that occur within 500m of the roadway intersections. Default inputs are specified for many of the input variables, allowing them to be bypassed. HYROAD permits the specification of up to five approach and five departure legs for the intersection, each of which can include up to seven lanes. The model can simulate up to a maximum of sixty receptors and fifty roadway segments. Overall, HYROAD has been designed to be used to model concentrations near complex intersection configurations with limited curved alignments, and dynamically varying emissions and traffic. The model operates in an IBM-compatible operating system or with the use of a graphical user interface (GUI) which runs under Windows® 98, 2000, XP and NT environments. The minimum configuration recommended is a 200 MHz Pentium® based PC with 64 megabytes of RAM and 400 megabytes of free hard disk space.

### *Availability*

The model code is available on EPA's SCRAM Internet website (see Introduction and Availability).

#### *a. Recommendations for Regulatory Use*

HYROAD can be used if it can be demonstrated to estimate concentrations equivalent to those provided by the preferred model for a given application. HYROAD should be executed in the equivalent mode.

HYROAD may also be used on a case-by-case basis in lieu of a preferred model if it can be demonstrated, using the criteria in Section 3.2 of the *Guideline*, that HYROAD is more appropriate for the specific application. In this case the model options/modes which are most appropriate for the application should be used.

#### *b. Input Requirements*

Traffic data requirements are: number of lanes, length and width of lanes, length of turning bays, lane restrictions, median width, mean free-flow speeds, signal cycle timing, turning and through movement volumes, and traffic volumes for each approach.

Emission data requirements: a matrix of MOBILE5 or MOBILE6 emission factors for a range of traffic speeds and ambient temperatures.

Meteorological data requirements: surface wind measurements, surface roughness, temperature, atmospheric stability class.

Receptor data requirements are: receptor coordinates and heights.

#### *c. Output*

Printed output options include:

- Program control parameters, traffic data, receptor locations;
- Meteorological data for each specified period;
- Average concentration calculated at each specified receptor location ;
- Screening mode analysis

#### *d. Type of Model*

The integrated air quality intersection dispersion modeling system consists of three modules (traffic, emissions, and dispersion) and a user interface. The traffic module simulates urban traffic flows over space and time based on traffic volumes, signalization, roadway geometry and vehicle movement through acceleration, deceleration, cruising and idling states. The module is based on the Traffic Network Simulation model (NETSIM). The emission module calculates vehicle emissions based on traffic flow outputs from the traffic module and emission factors from EPA's MOBILE5 or MOBILE6 model. The module calculates emissions using a weighted average composite emission factor, where the weights assigned to emission factors for different average speeds provide a best fit for the predicted speed distributions from the traffic module. Emissions are allocated temporally and spatially around the intersection based on vehicle operations predictions. The dispersion module uses a Gaussian puff approach in which dispersion processes are affected by induced traffic flows. A two-dimensional non-uniform wind and turbulence field is created based on the induced flows and ambient winds.

#### *e. Pollutant Types*

HYROAD can be used to model carbon monoxide pollutants. The model may also be applied to particulate exhaust emissions in the near roadway vicinity as well as primary emitted air toxics.

#### *f. Source-Receptor Relationships*

User specified locations are made for roadways and receptors. Receptors need not be at ground level. Only one intersection at a time can be modeled.

#### *g. Puff Behavior*

Puff models represent a continuous plume as a number of discrete packets of pollutant material. The contribution from each puff is sampled at a one-second time interval and then moves, evolving in size, until the next sampling step. The total concentration at a receptor is the sum of the contributions of all nearby puffs averaged for all sampling steps which are simulated for each possible traffic signalization. The integrated puff sampling approach used here was first developed for the MESOPUFF II model (Scire *et al.*, 1984) and then further refined and implemented in CALPUFF (Scire, 2000).

#### *h. Horizontal Winds*

HYROAD uses a fixed Cartesian grid of winds that is derived from both the input wind variables and perturbations due to traffic flows during each signal phase. A separate wind field is calculated for each signal phase. Vehicle-induced flows and turbulence are calculated using the algorithms from the vehicle wake theory of Eskridge and Hunt (1979), which superimposes a grid of cells over the roadway that is aligned with the wind direction. As this wind-axis grid in general will not align with the fixed grid, flows are interpolated to the centers of the fixed grid.

#### *i. Vertical Wind Speed*

The vertical wind speed is assumed to be zero.

#### *j. Horizontal Dispersion*

Initial puffs are assigned a minimum longitudinal length of 10 m (the smallest resolution of the emissions along each roadway). The cross-roadway dimension of the puff is assigned the mean lane width. Puffs within the roadway grow at the local rate of dispersion based on the local turbulent flow field and diffusivity as determined from Monin-Obukhov similarity theory with second moment closure (Binkowski, 1979). The local turbulent diffusivity,  $K_p$ , is then used in combination with the relationships between the crosswind concentration distribution  $\sigma_{xy}$  (Hanna *et al.*, 1977) and the non-dimensional function of travel time from Draxler (1976) for surface releases. After the puff has been initially dispersed, the rate of lateral dispersion is dependent upon the surface roughness and “urban” dispersion curves of the St. Louis study performed by McElroy and Pooler (1968). Briggs (1974) parameterized these values as a function of stability class. For areas in which the surface roughness is less than 50cm, the lateral dispersion is modified as a function of surface roughness.

### *k. Vertical Dispersion*

An initial value of 1.5 m is used for the initial vertical dispersion parameter. This value is held constant for all stability classes as Johnson (1974) showed that vertical dispersion near the roadway was independent of atmospheric stability. After the puff has been initially dispersed, the rate of vertical dispersion is dependent upon the surface roughness and the “urban” dispersion curves of the St. Louis study performed by McElroy and Pooler (1968). Smith (1973) developed power-law approximations to these values of vertical dispersion as a function of stability class and surface roughness.

### *l. Chemical Transformation*

Not treated.

### *m. Physical Removal*

Not treated.

### *n. Evaluation Studies*

Carr, E.L., R.G. Johnson, and R.G. Ireson, “HYROAD Model Formulation”, prepared by ICF Consulting for the National Cooperative Highway Research Program for the Transportation Research Board, National Research Council, July 2002, SYSAPP-02/074d.

### *o. Literature Cited*

Binkowski, F.S, 1979. A simple semi-empirical theory for turbulence in the atmospheric surface layer. *Atmos. Environ.*, 13:247-253.

Briggs, G.A., 1974. “Diffusion Estimation for Small Emissions in Environmental Research Laboratories.” Air Resources Atmosphere Turbulence and Diffusion Laboratory 1973 Annual Report; USAEC Report ATDL-106, National Report.

Carr, E.L. and R.G. Ireson, 1997. “Intersection Air Quality Modeling: Monitoring, Data Analysis and Assessment,” prepared by Systems Applications International for the National Cooperative Highway Research Program for the Transportation Research Board, National Research Council; January 1997.

Draxler, R.R, 1976. Determination of atmospheric diffusion parameters. *Atmos. Environ.*, 10(2):99-105.

Eskridge, R.E. and J.A. Catalano, 1987. *ROADWAY – A Numerical Model for Predicting Air Pollutants Near Highways – User’s Guide*; EPA/600/8-87/010, Atmospheric Sciences Research Laboratory; USEPA/ORD, Research Triangle Park, NC; March 1987.

Eskridge, R.E., Petersen, W.B. and S.T. Rao, 1991. Turbulent diffusion behind vehicles: effect of traffic speed on pollutant concentrations. *J. Air Waste Manage. Assoc.*, 41(3):312-317.

Eskridge, R.E. and J. C. R. Hunt, 1979. Highway modeling. Part I: Prediction of velocity and turbulence fields in the wakes of vehicles. *J. Appl. Meteorol.*, 18:387-400.

Eskridge, R.E. and S.T. Rao, 1983. Measurements and prediction of traffic-induced turbulence fields near roadways. *J. Appl. Meteorol.*, 22:1431-1443.

Eskridge, R.E. and S.T. Rao, 1986. Turbulent diffusion behind vehicles: experimentally determined turbulence mixing parameters. *Atmos. Environ.*, 22:1431-1443.

Hanna, S.R., Briggs, G.A., Deardorf, J., Egan, B.A., Gifford, F.A. and F. Pasquill, 1977. Workshop on stability classification schemes and sigma curves—Summary of recommendations. *Bull. Amer. Meteorol. Soc.*, 58:1305-1309.

Johnson, W.B, 1974. "Field Study of Near-Roadway Diffusion using a Fluorescent Dye Tracer." Symposia on Atmospheric Diffusion and Air Pollution, American Meteorological Society, Boston, MA; pp. 261-266.

McElroy, J.L.. and F. Pooler, 1968. The St. Louis Dispersion Study. U.S. Public Health Service, National Air Pollution Control Administration, Report AP-53.

Scire, J.S., Lurhmann, F.W., Bass, A. and S.R. Hanna, 1984 Development of the MESOPUFF II Dispersion Model, EPA-600/3-84-057; USEPA, Research Triangle Park, NC.

Scire, J.S., D.G. Strimaitis, and R.J. Yamartino, 2000. *A User's Guide for the CALPUFF Dispersion Model*, (Version 5); Earth Tech, Concord, MA.

Smith, F.B., 1973. A Scheme for Estimating the Vertical Dispersion of a Plume from a Source near Ground Level. In *Air Pollution - Modeling* No. 14, NATO/CEMS, - Third Meeting.

## Open Burn/Open Detonation Dispersion Model (OBODM)

### *Reference*

Bjorklund, J.R., J.F. Bowers, G.C. Dodd and J.M. White, 1998. Open Burn/Open Detonation Dispersion Model (OBODM) User's Guide, Vols. I and II. DPG Document No. DPG-TR-96-008a and 008b. U.S. Army Dugway Proving Ground, Dugway, UT.

### *Abstract*

OBODM is intended for use in evaluating the potential air quality impacts of the open burning and detonation (OB/OD) of obsolete munitions and solid propellants. OBODM uses cloud/plume rise, dispersion, and deposition algorithms taken from existing models for instantaneous and quasi-continuous sources to predict the downwind transport and dispersion of pollutants released by OB/OD operations. The model can be used to calculate peak concentration, time-mean concentration, dosage (time-integrated concentration), and particulate gravitational deposition for emissions from multiple OB/OD sources for either a single event or up to a year of sequential hourly source and meteorological inputs. OBODM includes a data base of empirical emissions factors for many explosives and propellants. The OBODM program is designed for use on IBM-compatible PCS using the MS-DOS<sup>®</sup> (Version 2.1 or higher) operating system and will also run under most WINDOWS<sup>®</sup> environments. OBODM requires 505 kilobytes of conventional memory, a math coprocessor, and a minimum of 3 megabytes of hard disk storage. Volume I of the user's guide contains instructions for installing and running the model and example problems. Volume II discusses the model's mathematical algorithms and default meteorological inputs.

### *Availability*

OBODM and the two-volume user's manual are available on the Dugway Proving Ground website at [www.dugway.army.mil](http://www.dugway.army.mil). Requests for the OBODM source code should be addressed to Meteorology & Obscurants Division, West Desert Test Center, Dugway Proving Ground, Dugway, UT 84022-5000.

#### *a. Recommendations for Regulatory Use*

There is no preferred model for application to the open burning and open detonation of obsolete or unsafe munitions and propellants. OBODM is specifically designed to predict the buoyant rise and dispersion of emissions from these instantaneous (open detonation) and short-term quasi-continuous (open burn) releases when a refined model is needed.

#### *b. Input Requirements*

OBODM source inputs include the source coordinates and physical dimensions, explosive or propellant type, pollutant species of interest, effective heat content of the explosive/propellant, burn rate for an open burn, total mass of explosive/propellant, and pollutant emissions factor. An OBODM data base provides much of this information for many explosives and propellants. For particulate matter, if the user wishes to consider gravitational settling and deposition, the particle density and particle size distribution (or particle mass-median diameter and geometric standard deviation) are also required. If the user wishes to consider the chemical transformation of a

gaseous pollutant, the pollutant half-life must be specified. When OBODM is used with sequential hourly meteorological inputs, hourly source inputs also can be used. OBODM allows up to 50 individual sources.

OBODM meteorological inputs consist of the mean wind speed and wind direction at 10 meters, standard deviations of the wind azimuth ( $\sigma_A$ ) and elevation ( $\sigma_E$ ) angles, longitudinal turbulence intensity, wind-profile exponent, mixing depth, vertical potential temperature gradient, relative humidity, vertical wind-direction shear (normally set to 0), and barometric pressure. OBODM uses the 10-meter wind speed and Pasquill stability category or net radiation index (NRI) to assign default values for any input not provided by the user except for the wind speed, wind direction, and ambient air temperature. The model will also calculate the NRI if cloud cover and height data are entered. OBODM can process from 1 to 8784 hours (1 year) of sequential meteorological inputs in a single run. Standard preprocessed meteorological input files for regulatory models such as ISCST3 can be used with OBODM.

OBODM uses a polar or Cartesian coordinate system for regular and discrete receptors. Receptor heights are required in open terrain. When OBODM is used in its complex terrain screening mode, all receptors are assumed to be at ground level and ground elevations are required. OBODM will accept a maximum of 10,000 receptors in a regular grid plus a maximum of 100 discrete receptors.

### *c. Output*

Printed output options include:

- Program control parameters, source data, and receptor data;
- Tables of hourly meteorological data for each specified day;
- "N"-day average concentration or total deposition calculated at each receptor for any desired source combinations;
- Concentration or deposition values calculated for any desired source combinations at all receptors for any specified day or time period within the day;
- Tables of highest and second-highest concentration or deposition values calculated at each receptor for each specified time period during an "N"-day period for any desired source combinations, and tables of the maximum 50 concentration or deposition values calculated for any desired source combination for each specified time period.

### *d. Type of Model*

OBODM uses a Gaussian puff model for open burns and a square-wave quasi-continuous Gaussian plume model for open burns. The square-wave quasi-continuous source model is an analytic solution to the integral of the Gaussian puff equation with respect to time over the duration of the release. That is, the quasi-continuous source model is the analytic equivalent of representing a quasi-continuous release by an overlapping series of Gaussian puffs.

### *e. Pollutant Types*

OBODM can be used to model primary pollutants. Settling and deposition of particulates are treated.

#### *f. Source-Receptor Relationships*

User specified locations are used for sources and receptors. Receptors need not be at ground level except in complex terrain. Receptor heights above ground-level must be the same for receptors in the regular array, but not for the discrete receptors.

#### *g. Plume Behavior*

Plume rise for quasi-continuous sources (open burns) is calculated by the Briggs (1971) equations as modified by Dumbauld *et al.* (1973) to account for the horizontal dimensions of large burns. Cloud rise for instantaneous sources (open detonations) is calculated using equations derived by Dumbauld *et al.* (1973) using assumptions analogous to those used to derive the Briggs (1971) equations for continuous sources.

The method of Weil and Brower (1984) is used to account for partial plume or cloud penetration into the stable layer above the surface mixing layer.

A tilted plume is used for particulates with settling velocities.

Partial reflection at the ground surface is assumed for particulates with settling velocities. OBODM computes the reflection coefficient as a function of settling velocity (Bowers *et al.*, 1979).

The SHORTZ/LONGZ complex terrain methodology (Bjorklund and Bowers, 1982) is used in the complex terrain screening mode.

#### *h. Horizontal Winds*

Winds are assumed to be horizontally uniform and steady-state. Default wind-profile exponents are based on wind speed and stability or wind speed and net radiation index.

#### *i. Vertical Wind Speed*

The vertical wind speed is assumed to be zero.

#### *j. Horizontal Dispersion*

OBODM uses semi-empirical Dugway Proving Ground (DPG) dispersion coefficients which directly relate plume and puff growth to atmospheric turbulence and vertical wind shear. The lateral dispersion coefficient, which differs for quasi-continuous and instantaneous sources, is from Cramer *et al.* (1972). The alongwind (longitudinal) dispersion coefficient is from Dumbauld and Bowers (1983). Plume/cloud growth by entrainment during buoyant rise is included (Bjorklund *et al.*, 1998). The horizontal dispersion coefficients depend on the cloud stabilization time for detonations and fast burns and on the concentration averaging time for lengthy burns.

#### *k. Vertical Dispersion*

OBODM uses the DPG vertical dispersion coefficient which relates vertical plume/cloud growth to the vertical turbulence intensity and includes the effects of entrainment during buoyant rise (Bjorklund *et al.*, 1998).

#### *l. Chemical Transformation*

Chemical transformations are approximated by exponential decay with the decay coefficient specified by the user.

#### *m. Physical Removal*

Dry deposition of particulates by gravitational fallout is treated using the methodology from the original ISC model (Bowers *et al.*, 1979).

#### *n. Evaluation Studies*

Bowers, J.F., J.E. Rafferty and J.M. White, 1990. Summary of Dugway Proving Ground Experience in Diffusion Development and Verification for MMW Obscurants. In Proceedings of Smoke/Obscurants symposium XIII, Program Manager Smoke/Obscurants, Aberdeen Proving Ground, MD.

Bowers, J.F. and J.E. Rafferty, 1991. Additional Verification of the Dugway Proving Ground Diffusion Model for MMW Obscurants. In Proceedings of Smoke/Obscurants Symposium XV, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD.

Cramer, H.E., J.R. Bjorklund, R.K. Dumbauld, J.E. Faulkner, F.A. Record, R.N. Swanson, and A.G. Tringle, 1972. Development of Dosage Models and Concepts. Document No. DTC-TR-72-609-1, U.S. Army Dugway Proving Ground, Dugway, UT.

#### *o. Literature Cited*

Bjorklund, J.R. and J.F. Bowers, 1982. User's Instruction for the SHORTZ and LONGZ Computer Programs, Vols. I and II. EPA Publication Nos. EPA-903/9-82-004a and 004b. U.S. Environmental Protection Agency, Region 3, Philadelphia, PA.

Bowers, J.F., J.R. Bjorklund, and C.S. Cheney, 1979. Industrial Source Complex (ISC) Dispersion Model User's Guide, Vols. I and II. Report Nos. EPA-450/4-79-030 and 031, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Briggs, G.A., 1971. Some Recent Analyses of Plume Rise Observations. Proceedings of the Second International Clean Air Congress. H.M. Englund and W.T. Berry, eds. Academic Press, New York, NY.

Cramer, H.E., J.R. Bjorklund, R.K. Dumbauld, J.E. Faulkner, F.A. Record, R.N. Swanson, and A.G. Tringle, 1972. Development of Dosage Models and Concepts, Vols I and II. Document Nos. DTC-TR-72-609-I and 609-II, U.S. Army Dugway Proving Ground, Dugway, UT.

Dumbauld, R.K., J.R. Bjorklund, and J.F. Bowers, 1973. NASA/MSFC Multilayer Diffusion Models and Computer Program for Operational Prediction of Toxic Fuel Hazards. NASA Contractor Report CR-129006, NASA George C. Marshall Space Flight Center, Huntsville, AL.

Dumbauld, R.K. and J.F. Bowers, 1983. Functional Methodologies for Characterizing Wind-Speed and Turbulence Profiles and Turbulent Diffusion Coefficients within and above Vegetative Canopies and Urban Domains. H.E. Cramer Company, Inc. Report No. Tr-83-341-01 prepared for U.S. Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM.

Weil, J.C. and R.P. Brower, 1984. An Updated Gaussian Plume Model for Tall Stacks. *Journal of the Air Pollution Control Association*, **34**: 818-827.

## PANACHE

### *Reference*

Transoft Group, 1994. User's Guide of Fluidyn-PANACHE, a Three-Dimensional Deterministic Simulation of Pollutants Dispersion Model for Complex Terrain; Cary, North Carolina.

### *Availability*

For a cost to be negotiated with the model developer, the computer code is available from: Transoft US, Inc., 1191 Crestmont Drive, Lafayette, CA 94549-3004; (925) 284-1200; Fax: (925) 284-1240. Internet: [www.fluidyn.com](http://www.fluidyn.com)

### *Abstract*

PANACHE<sup>®</sup> is an Eulerian (and Lagrangian for particulate matter), 3-dimensional finite volume fluid mechanics code designed to simulate continuous and short-term pollution dispersion in the atmosphere, in simple or complex terrain. For single or multiple sources, pollutant emissions from stack, point, area, volume, general sources and distant sources are treated. The model automatically treats obstacles, effects of vegetation and water bodies, the effects of vertical temperature stratification on the wind and diffusion fields, and turbulent shear flows caused by atmospheric boundary layer or terrain effects. The code solves Navier Stokes equations in a curvilinear mesh espousing the terrain and obstacles. A 2nd order resolution helps keep the number of cells limited in case of shearing flow. An initial wind field is computed by using a Lagrangian multiplier to interpolate wind data collected on site. The mesh generator, the solver and the numerical schemes have been adopted for atmospheric flows with or without chemical reactions. The model code operates on any workstation or IBM<sup>®</sup> - compatible PC (486 or higher). Gaussian and puff modes are available in PANACHE for fast, preliminary simulation.

#### *a. Recommendations for Regulatory Use*

On a case-by-case basis, PANACHE may be appropriate for the following types of situations: industrial or urban zone on a flat or complex terrain, transport distance from a few meters to 50km, continuous releases with hourly, monthly or annual averaging times, chemically reactive or non-reactive gases or particulate emissions for stationary or roadway sources.

#### *b. Input Requirements*

Data may be input directly from an external source (e.g., GIS file) or interactively. The model provides the option to use default values when input parameters are unavailable.

PANACHE<sup>®</sup> user environment integrates the pre- and post-processor with the solver. The calculations can be done interactively or in batch mode. An inverse scheme is provided to estimate missing data from a few measured values of the wind.

Terrain data requirements:

- Location, surface roughness estimates, and altitude contours.

- Location and dimensions of obstacles, forests, fields, and water bodies.

Source data requirements:

For all types of sources, the exit temperature and plume mass flow rates and concentration of each of the pollutants are required. External sources require mass flow rate. For roadways, estimated traffic volume and vehicular emissions are required.

Meteorological data requirements:

Hourly stability class, wind direction, wind speed, temperature, cloud cover, humidity, and mixing height data with lapse rate below and above it.

Primary meteorological variables available from the National Weather Service can be processed using PCRAMMET (see Section 8.3.3.2 of the *Guideline*) for creating an input file.

Data required at the domain boundary:

Wind profile (uniform, log or power law), depending on the terrain conditions (e.g., residential area, forest, sea, etc.).

Chemical source data requirements:

A database of selected species with specific heats and molecular weights can be extended by the user. For heavy gases the database includes a compressibility coefficients table.

Solar reflection:

For natural convection simulation with low wind on a sunny day, approximate values of temperature for fields, forests, water bodies, shadows and their variations with the time of the day are determined automatically.

### *c. Output*

Printed output option: pollutant concentration at receptor points, and listing of input data (terrain, chemical, weather, and source data) with turbulence and precision control data.

Graphical output includes: In 3-dimensional perspective or in any crosswind, downwind or horizontal plane: wind velocity, pollutant concentration, 3-dimensional isosurface. The profile of concentration can be obtained along any line on the terrain. The concentration contours can be either instantaneous or time integrated for the emission from a source or a source combination. A special utility is included to help prepare a report or a video animation. The user can select images, put in annotations, or do animation.

### *d. Type of Model*

The model uses an Eulerian (and Lagrangian for particulate matter) 3-dimensional finite volume model solving full Navier-Stokes equations. The numerical diffusion is low with appropriate turbulence models for building wakes. A second order resolution may be sought to

limit the diffusion. Gaussian and puff modes are available. The numerical scheme is self adaptive for the following situations:

- A curvilinear mesh or a chopped Cartesian mesh is generated automatically or manually;
- Thermal and gravity effects are simulated by full gravity (heavy gases), no gravity (well mixed light gases at ambient temperature), and Boussinesq approximation methods;
- $K_{diff}$ , K-e or a boundary layer turbulence models are used for turbulence calculations. The flow behind obstacles such as buildings, is calculated by using a modified K-e.
- For heavy gases, a 3-dimensional heat conduction from the ground and a stratification model for heat exchange from the atmosphere are used (with anisotropic turbulence).
- If local wind data are available, an initial wind field with terrain effects can be computed using a Lagrangian multiplier, which substantially reduces computation time.

#### *e. Pollutant Types*

- Scavenging, Acid Rain: A module for water droplets traveling through a plume considers the absorption and de-absorption effects of the pollutants by the droplet. Evaporation and chemical reactions with gases are also taken into account.
- Visibility: Predicts plume visibility and surface deposition of aerosol.
- Particulate matter: Calculates settling and dry deposition of particles based on a Probability Density Function (PDF) of their diameters. The exchange of mass, momentum and heat between particles and gas is treated with implicit coupling procedures.
- Ozone formation and dispersion: The photochemical model computes ozone formation and dispersion at street level in the presence of sunlight.
- Roadway Pollutants: Accounts for heat and turbulence due to vehicular movement. Emissions are based on traffic volume and emission factors.
- Odor Dispersion: Identifies odor sources for waste water plants.
- Radon Dispersion: Simulates natural radon accumulation in valleys and mine environments.

PANACHE may also be used in emergency planning and management for episodic emissions, and fire and soot spread in forested and urban areas or from combustible pools.

#### *f. Source-Receptor Relationship*

Simultaneous use of multiple kinds of sources at user defined locations. Any number of user defined receptors can identify pollutants from each source individually.

#### *g. Plume Behavior*

The options influencing the behavior are full gravity, Boussinesq approximation or no gravity.

#### *h. Horizontal Winds*

Horizontal wind speed approximations are made only at the boundaries based on National Weather Service data. Inside the domain of interest, full Navier-Stokes resolution with natural viscosity is used for 3-dimensional terrain and temperature dependent wind field calculation.

#### *i. Vertical Wind Speed*

Vertical wind speed approximations are made only at the boundaries based on National Weather Service data. The domain of interest is treated as for horizontal winds.

#### *j. Horizontal Dispersion*

Diffusion is calculated using appropriate turbulence models. A 2nd order solution for shearing flow can be sought when the number of meshes is limited between obstacles.

#### *k. Vertical Dispersion*

Dispersion by full gravity unless Boussinesq approximation or no gravity requested. Vertical dispersion is treated as above for horizontal dispersion.

#### *l. Chemical Transformation*

PANCHEM, an atmospheric chemistry module for chemical reactions, is available. Photochemical reactions are used for tropospheric ozone calculations.

#### *m. Physical Removal*

Physical removal is treated using dry deposition coefficients

#### *n. Evaluation Studies*

Goldwire, H.C. Jr, T.G. McRae, G.W. Johnson, D.L. Hipple, R.P. Koopman, J.W. McClure, L.K. Morris and R.T. Cederhall, 1985. Desert Tortoise Series Data Report: 1983 Pressurized Ammonia Spills. UCID 20562, Lawrence Livermore National Laboratory; Livermore, California.

Green, S.R., 1992. Modeling Turbulent Air Flow in a Stand of Widely Spaced Trees, The PHOENICS Journal of Computational Fluid Dynamics and Its Applications, **5**: 294-312.

Gryning, S.E. and E. Lyck, 1984. Atmospheric Dispersion from Elevated Sources in an Urban Area: Comparison Between Tracer Experiments and Model Calculations. *J. of Climate and Appl. Meteor.*, **23**: 651-660.

Havens, J., T. Spicer, H. Walker and T. Williams, 1995. Validation of Mathematical Models Using Wind-Tunnel Data Sets for Dense Gas Dispersion in the Presence of Obstacles.

University of Arkansas, 8th International Symposium-Loss Prevention and Safety Promotion in the Process Industries; Antwerp, Belgium.

McQuaid, J. (ed), 1985. Heavy Gas Dispersion Trials at Thorney Island. Proc. of a Symposium held at the University of Sheffield, Great Britain.

Pavitskiy, N.Y., A.A. Yakuskin and S.V. Zhubrin, 1993. Vehicular Exhaust Dispersion Around Group of Buildings. The PHOENICS Journal of Computational Fluid Dynamics and Its Applications, 6: 270-285.

Tripathi, S., 1994. Evaluation of Fluidyn-PANACHE on Heavy Gas Dispersion Test Case. Seminar on Evaluation of Models of Heavy Gas Dispersion Organized by European Commission; Mol, Belgium.

## Plume Visibility Model (PLUVUE II)

### *Reference*

Environmental Protection Agency, 1992. User's Manual for the Plume Visibility Model, PLUVUE II (Revised). EPA Publication No. EPA-454/B-92-008. U.S. Environmental Protection Agency, Research Triangle Park, NC. (NTIS PB 93-188233)

### *Availability*

This model code is available on the SCRAM Internet website and also on diskette (as PB 90-500778) from the National Technical Information Service (see [Introduction and Availability](#)).

### *Abstract*

The Plume Visibility Model (PLUVUE II) is used for estimating visual range reduction and atmospheric discoloration caused by plumes consisting of primary particles, nitrogen oxides and sulfur oxides emitted from a single emission source. PLUVUE II uses Gaussian formulations to predict transport and dispersion. The model includes chemical reactions, optical effects and surface deposition. Four types of optics calculations are made: horizontal and non-horizontal views through the plume with a sky viewing background; horizontal views through the plume with white, gray and black viewing backgrounds; and horizontal views along the axis of the plume with a sky viewing background.

#### *a. Recommendations for Regulatory Use*

The Plume Visibility Model (PLUVUE II) may be used on a case-by-case basis as a third level screening model. When applying PLUVUE II, the following precautions should be taken:

1. Treat the optical effects of NO<sub>2</sub> and particles separately as well as together to avoid cancellation of NO<sub>2</sub> absorption with particle scattering.
2. Examine the visual impact of the plume in 0.1 (or 0), 0.5, and 1.0 times the expected level of particulate matter in the background air.
3. Examine the visual impact of the plume over the full range of observer-plume sun angles.
4. The user should consult the appropriate Federal Land Manager when using PLUVUE II to assess visibility impacts in a Class I area.

#### *b. Input Requirements*

Source data requirements are: location and elevation; emission rates of SO<sub>2</sub>, NO<sub>x</sub>, and particulates; flue gas flow rate, exit velocity, and exit temperature; flue gas oxygen content; properties (including density, mass median and standard geometric deviation of radius) of the emitted aerosols in the accumulation (0.1 - 1.0 μm) and coarse (1.0 - 10 μm) size modes; and deposition velocities for SO<sub>2</sub>, NO<sub>x</sub>, coarse mode aerosol, and accumulations mode aerosol.

Meteorological data requirements are: stability class, wind direction (for an observer-based run), wind speed, lapse rate, air temperature, relative humidity, and mixing height.

Other data requirements are: ambient background concentrations of  $\text{NO}_x$ ,  $\text{NO}_2$ ,  $\text{O}_3$ , and  $\text{SO}_2$ , and background visual range of sulfate and nitrate concentrations.

Receptor (observer) data requirements are: location, terrain elevation at points along plume trajectory, white, gray, and black viewing backgrounds, the distance from the observer to the terrain observed behind the plume.

#### *c. Output*

Printed output includes plume concentrations and visual effects at specified downwind distances for calculated or specified lines of sight.

#### *d. Type of Model*

PLUVUE II is a Gaussian plume model. Visibility impairment is quantified once the spectral light intensity has been calculated for the specific lines of sight. Visibility impairment includes visual range reduction, plume contrast, relative coloration of a plume to its viewing background, and plume perceptibility due to its contrast and color with respect to a viewing background.

#### *e. Pollutant Types*

PLUVUE II treats  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{SO}_2$ ,  $\text{H}_2\text{SO}_4$ ,  $\text{HNO}_3$ ,  $\text{O}_3$ , primary and secondary particles to calculate effects on visibility.

#### *f. Source Receptor Relationship*

For performing the optics calculations at selected points along the plume trajectory, PLUVUE II has two modes: plume based and observer based calculations. The major difference is the orientation of the viewer to the source and the plume.

#### *g. Plume Behavior*

Briggs (1969, 1971, 1972) final plume rise equations are used.

#### *h. Horizontal Winds*

User-specified wind speed (and direction for an observer-based run) are assumed constant for the calculation.

#### *i. Vertical Wind Speed*

Vertical wind speed is assumed equal to zero.

#### *j. Horizontal Dispersion*

Constant, uniform (steady-state) wind is assumed for each hour. Straight line plume transport is assumed to all downwind distances.

*k. Vertical Dispersion*

Rural dispersion coefficients from Turner (1969) are used, with no adjustment for surface roughness. Six stability classes are used.

*l. Chemical Transformation*

The chemistry of NO, NO<sub>2</sub>, O<sub>3</sub>, OH, O(<sup>1</sup>D), SO<sub>2</sub>, HNO<sub>3</sub>, and H<sub>2</sub>SO<sub>4</sub> is treated by means of nine reactions. Steady state approximations are used for radicals and for the NO/NO<sub>2</sub>/O<sub>3</sub> reactions.

*m. Physical Removal*

Dry deposition of gaseous and particulate pollutants is treated using deposition velocities.

*n. Evaluation Studies*

Bergstrom, R.W., C. Seigneur, B.L. Babson, H.Y. Holman and M.A. Wojcik, 1981. Comparison of the Observed and Predicted Visual Effects Caused by Power Plant Plumes. *Atmos. Environ.*, **15**: 2135-2150.

Bergstrom, R.W., Seigneur, C.D. Johnson and L.W. Richards, 1984. Measurements and Simulations of the Visual Effects of Particulate Plumes. *Atmos. Environ.*, **18**: 2231-2244.

Seigneur, C., R.W. Bergstrom and A.B. Hudischewskyj, 1982. Evaluation of the EPA PLUVUE Model and the ERT Visibility Model Based on the 1979 VISTTA Data Base. EPA Publication No. EPA-450/4-82-008. U.S. Environmental Protection Agency, Research Triangle Park, NC.

White, W.H., C. Seigneur, D.W. Heinold, M.W. Eltgroth, L.W. Richards, P.T. Roberts, P.S. Bhardwaja, W.D. Conner and W.E. Wilson, Jr, 1985. Predicting the Visibility of Chimney Plumes: An Inter-comparison of Four Models with Observations at a Well-Controlled Power Plant. *Atmos. Environ.*, **19**: 515-528.

## Second-order Closure Integrated PUFF Model (SCIPUFF)

### *Reference*

Sykes, R.I., S.F. Parker, D.S. Henn, C.P. Cerasoli and L.P. Santos, 1998. PC-SCIPUFF Version 1.2PD Technical Documentation. ARAP Report No. 718. Titan Corporation, Titan Research & Technology Division, ARAP Group, P.O. Box 2229, Princeton, NJ, 08543-2229.

### *Availability*

SCIPUFF Version 1.2PD and its technical documentation are available for downloading from the the model developer's website ([www.titan.com/systems/prod.htm](http://www.titan.com/systems/prod.htm)) or by contacting: Dr. R. Ian Sykes, Titan Research & Technology, ARAP Group, P.O. Box 2229, Princeton, NJ 08543-2229. Phone: (609) 452-2950.

### *Abstract*

SCIPUFF is a Lagrangian puff dispersion model that uses a collection of Gaussian puffs to represent an arbitrary, three-dimensional, time-dependent concentration field. The turbulent diffusion parameterization is based on modern turbulence closure theory, specifically the second-order closure model of Donaldson (1973) and Lewellen (1977), which provides a direct relationship between the predicted dispersion rates and the measurable turbulent velocity statistics of the wind field. In addition to the average concentration value, the closure model also provides a prediction of the statistical variance in the concentration field resulting from the random fluctuations in the wind field. The closure approach also provides a direct representation for the effect of averaging time (Sykes and Gabruk, 1997).

Shear distortion is accurately represented using the full Gaussian spatial moment tensor, rather than simply the diagonal moments, and an efficient puff splitting/merging algorithm minimizes the number of puffs required for a calculation. In order to increase calculation efficiency, SCIPUFF uses a multi-level time-stepping scheme with an appropriately sized time-step for each puff. An adaptive multi-grid is used to identify neighboring puffs in the spatial domain, which greatly reduces the search time for overlapping puffs in the interaction calculation and puff-merging algorithm. Static puffs are used to represent the steady-state phase of the plume near the source and are updated only with the meteorology, also decreasing the number of puffs needed for the calculation.

SCIPUFF can model many types of source geometries and material properties. It can use several types of meteorological input, including surface and upper-air observations or three-dimensional gridded data. Planetary boundary layer turbulence is represented explicitly in terms of surface heat flux and shear stress using parameterized profile shapes. A Graphical User Interface (GUI) that runs on a PC is used to define the problem scenario, run the dispersion calculation and produce color contour plots of resulting concentrations. The GUI also includes an online 'Help'.

#### *a. Recommendations for Regulatory Use*

SCIPUFF is appropriate for modeling both short and long range (greater than 50km) transport, steady or non-steady state emissions of primary pollutants (gases or particles), buoyant

or neutral sources using time-dependent meteorological data (surface, profile, or gridded). Shear distortion, complex terrain, linear chemical transformations, gravitational settling and deposition are treated. In addition to the mean concentration, dose and deposition, SCIPUFF provides an estimate of the probability levels of the predicted values. The model may be used on a case-by-case basis.

### *b. Input Requirements*

#### Source Data:

1. Pollutant physical and chemical properties are input by the user, including the chemical decay rates and deposition velocities. Multiple pollutants may be defined for a single release and size distributions may be defined for particles.
2. Release types are specified, e.g., continuous (arbitrary duration), instantaneous, mobile, and stack sources. Input requirements for each source depend on the release type and include emission rate and duration for each material type and size group as well as source coordinates, elevation and size.

#### Meteorological Data (different forms of meteorological input can be used by SCIPUFF):

1. Fixed winds: Wind speed and direction is assumed constant.
2. Observational input: Time-dependent observations are combined from multiple surface stations and/or upper-air profiles. A pre-processor is available that can be used to convert input to the Industrial Source Complex Short Term (ISCST) model to SCIPUFF's input format for surface data.
3. Time-dependent 3-dimensional gridded input.

Terrain data can be included with the gridded meteorological input files or provided as a separate file for other input types.

#### Turbulence Data (two types of turbulence input may be specified optionally):

1. Planetary boundary layer: Vertical profiles of the boundary layer scale turbulent velocity fluctuations, heat flux and turbulence length scales can be provided as input by the user or modeled based on boundary layer characteristics. Options for treatment of the boundary layer include "calculated", "observed" or "simple diurnal". Input requirements depend on boundary layer treatment type.
2. Large scale variability: For long range transport, the mesoscale horizontal velocity fluctuations and turbulence length scale may be specified by the user, computed from a theoretical model or read from a meteorological observation file.

#### Other Input:

Receptor locations are provided by the user in a 'sampler' file that includes the receptor locations and heights and the name of the material to be sampled. Other data requirements

include the coordinates of the domain, duration of the calculation, averaging time and user-specified model options.

### *c. Output*

Color contour plots can be viewed upon completion of a run at user-specified times. Available plots include: horizontal instantaneous slice, vertical instantaneous slice, vertically integrated slice, integrated surface dose, and integrated surface deposition for either the mean concentration or probability levels. The user can input the desired location of the slices and view these locations one at a time after completion of the run. Plots can be animated over the simulation time based on user-specified time intervals. Tables of data (in ASCII-format) can be exported from the plots by clicking on desired locations with the mouse or a grid may be specified.

If a sampler (i.e., receptor) file was specified on input, an ASCII file of time-dependent concentrations at each sampler location is produced as output. Surface integrals of dose and deposition are stored as adaptive grid files with multiple time breaks in direct access binary format. The puff file is a binary file that contains the complete puff data at a number of time breaks.

### *d. Type of Model*

SCIPUFF is a time-dependent Gaussian puff model that employs second-order closure turbulence modeling techniques to relate the dispersion rate to velocity fluctuation statistics.

### *e. Pollutant Types*

SCIPUFF may be used to model the dispersion of primary pollutants (gases or particles) which are inert or undergo linear chemical reactions, e.g., CO, NO<sub>2</sub>, SO<sub>2</sub>, PM-10, PM-2.5.

### *f. Source-Receptor Relationships*

The time-dependent concentrations are calculated as the sum of the contribution from all puffs. The maximum number of continuous sources is 400. The maximum number of instantaneous sources is limited by the maximum number of puffs, which is 20,000. The maximum number of discrete receptors is 200. SCIPUFF uses an adaptive grid to compute concentrations on a plane and produces color contour plots upon the completion of a run. If desired, discrete receptors or grid receptor concentration values may be exported from the contour plot to an ASCII file. To obtain the individual contribution from each source, no additional runs are necessary, however, an extra pollutant needs to be released from each source which has the same properties as the pollutant of interest but a unique name.

### *g. Plume Behavior*

Plume rise is treated through the conservation of buoyancy and momentum. A turbulent entrainment model based on earlier work on power plant plume rise (Sykes *et al.*, 1988) relates the turbulent velocity to the vertical rise rate. Complex terrain is treated through the reflection in the local surface tangent plane. Fumigation is treated explicitly according to the modeled boundary layer behavior. Aerodynamic downwash is not treated.

#### *h. Horizontal Winds*

Horizontal winds may be specified by the user as constant, provided in a time-dependent 3-dimensional gridded meteorological file, or in multiple surface observations and/or upper-air profiles. Surface data and vertical profiles from multiple stations are interpolated in space and time. The arbitrary spatial locations at each observation time are interpolated onto a grid using a simple inverse square weighting. Velocity (and temperature) fields are then interpolated between the grid times to provide smoothly varying meteorology for the dispersion calculation. In the surface layer, a similarity profile which accounts for surface roughness and stability is used. A 3-dimensional mass-consistent wind field may be generated optionally.

#### *i. Vertical Wind Speed*

Unless provided in a time-dependent 3-dimensional gridded meteorological file, vertical wind speed is assumed zero. A 3-dimensional mass-consistent wind field may be generated optionally.

#### *j. Horizontal Dispersion*

Puff growth is based on second-order closure turbulence modeling involving the horizontal turbulent velocity fluctuations and length scales that are either provided as input or modeled. Wind shear effects are also treated. The effect of averaging time is explicitly represented by selectively filtering the assumed turbulence spectrum.

#### *k. Vertical Dispersion*

Puff growth is based on second-order closure turbulence modeling involving the vertical turbulent velocity fluctuations and length scales that are either provided as input or modeled. Turbulent vertical drift, buoyancy-forces and wind shear effects are also treated. Perfect reflection is assumed at the ground surface and, for a convective boundary layer, at the mixing height. The effect of averaging time is explicitly represented by selectively filtering the assumed turbulence spectrum.

#### *l. Chemical Transformation*

Linear chemical transformations are treated using exponential decay (decay rate is provided by the user).

#### *m. Physical Removal*

Deposition of gases and particles, and precipitation washout and gravitational settling of particles are treated. Gaseous dry deposition effects are based on a fixed deposition velocity provided by the user. Dry deposition of particles to vegetative canopies is based on the approach of Slinn (1982) which includes determining a particle deposition efficiency. Dry deposition of particles to non-vegetative rough surfaces and water is treated according to Lewellen and Sheng (1980). Gravitational settling effects are determined by the particle fall velocity which is obtained from the balance between gravitational acceleration and the aerodynamic drag force. Precipitation washout of particles is treated through the use of a scavenging coefficient that is a function of precipitation rate and particle size following the approach of Seinfeld (1986). Precipitation washout of gases is not treated.

*n. Evaluation Studies*

Sykes, R.I., W.S. Lewellen, S.F. Parker and D.S. Henn, 1988. A hierarchy of dynamic plume models incorporating uncertainty, Volume 4: Second-order Closure Integrated Puff, EPRI, EPRI EA-6095 Volume 4, Project 1616-28.

Sykes, R.I., S.F. Parker, D.S. Henn and W.S. Lewellen, 1993. Numerical simulation of ANATEX tracer data using a turbulence closure model for long-range dispersion. *J. Appl. Meteor.*, **32**: 929-947.

Sykes, R.I., D.S. Henn, S.F. Parker and R.S. Gabruk, 1996. SCIPUFF - A generalized hazard dispersion model. Preprint of the 76<sup>th</sup> AMS Annual Meeting, Ninth Joint Conference on the Applications of Air Pollution Meteorology with A&WMA, 184-188.

Sykes, R.I. and R.S. Gabruk, 1997. A second-order closure model for the effect of averaging time on turbulent plume dispersion. *J. Appl. Meteor.*, **36**: 165-184.

*o. Literature Cited*

Donaldson, C. du P., 1973. Atmospheric turbulence and the dispersal of atmospheric pollutants, AMS Workshop on Micrometeorology, D.A. Haugen (Ed.). Science Press, Boston. pp. 313-390.

Lewellen, W.S., 1977. Use of invariant modeling, Handbook of Turbulence, W. Frost and T.H. Moulden (Eds.). Plenum Press. pp. 237-280.

Lewellen, W.S. and Y.P. Sheng, 1980. Modeling of dry deposition of SO<sub>2</sub> and sulfate aerosols. EPRI, EPRI EA-1452, Project 1306-1.

Seinfeld, J.H., 1986. Atmospheric Chemistry and Physics of Air Pollution. Wiley, New York; p.738.

Slinn, W.G.N., 1982. Predictions for particle deposition to vegetative canopies. *Atmos. Environ.*, **16**: 1785-1794.

## Shoreline Dispersion Model (SDM)

### *Reference*

PEI Associates, 1988. User's Guide to SDM - A Shoreline Dispersion Model. EPA Publication No. EPA-450/4-88-017. U.S. Environmental Protection Agency, Research Triangle Park, NC. (NTIS No. PB 89-164305)

### *Availability*

The model code is available on the SCRAM Internet website (see [Introduction and Availability](#)).

### *Abstract*

SDM is a hybrid multi-point Gaussian dispersion model that calculates source impact for those hours during the year when fumigation events are expected using a special fumigation algorithm and the MPTER regulatory model for the remaining hours (see Appendix A).

#### *a. Recommendations for Regulatory Use*

SDM may be used on a case-by-case basis for the following applications:

- Tall stationary point sources located at a shoreline of any large body of water;
- Rural or urban areas;
- Flat terrain;
- Transport distances less than 50 km;
- 1-hour to 1-year averaging times.

#### *b. Input Requirements*

Source data: location, emission rate, physical stack height, stack gas exit velocity, stack inside diameter, stack gas temperature and shoreline coordinates.

Meteorological data: hourly values of mean wind speed within the Thermal Internal Boundary Layer (TIBL) and at stack height; mean potential temperature over land and over water; over water lapse rate; and surface sensible heat flux. In addition to these meteorological data, SDM access standard NWS surface and upper air meteorological data through the RAMMET preprocessor.

Receptor data: coordinates for each receptor.

#### *c. Output*

Printed output includes the MPTER model output as well as: special shoreline fumigation applicability report for each day and source; high-five tables on the standard output with "F" designation next to the concentration if that averaging period includes a fumigation event.

*d. Type of Model*

SDM is hybrid Gaussian model.

*e. Pollutant Types*

SDM may be used to model primary pollutants. Settling and deposition are not treated.

*f. Source-Receptor Relationships*

SDM applies user-specified locations of stationary point sources and receptors. User input stack height, shoreline orientation and source characteristics for each source. No topographic elevation is input; flat terrain is assumed.

*g. Plume Behavior*

SDM uses Briggs (1975) plume rise for final rise. SDM does not treat stack tip or building downwash.

*h. Horizontal Winds*

Constant, uniform (steady-state) wind is assumed for an hour. Straight line plume transport is assumed to all downwind distances. Separate wind speed profile exponents (EPA, 1980) for both rural and urban cases are assumed.

*i. Vertical Wind Speed*

Vertical wind speed is assumed equal to zero.

*j. Horizontal Dispersion*

For the fumigation algorithm coefficients based on Misra (1980) and Misra and McMillan (1980) are used for plume transport in stable air above TIBL and based on Lamb (1978) for transport in the unstable air below the TIBL. An effective horizontal dispersion coefficient based on Misra and Onlock (1982) is used. For nonfumigation periods, algorithms contained in the MPTER model are used (see Appendix A).

*k. Vertical Dispersion*

For the fumigation algorithm, coefficients based on Misra (1980) and Misra and McMillan (1980) are used.

*l. Chemical Transformation*

Chemical transformation is not included in the fumigation algorithm.

*m. Physical Removal*

Physical removal is not explicitly treated.

*n. Evaluation Studies*

Environmental Protection Agency, 1987. Analysis and Evaluation of Statistical Coastal Fumigation Models. EPA Publication No. EPA-450/4-87-002. U.S. Environmental Protection Agency, Research Triangle Park, NC. (NTIS PB 87-175519)

## SLAB

### *Reference:*

Ermak, D.L., 1990. User's Manual for SLAB: An Atmospheric Dispersion Model for Denser-than-Air Releases (UCRL-MA-105607), Lawrence Livermore National Laboratory.

### *Availability*

The computer code can be obtained from: Energy Science and Technology Center, P.O. Box 1020, Oak Ridge, TN 37830, Phone (615) 576-2606.

The User's Manual (as DE 91-008443) can be obtained from the National Technical Information Service. The computer code is also available on the SCRAM Internet website (see Introduction and Availability).

### *Abstract*

The SLAB model is a computer model, PC-based, that simulates the atmospheric dispersion of denser-than-air releases. The types of releases treated by the model include a ground-level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet and an instantaneous volume source. All sources except the evaporating pool may be characterized as aerosols. Only one type of release can be processed in any individual simulation. Also, the model simulates only one set of meteorological conditions; therefore direct application of the model over time periods longer than one or two hours is not recommended.

#### a. Recommendations for use

The SLAB model should be used as a refined model to estimate spatial and temporal distribution of short-term ambient concentration (e.g., 1-hour or less averaging times) and the expected area of exposure to concentrations above specified threshold values for toxic chemical releases where the release is suspected to be denser than the ambient air.

#### b. *Input Requirements*

The SLAB model is executed in the batch mode. Data are input directly from an external input file. There are 29 input parameters required to run each simulation. These parameters are divided into 5 categories by the user's guide: source type, source properties, spill properties, field properties, and meteorological parameters. The model is not designed to accept real-time meteorological data or convert units of input values. Chemical property data are not available within the model and must be input by the user. Some chemical and physical property data are available in the user's guide.

Source type is chosen as one of the following: evaporating pool release, horizontal jet release, vertical jet or stack release, or instantaneous or short duration evaporating pool release.

Source property data requirements are physical and chemical properties (molecular weight, vapor heat capacity at constant pressure; boiling point; latent heat of vaporization; liquid

heat capacity; liquid density; saturation pressure constants), and initial liquid mass fraction in the release.

Spill properties include: source temperature, emission rate, source dimensions, instantaneous source mass, release duration, and elevation above ground level.

Required field properties are: desired concentration averaging time, maximum downwind distance (to stop the calculation), and four separate heights at which the concentration calculations are to be made.

Meteorological parameter requirements are: ambient measurement height, ambient wind speed at designated ambient measurement height, ambient temperature, surface roughness, relative humidity, atmospheric stability class, and inverse Monin-Obukhov length (optional, only used as an input parameter when stability class is unknown).

### *c. Output*

No graphical output is generated by the current version of this program. The output print file is automatically saved and must be sent to the appropriate printer by the user after program execution. Printed output includes in tabular form:

Listing of model input data;

Instantaneous spatially-averaged cloud parameters - time, downwind distance, magnitude of peak concentration, cloud dimensions (including length for puff-type simulations), volume (or mole) and mass fractions, downwind velocity, vapor mass fraction, density, temperature, cloud velocity, vapor fraction, water content, gravity flow velocities, and entrainment velocities;

Time-averaged cloud parameters - parameters which may be used externally to calculate time-averaged concentrations at any location within the simulation domain (tabulated as functions of downwind distance);

Time-averaged concentration values at plume centerline and at five off-centerline distances (off-centerline distances are multiples of the effective cloud half-width, which varies as a function of downwind distance) at four user-specified heights and at the height of the plume centerline.

### *d. Type of Model*

As described by Ermak (1989), transport and dispersion are calculated by solving the conservation equations for mass, species, energy, and momentum, with the cloud being modeled as either a steady-state plume, a transient puff, or a combination of both, depending on the duration of the release. In the steady-state plume mode, the crosswind-averaged conservation equations are solved and all variables depend only on the downwind distance. In the transient puff mode, the volume-averaged conservation equations are solved, and all variables depend only on the downwind travel time of the puff center of mass. Time is related to downwind distance by the height-averaged ambient wind speed. The basic conservation equations are solved via a numerical integration scheme in space and time.

#### *e. Pollutant Types*

Pollutants are assumed to be non-reactive and non-depositing dense gases or liquid-vapor mixtures (aerosols). Surface heat transfer and water vapor flux are also included in the model.

#### *f. Source-Receptor Relationships*

Only one source can be modeled at a time.

There is no limitation to the number of receptors; the downwind receptor distances are internally-calculated by the model. The SLAB calculation is carried out up to the user-specified maximum downwind distance.

The model contains submodels for the source characterization of evaporating pools, elevated vertical or horizontal jets, and instantaneous volume sources.

#### *g. Plume Behavior*

Plume trajectory and dispersion is based on crosswind-averaged mass, species, energy, and momentum balance equations. Surrounding terrain is assumed to be flat and of uniform surface roughness. No obstacle or building effects are taken into account.

#### *h. Horizontal Winds*

A power law approximation of the logarithmic velocity profile which accounts for stability and surface roughness is used.

#### *i. Vertical Wind Speed*

Not treated.

#### *j. Vertical Dispersion*

The crosswind dispersion parameters are calculated from formulas reported by Morgan *et al.* (1983), which are based on experimental data from several sources. The formulas account for entrainment due to atmospheric turbulence, surface friction, thermal convection due to ground heating, differential motion between the air and the cloud, and damping due to stable density stratification within the cloud.

#### *k. Horizontal Dispersion*

The horizontal dispersion parameters are calculated from formulas similar to those described for vertical dispersion, also from the work of Morgan *et al.* (1983).

#### *l. Chemical Transformation*

The thermodynamics of the mixing of the dense gas or aerosol with ambient air (including water vapor) are treated. The relationship between the vapor and liquid fractions within the cloud

is treated using the local thermodynamic equilibrium approximation. Reactions of released chemicals with water or ambient air are not treated.

*m. Physical Removal*

Not treated.

*n. Evaluation Studies*

Blewitt, D.N., J.F. Yohn and D.L. Ermak, 1987. An Evaluation of SLAB and DEGADIS Heavy Gas Dispersion Models Using the HF Spill Test Data. Proceedings, AIChE International Conference on Vapor Cloud Modeling, Boston, MA, November, pp. 56-80.

Ermak, D.L., S.T. Chan, D.L. Morgan and L.K. Morris, 1982. A Comparison of Dense Gas Dispersion Model Simulations with Burro Series LNG Spill Test Results. *J. Haz. Matls.*, **6**: 129-160.

Zapert, J.G., R.J. Londergan and H. Thistle, 1991. Evaluation of Dense Gas Simulation Models. EPA Publication No. EPA-450/4-90-018. U.S. Environmental Protection Agency, Research Triangle Park, NC.

*o. Literature Cited*

Ermak, D.L., 1989. A Description of the SLAB Model, presented at JANNAF Safety and Environmental Protection Subcommittee Meeting, San Antonio, TX, April, 1989.

Morgan, D.L., Jr., L.K. Morris and D.L. Ermak, 1983. SLAB: A Time-Dependent Computer Model for the Dispersion of Heavy Gas Released in the Atmosphere, UCRL-53383, Lawrence Livermore National Laboratory, Livermore, CA.