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Office of Air Quality
Planning and Standards
Research Triangle Park, NC 27711

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A USER'S GUIDE FOR THE CALPUFF DISPERSION MODEL

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PREFACE

The Interagency Workgroup on Air Quality Modeling (IWAQM) was formed to provide a focus for development of technically sound, regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas. Meetings were held with personnel from interested Federal agencies, viz. the Environmental Protection Agency, the U.S. Forest Service, the National Park Service, and the U.S. Fish and Wildlife Service. The purpose of these meetings was to review respective regional modeling programs, to develop an organizational framework, and to formulate reasonable objectives and plans that could be presented to management for support and commitment. The members prepared a memorandum of understanding (MOU) that incorporated the goals and objectives of the workgroup and obtained signatures of management officials in each participating agency. Although no States are signatories, their participation in IWAQM functions is explicitly noted in the MOU.

This report describes the CALPUFF dispersion model and associated processing programs. The CALPUFF model described in this report reflects improvements to the model including 1) new modules to treat buoyant rise and dispersion from area sources (such as forest fires), buoyant line sources, and volume sources, 2) an improved treatment of complex terrain, 3) additional model switches to facilitate its use in regulatory applications, 4) an enhanced treatment of wind shear through puff splitting, and 4) an optional PC-based GUI. CALPUFF has been coupled to the Emissions Production Model (EPM) developed by the Forest Service through an interface processor. EPM provides time-dependent emissions and heat release data for use in modeling controlled burns and wildfires.

This report is the sixth document published by the IWAQM in an effort to provide the sponsoring agencies and other interested parties information on appropriate "off-the-shelf" methods for estimating long range transport impacts of air pollutants on Federal Class I areas and impacts on regional visibility. The IWAQM members anticipate issuing additional publications related to progress toward meeting the IWAQM goals and objectives, the results of model evaluation studies, proposed and final recommendations on modeling systems for regulatory applications, and other topics related to specific objectives in the MOU.

The Environmental Protection Agency must conduct a formal and public review before the Agency can recommend for routine use new algorithms in regulatory analyses. These reports are being released to establish a basis for reviews of the capabilities of this methodology and of the consequences resulting from use of this methodology in routine dispersion modeling of air pollutant impacts. These reports are one part of the overall information that must be considered before any formal changes can be adopted.

ACKNOWLEDGEMENTS

The members of IWAQM acknowledge the special efforts of Joseph S. Scire, Elizabeth M. Insley, Robert J. Yamartino and Mark E. Fernau of EARTH TECH. This report was prepared by EARTH TECH (formerly Sigma Research, Inc.) for W. W. Engineering and Science under Contract No. 53-56A6-3-00838 to the U. S. Department of Agriculture (USDA) Forest Service, with Richard W. Fisher as the Work Assignment Manager. This work was accomplished in partial fulfillment of Interagency Agreement DW12544201 between the USDA and EPA, with John S. Irwin as the Project Officer.

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1. INTRODUCTION

1.1 Background

As part of a study to design and develop a generalized non-steady-state air quality modeling system for regulatory use, Sigma Research Corporation developed the CALPUFF dispersion model and related models and programs, including the CALMET meteorological model. The original development of CALPUFF and CALMET was sponsored by the California Air Resources Board (CARB). Systems Application, Inc. (SAI) served as a subcontractor to Sigma Research with the responsibility for developing the wind field modeling component of the modeling system.

The original design specifications for the modeling system included: (1) the capability to treat time-varying point and area sources, (2) suitability for modeling domains from tens of meters to hundreds of kilometers from a source, (3) predictions for averaging times ranging from one-hour to one year, (4) applicability to inert pollutants and those subject to linear removal and chemical conversion mechanisms, and, (5) applicability for rough or complex terrain situations.

The modeling system (Scire et al., 1990a, 1990b) developed to meet these objectives consisted of three components: (1) a meteorological modeling package with both diagnostic and prognostic wind field generators, (2) a Gaussian puff dispersion model with chemical removal, wet and dry deposition, complex terrain algorithms, building downwash, plume fumigation, and other effects, and (3) postprocessing programs for the output fields of meteorological data, concentrations and deposition fluxes.

In July, 1987, CARB initiated a second project with Sigma Research to upgrade and modernize the Urban Airshed Model (UAM) to include state-of-the-science improvements in many of the key technical algorithms including the numerical advection and diffusion schemes, dry deposition, chemical mechanisms, and chemical integration solver. The new photochemical model, called CALGRID, was integrated into the CALMET/CALPUFF modeling framework to create a complete modeling system for both reactive and non-reactive pollutants. The CALPUFF and CALGRID models were designed to be compatible with the common meteorological model, CALMET, and share a postprocessor for the time-averaging and display of the modeling results.

The Interagency Workgroup on Air Quality Modeling (IWAQM) has reviewed various modeling approaches suitable for estimating pollutant concentrations at Class I areas, including

the individual and cumulative impacts of proposed and existing sources on Air Quality Related Values (AQRVs), Prevention of Significant Deterioration (PSD) increments, and National Ambient Air Quality Standards (NAAQS). IWAQM consists of representatives from the U.S. Environmental Protection Agency (EPA), U.S. Forest Service, National Park Service, and U.S. Fish and Wildlife Service. IWAQM released a Phase I report (EPA, 1993) which recommended using the MESOPUFF II dispersion model and MESOPAC II meteorological model for simulating regional air quality and visibility impacts. These recommendations were considered interim until more refined (Phase II) techniques could be identified and evaluated. As part of the Phase II work, IWAQM has reviewed and intercompared diagnostic wind field models, tested the use of coarse gridded winds fields from the Penn State/NCAR Mesoscale Model with four dimensional data assimilation (MM4-FDDA) as input into the diagnostic models, and evaluated the MESOPUFF II and CALPUFF modeling systems using tracer data collected during Cross-Appalachian Tracer Experiment (CAPTEX). The CAPTEX evaluation results (EPA, 1995) indicated that by using the CALMET/CALPUFF models with MM4-FDDA data, performance could be improved over that obtained with the interim Phase I modeling approach.

The CALMET and CALPUFF models have been enhanced as part of work for IWAQM, U.S. EPA, the U.S. Forest Service, the Environmental Protection Authority of Victoria (Australia), and private industry in the U.S. and Australia. The improvements to CALMET included modifications to make it more suitable for regional applications such as the use of a spatially variable initial guess field, an option for using hourly MM4-FDDA gridded fields as a supplement to observational data, the ability to compute Lambert conformal map factors, a modified mixing height scheme, an option to use similarity theory to extrapolate vertically surface wind observations, an enhanced algorithm to compute the three-dimensional temperature field over water bodies, and an optional PC-based Graphical User Interface to facilitate model setup and execution and to provide access to on-line Help files. Improvements to CALPUFF include new modules to treat buoyant rise and dispersion from area sources (such as forest fires), buoyant line sources, volume sources, an improved treatment of complex terrain, additional model switches to facilitate its use in regulatory applications, enhanced treatment of wind shear through puff splitting, and an optional PC-based GUI. CALPUFF has been coupled to the Emissions Production Model (EPM) developed by the Forest Service through an interface processor. EPM provides time-dependent emissions and heat release data for use in modeling controlled burns and wildfires.

1.2 Overview of the Modeling System

The overall modeling system configuration is presented in Figure 1-1. The meteorological modeling with the CALMET model is detailed in Figure 1-2. Note that the

preprocessors for the raw meteorological data are written to accommodate the U.S. National Climatic Data Center (NCDC) file formats. Figure 1-3 is the schematic of the CALPUFF dispersion model indicating the model input and output files. The postprocessing approach for the meteorological and dispersion modeling results is shown in Figure 1-4. The major components of the modeling system and interfaces to external programs are summarized below.

METSCAN is a meteorological preprocessor which performs quality assurance checks on the hourly surface meteorological data in the NCDC CD-144 format which is used as input to the SMERGE program.

READ56 and **READ62** are meteorological preprocessors which extract and process upper air wind and temperature data from standard data formats used by NCDC. READ56 and READ62 process TD-5600 and TD-6201 formatted data, respectively.

SMERGE is a meteorological preprocessor which processes hourly surface observations from a number of stations in NCDC CD-144 format and reformats the data into a single file with the data sorted by time rather than station.

PXTRACT is a meteorological preprocessor which extracts precipitation data for stations and a time period of interest from a fixed length, formatted precipitation data file in NCDC TD-3240 format.

PMERGE is a meteorological preprocessor responsible for reformatting the precipitation data files created by the PXTRACT program. PMERGE resolves "accumulation periods" into hourly values and flags suspicious or missing data. The output file can be formatted or binary, which can be directly input into the CALMET model, containing the precipitation data sorted by hour rather than station.

CSUMM (a version of the Colorado State University Mesoscale Model) is a primitive equation wind field model which simulates mesoscale airflow resulting from differential surface heating and terrain effects. The diagnostic wind field model within CALMET contains options that allow wind fields produced by CSUMM to be combined with observational data as part of the CALMET objective analysis procedure.

MM4-FDDA (Penn State/NCAR Mesoscale Model) is a prognostic wind field model with four dimensional data assimilation. CALMET has been modified to incorporate MM4-FDDA winds into its Diagnostic Wind Model (DWM).

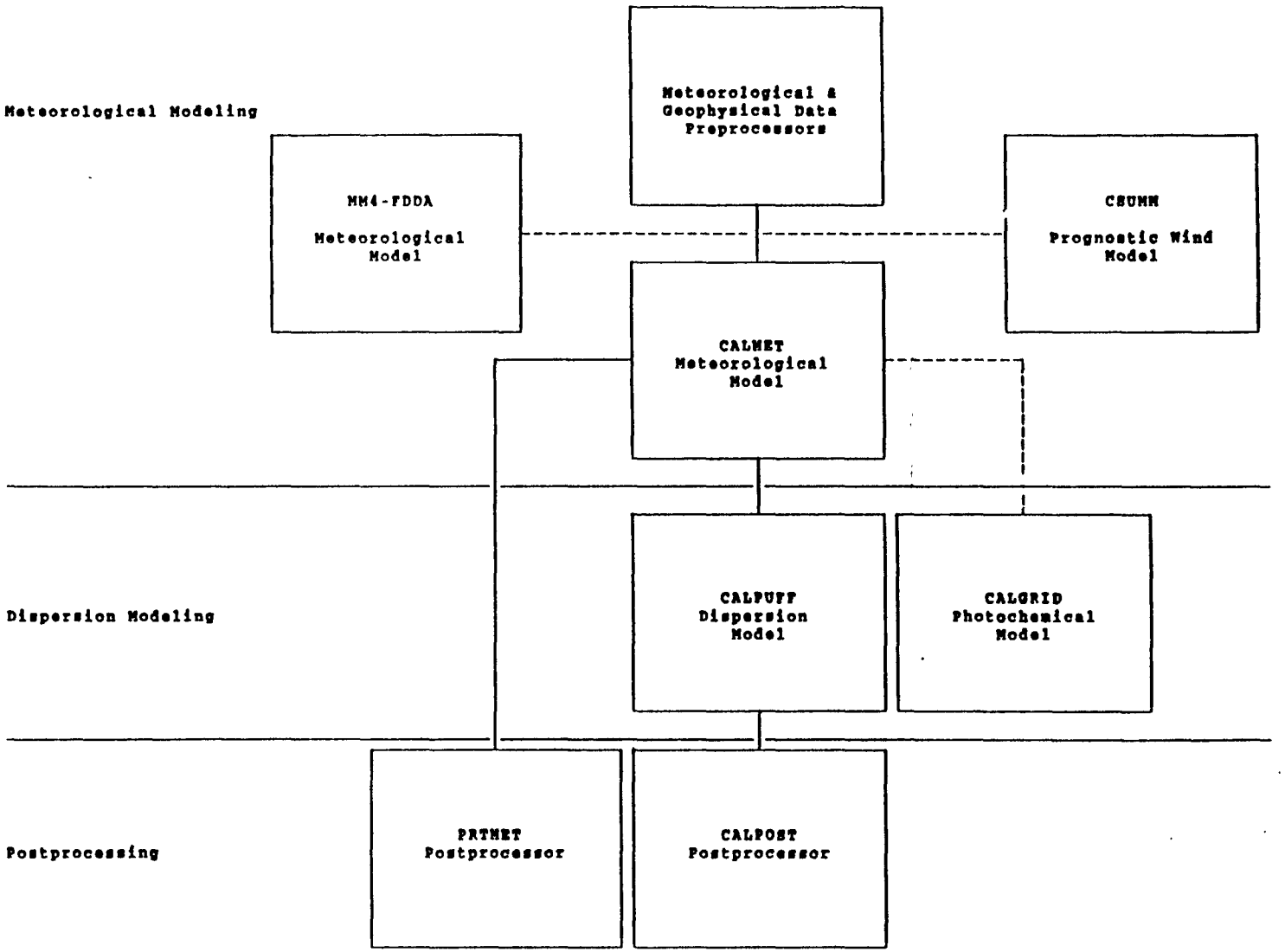


Figure 1-1. Overview of the program elements in the CALMET/CALPUFF modeling system. Also shown is the associated CALGRID photochemical model, and the MM4-FDDA and CSUMM meteorological models.

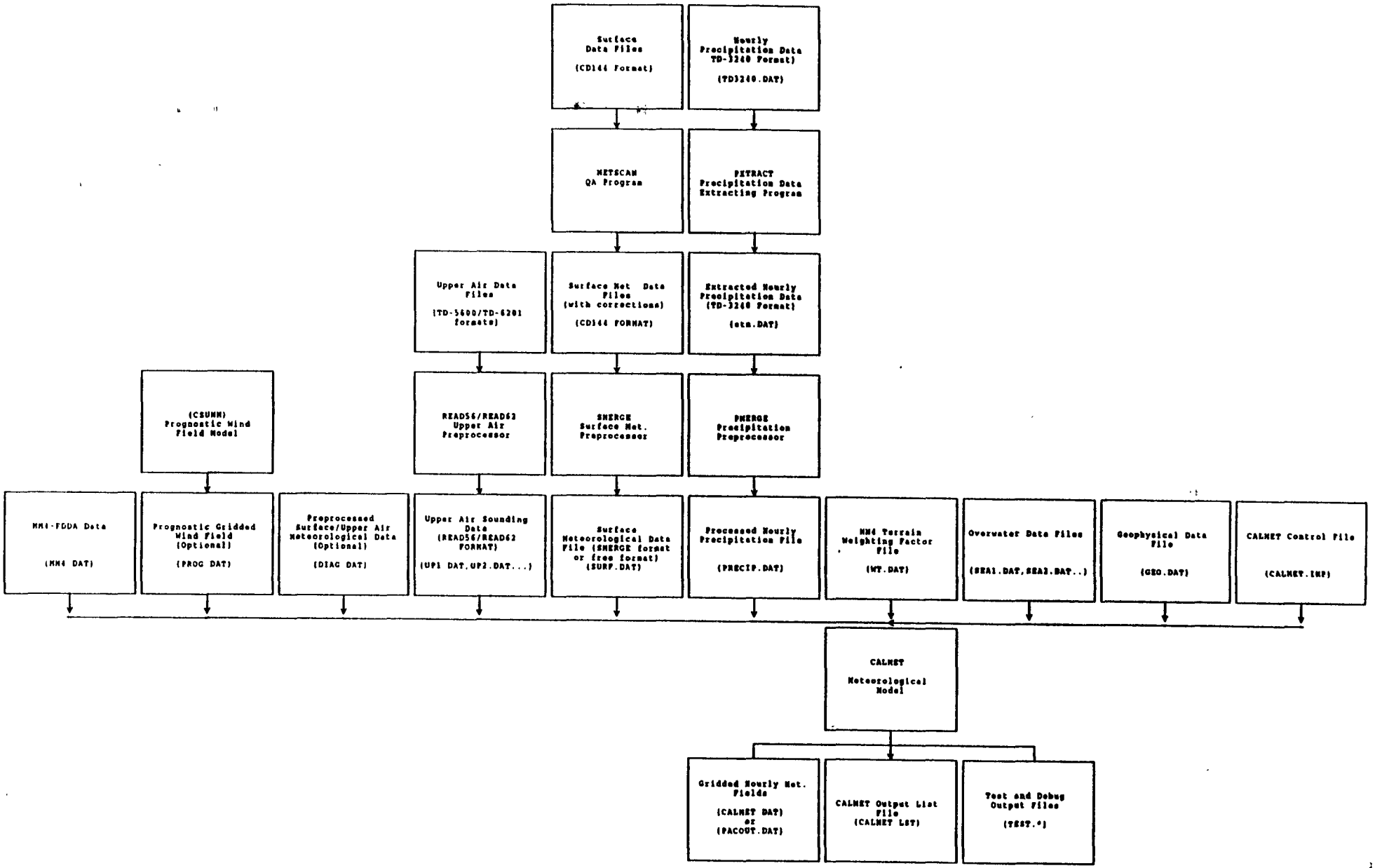


Figure 1-2. Meteorological modeling: CALMET modeling flow diagram.

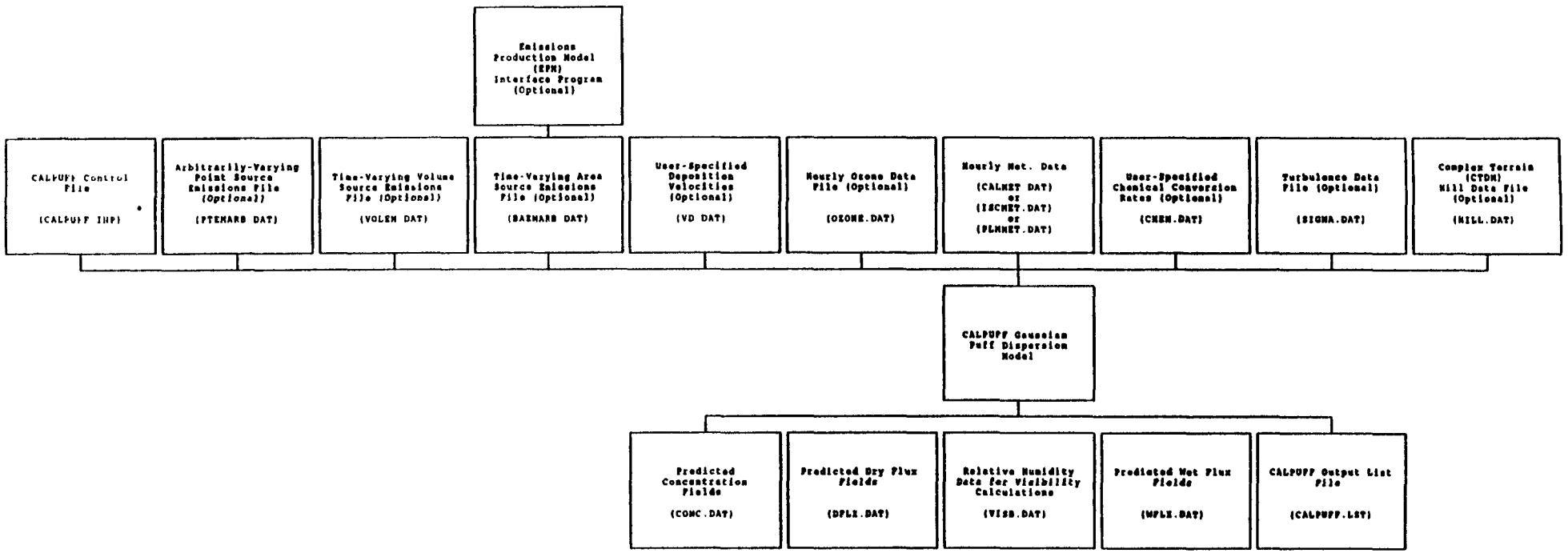


Figure 1-3. Dispersion Modeling: CALPUFF modeling flow diagram.

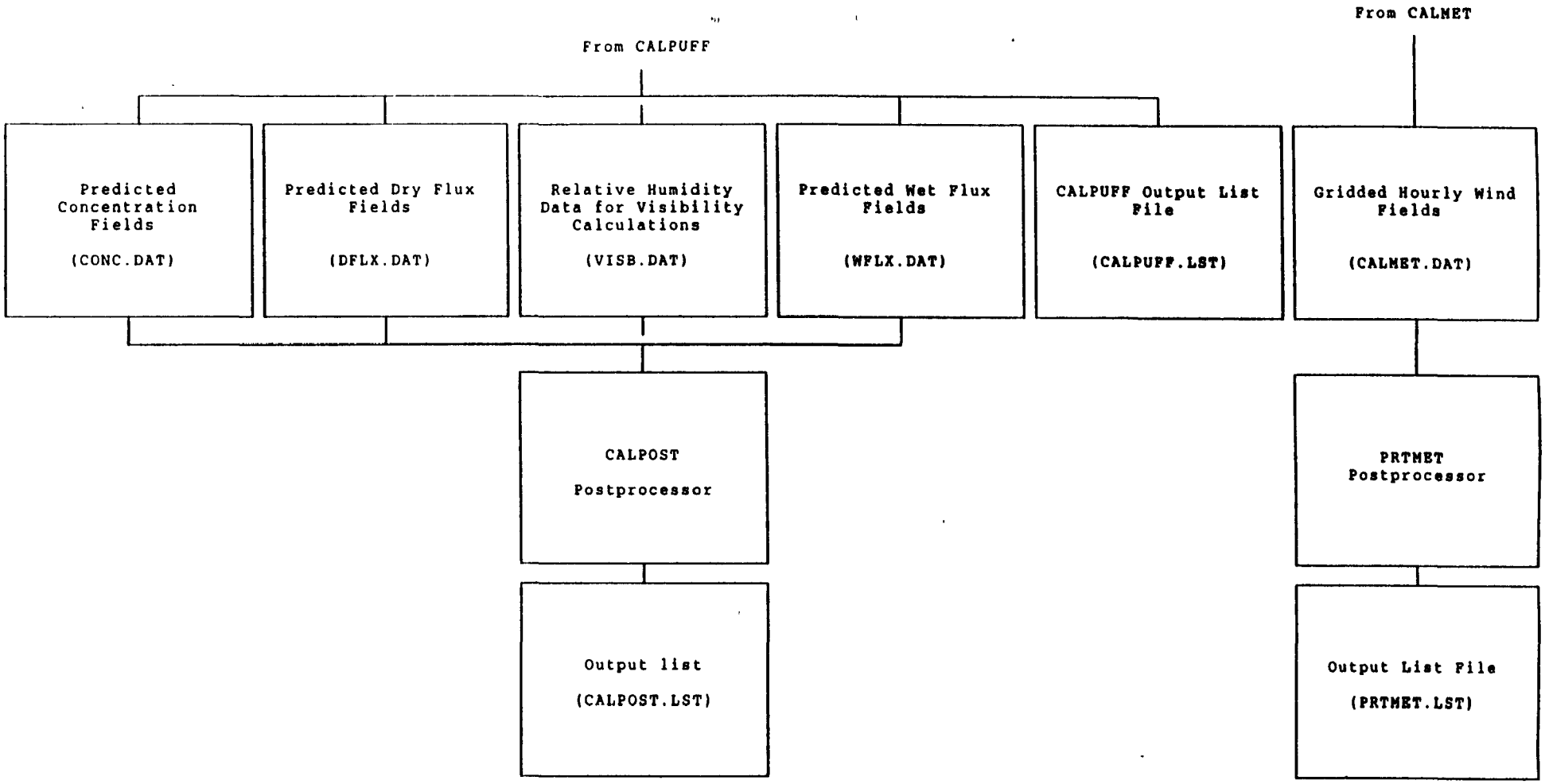


Figure 1-4. Postprocessing: CALPOST/PRTMET postprocessing flow diagram.

CALMET is a meteorological model which includes a diagnostic wind field generator containing objective analysis and parameterized treatments of slope flows, kinematic terrain effects, terrain blocking effects, and a divergence minimization procedure, and a micrometeorological model for overland and overwater boundary layers.

CALPUFF is a non-steady-state Lagrangian Gaussian puff model containing modules for complex terrain effects, overwater transport, coastal interaction effects, building downwash, wet and dry removal, and simple chemical transformation.

CALGRID is an Eulerian photochemical transport and dispersion model which includes modules for horizontal and vertical advection/diffusion, dry deposition, and a detailed photochemical mechanism.

OPTHILL is a processor program which uses topographical data (such as terrain maps) to develop hill shape factors that are used in the subgrid scale complex terrain (CTSG) module in CALPUFF.

PRTMET is a postprocessing program which displays user-selected portions of the meteorological data base produced by the CALMET meteorological model.

CALPOST is a postprocessing program with options for the computation of time-averaged concentrations and deposition fluxes predicted by the CALPUFF and CALGRID models. CALPOST will also compute visibility impacts in accordance with IWAQM recommendations.

This report describes the CALPUFF model and its related processors OPTHILL and CALPOST. Section 2 contains a description of the technical formulation of CALPUFF. The structure of the CALPUFF code is discussed in Section 3. The inputs and outputs of the CALPUFF model and the preprocessing and postprocessing programs are described in Section 4.

A series of companion reports describe other components of the modeling system. The technical formulation and user instructions for the revised CALMET model are contained in Scire et al. (1995). The prognostic wind field model, CSUMM, is described in a report by Kessler (1989). A stand-alone version of the Diagnostic Wind Model (DWM) used as the wind field module in CALMET is discussed by Douglas and Kessler (1988). Finally, the CALGRID model is documented in a paper by Yamartino et al. (1992) and reports by Yamartino et al. (1989) and Scire et al. (1989).

1.3 Major Model Algorithms and Options

CALPUFF is a multi-layer, multi-species non-steady-state puff dispersion model which can simulate the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. CALPUFF can use the three dimensional meteorological fields developed by the CALMET model, or simple, single station winds in a format consistent with the meteorological files used to drive the ISC2 (EPA, 1992) or AUSPLUME (Lorimer, 1976) steady-state Gaussian models. However, single-station ISC2 or AUSPLUME winds should be used with caution, because they do not allow CALPUFF to take advantage of its capabilities to treat spatially-variable meteorological fields.

CALMET includes a diagnostic wind field generator, and overland and overwater boundary layer modules. CALMET has the ability to combine the wind fields generated by the CSUMM prognostic wind field model or the MM4-FDDA model with observational data through an objective analysis procedure.

CALPUFF contains algorithms for near-source effects such as building downwash, transitional plume rise, partial plume penetration, subgrid scale terrain interactions as well as longer range effects such as pollutant removal (wet scavenging and dry deposition), chemical transformation, vertical wind shear, overwater transport and coastal interaction effects. It can accommodate arbitrarily-varying point source and gridded area source emissions. Most of the algorithms contain options to treat the physical processes at different levels of detail depending on the model application.

The major features and options of the CALPUFF model are summarized in Table 1-1. Some of the technical algorithms are briefly described below.

Dry Deposition: A full resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. Options are provided to allow user-specified, diurnally varying deposition velocities to be used for one or more pollutants instead of the resistance model (e.g., for sensitivity testing) or to by-pass the dry deposition model completely.

Wet Deposition: An empirical scavenging coefficient approach is used in CALPUFF to compute the depletion and wet deposition fluxes due to precipitation scavenging. The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).

Table 1-1
Major Features of the CALPUFF Model

- **Source types**
  - Point sources (constant or variable emissions)
  - Line sources (constant emissions)
  - Volume sources (constant or variable emissions)
  - Area sources (constant or variable emissions)

- **Non-steady-state emissions and meteorological conditions**
  - Gridded 3-D fields of meteorological variables (winds, temperature)
  - Spatially-variable fields of mixing height, friction velocity, convective velocity scale, Monin-Obukhov length, precipitation rate
  - Vertically and horizontally-varying turbulence and dispersion rates
  - Time-dependent source and emissions data

- **Efficient sampling functions**
  - Integrated puff formulation
  - Elongated puff (slug) formulation

- **Dispersion coefficient (σ_y, σ_z) options**
  - Direct measurements of σ_v and σ_w
  - Estimated values of σ_v and σ_w based on similarity theory
  - Pasquill-Gifford (PG) dispersion coefficients (rural areas)
  - McElroy-Pooler (MP) dispersion coefficients (urban areas)

- **Vertical wind shear**
  - Puff splitting
  - Differential advection and dispersion

- **Plume rise**
  - Partial penetration
  - Buoyant and momentum rise
  - Stack tip effects
  - Vertical wind shear
  - Building downwash effects

- **Building downwash**
  - Huber-Snyder method
  - Schulman-Scire method

(Continued)

Table 1-1 (Concluded)
Major Features of the CALPUFF Model

- **Subgrid scale complex terrain**
  - Dividing streamline, H_d:
    - Above H_d, puff flows over the hill and experiences altered diffusion rates
    - Below H_d, puff deflects around the hill, splits, and wraps around the hill

- **Interface to the Emissions Production Model (EPM)**
  - Time-varying heat flux and emissions from controlled burns and wildfires

- **Dry Deposition**
  - Gases and particulate matter
  - Three options:
    - Full treatment of space and time variations of deposition with a resistance model
    - User-specified diurnal cycles for each pollutant
    - No dry deposition

- **Overwater and coastal interaction effects**
  - Overwater boundary layer parameters
  - Abrupt change in meteorological conditions, plume dispersion at coastal boundary
  - Plume fumigation

- **Chemical transformation options**
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^=$, NO_x, HNO_3, and NO_3^- (MESOPUFF II method)
  - User-specified diurnal cycles of transformation rates
  - No chemical conversion

- **Wet Removal**
  - Scavenging coefficient approach
  - Removal rate a function of precipitation intensity and precipitation type

- **Graphical User Interface**
  - Click-and-point model setup and data input
  - Enhanced error checking of model inputs
  - On-line Help files

Chemical Transformation: CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme (SO_2, $SO_4^=$, NO_x, HNO_3, and NO_3^-) employed in the MESOPUFF II model or a set of user-specified, diurnally-varying transformation rates.

Subgrid Scale Complex Terrain: The complex terrain module in CALPUFF is based on the approach used in the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989). Plume impingement on subgrid scale hills is evaluated using a dividing streamline (H_d) to determine which pollutant material is deflected around the sides of a hill (below H_d) and which material is advected over the hill (above H_d). Individual puffs are split into up to three sections for these calculations.

Puff Sampling Functions: A set of accurate and computationally efficient puff sampling routines are included in CALPUFF which solve many of the computational difficulties with applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function is used. An integrated puff approached is used during less demanding conditions. Both techniques reproduce continuous plume results exactly under the appropriate steady state conditions.

Wind Shear Effects: CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport occur on the puffs generated from the original puff, which under some conditions, can substantially increase the effective rate of horizontal growth of the plume.

Building Downwash: The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions.

Overwater and Coastal Interaction Effects: Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in

meteorological and dispersion conditions, including the abrupt changes which occur at the coastline of a major body of water.

Dispersion Coefficients: Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements (σ_v and σ_w), the use of similarity theory to estimate σ_v and σ_w from modeled surface heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the Complex Terrain Dispersion Model (CDTM). Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients.

1.4 Summary of Data and Computer Requirements

Data Requirements

The input data sets used by CALPUFF are summarized in Table 1-2 (also see the modeling system flow diagram, Figure 1-1). CALPUFF reads user inputs from a "control file" with a default name of CALPUFF.INP. This file contains the user's selections for the various model options, technical input variables, output options, and other user-controllable options.

A meteorological data file (CALMET.DAT) contains hourly gridded fields of micrometeorological parameters and three-dimensional wind and temperature fields. The meteorological data file also contains geophysical data such as terrain heights and land use which are required by both the meteorological model (e.g., for terrain adjustment of the wind fields) and by the CALPUFF model. The contents of the CALMET.DAT input file and the other input data bases are summarized in Table 1-3. Options also exist for using single-station meteorological data in ISC2 or AUSPLUME data format. Note: CALPUFF requires the addition of three header records at the beginning of the ISC2 or AUSPLUME meteorological data (see Section 4.2.2).

Four files are provided for the input of emissions data. The control file, CALPUFF.INP includes point, line, volume and area source data for sources with constant emission parameters. Arbitrarily-varying point source data is read from a file with a default name of PTEMARB.DAT. Gridded, time-varying volume source emissions are obtained from the file VOLEM.DAT. Time-varying area source data is read from a file called BAEMARB.DAT.

Hourly observations of ozone data are used in the calculation of SO_2 and NO_x transformation rates if the MESOPUFF II chemical transformation scheme is selected. The hourly ozone data for one or more ozone stations are read from a data file called OZONE.DAT.

Table 1-2
Summary of CALPUFF Input Files

Default File Name	Contents	Unit* Number	Type
PUFFILES.DAT	File containing the filename and path for each of the input and output (I/O) files used in the current run. If an I/O filename is not specified in the PUFFILES.DAT file, the model uses the default filenames shown in this table	IO14	Formatted
CALPUFF.INP	Control file inputs	IO5	Formatted
CALMET.DAT	Geophysical and hourly meteorological data, created by the CALMET meteorological model	IO7	Unformatted
or ISCMET.DAT	Single-station ASCII meteorological data in slightly modified ISC2-format	IO7	Formatted
or PLMMET.DAT	Single-station ASCII meteorological data in slightly modified AUSPLUME format	IO7	Formatted
PTEMARB.DAT	Source and emissions data for point sources with arbitrarily-varying emission parameters (optional)	IO16	Unformatted
BAEMARB.DAT	Emissions data for area sources with time-varying emission parameters. Can be derived from EPM model files (optional)	IO17	Unformatted
VOLEM.DAT	Emissions data for volume sources with time-varying emission parameters (optional)	IO18	Formatted
VD.DAT	User-specified deposition velocities (optional)	IO20	Formatted
OZONE.DAT	Hourly ozone measurements at one or more ozone stations (optional)	IO22	Formatted
CHEM.DAT	User-specified chemical transformation rates (optional)	IO24	Formatted
SIGMA.DAT	Hourly turbulence measurements (σ_v, σ_w) (optional)	IO26	Formatted
HILL.DAT	Hill specifications from CTDM terrain processor (optional)	IO28	Formatted

* Variable shown is the parameter controlling the FORTRAN unit number associated with the file. Usually, the value assigned to the parameter is consistent with the name (i.e., IO7 = 7). However, the value can be easily changed in the parameter file to accommodate reserved unit numbers on a particular system.

Table 1-3
Summary of Input Data Used by CALPUFF

Geophysical Data (CALMET.DAT)

Gridded fields of:

- surface roughness lengths (z_o)
- land use categories
- terrain elevations
- leaf area indices

Meteorological Data (CALMET.DAT)

Gridded fields of:

- u, v, w wind components (3-D)
- air temperature (3-D)
- surface friction velocity (u_*)
- convective velocity scale (w_*)
- mixing height (z_i)
- Monin-Obukhov length (L)
- PGT stability class
- Precipitation rate

Hourly values of the following parameters at surface met. stations:

- air density (ρ_a)
- air temperature
- short-wave solar radiation
- relative humidity
- precipitation type

Emissions Data (CALPUFF.INP, PTEMARB.DAT, BAEMARB.DAT, VOLEM.DAT)

Point source emissions:

- Source and emissions data for point sources with constant emission parameters (CALPUFF.INP)
- Source and emissions data for point sources with arbitrarily-varying emission parameters (PTEMARB.DAT)

Area source emissions

- Emissions and initial size, height, and location for area sources with constant emission parameters (CALPUFF.INP)
- Gridded emissions data for buoyant area sources with time-varying emission parameters (BAEMARB.DAT)

(Continued)

Table 1-3 (Concluded)
Summary of Input Data Used by CALPUFF

Volume source emissions

- Emissions, height, size, and location of volume sources with constant emission parameters (CALPUFF.INP)
- Emissions data for volume sources with time-varying emission parameters (VOLEM.DAT)

Line source emissions

- Source and emissions data, height, length, location, spacing, and orientation of line sources with constant emission parameters (CALPUFF.INP)

Deposition Velocity Data (VD.DAT)

- Deposition velocity for each user-specified species for each hour of a diurnal cycle

Ozone Monitoring Data (OZONE.DAT)

- Hourly ozone measurements at one or more monitoring stations

Chemical Transformation Data (CHEM.DAT)

- Species-dependent chemical transformation rates for each hour of a diurnal cycle

Turbulence Observational Data (SIGMA.DAT)

- Hourly measurements of turbulence (σ_v, σ_w) at an onsite meteorological tower

Hill Data (HILL.DAT)

- Hill shape and height parameters for use in the subgrid-scale complex terrain module (CTSG)

Two additional input files, VD.DAT and CHEM.DAT, contain diurnal cycles of user-specified deposition velocities and chemical transformation rates, respectively. These files are necessary only if the user wishes to substitute the values normally computed internally by the deposition and chemical models with sets of time-varying but spatially-uniform externally specified values.

Another optional input file, SIGMA.DAT, contains hourly observations of σ_v and σ_w. These parameters can be used to compute the plume dispersion coefficients σ_y and σ_z.

The structure, format and contents of each CALPUFF input data set are described in Section 4.2. The CALPUFF output files are summarized in Table 1-4. The list file contains a copy of the inputs used in the run, optional output fields of gridded and discrete receptor concentrations, wet deposition fluxes, and dry deposition fluxes and other run data. The CONC.DAT, WFLX.DAT, and DFLX.DAT files contain the output concentrations, wet and dry fluxes, respectively, in an unformatted form suitable for further processing by the postprocessing program, CALPOST. The VISB.DAT file contains relative humidity information which is required by CALPOST in order to perform certain visibility-relative computations.

Computer Requirements

The memory management scheme used in CALPUFF is designed to allow the maximum array dimensions in the model to be easily adjusted to match the requirements of a particular application. An external parameter file contains the maximum array size for all of the major arrays. A re-sizing of the program can be accomplished by modifying the appropriate variable or variables in the parameter file and re-compiling the program. All appropriate arrays in the model will be automatically re-sized by the updated parameter values. For example, the maximum number of horizontal grid cells allowed in the model, MXNX and MXNY, are two of the variables which can be adjusted within the parameter file. However, no change to the parameter file is necessary if a particular application requires a smaller array size than the maximum values specified in the parameter file.

The memory required by CALPUFF will be a strong function of the specified maximum array dimensions in the parameter file. However, as an example, CALPUFF required approximately 300 K bytes of memory for a test run with a 10 x 10 horizontal grid, with 5 vertical layers, and a maximum number of puffs of 100. This type of configuration may be suitable for

Table 1-4
Summary of CALPUFF Output Files

Default File Name	Contents	Unit* Number	Type
CALPUFF.LST	List file produced by CALPUFF	IO6	Formatted
CONC.DAT	One-hour averaged concentrations (g/m^3) at the gridded and discrete receptors for species selected by the user in the control file (optional)	IO8	Unformatted
DFLX.DAT	One-hour averaged dry deposition fluxes ($g/m^2/s$) at the gridded and discrete receptors for species selected by the user in the control file (optional)	IO9	Unformatted
WFLX.DAT	One-hour averaged wet deposition fluxes ($g/m^2/s$) at the gridded and discrete receptors for species selected by the user in the control file (optional)	IO10	Unformatted
VISB.DAT	Relative humidity data required for visibility-related postprocessing (optional)	IO11	Unformatted
DEBUG.DAT	Tables of detailed puff/slug data useful for debugging (optional)	IO30	Formatted

* Variable shown is the parameter controlling the FORTRAN unit number associated with the file. Usually, the value assigned to the parameter is consistent with the name (i.e., IO8 = 8). However, the value can be easily changed in the parameter file to accommodate reserved unit numbers on a particular system.

evaluating the near-field impact of a small number of point sources. For studies involving long-range transport, memory requirements will typically be at least 8 megabytes, with more required for simulations involving large numbers of sources.

The run time of CALPUFF will vary considerably depending on the model application. Variations of factors of 10-20 are likely depending of the size of the domain, the number of sources, selection of technical options, and meteorological variables such as the mean wind speed. Because each puff is treated independently, any factor which influences the number and residence time of puffs on the computational grid will affect the run time of the model.

Program Execution

CALPUFF (Version 3.0 and above) can be executed with the following DOS command line:

CALPUF3 filename

where it is assumed that the executable file is called CALPUF3.EXE and the "filename" is the name of the file (up to 70 characters in length) containing the input and output (I/O) files to be used in the run. The default I/O file name is PUFFILES.DAT. In the I/O file the user can change the name of any of the input and output files from their default names, and change the directory from which the files will be accessed by specifying the file's full pathname (see Section 4.2).

2. TECHNICAL DISCUSSION

2.1 Solution of the Puff Equations

Puff models represent a continuous plume as a number of discrete packets of pollutant material. Most puff models (e.g., Ludwig et al., 1977; van Egmond and Kesseboom, 1983; Peterson, 1986) evaluate the contribution of a puff to the concentration at a receptor by a "snapshot" approach. Each puff is "frozen" at particular time intervals (sampling steps). The concentration due to the "frozen" puff at that time is computed (or sampled). The puff is then allowed to move, evolving in size, strength, etc., 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 within the basic time step. Depending on the model and the application, the sampling step and the time step may both be one hour, indicating only one "snapshot" of the puff is taken each hour.

A traditional drawback of the puff approach has been the need for the release of many puffs to adequately represent a continuous plume close to a source. Ludwig et al. (1977) have shown that if the distance between puffs exceeds a maximum of about 2 σ_y, inaccurate results may be obtained (see Figure 2-1). Better results are obtained if the puff separation is reduced to no more than one σ_y. If the puffs do not overlap sufficiently, the concentrations at receptors located in the gap between puffs at the time of the "snapshot" are underestimated, while those at the puff centers are overestimated.

Ludwig et al. (1977) recommend spacing puffs uniformly in space rather than in time with a puff merging/purging scheme to reduce the total number of puffs. Zannetti (1981) suggests tracking fewer puffs than necessary for adequate sampling, but then saturating the area near a receptor with artificially generated puffs to provide the required puff overlap (see Figure 2-2). Although both schemes act to reduce the number of puffs carried by the model, the snapshot sampling method still requires that an uneconomically large number of puffs be generated near the source. For example, at a receptor 100 meters from a source, and assuming PGT dispersion rates, puffs at a density corresponding to a release rate of over 1300 puffs/hour are required to meet the 2 σ_y criterion for F stability, 3 m/s wind conditions. During high wind speed, neutral conditions (10 m/s, D stability), nearly 2200 puffs/hour are needed. The more stringent one σ_y criterion would double the number of puffs required.

Two alternatives to the conventional snapshot sampling function are discussed below. The first is based on the integrated sampling function in the MESOPUFF II model (Scire et al.,

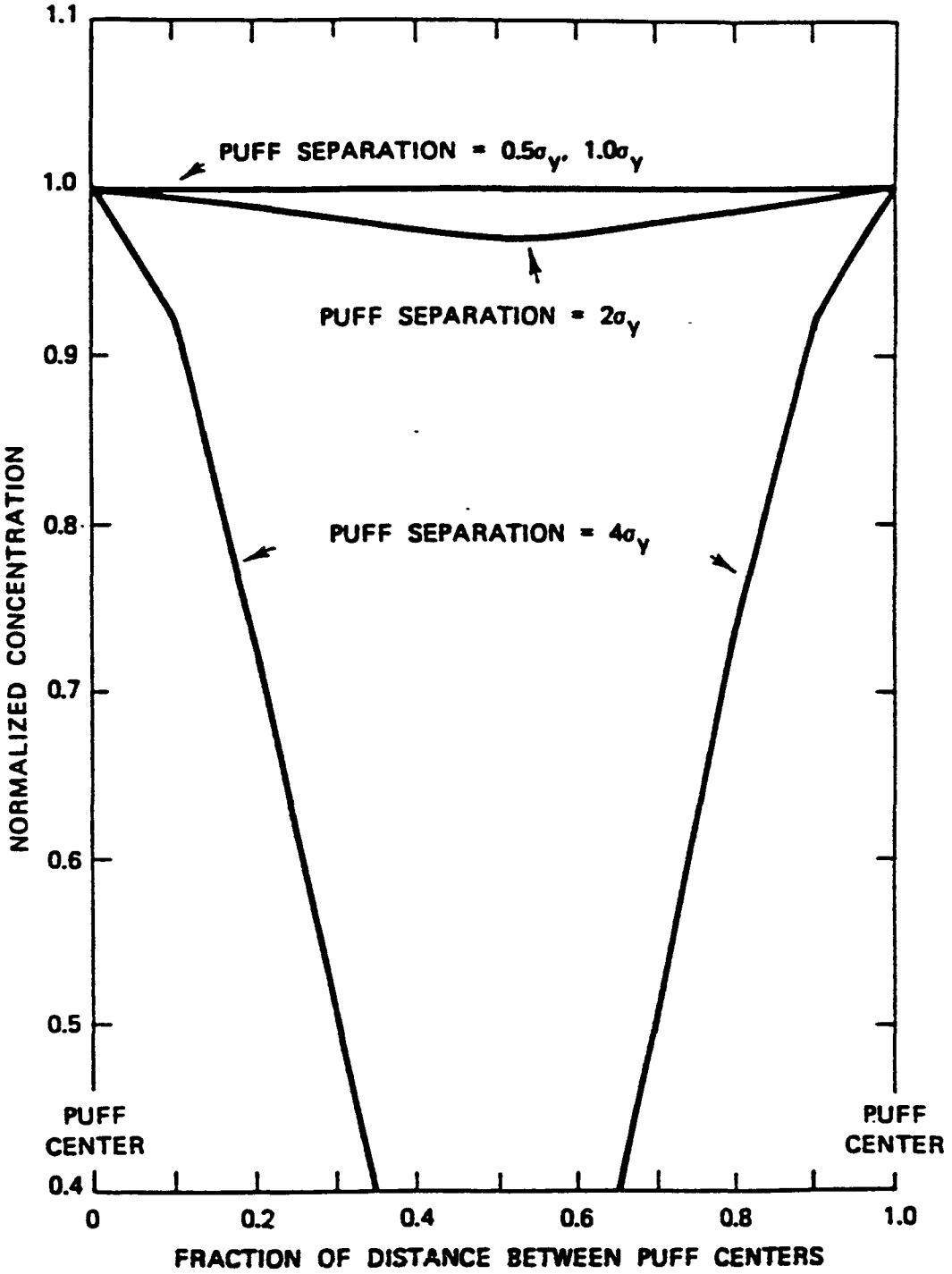


Figure 2-1. Normalized concentration between two puffs in a string of puffs of equal size and spacing. [From Ludwig et al. (1977)].

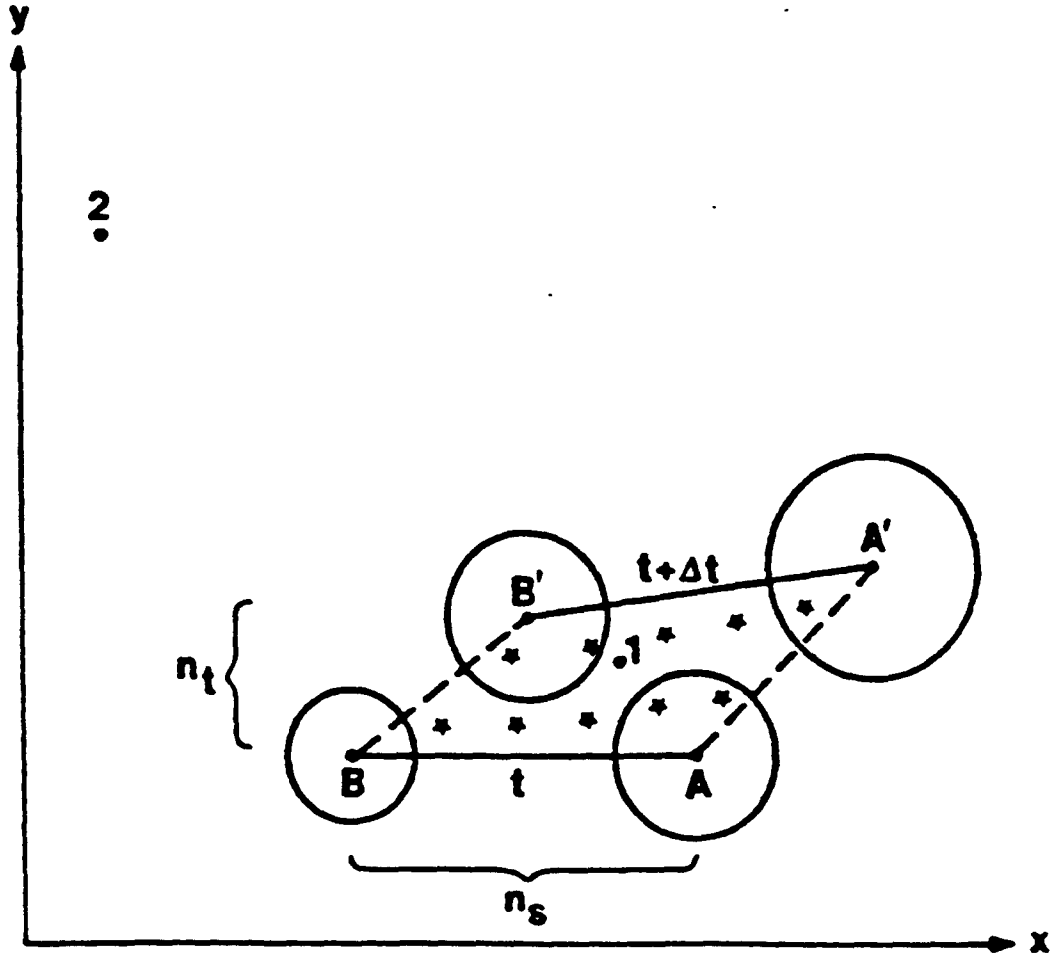


Figure 2-2. Illustration of the puff generation scheme of Zannetti (1981). The advected puffs (A → A', B → B') in the vicinity of Receptor 1 are not sufficient to resolve the plume. The mass from the original puffs is redistributed into n_t x n_s new puffs (asterisks) for sampling purposes. [From Zannetti (1981)].

1984a,b), with modifications for near-field applications. The second scheme uses a non-circular puff (slug) elongated in the direction of the wind to eliminate the need for frequent releases of puffs. The performances of the original and modified integrated sampling functions and the slug model are evaluated for unsteady and steady-state conditions. The sampling scheme used in CALPUFF is a hybrid circular puff/elongated slug method taking advantage of the strengths of each algorithm.

2.1.1 Integrated Puff Sampling Function Formulation

The basic equation for the contribution of a puff at a receptor is:

$$C = \frac{Q}{2\pi\sigma_x\sigma_y} g \exp\left[-d_a^2/\left(2\sigma_x^2\right)\right] \exp\left[-d_c^2/\left(2\sigma_y^2\right)\right] \quad (2\text{-}1)$$

$$g = \frac{2}{(2\pi)^{1/2}\sigma_z} \sum_{n=-\infty}^{\infty} \exp\left[-(H_e + 2nh)^2/\left(2\sigma_z^2\right)\right] \quad (2\text{-}2)$$

where, C is the ground-level concentration (g/m^3),
Q is the pollutant mass (g) in the puff,
σ_x is the standard deviation (m) of the Gaussian distribution in the along-wind direction,
σ_y is the standard deviation (m) of the Gaussian distribution in the cross-wind direction,
σ_z is the standard deviation (m) of the Gaussian distribution in the vertical direction,
d_a is the distance (m) from the puff center to the receptor in the along-wind direction,
d_c is the distance (m) from the puff center to the receptor in the cross-wind direction,
g is the vertical term (m) of the Gaussian equation,
H is the effective height (m) above the ground of the puff center, and,
h is the mixed-layer height (m).

The summation in the vertical term, g, accounts for multiple reflections off the mixing lid and the ground. It reduces to the uniformly mixed limit of 1/h for $\sigma_z > 1.6$ h. In general, puffs within the convective boundary layer meet this criterion within a few hours after release.

For a horizontally symmetric puff, with $\sigma_x = \sigma_y$, Eqn. (2-1) reduces to:

$$C(s) = \frac{Q(s)}{2\pi\sigma_y^2(s)}\, g(s)\, \exp\left[-R^2(s)/\left(2\sigma_y^2(s)\right)\right] \qquad (2\text{-}3)$$

where, R is the distance (m) from the center of the puff to the receptor, and,
s is the distance (m) traveled by the puff.

The distance dependence of the variables in Eqn. (2-3) is indicated (e.g., C(s), $\sigma_y(s)$, etc.). Integrating Eqn. (2-3) over the distance of puff travel, ds, during the sampling step, dt, yields the time averaged concentration, $\bar{C}$.

$$\bar{C} = \frac{1}{ds}\int_{s_o}^{s_o+ds} \frac{Q(s)}{2\pi\sigma_y^2(s)}\, g(s)\, \exp\left[-R^2(s)/2\sigma_y^2(s)\right]ds \qquad (2\text{-}4)$$

where s_o is the value of s at the beginning of the sampling step.

If it is assumed that the most significant s dependencies during the sampling step are in the R(s) and Q(s) terms, an analytical solution to this integral can be obtained. Figure 2-3 illustrates the movement of a puff from coordinates (x_1,y_1) to (x_2,y_2). Assuming the trajectory segment is a straight line, and transforming s to a dimensionless trajectory variable, p, the radial distance to the receptor at (x_r,y_r) is:

$$R(s) = \left[(x_1 - x_r + p\, dx)^2 + (y_1 - y_r + p\, dy)^2\right]^{1/2} \qquad (2\text{-}5)$$

where, p is zero at the beginning of the trajectory segment (i.e., at (x_1,y_1)),
p is one at the end of the trajectory segment (i.e., at (x_2,y_2)), and,
dx, dy are the incremental X and Y distances travelled by the puff (i.e., $dx = x_2 - x_1$, and $dy = y_2 - y_1$).

The exponential variation of Q due to removal and chemical transformation processes is expressed as a linear function of the sampling interval:

$$Q(s) = Q(s_o) + p\,[Q(s_o + ds) - Q(s_o)] \qquad (2\text{-}6)$$

Using Eqn. (2-6), and transforming to p coordinates, Eqn. (2-4) becomes:

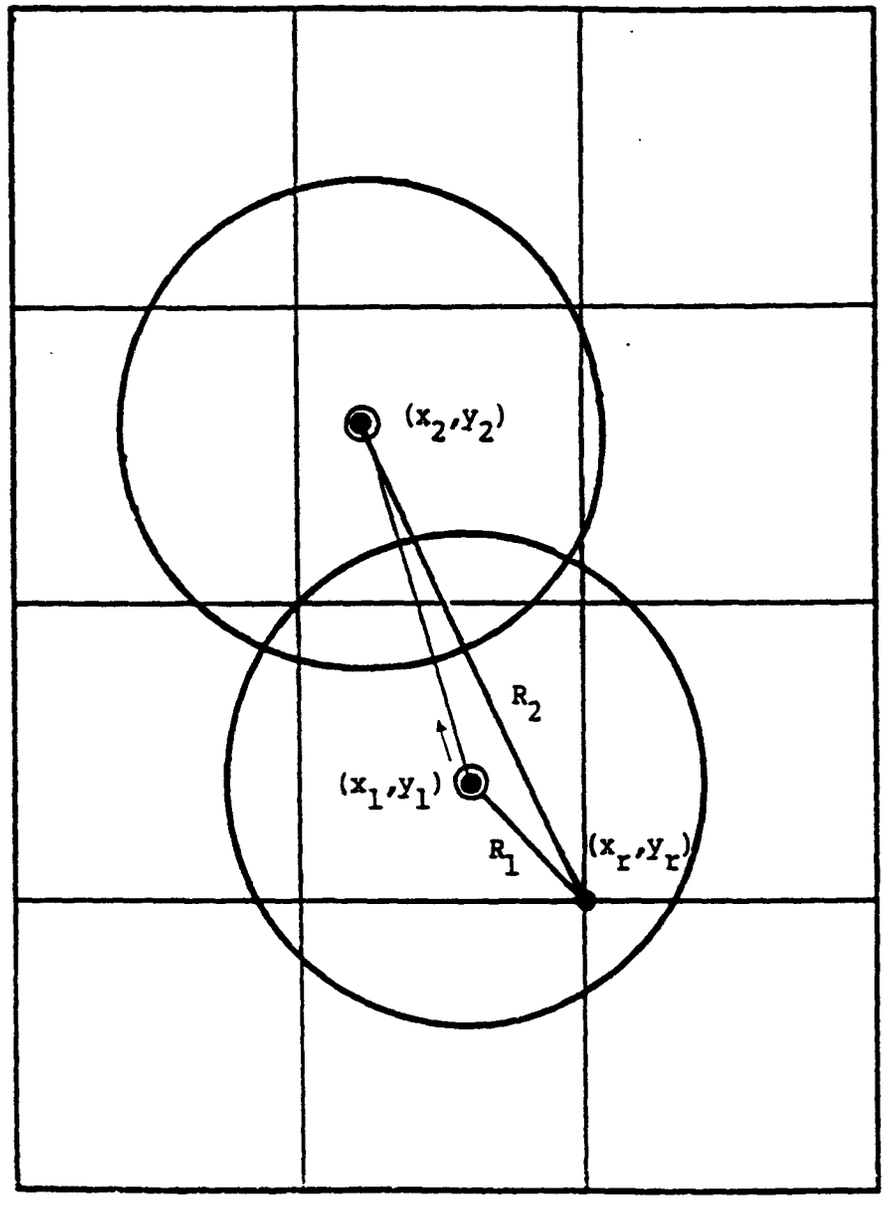


Figure 2-3. Illustration of the puff movement during the sampling step and the associated changes in the puff-receptor distance.

$$C = \frac{g}{2\pi\ \sigma_y^2}\left\{Q(s_o)\int_0^1 \exp\left[-R^2(p)/\left(2\sigma_y^2\right)\right]\,dp + \right.$$
$$\left.[Q(s_o + ds) - Q(s_o)]\int_0^1 p\,\exp\left[-R^2(p)/\left(2\sigma_y^2\right)\right]\,dp\right\} \qquad (2\text{-}7)$$

The solution of the integrals in Eqn. (2-7) is expressed in terms of error functions and exponentials:

$$\overline{C} = \frac{g}{2\pi\sigma_y^2}\{Q(s_o)\ I_1 + [Q(s_o + ds) - Q(s_o)]\ I_2\} \qquad (2\text{-}8)$$

$$I_1 = \left[\frac{\pi}{2a}\right]^{1/2}\exp\left[\frac{b^2}{2a} - \frac{c}{2}\right]\left\{erf\left[\frac{a+b}{(2a)^{1/2}}\right] - erf\left[\frac{b}{(2a)^{1/2}}\right]\right\} \qquad (2\text{-}9)$$

$$I_2 = \frac{-b\ I_1}{a} + \frac{1}{a}\exp\left[\frac{b^2}{2a} - \frac{c}{2}\right]\left\{\exp\left[\frac{-b^2}{2a}\right] - \exp\left[\frac{-1}{2}\left(a + 2b + \frac{b^2}{a}\right)\right]\right\} \qquad (2\text{-}10)$$

$$a = (dx^2 + dy^2)/\sigma_y^2 \qquad (2\text{-}11)$$

$$b = [dx(x_1 - x_r) + dy(y_1 - y_r)]/\sigma_y^2 \qquad (2\text{-}12)$$

$$c = [(x_1 - x_r)^2 + (y_1 - y_r)^2]/\sigma_y^2 \qquad (2\text{-}13)$$

The horizontal dispersion coefficient, σ_y, and the vertical term, g, are evaluated and held constant throughout the trajectory segment. In MESOPUFF II, σ_y and g are computed at the mid-point of the trajectory segment (p = 0.5). At mesoscale distances, the fractional change in the puff size during the sampling step is usually small, and the use of the mid-point values of σ_y and g is adequate. This assumption reduces the number of times that the dispersion coefficients and vertical reflection terms need be computed to one per sampling step (independent of the number of receptors). This optimization for mesoscale distances, however, may not be appropriate in the near-field, where the fractional puff growth rate can be rapid and plume height may vary. For this reason, the integrated sampling function has been also tested with receptor-specific values of σ_y and g, evaluated at the point of closest approach of the puff to

each receptor. The results of the test runs of both puff models as well as the slug model described in the next subsection are discussed below.

2.1.2 Slug Formulation and Sampling Functions

In the slug model, the "puffs" consist of Gaussian packets of pollutant material stretched in the along-wind direction. A slug can be visualized as a group of overlapping circular puffs having very small puff separation distances. In fact, the slug represents the continuous emission of puffs, each containing the infinitesimal mass q dt. The length of the main body of the slug is $u\ \Delta t_e$, where u is the wind speed, and Δt_e is the time of emission of the pollutant. The concentration due to the presence of a slug can be described as:

$$C(t) = \frac{Fq}{(2\pi)^{1/2}\, u' \sigma_y}\, g\, \exp\left[\frac{-d_c^2}{2\sigma_y^2}\,\frac{u^2}{u'^2}\right] \qquad (2\text{-}14)$$

$$F = \frac{1}{2}\left\{ erf\left[\frac{d_{a2}}{\sqrt{2}\ \sigma_{y2}}\right] - erf\left[\frac{-d_{a1}}{\sqrt{2}\ \sigma_{y1}}\right]\right\} \qquad (2\text{-}15)$$

where, u is the vector mean wind speed (m/s),

u' is the scalar wind speed (defined as $u' = (u^2 + \sigma_v^2)^{1/2}$ with σ_v = wind speed variance),

q is the source emission rate (g/s),

F is a "causality" function, and

g is the vertical coupling factor of Eqn. 2-2.

The quantities d_c and d_a are cross-slug (i.e., perpendicular to the slug axis) and along-slug distances, respectively, to the receptor. In particular, d_{a2} is the distance from slug end 2 (with $d_{a2} > 0$ in the direction of end 1), whereas the distance from slug end 1 is defined as $-d_{a1} \equiv d_{a2} - \ell_{xy}$, with ℓ_{xy} being the length of the slug projection in the x-y plane. The subscripts 1 and 2 on the dispersion coefficients refer to values at the oldest and youngest ends of the slug, respectively. The absence of a numerical subscript indicates a value defined at the receptor.

This "slug" formulation retains many of the important properties of the circular puff model, while significantly reducing puff overlap problems associated with snapshot sampling of circular puffs. The concentration distribution within the body of the slug, away from the slug endpoints, approaches that of the Gaussian plume result under the appropriate steady-state conditions. The concentrations near the endpoints of the slug (both inside and outside of the

body of the slug) fall off in such a way that if adjacent slugs are present, the plume predictions will be reproduced when the contributions of those slugs are included (again, during steady-state conditions). Eqn. (2-14) can be explicitly shown to conserve mass. As with circular puffs, each slug is free to evolve independently in response to the local effects of dispersion, chemical transformation, removal, etc. However, unlike puffs, we constrain the end points of adjacent slugs to remain connected. This ensures continuity of a simulated plume without the gaps associated with puff or segmented plume models.

The "causality" function, F, accounts for edge effects near the endpoints of the slug. For long emission times such that $u\,\Delta t_e > \sigma_x$, and points well inside the body of the slug, evaluation of the error functions in Eqn. (2-15) produces F = 0.5(1 - (-1)) = 1 (i.e., no edge effects). For receptors well outside the slug, F becomes zero, indicating that the pollutant material has not yet reached the receptor or has already passed it by. Near the endpoints, the causality factor produces a leading/trailing Gaussian tail on the distribution.

The factor (u/u') allows low wind speed and calm conditions to be properly treated. As u approaches zero, the exponential crosswind term becomes unity and F approaches $-\text{erf}\{d_s/[(\sqrt{2}\,\sigma_y]\}$. Under these conditions, the radial concentration dependence of the distribution is determined by the causality factor. For u greater than a few meters per second, (u/u') is very close to one, so that this ratio becomes unimportant. The factors (u/u') and F make the slug model more "puff-like" than segmented plume models (e.g., Hales et al., 1977; Benkley and Bass, 1979). Unlike the slug model, segmented plume models generally do not properly treat low wind speed conditions or segment edge effects.

Eqn. (2-14) represents a "snapshot" description of the elongated puff at time t. Figure 2-4 displays the concentration isopleths of two such slug snapshots. As with the "snapshot" puff equation, Eqn. (2-14) must be integrated during the sampling step to produce a time-averaged concentration. In the case where the emission rate and meteorological conditions do not vary during the sampling step, a generalized analytical solution to the integral can be obtained for "emitting" slugs (i.e., the endpoint of the "youngest" end of the slug is at the source):

$$\overline{C} = \frac{\overline{F}q}{\sqrt{2\pi}u'\sigma_y}\, g\, \exp\left[\frac{-d^2}{2\sigma_y^2}\,\frac{u^2}{u'^2}\right] \qquad (2\text{-}16)$$

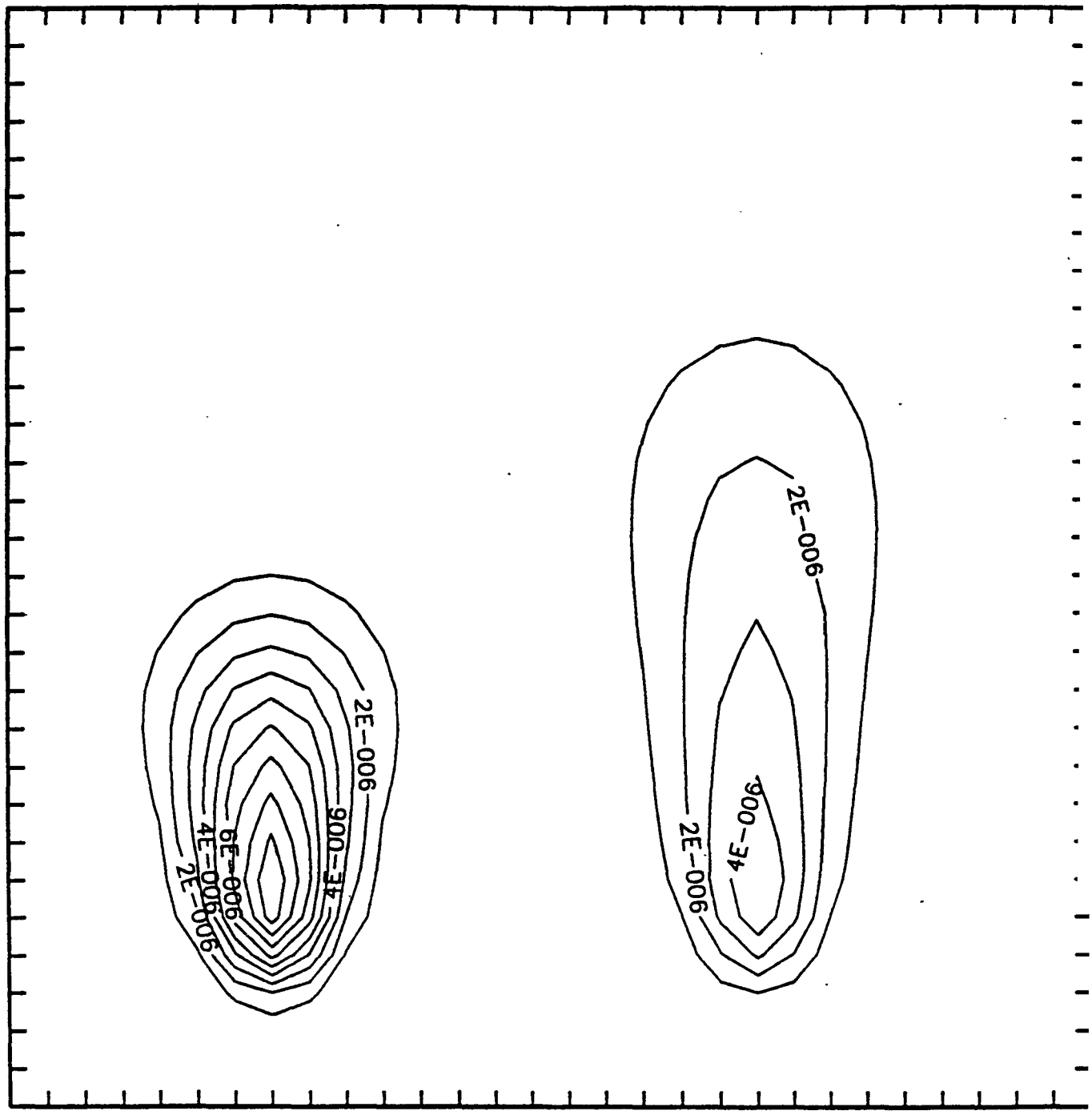


Figure 2-4. Isopleths of two slug "snapshots." The slug snapshot at left represents the slug at the beginning of a time step whereas the snapshot at right shows the instantaneous distribution at the end of the time step. During the time step, the slug experienced advection (to the right), diffusion, and some along-slug stretching due to wind shear.

$$\bar{F} = \frac{1}{2}\, erf(\phi_2) + \frac{1}{2}\,\frac{\sqrt{2}\,\sigma_y}{u\Delta t_s}\left\{\left[\xi_e\, erf(\xi_e) - \xi_b\, erf(\xi_b)\right] + \frac{1}{2}\left[\exp\left(\xi_e^2\right) - \exp\left(\xi_b^2\right)\right]\right\} \quad (2\text{-}17)$$

where

$$\xi_e = \frac{d_{a2} - u\Delta t_s}{\sqrt{2}\sigma_y} \quad (2\text{-}18)$$

represents the situation at the <u>end</u> of the time step Δt_s.

$$\xi_b = \frac{d_{a2}}{\sqrt{2}\sigma_y} \quad (2\text{-}19)$$

represents the situation at the <u>beginning</u> of the time step,

$$\phi_2 = \frac{d_{a2}}{\sqrt{2}\sigma_{y2}} \quad (2\text{-}20)$$

represents the steady state conditions at the source, and where Δt_s is the duration of the sampling step.

For Eqn. (2-16) to apply, the sampling interval must correspond to the emission interval, as is normally the case for fresh emissions. The value of σ_{y2} used is the initial lateral spread (if any) of the emissions at the source. For older slugs, the endpoint of the slug is no longer fixed at the source and the long axis of the slug is not likely to be along the advecting wind direction. An analytical integration of Eqn. (2-14) is not possible for these slugs unless restrictive conditions are imposed on the form of the puff growth equations. Because of the importance of generality in the puff growth equations, the time-averaged concentrations of older/ slugs are determined by numerical integration of Eqn. (2-14). As discussed in the next subsection, this integration can be accomplished at reasonable computation cost. Figure 2-5 shows the result of such integral averaging for the situation where the Figure 2-4 "snapshots" depict the start and end slug states of the averaging period.

The above development also ignores the effect of loss or production mechanisms; however, this can be handled in much the same "linearized" manner that MESOPUFF II invokes. This is accomplished by allowing the effective emission rate, q, to vary linearly over time as:

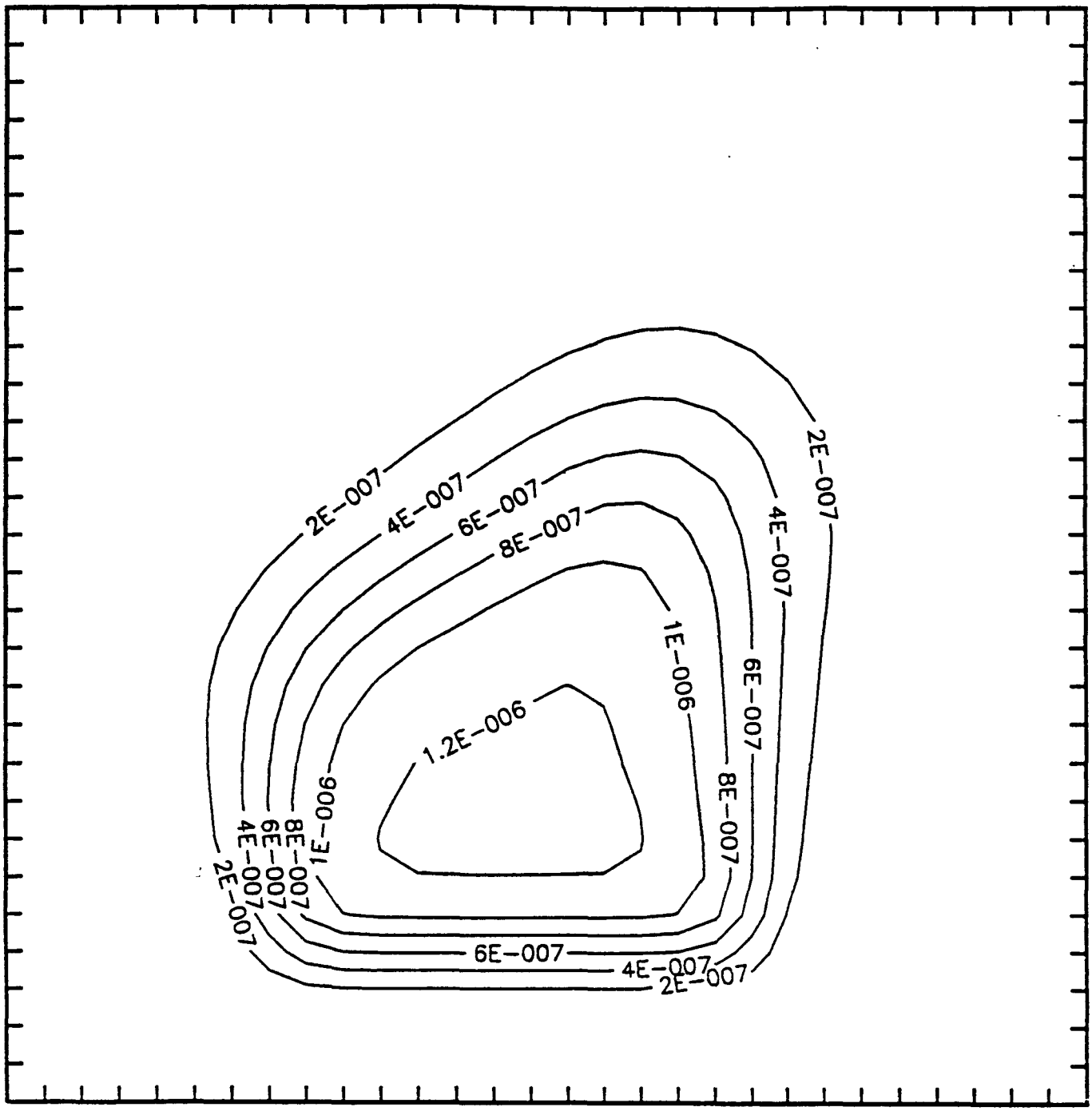


Figure 2-5. Receptor-time averaged concentrations resulting from the transport and evolution of the slug depicted in Figure 2-4 from its initial (left "snapshot") to final (right "snapshot") state. The tick marks on the border suggest the 2-d mesh of receptors considered.

$$q(t) = q_b + (q_e - q_b) \cdot (t/\Delta t_s) \tag{2-21}$$

where, q_b is the effective emission rate for the slug at the beginning of the time step (n.b., q_b = q for fresh emissions),

q_e is the effective emission rate including loss or production which occurs during the time step, and,

Δt_s is the duration of the time step.

The variable ξ is also the function

$$\xi = \frac{d_{a2} - u\Delta t_s \cdot (t/\Delta t_s)}{\sqrt{2}\sigma_y} \tag{2-22}$$

of the dimensionless time variable $t/\Delta t_s$, where $0 \le t/\Delta t_s \le 1$, such that

$$\xi = \xi_b + (\xi_e - \xi_b) \cdot (t/\Delta t_s) \tag{2-23}$$

and the causality function becomes

$$F(\xi) = \frac{1}{2}\{erf(\phi_2) - erf(\xi)\} \tag{2-24}$$

Thus, the time averaging process yields

$$\overline{C} = \frac{g}{\sqrt{2\pi}u'\sigma_y}\left\{\exp\left[\frac{-d^2_c}{2\sigma_y^2} \cdot \frac{u^2}{u'^2}\right]\right\}\{q_b F_o + (q_e - q_b) F_1\} \tag{2-25}$$

where F_o is just $\overline{F}$ from Eqn. (2-17) and

$$F_1 = \int_0^{\Delta t_s} \frac{dt}{\Delta t_s}(t/\Delta t_s) F(t) = \frac{1}{\Delta\xi}\int_{\xi_b}^{\xi_e} d\xi \frac{\xi - \xi_b}{\Delta\xi} F(\xi) \tag{2-26}$$

with $\Delta\xi \equiv \xi_e - \xi_b = \dfrac{-u\Delta t_s}{\sqrt{2}\sigma_y}$

Substituting in Eqn. (2-24) then yields

$$F_1 = \frac{1}{4} erf(\phi_2) - \frac{1/2}{(\Delta\xi)^2}\left\{\int_{\xi}^{\xi_c} d\xi\ \xi\ erf(\xi) - \xi_b \int_{\xi}^{\xi_c} d\xi\ erf(\xi)\right\} \quad (2\text{-}27)$$

where $$\int dx\ erf(x) = x\ erf(x) + \frac{1}{\sqrt{\pi}} \exp(-x^2) \quad (2\text{-}28)$$

has already been used to obtain Eqn. (2-17) and where

$$\int dx\ x\ erf(x) = \frac{1}{2}x^2\ erf(x) + \frac{1}{2}\frac{x}{\sqrt{\pi}} \exp(-x^2) - \frac{1}{4} erf(x) \quad (2\text{-}29)$$

is a special case of the more general expression developed by Geller and Ng (1971) in terms of the generalized hypergeometric function ${}_2F_2$.

Generalizing the problem of dealing with older slugs is trivial if one deals with a numerical integration (i.e., time average) of Eqn. (2-14). The time dependent expression q(t) given by Eqn. (2-21), simply replaces q and the numerical integration proceeds.

This numerical integration process has itself received special attention because it greatly influences the computing time needs of the slug model. First, all receptors lying outside of the slug's $\pm\ 3\sigma_y$ envelope during the entire averaging time interval are eliminated from consideration. Second, for those receptors remaining, integration time limits are computed such that sampling is not performed when the receptor is outside of the $\pm\ 3\sigma_y$ envelope. As the endpoints of the slug are advected separately such that the slug may "tumble", the algebra for finding the appropriate time limits involves the roots of cubic equations, but is otherwise straightforward and is not discussed further.

Invocation of the "frozen σ" methodology (i.e., σ_y and σ_z are fixed at receptor specific values throughout the averaging time period) creates another class of situations which can be integrated analytically; however, the most general case involves indefinite integrals of the form

$$\int dt\ \exp(-\beta^2 t^2)\ erf(a + bt), \quad (2\text{-}30)$$

which defy solution except in a few simple cases (e.g., a = 0 and b = β). In fact, integrability has proven not to be the sole criteria in these slug sampling problems. For example, the preceding work on linear time variation of loss (or production) mechanisms can also be evaluated for the more realistic exponential process; however, the analytic forms are found to be

very volatile on a computer because subtraction of large numbers to obtain small numbers is required.

One tractable case involves the quite physical scenario of a slug passing rapidly over a receptor and with slug endpoints sufficiently far away that the along-slug causality factor, F(t), is time independent. In this case the causality factor also becomes fixed and can be taken outside the integral and approximated as

$$\overline{F} = \frac{1}{2}\left(F_b + F_e\right) \quad , \tag{2-31}$$

which is just the average of values at the beginning and end of the time step. This approximation is, however, made only if F_b and F_e are within a specified fractional tolerance of each other. A similar procedure enables one to move the vertical coupling factor, g, outside the integral and replace it with the mean value $\overline{g}$. The tolerance factor for both causality and vertical coupling coefficient variation is currently set at a conservative 0.02 (i.e., 2%). Finally the variability of the lateral coupling term,

$$Y(t) = \exp\left(-\eta(t)^2\right) \quad , \tag{2-32}$$

where $\eta(t) = \dfrac{d_c(t)}{\sqrt{2}\sigma_y} \cdot \dfrac{u}{u'}$

and $d_c(t)$ is the time dependent crosswind distance, is checked and the integrals

$$I_m = \int_0^{\Delta t_s} \frac{dt}{\Delta t_s}\left(t/\Delta t_s\right)^m Y(t) \tag{2-33}$$

evaluated for m = 0 and 1.

These integrals can be solved to yield

$$I_0 = \frac{\sqrt{\pi}}{2}\left[erf(\eta_e) - erf(\eta_b)\right]/\left(\eta_e - \eta_b\right) \tag{2-34}$$

and

$$I_1 = \frac{1}{2}\left[\exp\left(-\eta_b^2\right) - \exp\left(-\eta_e^2\right)\right]/\left(\eta_e - \eta_b\right)^2 - \eta_b I_0/\left(\eta_e - \eta_b\right) \tag{2-35}$$

so that the final time-averaged concentrations can be written as

$$\overline{C} = \frac{\overline{g}\,\overline{F}}{\sqrt{2\pi}u'\sigma_y}\left\{q_b I_0 + (q_e - q_b) I_1\right\} \qquad (2\text{-}36)$$

as an alternative to numerical integration for the older slugs.

Computations are also performed for the vertically integrated counterparts to Eqns. (2-25 and 2-36) as these are required for evaluation of wet removal and wet fluxes at a ground level receptor; however, Gaussian normalization dictates that this is accomplished simply by replacing g with 1.0 in Eqn. (2-25) or $\overline{g}$ with 1.0 in Eqn. (2-36).

2.1.3 Sampling Function Testing

The slug model and two versions of the integrated (circular) puff model have been subjected to several sensitivity tests in order to:

- evaluate the performance of each formulation in reproducing the known steady-state plume solution under the appropriate emission and meteorological conditions;
- demonstrate and intercompare the models' capabilities under non-steady conditions;
- assess the cost-effectiveness of the different algorithms;
- demonstrate the consistency of the circular puff/elongated slug models and the feasibility of the proposed hybrid approach.

Tables 2-1 (a,b) and 2-2 (a,b) present the plume, puff, and slug results for two sets of steady-state emission and meteorological conditions. Plume centerline values are presented at receptors from 100 m to 10 km from the source. A constant emission rate of 1 g/s from a 10 m high source is assumed. The first set of results assume neutral (D class) stability conditions with 10 m/s winds. Stable (F class) conditions with 3 m/s winds are applied in the second set of runs. Puff model #1 employs the integrated puff sampling function with trajectory mid-point values of σ_y and g. The puff release rate and sampling rate were varied from 100/hr to 500/hr for the puff model #1 simulations. Puff model #2 uses the same integrated sampling function as #1, except receptor-specific values of σ_y and g are used instead of trajectory mid-point values.

Table 2-1 (a)
Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed: 10 m/s, Stability Class: D, Stack Height: 10 m,
Unlimited Mixing Height, Emission Rate: 1 g/s)

Distance (m)	Plume Model (g/m^3)	Puff Model #1		
		100 puffs/hr 100 samp./hr	300 puffs/hr 300 samp./hr	500 puffs/hr 500 samp./hr
100	8.273×10^{-5}	1.266×10^{-4}	1.749×10^{-4}	9.618×10^{-5}
200	1.204×10^{-4}	1.266×10^{-4}	1.295×10^{-4}	1.306×10^{-4}
300	8.270×10^{-5}	1.288×10^{-4}	8.341×10^{-5}	7.929×10^{-5}
400	5.711×10^{-5}	3.164×10^{-5}	5.183×10^{-5}	5.682×10^{-5}
500	4.145×10^{-5}	3.693×10^{-5}	3.976×10^{-5}	4.176×10^{-5}
600	3.144×10^{-5}	3.733×10^{-5}	3.212×10^{-5}	3.145×10^{-5}
700	2.469×10^{-5}	3.189×10^{-5}	2.529×10^{-5}	2.467×10^{-5}
800	1.995×10^{-5}	1.559×10^{-5}	2.002×10^{-5}	1.995×10^{-5}
900	1.648×10^{-5}	1.658×10^{-5}	1.644×10^{-5}	1.648×10^{-5}
1000	1.387×10^{-5}	1.654×10^{-5}	1.394×10^{-5}	1.393×10^{-5}
2000	4.863×10^{-6}	4.871×10^{-6}	4.853×10^{-6}	4.856×10^{-6}
3000	2.616×10^{-6}	2.613×10^{-6}	2.614×10^{-6}	2.612×10^{-6}
4000	1.702×10^{-6}	1.704×10^{-6}	1.699×10^{-6}	1.698×10^{-6}
5000	1.219×10^{-6}	1.219×10^{-6}	1.217×10^{-6}	1.217×10^{-6}
6000	9.284×10^{-7}	9.280×10^{-7}	9.270×10^{-7}	9.268×10^{-7}
7000	7.374×10^{-7}	7.372×10^{-7}	7.364×10^{-7}	7.359×10^{-7}
8000	6.040×10^{-7}	6.029×10^{-7}	6.023×10^{-7}	6.022×10^{-7}
9000	5.066×10^{-7}	5.060×10^{-7}	5.055×10^{-7}	5.053×10^{-7}
10000	4.329×10^{-7}	4.326×10^{-7}	4.324×10^{-7}	4.321×10^{-7}
Compaq-286 CPU time (s)	1.0	249.4	2054.3	5592.4

Table 2-1 (b)
Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed: 10 m/s, Stability Class: D, Stack Height: 10 m,
Unlimited Mixing Height, Emission Rate: 1 g/s)

		—— CALPUFF MODULES ——	
Distance (m)	Plume Model (g/m^3)	Integrated Puff Model* (g/m^3)	Slug Model* (g/m^3)
100	8.273×10^{-5}	8.273×10^{-5}	8.273×10^{-5}
200	1.204×10^{-4}	1.204×10^{-4}	1.204×10^{-4}
300	8.270×10^{-5}	8.270×10^{-5}	8.270×10^{-5}
400	5.711×10^{-5}	5.711×10^{-5}	5.711×10^{-5}
500	4.145×10^{-5}	4.145×10^{-5}	4.145×10^{-5}
600	3.144×10^{-5}	3.144×10^{-5}	3.144×10^{-5}
700	2.469×10^{-5}	2.469×10^{-5}	2.469×10^{-5}
800	1.995×10^{-5}	1.995×10^{-5}	1.995×10^{-5}
900	1.648×10^{-5}	1.648×10^{-5}	1.648×10^{-5}
1000	1.387×10^{-5}	1.387×10^{-5}	1.387×10^{-5}
2000	4.863×10^{-6}	4.863×10^{-6}	4.863×10^{-6}
3000	2.616×10^{-6}	2.616×10^{-6}	2.616×10^{-6}
4000	1.702×10^{-6}	1.702×10^{-6}	1.702×10^{-6}
5000	1.219×10^{-6}	1.219×10^{-6}	1.219×10^{-6}
6000	9.284×10^{-7}	9.284×10^{-7}	9.284×10^{-7}
7000	7.374×10^{-7}	7.374×10^{-7}	7.374×10^{-7}
8000	6.040×10^{-7}	6.040×10^{-7}	6.040×10^{-7}
9000	5.066×10^{-7}	5.066×10^{-7}	5.066×10^{-7}
0000	4.329×10^{-7}	4.329×10^{-7}	4.329×10^{-7}
Compaq-286 CPU time (s)	1.0	1.8	1.2-5.7

* Same as plume model to four places of accuracy.

Table 2-2 (a)
Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed: 5 m/s, Stability Class: F, Stack Height: 10 m,
Unlimited Mixing Height, Emission Rate: 1 g/s)

Distance (m)	Plume Model (g/m^3)	Puff Model #1		
		100 puffs/hr 100 samp./hr	300 puffs/hr 300 samp./hr	500 puffs/hr 500 samp./hr
100	6.495×10^{-7}	1.379×10^{-7}	1.379×10^{-7}	5.814×10^{-5}
200	1.017×10^{-4}	1.823×10^{-4}	1.159×10^{-4}	1.018×10^{-4}
300	2.075×10^{-4}	1.869×10^{-4}	2.033×10^{-4}	2.046×10^{-4}
400	2.255×10^{-4}	2.171×10^{-4}	2.313×10^{-4}	2.242×10^{-4}
500	2.076×10^{-4}	2.234×10^{-4}	2.027×10^{-4}	2.078×10^{-4}
600	1.816×10^{-4}	1.733×10^{-4}	1.818×10^{-4}	1.813×10^{-4}
700	1.567×10^{-4}	1.736×10^{-4}	1.575×10^{-4}	1.566×10^{-4}
800	1.357×10^{-4}	1.337×10^{-4}	1.351×10^{-4}	1.355×10^{-4}
900	1.184×10^{-4}	1.197×10^{-4}	1.185×10^{-4}	1.183×10^{-4}
1000	1.042×10^{-4}	1.062×10^{-4}	1.041×10^{-4}	1.040×10^{-4}
2000	4.154×10^{-5}	4.135×10^{-5}	4.153×10^{-5}	4.154×10^{-5}
3000	2.397×10^{-5}	2.401×10^{-5}	2.398×10^{-5}	2.394×10^{-5}
4000	1.644×10^{-5}	1.644×10^{-5}	1.641×10^{-5}	1.641×10^{-5}
5000	1.224×10^{-5}	1.224×10^{-6}	1.223×10^{-5}	1.222×10^{-5}
6000	9.612×10^{-6}	9.609×10^{-6}	9.592×10^{-6}	9.594×10^{-6}
7000	7.830×10^{-6}	7.832×10^{-6}	7.822×10^{-6}	7.818×10^{-6}
8000	6.596×10^{-6}	6.584×10^{-6}	6.581×10^{-6}	6.580×10^{-6}
9000	5.669×10^{-6}	5.661×10^{-6}	5.659×10^{-6}	5.658×10^{-6}
10000	4.950×10^{-6}	4.945×10^{-6}	4.939×10^{-6}	4.940×10^{-6}
Compaq-286 CPU time (s)	1.1	309.8	2566.7	7049.5

Table 2-2 (b)
Comparison of Plume, Puff, and Slug Models for Steady-State Conditions

(Wind Speed: 5 m/s, Stability Class: F, Stack Height: 10 m,
Unlimited Mixing Height, Emission Rate: 1 g/s)

		CALPUFF MODULES	
Distance (m)	Plume Model (g/m^3)	Puff Model* (g/m^3)	Integrated Slug Model* (g/m^3)
100	6.495×10^{-7}	6.495×10^{-7}	6.495×10^{-7}
200	1.017×10^{-4}	1.017×10^{-4}	1.017×10^{-4}
300	2.075×10^{-4}	2.075×10^{-4}	2.075×10^{-4}
400	2.255×10^{-4}	2.255×10^{-4}	2.255×10^{-4}
500	2.076×10^{-4}	2.076×10^{-4}	2.076×10^{-4}
600	1.816×10^{-4}	1.816×10^{-4}	1.816×10^{-4}
700	1.567×10^{-4}	1.567×10^{-4}	1.567×10^{-4}
800	1.357×10^{-4}	1.357×10^{-4}	1.357×10^{-4}
900	1.184×10^{-4}	1.184×10^{-4}	1.184×10^{-4}
1000	1.042×10^{-4}	1.042×10^{-4}	1.042×10^{-4}
2000	4.154×10^{-6}	4.154×10^{-6}	4.154×10^{-6}
3000	2.397×10^{-6}	2.397×10^{-6}	2.397×10^{-6}
4000	1.644×10^{-6}	1.644×10^{-6}	1.644×10^{-6}
5000	1.224×10^{-6}	1.224×10^{-6}	1.224×10^{-6}
6000	9.612×10^{-6}	9.613×10^{-8}	9.613×10^{-8}
7000	7.830×10^{-6}	7.830×10^{-6}	7.830×10^{-6}
8000	6.596×10^{-6}	6.596×10^{-6}	6.596×10^{-6}
9000	5.669×10^{-6}	5.669×10^{-6}	5.669×10^{-6}
10000	4.950×10^{-6}	4.950×10^{-6}	4.950×10^{-6}
Compaq-286 CPU time (s)	1.1	1.5	1.3-5.7

* Same as plume model to four places of accuracy.

The puff release rate and sampling rate in the puff model #2 runs were both 1/hr. Operationally, the slug model would employ the efficient time-integrated relationship (Eqn. 2-16) for the slug originating at the source; however, these concentrations will always be slightly less than the plume concentrations, but do approach them asymptotically as $\Delta t_s \rightarrow \infty$. Instead, the slug model was evaluated by considering the slugs as being "old", and both the numerical integration technique of Eqn. (2-14) and the approximate, factored form of Eqn. (2-36) were considered. Both of these "old" slug methods gave predictions identical to the plume model for the four significant digits displayed. (It should be noted that numerical integration was not necessary in this special case of steady-state conditions, but was performed anyway to demonstrate the more general technique and allow its evaluation in terms of its consistency with the plume solution and its cost effectiveness.)

The results indicate that a large number of puffs/samples are necessary to adequately reproduce the plume solution at near-field receptors when the puff model #1 assumptions are employed. The errors are associated with the use of the trajectory mid-point values of σ_y and g. This model is optimized for source-receptor distances on scales from tens to hundreds of kilometers, and is not cost effective for application close to the source. Puff model #2, using receptor-specific dispersion coefficients and the integrated sampling function, reproduces the plume solution exactly with a computational cost less than 1% of that required for puff model #1. In fact, its CPU requirements are competitive with those needed to solve the steady-state plume equation. The CPU costs of the slug model are comparable to the plume model when the analytic form is used, but is somewhat more costly than puff model #2 when the 40 iteration, numerical solver is selected. Additional test runs of the puff and slug models under a range of different meteorological conditions produced similar results.

The slug and puff (#2) models were also used to simulate a case of non-steady emissions. An emission rate of 1 g/s for a duration of one hour was modeled. Although a one-hour release was used in this demonstration run, either model is capable of handling arbitrary variations in emission rates, including those on time scales of less than one hour. B stability, 1 m/s winds were the assumed meteorological conditions. The results are presented in Figures 2-6 and 2-7 along with the steady-state plume solution. The puff and slug model results intercompare well (within a few percent, except at the tails of the distribution with very low concentration values). The puff/slug predictions approach the steady-state results when the center of the pollutant cloud passes the receptor, but clearly show the causality and edge effects of the approaching/passing distribution. The puff model lumps the pollutant mass into n packets (puffs), each with 1/n of the total emission (n = 100 in this test). The mass actually release from time t = 0 to t = dt/n is packaged into the puff released at t = 0. The puff lumping effect tends to result in a slightly premature arrival/departure of the pollutant, which is

not seen in the case of steady emissions. In the non-steady runs, because the correct puff causality is obtained by increasing the puff release rate, the slug model is more computationally efficient.

In order to provide a cost-effective sampling scheme for a range of meteorological, emission, and source-receptor configurations, a hybrid circular puff/elongated slug scheme is proposed. The model will store information on the trailing endpoint of the emission cloud (required for the slug model) in addition to the data describing the leading edge (used in both the puff and slug models), at least initially, when the ratio $\sigma_y/(u\ dt_s)$ is small. In the far-field, the initial elongation of the slug becomes unimportant, and puff sampling is nearly always the most efficient. For near-field receptors, however, if the emission rate changes rapidly, or a large wind direction change results in advection of a slug segment at a large angle to its long axis, the slug model is more cost effective. Therefore, internal checks will be performed to select the most appropriate sampling scheme. Although an all-slug or all-puff model could be engineered to produce appropriate results under all conditions, this hybrid approach, which takes advantage of the strengths of each algorithm, can produce the same results at lower computational cost.

2.2 Dispersion Coefficients

A key modeling consideration is the specification of the horizontal and vertical Gaussian dispersion coefficients, σ_y and σ_z. The dispersion coefficients n time steps from the source each consist of a number of different components:

$$\sigma_{y,n}^2 = \sigma_{yt}^2 \left(\xi_{n-1} + \Delta\xi\right) + \sigma_{yt}^2 + \sigma_{yb}^2 \qquad (2\text{-}37)$$

where ξ_{n-1} is defined implicitly by the relation $\sigma_{yt}(\xi_{n-1}) = \sigma_{y,n-1}$ and ξ_o is defined implicitly by the relation $\sigma_{yt}^2(\xi_o) = v_{yo}^2$, and

$$\sigma_{z,n}^2 = \sigma_{zt}^2 \left(\xi_{n-1} + \Delta\xi\right) + \sigma_{zb}^2 \ , \qquad (2\text{-}38)$$

where $\sigma_{zt}(\xi_{n-1}) = \sigma_{z,n-1}$ defines ξ_{n-1} implicitly and $\sigma_{zt}^2(\xi_o) = v_{zo}^2$ defines ξ_o implicitly, and

where, $\sigma_{y,n}, \sigma_{z,n}$ are the total horizontal and vertical dispersion coefficients at the end of n time steps,

σ_{yt}, σ_{zt} are the functional forms of the components (m) of σ_y and σ_z due to atmospheric turbulence,

σ_{yb}, σ_{zb} are the components (m) of σ_y and σ_z due to plume buoyancy,

σ_{yo}, σ_{zo} are the initial values (m) of σ_y and σ_z due to the nature of the source (e.g., area source) or the rapid initial dilution associated with building downwash of point sources,

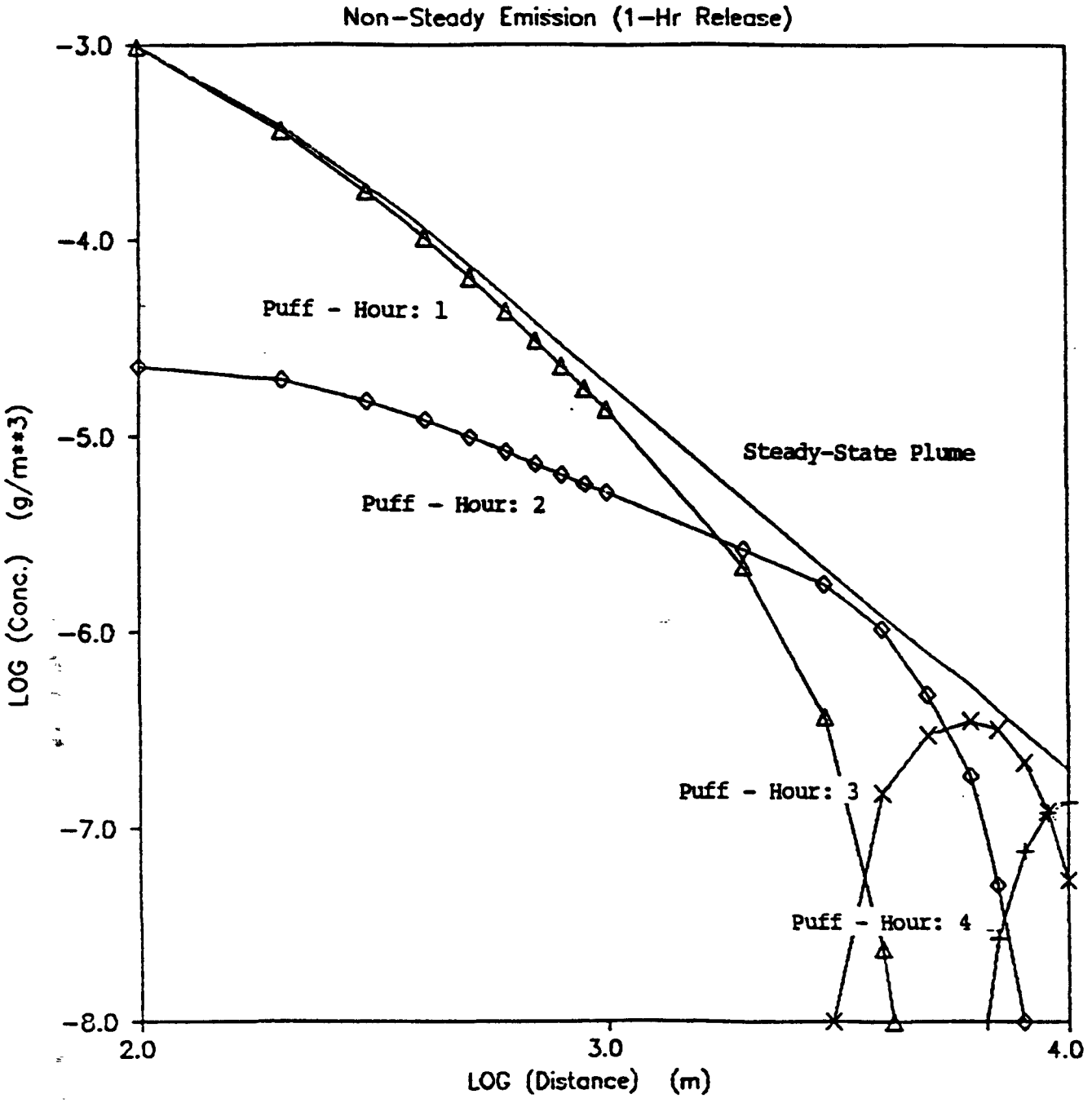


Figure 2-6. Concentration predictions of puff model #2 for non-steady emission conditions. Emission rate: 1 g/s, Emission duration: 1 hour, Wind speed: 1 m/s, Stability class: B, Stack height: 10 m, Mixing height: unlimited.

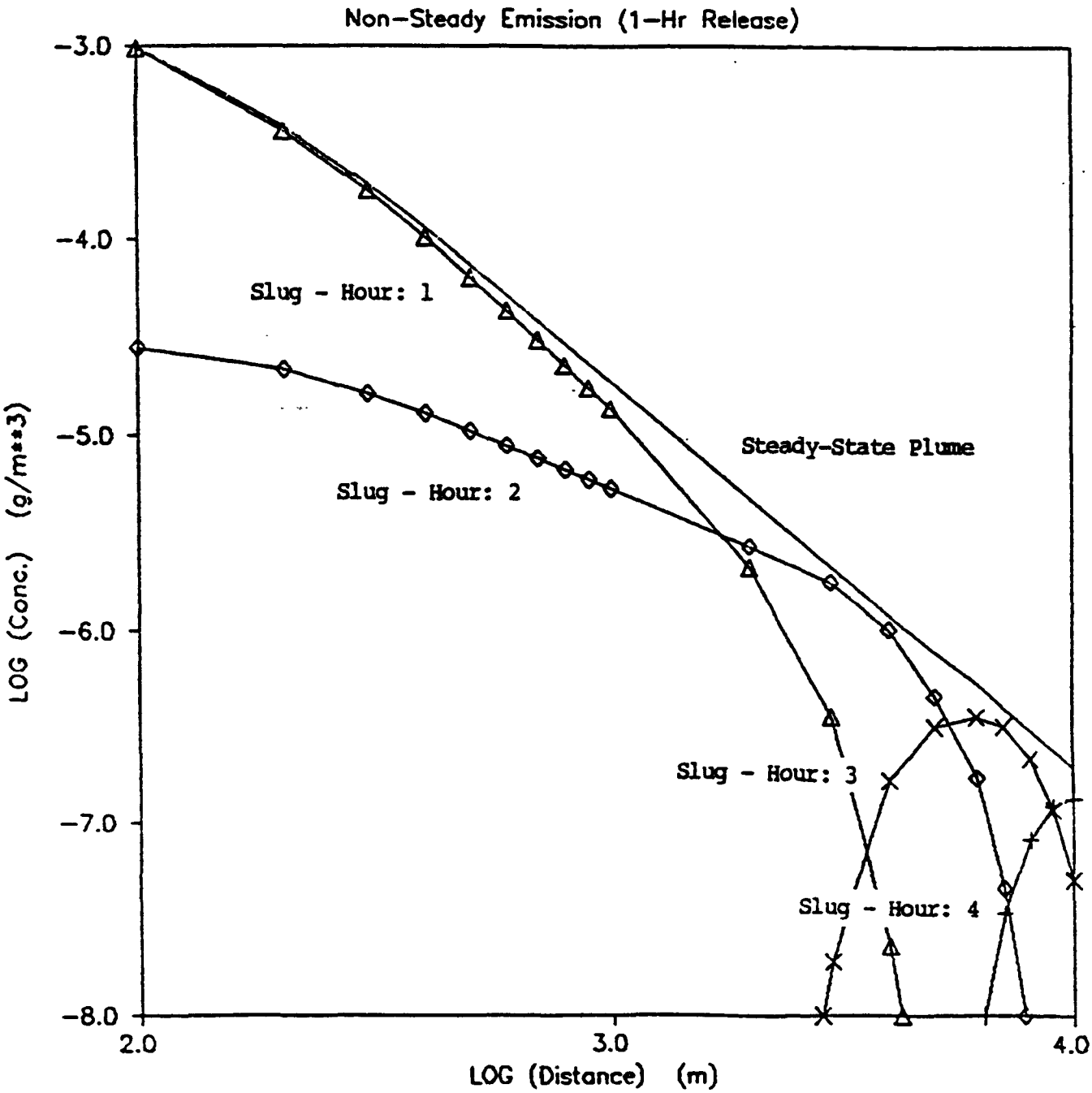


Figure 2-7. Concentration predictions of the slug model for non-steady emission conditions. Emission rate: 1 g/s, Emission duration: 1 hour, Wind speed: 1 m/s, Stability class: B, Stack height: 10 m, Mixing height: unlimited.

σ_{ys} is the component of the horizontal dispersion coefficient (m) due to vertical wind shear effects,

ξ_{n-1} is the pseudo-value based on the previous time step's total sigma,

$\Delta\xi$ is the incremental transport distance or time variable, and,

ξ_o is the initial pseudo-value of this variable and is defined implicitly and separately for y and z.

Thus, quadratic addition of initial dispersion components is assumed, but subsequent growth of the puff or slug is accomplished using the pseudo-distance or pseudo-transport time approach. This pseudo-variable approach is necessary if current puff growth is to be dependent only on the current size of the puff and not on how it reached that size.

2.2.1 Atmospheric Turbulence Components

The basic strategy in the design of the dispersion module is to allow the use of the most refined data available in the calculation of σ_{yt} and σ_{zt} while providing for backup algorithms not requiring specialized data for situations in which these data are not available. Three levels of input data will be allowed:

(1) Direct measurements of turbulence, σ_v and σ_w, (Option 1)

(2) Micrometeorological scaling parameters u_*, w_*, L, and h, from CALMET or other meteorological model yielding internally computed estimates of the crosswind and vertical components of turbulence based on similarity theory, (Option 2), or

(3) Pasquill-Gifford-Turner (PGT) class and user choice of either ISC or AUSPLUME dispersion coefficients (Option 3) or the MESOPUFF II implementation of PGT rural dispersion coefficients (Option 4).

The general forms of σ_{yt} and σ_{zt} (Hanna et al., 1977) for Options (1) and (2) are:

$$\sigma_{yt} = \sigma_v \, t \, f_y(t/t_{by}) \tag{2-39}$$

$$\sigma_{zt} = \sigma_w \, t \, f_z(t/t_{bz}) \tag{2-40}$$

where, σ_v is the standard deviation (m/s) of the horizontal crosswind component of the wind,

σ_w is the standard deviation (m/s) of the vertical component of the wind,

t is the travel time (s) of the plume to the receptor, and,

t_{ty}, t_{tz} are the horizontal and vertical Lagrangian time scales (s).

Equations (2-39) and (2-40) can be expressed in terms of the horizontal and vertical components (i_y and i_z) of the turbulence intensity using the following relationships.

$$i_y = \sigma_v / u \approx \sigma_\theta \tag{2-41}$$

$$i_z = \sigma_w / u \approx \sigma_\phi \tag{2-42}$$

where, u is the wind speed (m/s),

σ_θ is the standard deviation (m/s) of the horizontal wind angle, and,

σ_ϕ is the standard deviation (m/s) of the vertical wind angle.

The most desirable approach is to relate the dispersion coefficients directly to the measured turbulence velocity variances (σ_v and σ_w) or intensity components (i_y and i_z). However, it is important that the quality of the observational data be considered in the selection of the method for computing the dispersion coefficients. For example, inaccurate observations of i_z, which is difficult to measure, may lead to less accurate modeling results that predictions based on more routine data. It is recommended that the default selection be Option 2, which uses similarity theory and micrometeorological variables derived from routinely available meteorological observations and surface characteristics. Many laboratory experiments, field studies, and numerical simulations (e.g., Deardorff and Willis, 1975; Caughey, 1981; Lamb, 1981) have shown the importance and utility of convective scaling in the convective boundary layer. Convective scaling has been successfully applied to data collected at a wide variety of sites, including oceans, rural land surfaces (e.g., Hicks, 1985) and urban areas (Ching et al., 1983). Similarly, in the stable boundary layer, local scaling has been shown to apply (e.g., Hunt, 1982; Nieuwstadt, 1984). The micrometeorological model, (see Section 4) explicitly relates the aerodynamic and thermal characteristics of the surface to the sensible heat flux and momentum transfer rates that are used in the computation of the dispersion coefficients.

Weil (1985) and Briggs (1985) provide reviews on the use of similarity theory in diffusion models. In the convective boundary layer, Weil describes the turbulence characteristics in three layers:

(1) Surface layer - $z \leq 0.1$ h; $\sigma_v \sim$ constant with height, σ_w increases with height

(2) Mixed layer - $0.1h < z < 0.8h$; $\sigma_v \sim$ constant with height, $\sigma_w \sim$ constant with height

(3) Entrainment layer - $z > 0.8h$; σ_v decreases with height, σ_w decreases with height.

In the surface layer, Panofsky et al. (1977) propose the following relations.

$$\sigma_v = u_* \left[4 + 0.6(-h/L)^{2/3}\right]^{1/2} \tag{2-43}$$

$$\sigma_w = u_* \left[1.6 + 2.9\ (-z/L)^{2/3}\right]^{1/2} \tag{2-44}$$

where, u_* is the surface friction velocity (m/s), and
L is the Monin-Obukhov length (m).

Hicks (1985) suggests the following for the mixed layer (0.1 to 0.8 h).

$$\sigma_v = \left(3.6\ u_*^2 + 0.35\ w_*^2\right)^{1/2} \tag{2-45}$$

$$\sigma_w = \left(1.2\ u_*^2 + 0.35\ w_*^2\right)^{1/2} \tag{2-46}$$

In the neutral boundary layer, Arya (1984) reports monotonically decreasing values of σ_v and σ_w throughout the mixed layer. Using Blackadar and Tennekes (1968) relationship for the neutral boundary layer height, Arya's results can be expressed as:

$$\sigma_v = 1.8\ \exp\ (-0.9\ z/h) \tag{2-47}$$

$$\sigma_w = 1.3\ \exp\ (-0.9\ z/h) \tag{2-48}$$

In the stable boundary layer, Nieuwstadt (1984) finds that σ_v and σ_w bear constant ratios with the local friction velocity.

$$\sigma_v / u_{*\ell} = C_v \tag{2-49}$$

$$\sigma_w / u_{*\ell} = C_w \tag{2-50}$$

where, $u_{*\ell}$ is the local friction velocity (m/s), and,
C_v and C_w are constants.

Hanna et al. (1986) suggest that $C_v = 1.6$. C_w has a value = 1.3 (Nieuwstadt, 1984). The local friction velocity, u_{*l}, can be expressed (Nieuwstadt, 1984) as:

$$u_{*l} = u_* \, (1 - z/h)^{3/4} \tag{2-51}$$

The modeling requires a formulation that yields the proper values and vertical variations for σ_v and σ_w in the convective, neutral, and stable limits, and one that provides a mechanism for interpolating the results for intermediate conditions without physically unrealistic discontinuities. The following equations for the neutral-convective boundary layer are based on the data discussed above and satisfy these conditions. The formulation for the entrainment layer is based on data reported by Caughey (1981).

Surface Layer: $z \le 0.1$ h ($L \le 0$)

$$\sigma_v = \left[4 \, u_*^2 \, a_n^2 + 0.35 \, w_*^2\right]^{1/2} \tag{2-52}$$

$$\sigma_w = \left[1.6 \, u_*^2 \, a_n^2 + 2.9 \, u_*^2 \, (-z/L)^{2/3}\right]^{1/2} \tag{2-53}$$

$$a_n = \exp\left[-0.9 \, (z/h)\right] \tag{2-54}$$

Mixed-Layer: $z = 0.1$-0.8 h ($L \le 0$)

$$\sigma_v = \left[4 \, u_*^2 \, a_n^2 + 0.35 \, w_*^2\right]^{1/2} \tag{2-55}$$

$$\sigma_w = \left[1.15 \, u_*^2 \, a_n^2 + 0.35 \, w_*^2\right]^{1/2} \tag{2-56}$$

Entrainment Layer: $z > 0.8$ h ($L \le 0$)

$$\sigma_v = \left[4 \, u_*^2 \, a_n^2 + 0.35 \, w_*^2\right]^{1/2} \tag{2-57}$$

for $z = 0.8$ to 1.0 h

$$\sigma_w = \left[1.15 \, u_*^2 \, a_n^2 + a_{cl} \, 0.35 \, w_*^2\right]^{1/2} \tag{2-58}$$

$$a_{cl} = \left[1/2 + (h - z)/(o.4h)\right] \tag{2-59}$$

for $z = 1.0$ to 1.2 h

$$\sigma_w = \left[1.15\ u_*^2\ a_n^2 + a_{c2}\ 0.35\ w_*^2\right]^{1/2} \quad (2\text{-}60)$$

$$a_{c2} = [1/3 + (1.2h - z)/(1.2h)] \quad (2\text{-}61)$$

In the neutral-stable boundary layer, the following equations can be used to interpolate vertical profiles of σ_v and σ_w as a function of stability. As with the neutral-convective equations, they provide the proper values in the appropriate stability limits.

$$\sigma_v = u_*\left[(1.6\ C_s\ (z/L) + 1.8\ a_n)/(1 + z/L)\right] \quad (L > 0) \quad (2\text{-}62)$$

$$\sigma_w = 1.3\ u_*\left[(C_s\ (z/L) + a_n)/(1 + z/L)\right] \quad (L > 0) \quad (2\text{-}63)$$

$$C_s = (1 - z/h)^{3/4} \quad (L > 0) \quad (2\text{-}64)$$

It is assumed that the similarity-based values of σ_v, σ_w from which σ_y, σ_z are derived, are representative of one-hour average values. In order to provide for non-zero plume growth rates above the mixing height and to prevent numerical problems associated with near-zero plume dimensions, minimum σ_v and σ_w values are applied. Hanna et al. (1986) suggest an appropriate minimum one-hour average σ_v value is ~ 0.5 m/s. This is significantly higher than σ_v expected based on PGT E and F stability curves. Appropriate default minimum values for σ_v and σ_w can be input by the user.

Equation (2-52) to (2-61) have been tested with the original data providing the basis for the Panofsky et al. (1977) and Hicks (1985) formulations. The results (summarized in Table 2-3) indicate that the modified equations compare well with the original equations and the observational data. The modified equations have the advantage of allowing a smooth and continuous transition to the neutral stability results of Arya (1984).

Irwin (1983) has evaluated several schemes for determining the f_y and f_z functions. It was concluded that a parameterization suggested by Draxler (1976) performed best overall.

$$f_y = [1 + 0.9\ (t/1000)^{1/2}]^{-1} \quad (2\text{-}65)$$

$$f_z = \left[1 + 0.9\ (t/500)^{1/2}\right]^{-1} \quad L < 0 \quad (2\text{-}66)$$

$$f_z = \left[1 + 0.945\ (t/100)^{.806}\right]^{-1} \quad L > 0 \quad (2\text{-}67)$$

Table 2-3
Comparison of Panofsky et al. (1977)/Hicks (1985)
σ_v, σ_w Formulations with Eqns. (2-52) to (2-61)

Panofsky et al. data	Observed σ_v vs. Panofsky	Observed σ_v vs. Eqns. (2-52) to (2-61)	Panofsky σ_v vs. Eqns. (2-52) to (2-61)
Average	(1.14, 1.20)	(1.14, 1.21)	(1.20, 1.21)
Corr. Coef.	.81	.84	.992
Average Bias	.07	.07	.00
Average Abs. Error	.10	.09	.02
RMSE	.13	.12	.02

Hicks 1985 data	Observed σ_v vs. Hicks	Observed σ_v vs. Eqns. (2-52) to (2-61)	Hicks σ_v vs. Eqns. (2-52) to (2-61)
Average	(1.17, 1.12)	(1.17, 1.06)	(1.12, 1.06)
Corr. Coef.	.79	.77	.998
Average Bias	-.05	-.11	.06
Average Abs. Error	.20	.23	.06
RMSE	.27	.30	.08

Hicks 1985 data	Observed σ_w vs. Hicks	Observed σ_w vs. Eqns. (2-52) to (2-61)	Hicks σ_w vs. Eqns. (2-52) to (2-61)
Average	(.98, 1.01)	(.98, .98)	(1.01, .98)
Corr. Coef.	.91	.91	.998
Average Bias	.03	.00	-.03
Average Abs. Error	.12	.11	.03
RMSE	.15	.14	.04

At longer transport distances, an option is provided to switch to the Heffter (1965) equations (i.e., $\sigma_{yt} \propto t$, $\sigma_{zt} \propto t^{1/2}$). The transition from distance-dependent to time-dependent (i.e., Heffter) dispersion coefficients occurs in CALPUFF when the lateral dimensions of the plume reach a critical size, defined by the variable SYTDEP in Input Group 12 of the control file. The default value of SYTDEP is 550 m. Assuming PG dispersion rates under neutral conditions, a plume's σ_y will reach 550 m after approximately 10 km of travel distance.

The user may also wish to have puff growth determined on the basis of gridded input fields of PGT class. The approach is particularly useful if one is trying to compare the modeling results with steady-state regulatory model predictions or attempting to achieve compatibility with regulatory requirements. The user may select either AUSPLUME (Lorimer, 1986) or ISC2 model (U.S. EPA, 1992) dispersion methodology (Option 3) or the MESOPUFF II (Scire et al., 1984b) implementation of the PGT dispersion curves (Option 4).

Option 3 also requires the specification of gridded land use type, which in turn determines whether the ISC "rural" or "urban" dispersion curves are used. The "rural" dispersion equations and parameters are presented in Tables 2-4 and 2-5 for σ_y and σ_z respectively and are based on parameterizations of the PGT curves. The "urban" dispersion equations and parameter values are based on Briggs' (as reported in Gifford, 1976) parameterizations of the St. Louis dispersion data analyzed by McElroy and Poole (1968) and are presented in Tables 2-6 and 2-7 for σ_y and σ_z respectively.

If the MESOPUFF II form of the PGT stability-dependent dispersion curves is selected (Option 4), the puff growth functions are of the form:

$$\sigma_y = a_y x^{b_y} \tag{2-68}$$

$$\sigma_z = a_z x^{b_y} \tag{2-69}$$

where a_y, b_y, a_z, b_z are the stability dependent coefficients presented in Table 2-8.

The regulatory modeling guidance from the US EPA indicates that the PG dispersion curves, as defined above, are suitable for predicting one-hour average concentrations. The EPA of Victoria (Australia) bases the PG dispersion curves on a 3-minute averaging time and a surface roughness length (z_o) of 0.03 m. CALPUFF has the option to scale the PG dispersion coefficients for different averaging times or surface roughness lengths. The averaging time adjustment applies only to σ_y and is of the form:

Table 2-4
Parameters Used to Calculate Pasquill-Gifford σ_y

	$\sigma_y = 465.11628\ (x) \tan (\theta)$** $\theta = 0.017453293\ (c - d \ln x)$	
Pasquill Stability Class	c	d
A	24.1670	2.5334
B	18.3330	1.8096
C	12.5000	1.0857
D	8.3330	0.72382
E	6.2500	0.54287
F	4.1667	0.36191

* Source: U.S. EPA (1992)
** Where σ_y is in meters and x is in kilometers

Table 2-5

Parameters Used to Calculate Pasquill-Gifford σ_z*

Pasquill Stability Class	x (km)	σ_y (meters) = a x^b	
		c	d
A**	< .10	122.800	0.94470
	0.10 - 0.15	158.080	1.05420
	0.16 - 0.20	170.220	1.09320
	0.21 - 0.25	179.520	1.12620
	0.26 - 0.30	217.410	1.26440
	0.31 - 0.40	258.890	1.40940
	0.41 - 0.50	346.750	1.72830
	0.51 - 3.11	453.850	2.11660
	> 3.11	**	**
B**	< .20	90.673	0.93198
	0.21 - 0.40	98.483	0.98332
	> 0.40	109.300	1.09710
C**	All	61.141	0.91465
D	< .30	34.459	0.86974
	0.31 - 1.00	32.093	0.81066
	1.01 - 3.00	32.093	0.64403
	3.01 - 10.00	33.504	0.60486
	10.01 - 30.00	36.650	0.56589
	> 30.00	44.053	0.51179
E	< .10	24.260	0.83660
	0.10 - 0.30	23.331	0.81956
	0.31 - 1.00	21.628	0.75660
	1.01 - 2.00	21.628	0.63077
	2.01 - 4.00	22.534	0.57154
	4.01 - 10.00	24.703	0.50527
	10.01 - 20.00	26.970	0.46713
	20.01 - 40.00	35.420	0.37615
	> 40.00	47.618	0.29592
F	< .20	15.209	0.81558
	0.21 - 0.70	14.457	0.78407
	0.70 - 1.00	13.953	0.68465
	1.01 - 2.00	13.953	0.63227
	2.01 - 3.00	14.823	0.54503
	3.01 - 7.00	16.187	0.46490
	7.01 - 15.00	17.836	0.41507
	15.01 - 30.00	22.651	0.32681
	30.01 - 60.00	27.074	0.27436
	> 60.00	34.219	0.21716

* Source: U.S. EPA (1992)

** If the calculated value of σ_z exceeds 5000 m, σ_z is set equal to 5000 m

Table 2-6
Briggs Formulas Used to Calculate McElroy-Pooler σ_y*

Pasquill Stability Category	σ_y (meters)**
A	$0.32\ x\ (1.0 + 0.0004\ x)^{-1/2}$
B	$0.32\ x\ (1.0 + 0.0004\ x)^{-1/2}$
C	$0.22\ x\ (1.0 + 0.0004\ x)^{-1/2}$
D	$0.16\ x\ (1.0 + 0.0004\ x)^{-1/2}$
E	$0.11\ x\ (1.0 + 0.0004\ x)^{-1/2}$
F	$0.11\ x\ (1.0 + 0.0004\ x)^{-1/2}$

* Source: U.S. EPA (1992)
** where x is in meters

Table 2-7
Briggs Formulas Used to Calculate McElroy-Pooler σ_z*

Pasquill Stability Category	σ_z (meters)**
A	$0.24\,x\,(1.0 + 0.001\,x)^{+1/2}$
B	$0.24\,x\,(1.0 + 0.001\,x)^{+1/2}$
C	$0.20\,x$
D	$0.14\,x\,(1.0 + 0.0003\,x)^{-1/2}$
E	$0.08\,x\,(1.0 + 0.0015\,x)^{-1/2}$
F	$0.08\,x\,(1.0 + 0.0015\,x)^{-1/2}$

* Source: U.S. EPA (1992)
** where x is in meters

Table 2-8
MESOPUFF II Growth Rate Coefficients a_y, b_y, a_z, b_z*

Stability Class	a_y	b_y	a_z	b_z
A	0.36	0.9	0.00023	2.10
B	0.25	0.9	0.058	1.09
C	0.19	0.9	0.11	0.91
D	0.13	0.9	0.57	0.58
E	0.096	0.9	0.85	0.47
F	0.063	0.9	0.77	0.42

* Source: Scire et al. (1984b)

$$\sigma_y(\tau_{ave}) = \sigma_y(\tau_{base})\left(\frac{\tau_{ave}}{\tau_{base}}\right)^{0.2} \quad (2\text{-}72)$$

where τ_{base} is the averaging time (minutes) assumed for the standard PG curves (e.g., 60 minutes by U.S. EPA, 3 minutes in Australia).

τ_{ave} is the averaging time (minutes) of the concentrations predicted by CALPUFF ($\tau_{ave} \leq 60$ minutes).

$\sigma_y(\tau_{base})$, $\sigma_y(\tau_{ave})$ are the values of σ_y assumed for averaging times of τ_{base} and τ_{ave} minutes, respectively.

The values of τ_{base} is defined as 60 minutes in CALPUFF. The τ_{ave} variable is specified by the user in Input Group 1 of the control file (see the variable AVET). The value of τ_{ave} should not exceed 60 minutes, because multi-hour average concentrations are computed explicitly by time-averaging hourly values in CALPUFF.

The roughness length adjustment to the PG σ_z curves is based on Smith (1972), as implemented in the AUSPLUME model (Lorimer, 1986). This adjustment is most appropriate for near-surface releases and is not recommended for tall stack emissions (e.g., sources above 100 m). The adjusted value of σ_z is

$$\sigma_z' = a' x^{b'} \quad (2\text{-}73)$$

where

$$a' = a \cdot \left\{1.585(1000)^{\beta} z_o^{0.1301}\right\} \quad (2\text{-}74a)$$

$$b' = b - \beta \quad (2\text{-}74b)$$

$$\beta = 0.0777 + 0.0215 \ln(z_o) \quad (2\text{-}74c)$$

and z_o is the surface roughness length (m),

x is the downwind distance (m),

σ_z' is the roughness adjusted value of σ_z, and

a, b are the PG dispersion curve parameters (see Table 2-5).

For σ_y, the roughness length adjustments is:

$$\sigma_y' = \sigma_y \, (z_o / z_{o(ref)})^{0.2} \tag{2-75}$$

where the reference roughness length ($z_{o(ref)}$) is 0.03 meters, and the prime indicates the roughness length adjusted value of σ_y.

It is recommended that the surface correction be limited to surface roughness lengths no greater than one meter. The time average and surface roughness adjustments can be applied to either the ISC2 or MESOPUFF II PG rural dispersion curves. Adjustments are not made to the McElroy-Pooler urban curves or the similarity-based dispersion curves, which have the effects of roughness implicitly included.

2.2.2 Plume Buoyancy Components

The effect of plume buoyancy on the dispersion coefficients are parameterized in terms of the plume rise (Pasquill, 1976; Irwin, 1979).

$$\sigma_{yb} = \Delta H / 3.5 \tag{2-76}$$

$$\sigma_{zb} = \Delta H / 3.5 \tag{2-77}$$

where ΔH is the plume rise (m).

2.2.3 Initial Plume Size

The initial size of puffs emitted by volume sources is determined by user-specified initial dispersion coefficients, σ_{yo} and σ_{zo}. The volume source option allows the emissions from a number of smaller sources in a given area (e.g., a grid cell) to be combined into a single source. The volume source emissions are immediately spread over a volume described by σ_{yo} and σ_{zo}. The subsequent growth of the volume source puff is computed in the same manner as the point source puffs, using a virtual source to match the initial values of σ_y and σ_z.

Point source emissions subject to building downwash effects experience a rapid initial growth due to the high building-induced turbulence intensity in the lee of the building. A building downwash model (described in Section 2.3) is used to internally compute initial plume dimensions for downwashed point source emissions as a function of building dimensions, stack height, momentum flux, and meteorological conditions.

2.2.4 Vertical Wind Shear

Vertical wind shear can sometimes be an important factor affecting plume transport and dispersion. The change of wind speed and wind direction with height causes a differential advection of pollutant material emitted at different heights. Even for material emitted at a given height, when plumes become large enough, across-plume shear may transport the upper portion of a plume in a different direction than the lower portion. When vertical mixing brings the entire plume to the ground, the effective horizontal dispersion of the plume may be significantly enhanced as a result of the differential transport. CALPUFF explicitly models wind shear effects on different puffs by allowing each puff to be independently advected by its *local* wind speed and direction, and independently mixed vertically to the ground. For example, puffs emitted from two sources co-located in the horizontal, but with different release heights will be transported in CALPUFF in different directions and at different speeds if the wind fields indicate such a shear exists. Shear across a single puff is handled in CALPUFF by allowing the puff to split into two pieces when across-puff shear becomes important. Each portion of the puff is then independently transported and dispersed. A single puff may be split multiple times if it remains in the modeling domain long enough. Because across-puff wind shear effects are not likely to be important in all applications, and because puff splitting increases computational requirements, the puff splitting feature is an option that can be turned off. It is controlled by the MSPLIT variable in Input Group 2 of the control file.

2.3 Building Downwash

The dispersion and buoyant rise of plumes released from short stacks can be significantly modified by the presence of buildings or other obstacles to the flow. Hosker (1984) provides a description of the flow patterns in three regions near buildings. Figure 2-8 shows (1) a displacement zone upwind of the buildings, where the flow is influenced by the high pressure along the upwind building face, (2) a cavity zone characterized by recirculating flow, high turbulence intensity, and low mean wind speed, and (3) a turbulent wake region where the flow characteristics and turbulence intensity gradually approach the ambient values.

The parameterization of building downwash in CALPUFF is appropriate for use in the turbulent wake region and is based on the procedures used in the ISC2 model. ISC2 contains two building downwash algorithms:

- Huber-Snyder model (Huber and Snyder, 1976; Huber, 1977). In ISC2, this model is applied when the source height is greater than the building height (H_b) plus one-half of the lesser of the building height or projected width (L_b). It applies either a full building wake effect or none at all, depending on the effective height of the emitted plume.

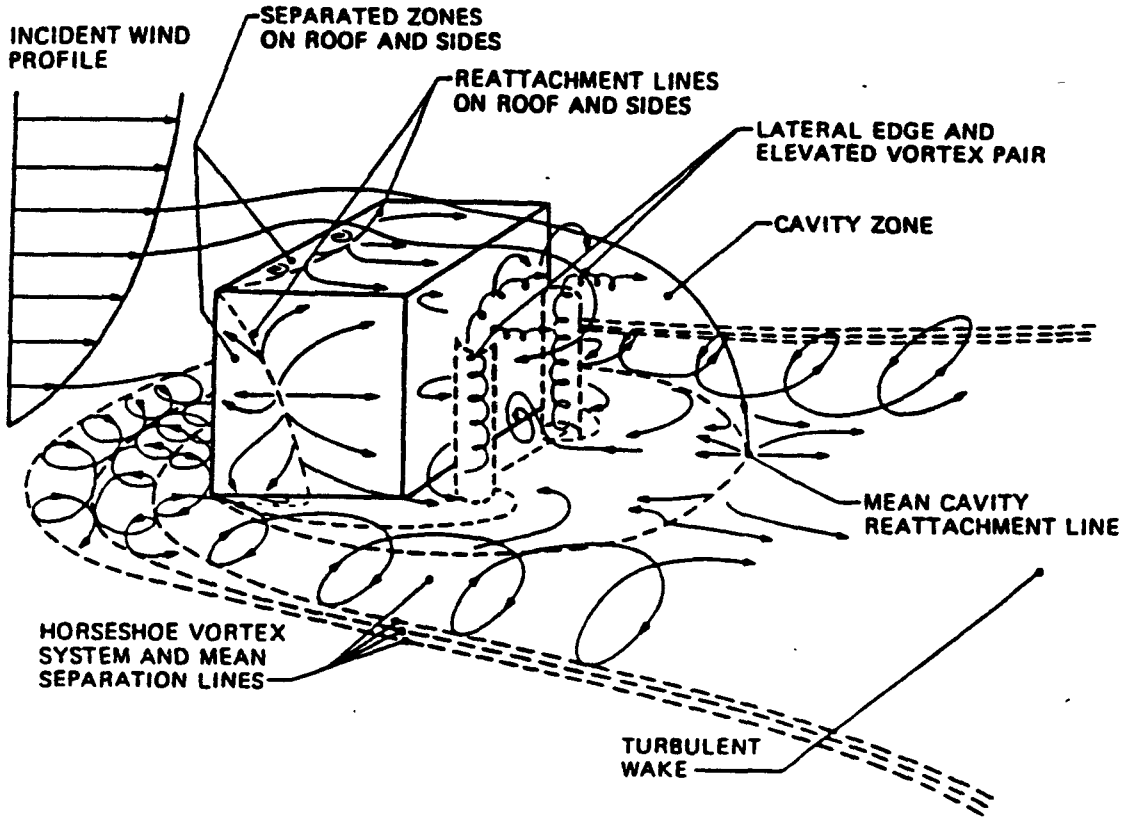


Figure 2-8. Flow near a sharp-edged building in a deep boundary layer. [From Hosker, (1984)]

- Schulman-Scire model (Scire and Schulman, 1980; Schulman and Hanna, 1986). This model applies a linear decay factor to the building-induced enhancement of the dispersion coefficients and accounts for the effect of downwash on plume rise. It is used in ISC2 for stacks lower in height than $H_b + 0.5\ L_b$.

The main difference in the treatment of downwash between ISC2 and CALPUFF is that the height threshold determining which model is used is an input variable. This option allows the user to apply one of the models for all stacks, which has the desirable effect of eliminating the discontinuity of the ISC2 approach at stack heights of $H_b + 0.5\ L_b$. Thus, in CALPUFF, the Huber-Snyder technique is used for stacks greater than $H_b + T_{bd}\ L_b$, where T_{bd} has a default value of 0.5. A negative value of T_{bd} indicates the Huber-Snyder method is used for all stacks, and a value of 1.5 results in the Schulman-Scire method being always used. If T_{Tb} is set equal to 0.5 (its default value), the CALPUFF treatment will be equivalent to than in ISC2.

Both downwash methods use wind direction-specific building dimensions (i.e., H_b, H_w, L_b). CALPUFF, like the short-term version of ISC2, uses 36 wind direction-specific values of the building dimensions, corresponding to wind vectors from 10° to 360° in increments of 10°. The EPA Building Profile Input Program (BPIP) (EPA, 1993) can be used to develop the wind direction-specific building dimensions for CALPUFF and determine Good Engineering Practice (GEP) stack height associated with one or more buildings.

2.3.1 Huber-Snyder Downwash Procedure

If the stack height exceeds $H_b + T_{bd}L_b$, the Huber-Snyder algorithm is applied. The first step is to compute the effective plume height, H_e, due to momentum rise at a downwind distance of two building heights. If H_e exceeds $H_b + 1.5\ L_b$ (where H_b and L_b are the wind direction specific values), building downwash effects are assumed to be negligible. Otherwise, building-induced enhancement of the plume dispersion coefficients is evaluated. For stack heights, H_s, less than $1.2H_b$, both σ_y and σ_z are enhanced. Only σ_z is enhanced for stack heights above $1.2\ H_b$ (but below $H_b + 1.5\ L_b$).

A building is defined as a squat building if the projected building width, H_w, exceeds the building height (i.e., $H_w \geq H_b$). A tall building is defined as one for which $H_w < H_b$. Because both the controlling building height and projected width can vary with wind direction, the classification of a building as squat or tall can also vary by direction. For a squat building, the enhanced σ_z is:

$$\sigma_z' = 0.7\ H_b + 0.067\ (x - 3H_b) \qquad (2\text{-}78)$$

where x is the downwind distance (in meters).

For a tall building,

$$\sigma_z' = 0.7\ H_w + 0.067\ (x - 3H_w) \quad 3H_w < x < 10H_w \tag{2-79}$$

If the ratio H_s/H_b is less than or equal to 1.2, the horizontal dispersion coefficient, σ_y, is enhanced. For a squat building with a projected width to height ratio (H_w/H_b) less than 5, the equation for σ_y is:

$$\sigma_y' = 0.35\ H_w + 0.067\ (x - 3H_b) \quad 3H_b < x < 10H_b \tag{2-80}$$

For buildings with (H_w/H_b) greater than 5, two options are provided for σ_y.

$$\sigma_y' = 0.35\ H_b + 0.067\ (x - 3H_b) \quad 3H_b < x < 10H_b \tag{2-81}$$

or,

$$\sigma_y' = 1.75\ H_b + 0.067\ (x - 3H_b) \quad 3H_b < x < 10H_b \tag{2-82}$$

Eqn. (2-81) results in higher centerline concentrations than Eqn. (2-82), and is considered as an upper bound estimate of the impacts of the source. The ISC2 manual suggests that Eqn. (2-82) is most appropriate if the source is located within 2.5 H_b of the end of the building. Eqn. (2-81) is a better estimate if the source is located near the center of the building. However, in practice, the more conservative Eqn. (2-81) is usually used for regulatory applications regardless of the position of the stack.

For a tall building, the equation for σ_y is:

$$\sigma_y' = 0.35\ H_w + 0.067\ (x - 3H_w) \quad 3H_w < x < 10H_w \tag{2-83}$$

2.3.2 Schulman-Scire Downwash Procedure

The main features of the Schulman-Scire algorithm are that the effects of building downwash on reducing plume rise are incorporated, and the enhancement of σ_z is a gradual function of effective plume height rather than a step function. As noted above, both schemes use wind direction specific building dimensions.

The plume rise equations incorporating building downwash effects are discussed in Section 2.4.4. Wind tunnel studies of buoyant emissions from sub-GEP height stacks have shown that plume rise is decreased during downwash conditions (e.g. Huber and Snyder, 1976). The increased mechanical turbulence in the building wake leads to enhanced plume dispersion (reflected in the enhanced dispersion coefficients), which causes a rapid dilution of the plume.

This dilution reduces the rate of rise of the plume and results in lower plume heights. As discussed in Section 2.4.4, the initially high dilution rate is modeled by applying an initial "dilution radius" to the plume. The inclusion of downwash effects in the plume rise equations is a key part of the Schulman-Scire downwash method.

The second component of the model is the linear decay function which is applied to the enhancement of σ_z. The vertical dispersion coefficient is determined as:

$$\sigma_z'' = A\ \sigma_z' \tag{2-84}$$

where σ_z' is determined from Eqns. (2-78) and (2-79), and,

$$A = \begin{cases} 1 & H_e \le H_b \\ (H_b - H_e)/(2\ L) + 1 & H_b < H_e \le H_b + 2L \\ 0 & H_b + 2L < H_e \end{cases} \tag{2-85}$$

2.4 Plume Rise

The plume rise relationships in the CALPUFF model are generalized to apply to a variety of source types and plume characteristics. The following effects are included in the plume rise algorithm:

- Plume buoyancy and momentum
- Stable atmospheric stratification
- Partial penetration of the plume into an elevated stable inversion layer
- Building downwash and stack-tip downwash effects
- Vertical wind shear
- Area source plume rise
- Line source plume rise

2.4.1 Basic Plume Rise Equations

The basic point source plume rise relationships are based on the Briggs (1975) equations. The plume rise due to buoyancy and momentum during neutral or unstable conditions, z_n is:

$$z_n = \left[3F_m x/\left(\beta_j^2 u_s^2\right) + 3Fx^2/\left(2\beta_1^2 u_s^3\right)\right]^{1/3} \tag{2-86}$$

where, F_m is the momentum flux (m^4/s^2),
F is the buoyancy flux (m^4/s^3),

u is the stack height wind speed (m/s),
x is the downwind distance (m),
β_1 is the neutral entrainment parameter (~ 0.6),
β_j is the jet entrainment coefficient ($\beta_j = 1/3 + u_s/w$), and,
w is the stack gas exit speed (m/s).

The distance to final plume rise, x_f, is:

$$x_f = \begin{cases} 3.5x^* & F > 0 \\ 4D\,(w + 3u_s)^2 / (u_s w) & F = 0 \end{cases} \quad (2\text{-}87)$$

$$x^* = \begin{cases} 14\,F^{5/8} & F \le 55 m^4/s^3 \\ 34\,F^{2/5} & F > 55\ m^4/s^3 \end{cases} \quad (2\text{-}88)$$

where D is the stack diameter (m).

During stable conditions, the final plume rise, z_{sf}, is determined by:

$$z_{sf} = \left[3F_m / \left(\beta_j^2 u_s S^{1/2}\right) + 6F / \left(\beta_2^2 u_s S\right)\right]^{1/3} \quad (2\text{-}89)$$

where, β is the stable entrainment parameter (~ 0.6),
S is a stability parameter [$(g/T_a)(d\theta/dz)$,
g is the acceleration due to gravity (m/s^2),
T_a is the ambient temperature (deg. K), and,
$d\theta/dz$ is the potential temperature lapse rate (deg. K/m).

Transitional plume rise during stable conditions is computed by Eqn. (2-86) up to the point at which $z_n = z_{sf}$. For low wind speed and calm conditions, the following equation (Briggs, 1975) is used to compute the plume centerline rise:

$$z_{sf} = 4\,F^{1/4} / S^{3/8} \quad (2\text{-}90)$$

2.4.2 Stack-tip Downwash

If the ratio of the stack gas exit speed to the ambient wind speed is less than 1.5, the plume may be drawn into the lee of the stack. Briggs (1973) suggests modifying the stack height to adjust for this stack-tip effect:

$$h_s' = \begin{cases} h_s + 2D(w/u_s - 1.5) & w/u_s < 1.5 \\ h_s & w/u_s \geq 1.5 \end{cases} \quad (2\text{-}91)$$

where h_s' is the adjusted stack top height.

2.4.3 Partial Plume Penetration

Plumes from tall stacks may frequently interact with the capping inversion at the top of the mixed layer. A fraction of the plume mass may penetrate the inversion, and therefore be unavailable for immediate mixing to the ground. Manins (1979) developed a procedure for estimating partial plume penetration into an elevated inversion using water tank experimental data. This scheme is adopted for use in CALPUFF.

A penetration parameter, P, is defined as:

$$P = \frac{F_b}{u\, b_i\, \Delta h_i^2} \quad (2\text{-}92a)$$

where u is the stack height wind speed,
F_b is the initial buoyancy of the stack emissions,
Δh_i is the height of the inversion (h) above the stack top (h_s), (i.e., $\Delta h_i = h - h_s$)
b_i is the strength of the inversion ($b_i = g\Delta T_i/T_a$),
ΔT_i is the temperature jump across the inversion,
T_a is the ambient air temperature, and
g is the acceleration due to gravity.

The fraction, f, of the plume remaining below the inversion is:

$$f = \begin{cases} 1 & (P < 0.08) \\ \dfrac{0.08}{P} - P + 0.08 & (0.08 < P \leq 0.3) \\ 0 & (P > 0.3) \end{cases} \quad (2\text{-}92b)$$

Thus, no penetration is predicted for P < 0.08, and nearly full penetration is suggested for P = 0.3 and above. Manins (1979) compared this scheme with the partial penetration

Thus, no penetration is predicted for $P < 0.08$, and nearly full penetration is suggested for $P = 0.3$ and above. Manins (1979) compared this scheme with the partial penetration methods of Briggs (1969) and Briggs (1975) using water tank data. He found that the Briggs (1969) model underestimates the amount of penetration into the inversion layer, while the Briggs (1975) method tends to overestimate it. Field data collected at the Gladstone power station in Queensland, Australia, also supported these conclusions (Manins, 1984).

Knowing f from Eqn. (2-92b), the effective final height of the plume trapped below the inversion can be estimated as the minimum of (Δh, Δh_1) where Δh is evaluated at $x = x_f$ and Δh_1 is defined below.

$$\Delta h_1 = \left(1 - \frac{f}{3}\right) \Delta h_i \qquad (2\text{-}93a)$$

Note that Δh, Δh_1, and Δh_i are all measured above the stack top height.

The effective height of the portion of the plume above the inversion base is (Hanna and Chang, 1991):

$$\Delta h_2 = (2 - f)(\Delta h_i) \qquad (2\text{-}93b)$$

where Eqns. (2-93a) and (2-93b) apply only for plumes which partially penetrate the inversion.

2.4.4 Building Downwash

Wind tunnel observations of plume dispersion and plume rise indicate that plume rise can be significantly reduced by building downwash. Huber and Snyder (1982) found that during downwash conditions, plume rise was reduced by one-third below the value obtained in the absence of the building. In an analysis of plume rise observations, Rittmann (1982) found lower plume rise than predicted by the 2/3 law (a form of Eqn. 2-86) for smaller sources which are most likely to be affected by downwash. Several studies (e.g., Bowers and Anderson, 1981; Scire and Schulman, 1981; Thuillier, 1982) with the original version of the ISC building downwash algorithm, which did not account for the effects of building downwash on plume rise, showed that neglecting building downwash effects on plume rise can significantly underestimated peak concentrations during downwash conditions.

The increased mechanical turbulence in the building wake which leads to enhanced plume dispersion, causes a rapid dilution of the plume. This dilution reduces the rate of rise of the plume and leads to lower plume heights. One method of treating the initially high dilution rate is to assume an initial "dilution radius" for the plume (Scire and Schulman, 1980). This

rate is to assume an initial "dilution radius" for the plume (Scire and Schulman, 1980). This technique is incorporated in the Buoyant Line and Point Source (BLP) model (Schulman and Scire, 1980) and a modified version of the ISC model. It has been shown (Schulman and Hanna, 1986), to produce more realistic estimates of ground-level concentrations during building downwash conditions.

The plume rise of a downwashed plume with $\sigma_{yo} \leq \sigma_{zo}$ during neutral-unstable conditions is given by:

$$z_d^3 + \left(3R_o z_d / \beta_1 + 3R_o^2 / \beta_1^2\right) z_d = \left[3F_m x / \left(\beta_j^2 u_s^2\right) + 3Fx^2 / \left(2\beta_1 2u_s^3\right)\right] \quad (2\text{-}94)$$

where R_o is the dilution radius [$R_o = (2)^{1/2}\sigma_{zo}$], and σ_{yo}, σ_{zo} are the horizontal and vertical dispersion coefficients, respectively, at a downwind distance of $3H_b$ (see Section 2.3). The factor of $(2)^{1/2}$ in the R_o equation converts the Gaussian dispersion coefficient into an effective top-hat distribution for the plume rise calculations.

Final stable plume rise is:

$$z_d^3 + \left(3R_o z_d / \beta_2 + 3R_o^2 / \beta_2^2\right) z_d = \left[3F_m / \left(\beta_j^2 u_s S^{1/2}\right) + 6F / \left(\beta_2^2 u_s S\right)\right] \quad (2\text{-}95)$$

Transitional plume rise during stable conditions is computed with Eqn. (2-94) until the final plume height predicted by Eqn. (2-95) is obtained.

When horizontal mixing of the plume in the building wake causes $\sigma_{yo} > \sigma_{zo}$, it is necessary to account for the elongated shape of the plume. The plume can be represented as a finite line source. The plume rise for a line source of length L_e during neutral-unstable conditions is:

$$z_d^3 + \left[3L_e / (\pi\beta_1)\right] z_d^2 + \left[3R_o z_d / \beta_1 + 6R_o L_e / \left(\pi\beta_1^2\right) + 3R_o^2 / \beta_1^2\right] z_d = \left[3F_m x / \left(\beta_j^2 u_s^2\right) + 3Fx^2 / \left(2\beta_1^2 u_s^3\right)\right] \quad (2\text{-}96)$$

and, for final stable plume rise:

$$z_d^3 + \left[3L_e / (\pi\beta_1)\right] z_d^2 + \left[3R_o z_d / \beta_1 + 6R_o L_e / \left(\pi\beta_1^2\right) + 3R_o^2 / \beta_1^2\right] z_d = \left[3F_m / \left(\beta_j^2 u_s S^{1/2}\right) + 6F / \left(\beta_2^2 u_s S\right)\right] \quad (2\text{-}97)$$

The effective line length, L_e, is $(2\pi)^{1/2}$ $(\sigma_{yo} - \sigma_{zo})$ if $\sigma_{yo} > \sigma_{zo}$. Otherwise, $L_e = 0$, and Eqns. (2-96) and (2-97) reduce to Eqns. (2-94) and (2-95).

As described in Section 2.3, the enhanced dispersion coefficients, σ_{zo} and σ_{yo}, vary with stack height, momentum rise, and building dimensions. The variation of R_o with for several stack heights is illustrated in Figure 2-9. As σ_{zo} and σ_{yo} approach zero (i.e., building downwash effects become negligible), Eqns (2-94) to (2-97) approach the unmodified Briggs equations. The effect of R_o and L_e is always to lower the plume height, thereby tending to increase the predicted maximum ground-level concentration.

2.4.5 Vertical Wind Shear

The variation of wind speed up to stack height is usually accounted for in plume rise algorithms by the use of the stack height wind speed in the plume rise equations. Most formulations assume that the wind speed is constant above the stack top. This assumption is reasonable for mid-sized and tall stacks. However, the variation of wind speed above the stack top can have a significant effect on reducing the plume rise of buoyant releases from short stacks imbedded in the surface (shear) layer of the atmosphere (Scire and Schulman, 1980). Assuming the vertical wind speed profile above the stack can be approximated as $u(z) = u_s(z/h_s)^p$, where u_s is the wind speed at the stack top, h_s, and u(z) is the wind speed at height z, the plume rise from a short stack can be represented during neutral and unstable conditions as:

$$z_w = \left[\left[e^2/(6 + 2p)\right]\left(F\, z_m^{3p}\right)/\left(\beta_1^2\, u_m^3\right)\right]^{1/e} x^{2/e} \qquad (2\text{-}98)$$

$$e = 3 + 3p \qquad (2\text{-}99)$$

where p is the wind speed power law exponent.

During stable conditions, the final plume height is:

$$z_w = \left[\left[2\,(3 + p) z_m^p\, F\right]/\left(\beta_2^2\, u_m\, S\right)\right]^{1/(3+p)} \qquad (2\text{-}100)$$

The wind shear exponent can be estimated from the atmospheric stability class or computed from the vertical wind data generated from the wind field model. It should be noted that Eqns. (2-98) and (2-100) both reduce to the Briggs buoyant plume rise equations when there is no wind shear above the stack top (i.e., p = 0).

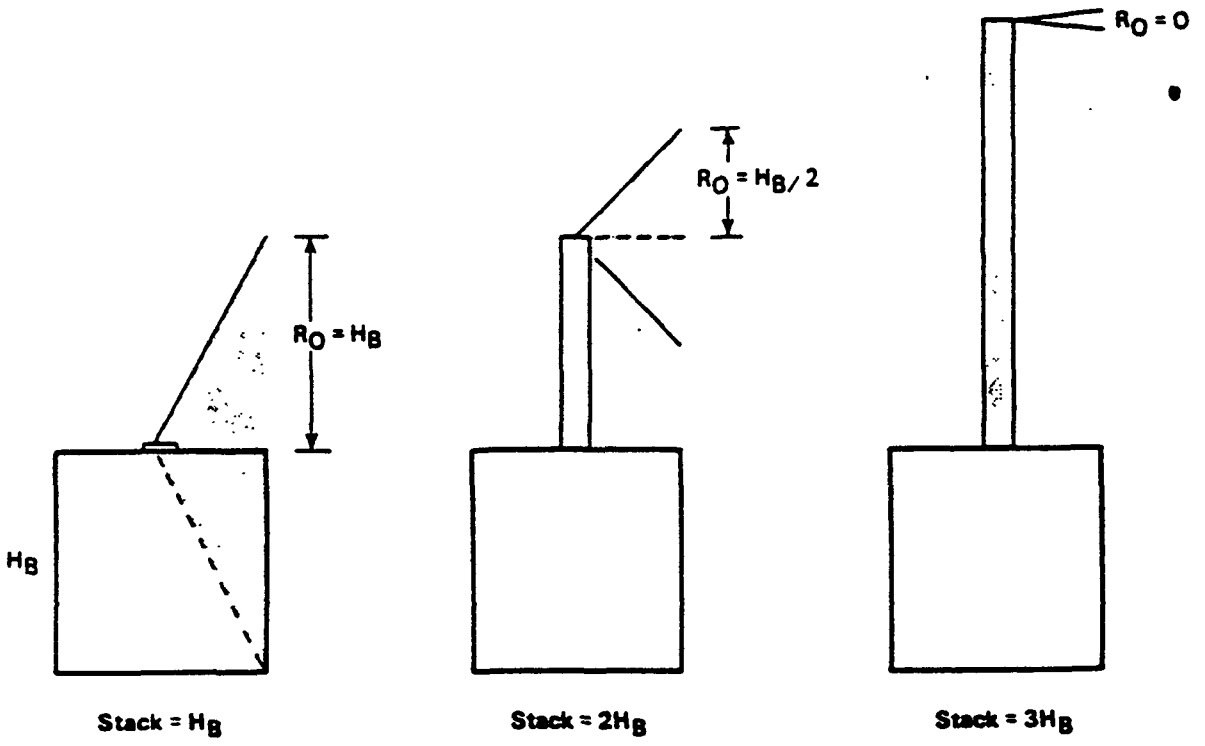


Figure 2-9. Illustration of the initial dilution radius, R_o, as a function of stack height for a squat building (from Schulman and Scire (1981)). Momentum plume rise is neglected in the figure.

The assumption of $u(z) = u_s (z/h_s)^p$ is most valid for short stacks where the shear effect is expected to be the greatest. However, it breaks down for taller stacks. Therefore, Eqns. (2-98) and (2-100) are used to provide an upper limit of the plume height for short stacks, i.e., that the actual plume height be taken as the minimum of the predictions of the shear, downwash, and no-shear predictions, as appropriate.

2.4.6 Area Source Plume Rise

The treatment of plume rise from large buoyant area sources requires special considerations that include effects of vertical wind shear, large initial plume size, and potentially large density differences between the plume and ambient air.

The area source plume rise model in CALPUFF is formulated to calculate the rise of buoyant plumes resulting from forest fires, the burning of leaking oil, and other type of buoyant area sources. The model is designed to be general, with applicability to the following conditions:

(a) all types of ambient temperature stratifications;
(b) all types of wind stratifications;
(c) any size of finite emission source;
(d) includes the effects of plume radiative heat loss; and
(e) is free of the limitations of the Boussinesq approximation.

All these factors may be important in large forest fire plumes. Due to the complex mountainous terrain in many forested areas and the strong influence it has on meteorological conditions, complex temperature and wind patterns may exist. The ambient temperature stratification is usually more complicated than linear stratification which is normally assumed in most plume rise models. Wind shear is important because the forest fire plume starts at ground where there is a zone of large velocity gradients in the vertical. Therefore, it is necessary to allow for arbitrary profiles of winds and temperatures to be accounted for in the plume rise, including potential stability and wind reversals in the vertical. The initial fire size may be large, of the order of ten or more kilometers in radius. Since the plume temperature near the burning source is much higher than the ambient air temperature, up to 1600 °K, radiative heat loss will reduce the heat flux which is carried by the plume along its trajectory. This reduction of heat flux also reduces the buoyancy flux and thus eventually reduces the final plume rise. Also, since the initial temperature of the plume is high, and the initial density difference between the plume and ambient air is large, the application of Boussinesq approximation becomes questionable.

The source parameters of a forest fire are usually not constant. The life cycle of a forest fire includes an initial developing stage with large increases in heat generation and pollutant emission rates, followed by a stage of decreasing values. The magnitude of the variation in heat generation and emission rates may be two orders of magnitude over the course of burn. The resulting time dependency to the plume rise can be calculated assuming that the plume motion is quasi-steady so that the input of source condition is time-dependent but the time-derivatives in the governing equations are neglected. This assumption is reasonable because the time scale for plume rise is much shorter than that of the fire life-span.

The derivation of the governing equations are similar to the one given by Weil (1988) except that the Boussinesq approximation has not been applied. The Boussinesq approximation simplifies the plume rise equations by assuming that the plume density is close enough to the ambient density that density variations, other than in the buoyancy term, can be neglected. The plume cross section is assumed to be circular with radius r. (Although the plume cross section, as it rises, appears to be dominated by a pair of counter-rotating line vortices, its effect on the plume rise trajectory can still be well quantified by integral models (Zhang, 1993)). All the physical quantities are assumed to be uniform within this cross section. The mass conservation law can be expressed in terms of entrainment hypothesis, which accounts for the entrainment of the ambient air flowing both parallel and cross the plume centerline (Hoult and Weil, 1972),

$$\frac{d}{ds}\left(\rho U_{sc} r^2\right) = 2 r \alpha \rho_a \left|U_{sc} - U_a \cos\phi\right| + 2 r \beta \rho_a \left|U_a \sin\phi\right| \qquad (2\text{-}101)$$

where $\alpha = 0.11$ and $\beta = 0.6$ are the entrainment parameters corresponding to the differences of velocity components between the wind and the plume in directions parallel and normal to the plume centerline, respectively (Weil, 1988); $U_a(z)$ is the ambient horizontal wind speed, which can be an arbitrary function of height; and

$$U_{sc} = \sqrt{u^2 + w^2} \qquad (2\text{-}102)$$

is the velocity of the plume cross section along its centerline, with two components u and w in the horizontal and vertical directions, ρ and ρ_a are the plume density and air density, respectively, s is the length of the plume centerline measured from the emission source, and ϕ is the centerline inclination. See Figure 2-10 for a schematic view of the plume rise and various variables.

The momentum equation in the wind direction is

$$\frac{d}{ds}\left(\rho U_{sc} r^2 \left(u - U_a\right)\right) = -r^2 \rho w \frac{dU_a}{dz} \qquad (2\text{-}103)$$

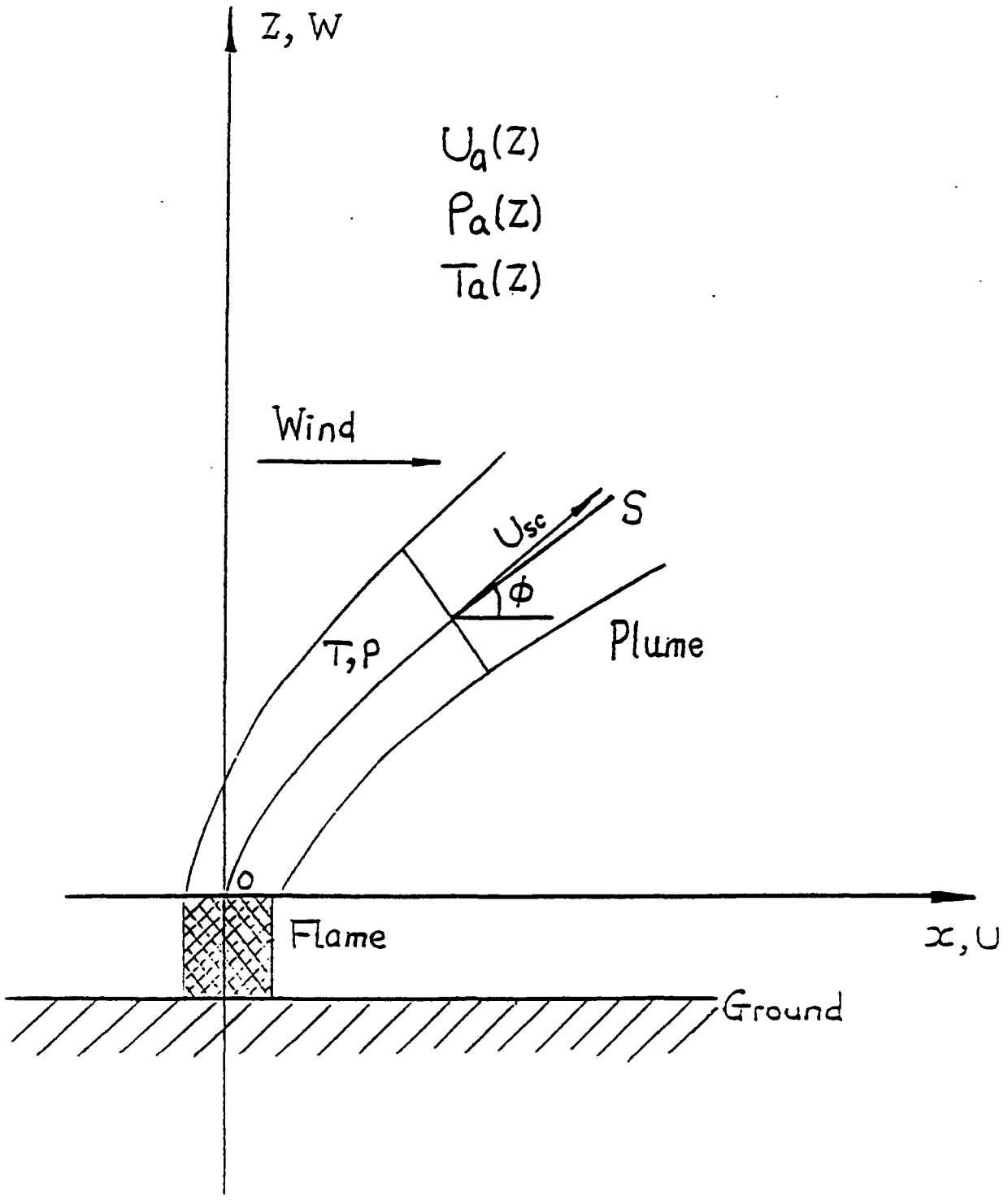


Figure 2-10. Schematic and nomenclature for plume in a crosswind.

where the right hand side is related with the wind shear. The momentum equation in the vertical direction is a balance among inertial acceleration, entrained momentum, and buoyancy:

$$\frac{d}{ds}\left(\rho\ U_{sc}\ r^2\ w\right) = g\,r^2\left(\rho_a - \rho\right) \tag{2-104}$$

where g is the gravitational acceleration. The energy equation can be written as

$$\frac{d}{ds}\left(\rho\ U_{sc}\ r^2\left(T - T_a\right)\right) = \rho\ \frac{d\eta_a}{dz}\ w r^2 + \frac{Q}{c_p}\ r^2 \tag{2-105}$$

where

$$\frac{d\ \eta_a}{dz} = \frac{dT_a}{dz} + \frac{g}{c_p}$$

is the vertical lapse rate of the ambient potential temperature. The constant on the right hand side is

$$\frac{g}{c_p} = 9.76\ x\ 10^{-3}\ °\text{K/m} \tag{2-106}$$

where c_p is the specific heat of the ambient air.

The last term in Eqn. (2-105) corresponds to the radiative heat loss from the plume to the ambient air. This term is expected to be important only initially when the plume temperature is high. Q is the heat loss per unit volume of the plume. This last term can be estimated by

$$\frac{Q}{c_p}\ r^2 = -\ 2\,\pi\,\epsilon\,\sigma\,r\left(T^4 - T_a^4\right)/c_p = -R_p\,r\left(T^4 - T_a^4\right) \tag{2-107}$$

where σ and ϵ are the Stefan-Boltzmann constant and the emissivity respectively, and $R_p = \frac{2\,\pi\,\epsilon\,\sigma}{c_p}$ is a variable which characterizing the radiation properties. If we choose,

$$c_p = 10^3\ \text{J/kg·K},\ \sigma = 5.67\ x\ 10^{-8}\ \frac{\text{W}}{\text{m}^2\text{K}^4}$$

and let ϵ = 0.8, then $R_p = 9.1 \times 10^{-11}$ kg/m^{2}K^{3}s. The energy equation finally becomes

$$\frac{d}{ds}\left[\rho U_{sc} r^2 (T - T_a)\right] = -\left(\frac{dT_a}{dz} + \frac{g}{c_p}\right)\rho w r^2 - R_p r\left(T^4 - T_a^4\right) \qquad (2\text{-}108)$$

It is expected that the radiative heat loss is large for high T and small r.

In deriving equations (2-103) and (2-105), it is assumed that the ambient wind is horizontal and the vertical gradients of ambient properties $\frac{dU_a}{dz}, \frac{dT_a}{dz}$ do not vary significantly across the plume cross section.

To close the equation set, two geometric relations are needed:

$$\frac{dz}{ds} = \frac{w}{U_{sc}} = \sin\phi \qquad (2\text{-}109)$$

$$\frac{dx}{ds} = \frac{u}{U_{sc}} = \cos\phi \qquad (2\text{-}110)$$

These equations can be solved subject to the following initial conditions and ambient meteorological conditions. Initial conditions are specified at the source location s = 0, where x = 0. The following information is needed as input: plume density, ρ_o; vertical velocity, w_o; plume radius, r_o; and temperature, T_o. The ambient conditions are specified in terms of horizontal wind profile, $U_a(z)$, and air temperature profile, $T_a(z)$. (In the case of a forest fire plume, the source parameters are to be provided by EPM and the meteorological conditions by the CALMET model.)

Most meteorological observations give the atmospheric stratification in the form of temperature distribution versus pressure. To obtain relations of air density versus height, and plume density versus height, it is assumed that the atmospheric pressure distribution can be approximated as that of an adiabatic atmosphere.

$$p = p_o\left[1 - \frac{\gamma - 1}{\gamma}\frac{gz}{RT_{ao}}\right]^{\frac{\gamma}{\gamma-1}} \qquad (2\text{-}111)$$

where T_{ao} is the ground level air temperature. Based on (2-111), if the air temperature and plume temperature are T_a and T respectively at height z, the corresponding densities can be obtained as

$$\rho_a = \frac{p(z)}{RT_a} \text{ and } \rho = \frac{p(z)}{RT} \qquad (2\text{-}112)$$

where R is the gas constant of the ambient air and the plume.

The equations described above are solved numerically using a second order, marching in s, Heun's predictor-corrector scheme.

$$\frac{dy}{ds} = f(s,y)$$

$$y^* = y^n + f(s^n, y^n)\,\Delta s$$

$$y^{n+1} = y^n + \frac{1}{2}\left[f(s^n,y^n) + f(s^*,y^*)\right]\Delta s$$

2.5 Overwater and Coastal Dispersion

There are important differences in the structures of the marine and continental boundary layers which can have significant effects on plume dispersion in the overwater and coastal environments. These differences arise for three basic reasons (LeMone, 1978):

- Water has a high heat capacity and is partially transparent to solar radiation, resulting in a relatively small diurnal temperature range (~ 0.5 deg. C).
- The sea surface is generally more uniform and less aerodynamically rough than typical land surfaces.
- There is a constant source of moisture in the marine boundary layer.

As a result of these differences, the sensible heat flux over the open water is typically more than an order of magnitude less than over land. The absence of a strong sensible heat flux to drive the marine mixed-layer and the small surface roughness result in relatively low mixing heights that offer the potential for significant plume trapping effects. LeMone (1978) indicates that the typical marine mixing depth is only about 500 m. Data from three offshore and coastal experiments reported by Hanna et al. (1985) (two of which were conducted in California) show many hours with mixing heights less than 100 m.

Another result is that the diurnal and annual variations of stability over water are completely unrelated to the typical overland behavior. For example, North Sea observations of water and air temperatures reported by Nieuwstadt (1977) (Figure 2-11) show that temperature inversions typically persist most of the day in June, while unstable conditions occur all day in January. During other times of the year, the overwater diurnal stability cycle is out of phase with the overland cycle (i.e., stable over water during the day and unstable at night).

The techniques used in the CALMET meteorological model for determining overwater mixing height, stability, and turbulence levels based on the air-sea temperature difference, wind speed, and the specific humidity have been discussed in Scire et al. (1995). These methods are applied by CALMET to the portions of the modeling domain over water. At the land-sea interface, rapid changes in the dispersion characteristics may occur which can significantly affect the ground-level concentrations from coastal sources. The puff model formulation is well-suited to accommodate these spatial changes in the coastal transition zone.

A typical situation during stable onshore flow conditions is shown in Figure 2-12. A narrow plume imbedded in the stable layer above the shallow mixed-layer is intercepted by a growing Thermal Internal Boundary Layer (TIBL). The growth of the TIBL is caused by the sensible heat flux associated with solar heating of the land surface. The convective overland conditions can rapidly bring the elevated pollutant to the ground, causing locally high ground-level concentrations. Many coastal fumigation models assume immediate mixing of the pollutant intercepted by the TIBL to the ground (e.g., Lyons and Cole, 1973, Misra, 1980). Deardorff and Willis (1982), based on laboratory experiments, suggest the importance of turbulent fluctuations in the TIBL height and indicate the plume does not become well-mixed immediately. In the Offshore and Coastal Dispersion (OCD) model, Hanna et al. (1985) use the minimum concentration predicted by a virtual source technique or that predicted by the Deardorff and Willis model to describe shoreline fumigation.

In CALPUFF, the land-sea interface is resolved on the scale of the computational grid. The CALPUFF model provides the turbulence and dispersion characteristic of the overwater as well as the overland boundary layers. The transition from marine to continental dispersion rates is assumed to occur at the coastal boundary determined from the gridded land use data. Once a puff within a marine layer encounters the overland mixed layer height, the puff growth is changed from that appropriate for the marine layer to that appropriate for the overland boundary layer.

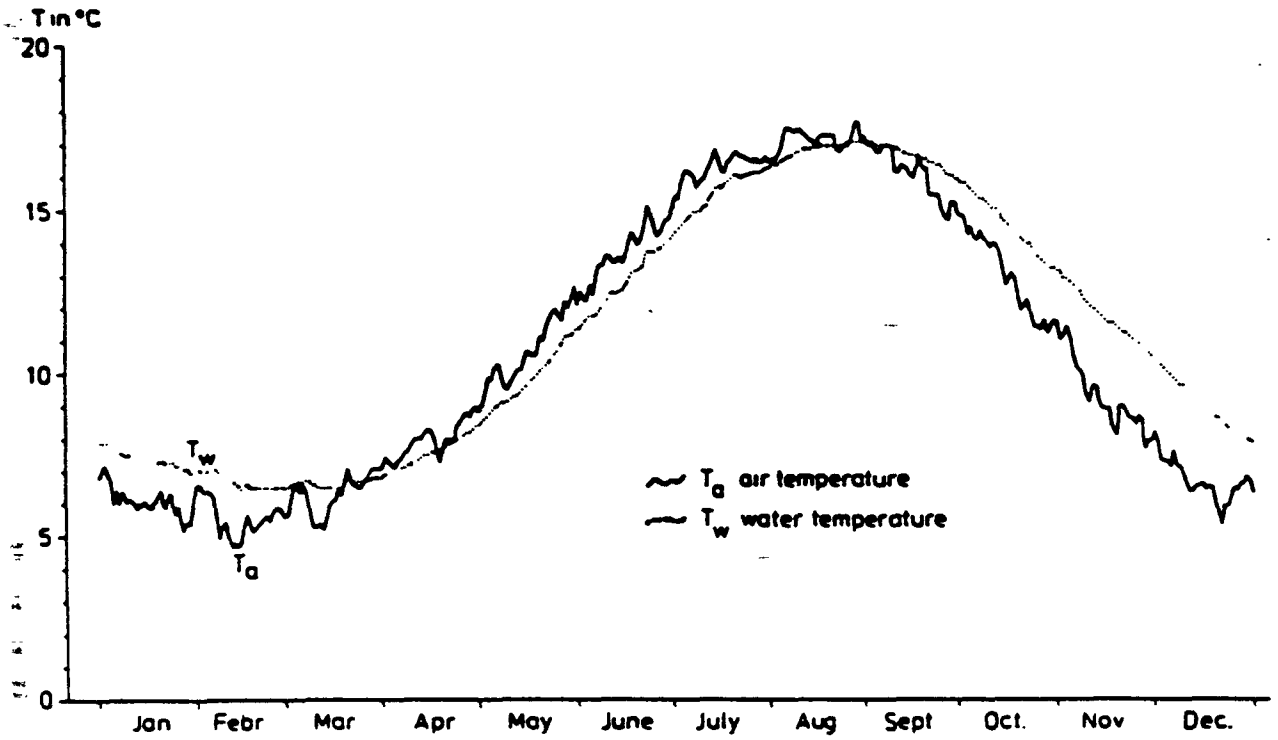


Figure 2-11. Daily average air and water temperatures measured in the North Sea (from Nieuwstadt (1977)).

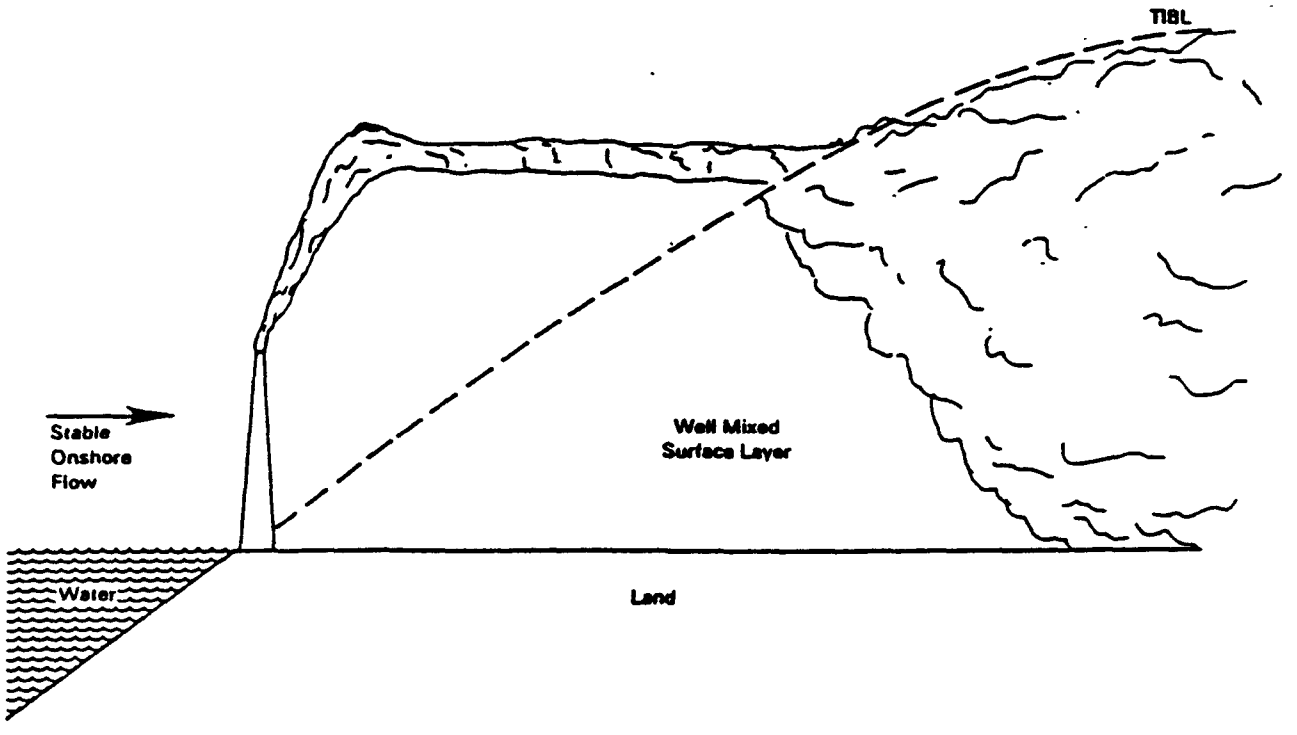


Figure 2-12. Schematic illustration of a typical coastal fumigation condition (from Hanna et al., (1985)).

2.6 Complex Terrain

The effect of terrain on ground-level concentrations is simulated in CALPUFF in three ways:

1. Adjustment of the wind field to large-scale terrain features;

2. Explicit simulation of puff-terrain interaction for distinct features too small to influence the large-scale wind field;

3. "Simplified" treatment for puff-terrain interaction with both large and small-scale features.

This allows CALPUFF to respond to the presence of terrain on two scales. Options are available in CALMET for invoking either a diagnostic or prognostic wind field model to simulate the response of the large-scale flow to the presence of terrain. The effect of terrain that extends over a scale large enough to be resolved by the grid used in CALMET will be manifest in the boundary conditions for the flow field. A puff embedded in this flow will either rise with the flow along the surface of the terrain, or it will be steered by the flow along the terrain, depending on the degree of stratification. Smaller-scale terrain features encountered by a puff in this flow can then be simulated explicitly by a separate subroutine, CTSG (COMPLEX TERRAIN ALGORITHM FOR SUB-GRID SCALE FEATURES), that embodies the methods used in the Complex Terrain Dispersion Model (CTDM). Concentration estimates on any terrain features not treated by CTSG (this is an option in CALPUFF) include simpler adjustments to the effective height of the puff above the ground that are consistent with the procedures used in ISC. As an alternative option, we have also included a more elaborate terrain adjustment which does draw on CTDM concepts, without requiring the terrain description procedures of CTSG. Section 2.6.1 provides a complete description of the CTSG module, and Section 2.6.2 describes the alternative "simple" terrain adjustment procedures.

2.6.1 COMPLEX TERRAIN ALGORITHM FOR SUB-GRID SCALE FEATURES (CTSG)

CTSG accepts the flow field produced by the flow model (both the wind and temperature structure) in the vicinity of a terrain feature as the incident flow toward that feature. It then proceeds to simulate changes in the flow and in the rate of dispersion that are induced by that terrain feature. At the core of CTSG is the modeling approach adopted in CTDM, the complex terrain model developed in EPA's Complex Terrain Model Development program. Our goal in

designing CTSG is to produce a puff algorithm that contains those elements of the CTDM approach that have the greatest impact on ground-level concentrations.

Figure 2-13 illustrates the intended role of CTSG in the CALPUFF system. In the upper panel of the figure, a cross-section of steep terrain rising with distance inland from a coast is depicted. The vertical dashed lines show the boundaries of a grid used by the wind-field model. The idealized terrain consists of a nearly uniform slope over much of the grid-square, plus a secondary feature right at the coast. At night, one might imagine a puff of material traveling down this slope in a drainage flow toward the secondary feature. The interaction of the puff with this secondary feature would be simulated by CTSG.

In the lower panel, the puff is shown as it is "seen" in the modeling system. The wind model provides the transport speed and direction for the puff, and concentrations are computed at receptors beneath the puff as if the terrain were flat. However, the secondary feature is now represented as an obstacle to the flow, and CTSG produces concentrations at receptors on this feature using methods developed for CTDM.

2.6.1.1 Modeling Regions

A central feature of CTDM adopted for use in CTSG is the dividing-streamline concept. The flow is taken to be composed of two layers. In the upper layer, the approach flow has sufficient energy to transport a fluid parcel up and over the hill against a stable potential density gradient. In the lower layer, the flow is constrained to travel around the hill. This concept was suggested by theoretical arguments of Drazin (1961) and Sheppard (1956) and was demonstrated through laboratory experiments by Riley et al. (1976), Brighton (1978), Hunt and Snyder (1980), Snyder (1980), and Snyder and Hunt (1984).

H_d, the dividing-streamline height (m), is obtained from profiles of wind speed (m/s) and temperature (as the Brunt-Vaisala frequency, N (1/s)). H_d is computed for each hill by locating the lowest height at which the kinetic energy of the approach flow just balances the potential energy attained in elevating a fluid parcel from this height to the top of the hill. The statement that defines this balance is:

$$.5\ u^2(H_d) = \int_{H_d}^{H} N^2(z)\ [H - z]\, dz \qquad (2\text{-}113)$$

where $u(H_d)$ is the wind speed at $z = H_d$, H is the elevation of the top of the hill, and N(z) is the Brunt-Vaisala frequency at height z. In practice, the value of H_d is obtained by rewriting the

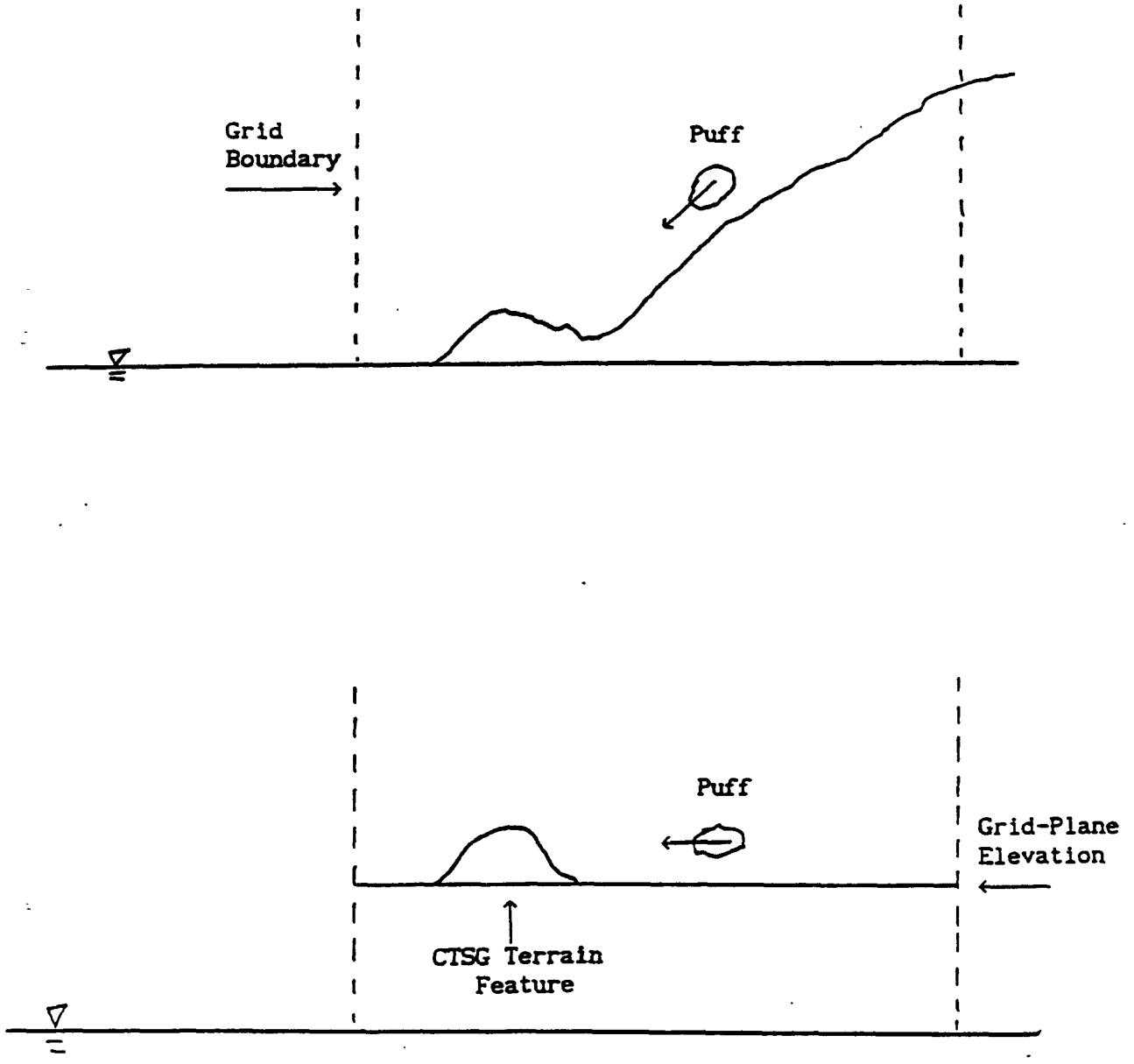


Figure 2-13. Depiction of the intended use of CTSG. The lower panel illustrates the portion of the terrain present in the upper panel that can be simulated by CTSG, and it illustrates the relationship between the gridded terrain, the modeled winds, and the CTSG terrain feature.

integral on the right-hand side (RHS) of Eqn. (2-113) as a sum over layers of constant N. For layer n,

$$RHS_n = RHS_{n+1} + \int_{z_n}^{z_{n+1}} N_n^2 (H - z)\, dz = N_1^2 (H - z_{mn}) (z_{n+1} - z_n) \qquad (2\text{-}114)$$

where z_{mn} denotes the mean height of the layer, 0.5 $(z_{n+1} + z_n)$. The layer that contains H_d is found by comparing the LHS of Eqn. (2-113) at each measurement height n with the corresponding RHS_n, starting with the layer that contains the top of the hill. If LHS_n exceeds RHS_n, then H_d must lie below z_n, and so the process is repeated until the lowest layer is found in which the LHS becomes less than the RHS (in the layer above, the LHS is greater than the RHS). This then identifies the layer that contains H_d.

H_d is then computed within this layer by assuming that the wind speed follows a linear profile. Denote this as layer j, where the elevations at the top and bottom of the layer are z_{n+1} and z_j, respectively. Denote u(z) in the layer as

$$u(z) = a_j + b_j z$$

then Eqn. (2-113) becomes

$$\frac{1}{2} (a_j + b_j H_d)^2 = N_j^2 (H - 1/2[z_{j+1} + H_d]) (z_{j+1} - H_d) + RHS_{j+1} \qquad (2\text{-}115)$$

where the last term, RHS_{j+1}, denotes the value of the RHS from z_{j+1} to the top of the hill. Eqn. (2-115) is quadratic in H_d, and is readily solved for H_d.

Once H_d is computed for a hill, the stratification length scale for the flow above H_d is computed as u_m/N_m where u_m and N_m are average values between H_d and the first model-layer above the top of the hill. This length scale characterizes the degree of stratification of the flow above H_d. Note that N_n is computed from the temperature difference across the layer.

Puff material above H_d, the dividing-streamline height, experiences an altered rate of diffusion in the deformed flow field over the hill. It is this change in the effective dispersion that leads to increased ground-level concentrations (GLC's) observed over hills when H_d is zero. When H_d is not zero, only that portion of the puff that lies above H_d as the puff encounters the hill travels over the hill. The puff is modeled as if it were sheared off at H_d so that material nearer the center of the puff may reach the surface without further dilution. The theory of

diffusion of narrow plumes embedded in a deforming flow field (Hunt and Mulhearn 1973) provides the basis for estimating GLC values in the upper layer (subroutine UPPER).

Puff material below H_d is deflected around the hill, being embedded in a horizontal two-dimensional flow. The stagnation streamline in this flow forms the boundary of the hill and therefore separates portions of the puff which travel around one side or the other. The center of the puff is able to impinge on the hillside only if the puff is centered on the stagnation streamline, and lies below H_d. Concentration estimates from subroutine LOWER are based on the analysis of Hunt et al. (1979) which indicates that the GLC near the impingement point is essentially that obtained by sampling the puff (in the absence of the hill) along the stagnation streamline at the elevation of the receptor. As the puff encounters the hill, the lateral distribution of material in the puff is separated along the stagnation streamline, and each segment is allowed to travel around the hill with complete reflection at the plane $z=0$ as well as $y=Y_d$ (stagnation streamline), i.e., the hillside. Figure 2-14 illustrates how the puff material is treated in CTSG. For the sake of illustration, the outline of a continuous series of puffs is portrayed as a plume and the height of the center of the plume exceeds H_d.

Three regions are identified in the figure. Boundaries between these three regions are defined differently in the upper and lower layers, as discussed later. For illustration, we will consider the boundaries identical, as drawn in Figure 2-14. The distinction between the upper flow and the lower flow as described above is strictly applied in region 2. Prior to this, in region 1, the portion of the puff above H_d has not reached the hill (at $z = H_d$) and so the vertical structure remains continuous. Concentrations are estimated as if receptors in this region were positioned on poles. Receptors below H_d in region 1 are placed on poles to simulate an impingement calculation. The pole height is equal to the height of the receptor above the base of the hill, and the lateral position of the pole is shifted to the location of the stagnation streamline. In essence, the flow below H_d in region 1 is turned much as it is in region 2, but no reflection from the side of the hill is included. Receptors may also be located above H_d in region 1. Figure 2-15 depicts a situation in which departures in shape between the actual terrain feature and the simplified hill used in CTSG cause ground-level receptors to be placed above H_d in region 1. In this case receptor 2 is also modeled as a receptor-on-a-pole, but the height of this pole is set to H_d, and its lateral position is the same as that of the receptor. This approach assumes that flow above H_d is deflected in the vertical, but not in the lateral direction. No alterations are made to the dispersion rates. Differences in the way receptors in region 1 are treated can be summarized as follows: the flow above H_d is considered to be terrain-following in the vertical, with no horizontal deflection, and the flow below H_d is considered to be terrain-following in the horizontal, with no vertical deflection. Note that the stagnation streamline defines the boundary that shifts the flow left or right in the horizontal. Using H_d in this way

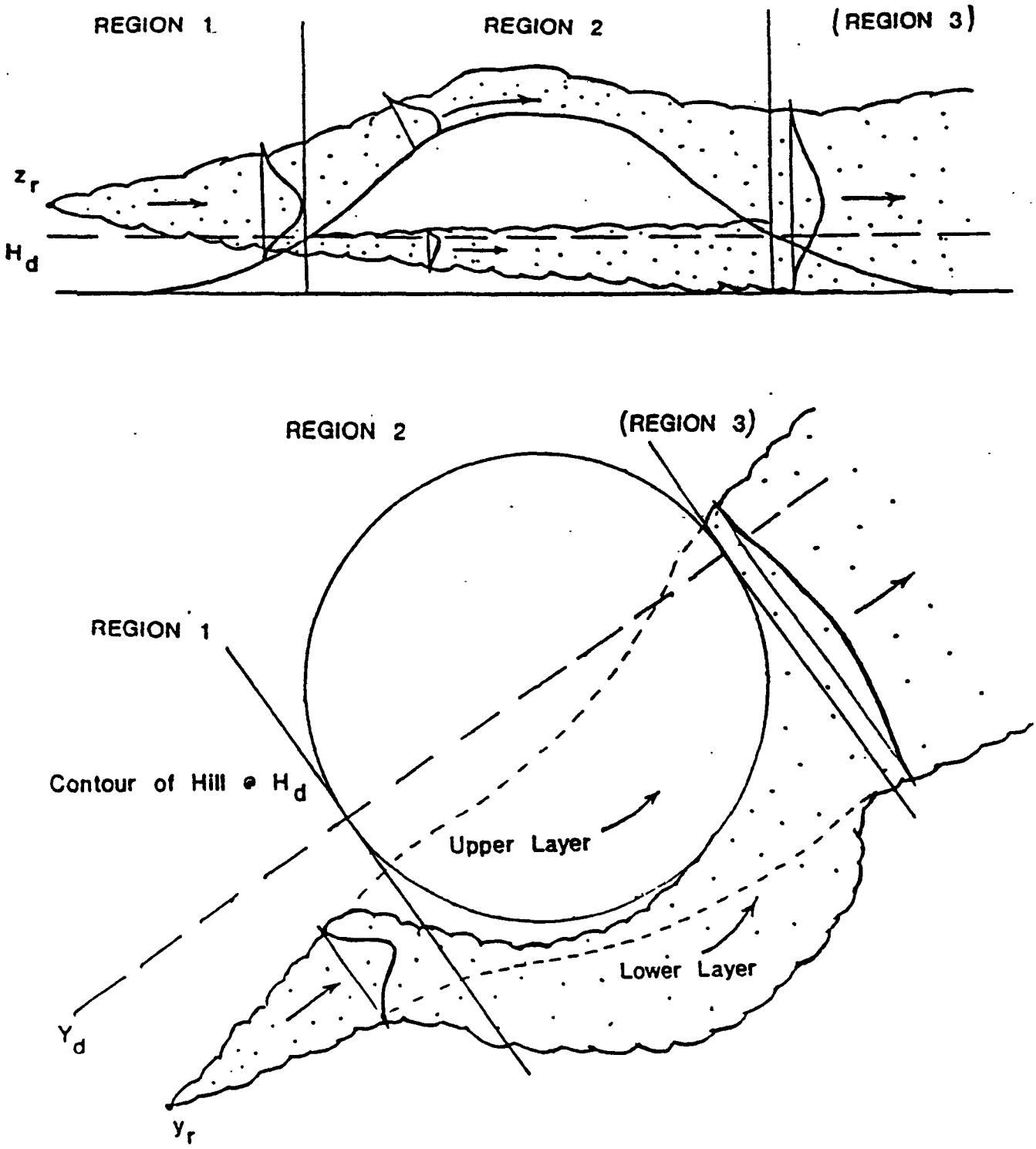


Figure 2-14. Illustration of modeling regions and partitioning of the flow above and below the dividing-streamline height H_d.

enforces a clear and sometimes abrupt distinction in the way concentrations may be obtained at nearby receptors. This can lead to discontinuities in concentrations determined at receptors that straddle H_d just upwind of the hill, when the puff is located "far" from the stagnation streamline of the flow below H_d, yet travels toward the hill in the layer above H_d. Subroutine PUFFC performs these calculations in region 1. Details of the model for regions 2 and 3 are provided in the following subsections.

The CTSG algorithm may be invoked whenever concentration estimates are needed at receptors that are located on terrain elements that are not resolved by the grid in the flow-field model. It specifies the relationship between a single puff and all receptors on a single terrain feature for the current averaging/transport time-period. Consequently, CTSG is called for each puff/terrain-element pair during each time-step. Some reduction in execution time is be gained by screening out puff/terrain-element pairs for combinations of puff size and position, relative to those of the terrain feature, that exhibit minimal terrain influence. These combinations are then modeled as if the terrain were absent.

When the "slug" representations of the cloud is employed (i.e., at times small enough that the turbulent spread at the end-points of the slug are less than the length of the slug), the puff/terrain formulation cannot be applied directly. Instead, the slug is partitioned into an equivalent series of overlapping puffs and each of these is modeled separately for the time-step.

2.6.1.2 Description of Terrain Features

CTSG uses simple analytical obstacle shapes to represent sub-grid scale terrain features. Below H_d, CTSG uses an elliptical cylinder to represent the hill. The axes and orientation of this ellipse represent the overall scale and orientation of the terrain feature at the minimum of the elevation of the puff, or H_d. Above H_d, CTSG uses a Gaussian shape to represent the hill. The height of the Gaussian hill is equal to the difference in height from the peak of the hill to H_d. The horizontal length scales and orientation of the hill are chosen so that the lateral extent of the Gaussian hill at one half its height is representative of the scale of the terrain feature half way between H_d and the top of the hill. When the major axis of the hill lies along the x-axis of the coordinate system, these shapes are defined by

$$\text{ellipse:} \quad 1 = \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right) \tag{2-116a}$$

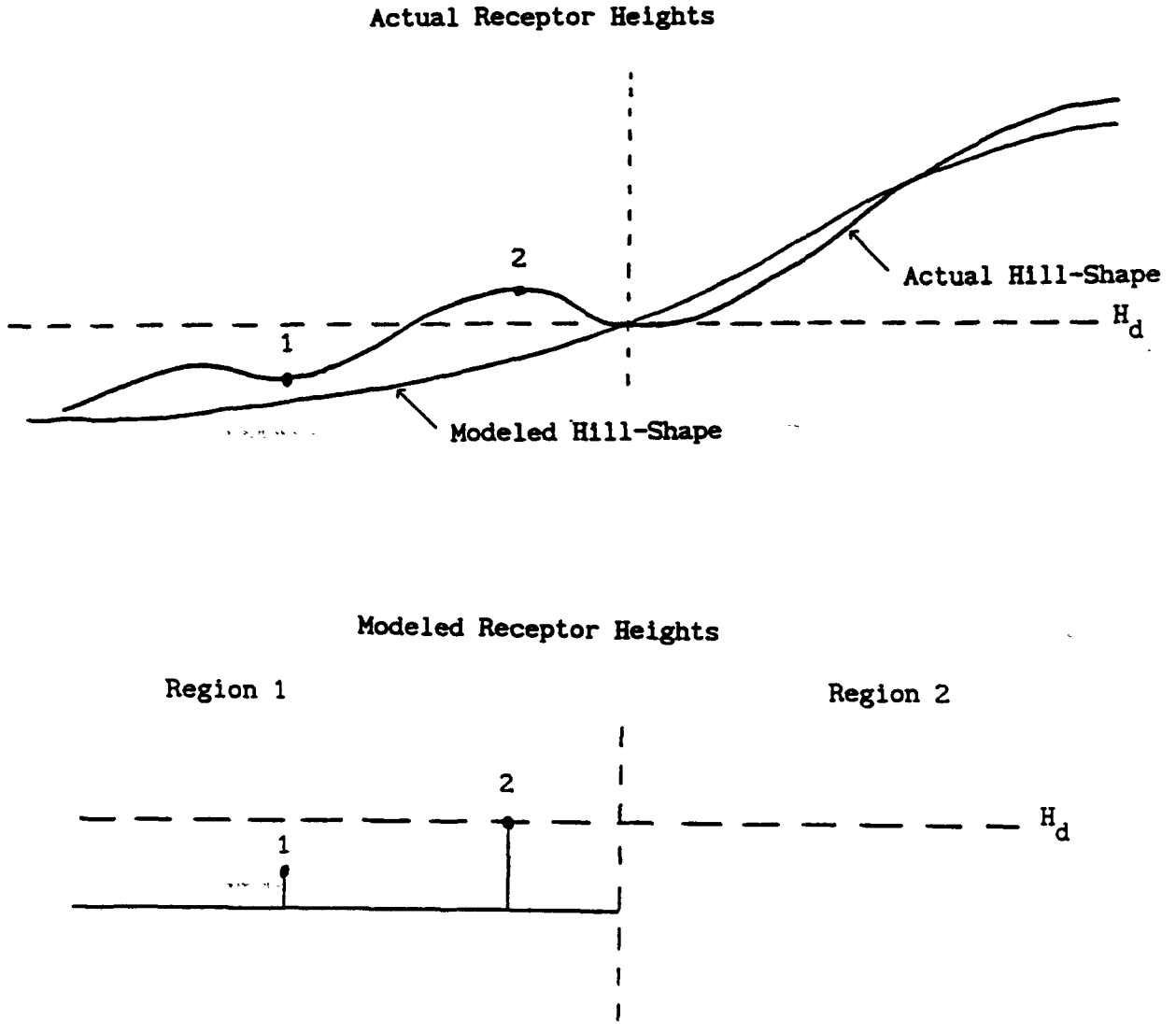


Figure 2-15. Treatment of height of receptors located upwind of the impingement point (Region 1).

$$\textit{Gaussian:} \quad h = H\, e^{-(x/L_x)^2}\, e^{-(y/L_y)^2} \tag{2-116b}$$

where (a,b) are the semi-axis lengths of the horizontal cross-section of the elliptical cylinder below H_d, and (L_x,L_y) are the Gaussian length scales along the two axes of the hill above H_d. For each puff, hill, and value of H_d, the model selects a particular elliptic cylinder and Gaussian-shaped hill.

To do this, the user must describe each terrain feature as an inverse polynomial hill (Figure 2-16). For each axis, the shape that must be fit to the height-profile of the terrain feature has the functional form:

$$ht = \text{relief}\left[\frac{1 - (|x| \,/\, axmax)^{expo}}{1 + (|x| \,/\, scale)^{expo}}\right] \tag{2-117a}$$

where "ht" is the elevation of a point on the hill above the grid-plane, "|x|" is the unsigned distance from the center of the hill to the inverse polynomial profile at the elevation "ht", "axmax" is the value of "|x|" at which "ht" equals zero (the base of the hill), "relief" is the height of the hill above the grid-plane, "scale" is the length scale of the polynomial function which is half the span of the function at one half the peak of the function, and "expo" is the power (exponent) of the function.

Given this description of the hill, CTSG solves for "x" at specific elevations "ht" along each axis of the hill to obtain the semi-axes for the elliptic cylinder and the Gaussian hill:

$$\text{axis } (ht) = \text{scale}\left[\frac{1 - ht \,/\, \text{relief}}{ht \,/\, \text{relief} + (\text{scale} \,/\, axmax)^{expo}}\right]^{1/expo} \tag{2-117b}$$

Below H_d, the height used to obtain the axes of the elliptic cylinder is the minimum of H_d and the puff height. Above H_d, the length scales are obtained halfway between H_d and the top of the hill, and the corresponding length scales for the Gaussian hill are formed by multiplying these scales by 1.20. The factor 1.20 is obtained by demanding that the Gaussian hill and the polynomial hill function have the same span at an elevation halfway between H_d and the top of the hill (Figure 2-17).

Alternatively, the user may elect to use a terrain feature description file that is identical to the one used in CTDMPLUS. The file, named "TERRAIN" (as in CTDMPLUS), provides

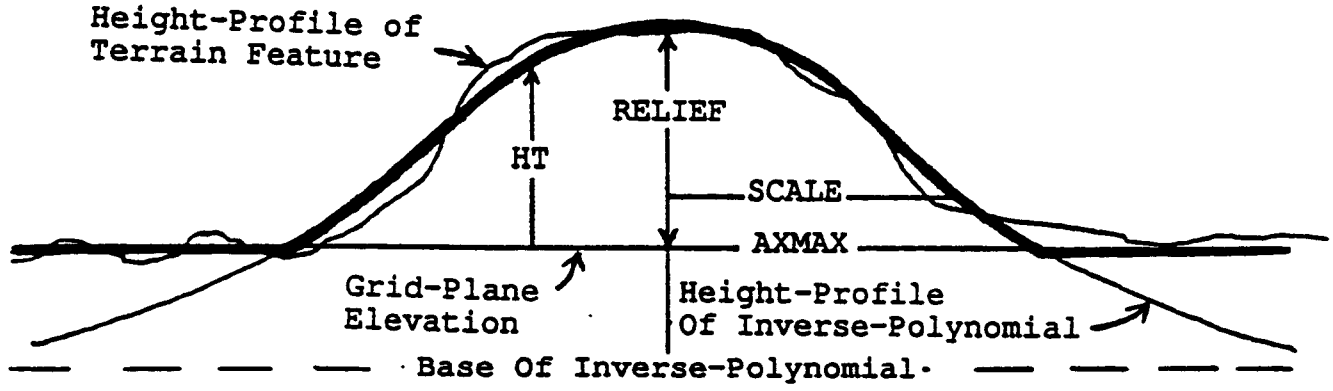


Figure 2-16. Profile of a terrain feature along one of its two axes. A best-fit inverse polynomial function describes this profile to CTSG.

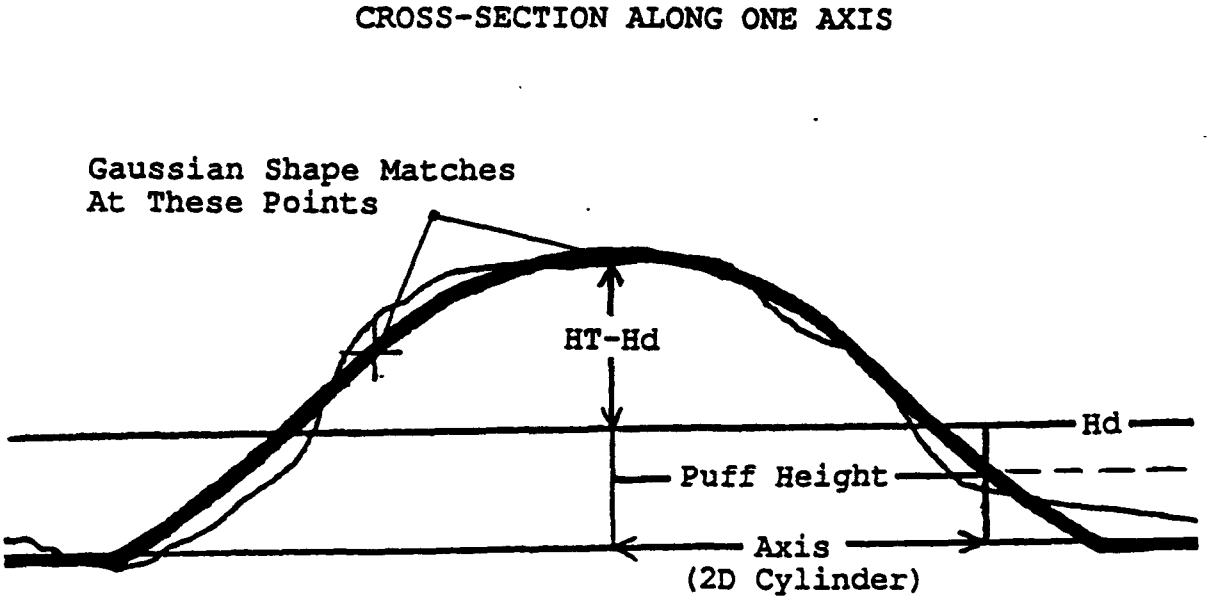


Figure 2-17. Use of hill profile function within CTSG. The model extracts the length scales for a Gaussian profile above H_d, and an elliptical cylinder below H_d.

the model with a series of parameters that define ellipses and polynomial hill profiles which have been fit to the terrain feature at a series of H_d's. With this option, CALPUFF uses the interpolation functions of CTDMPLUS to obtain the ellipse and Gaussian hill information appropriate to a specific value of H_d. An example of the format of this file can be found in Section 4.2. Anyone wishing to use this option should be familiar with the contents of the CTDMPLUS users guide (Perry et al., 1989).

2.6.1.3 Upper Layer

An estimate of the concentration (g/m_3) at a receptor at the surface of a hill in region 2, due to a plume whose initial position is (z_p,y_p), is given by

$$C(t_R y_R 0; t_o) = qF_z F_y / [2\pi u \sigma_{ze} \sigma_{ye}] \qquad (2\text{-}118)$$

where t_R is the travel-time (s) from the source to the receptor, t_o is the travel-time along the plume centerline from the source to the upwind base of the hill (if H_d is non-zero, t_o is the time to the point where the flow first encounters the hill at an elevation equal to the lesser of z_p and H_d), y_R is the cross-wind location (m) of the receptor, q is the mass flux (g/s), F_z and F_y are the vertical and horizontal distribution functions, u is the mean wind speed (m/s) at the elevation of the center of the plume, and σ_{ze} and σ_{ye} are the effective dispersion parameters (m) given by

$$\sigma_{ze}^2 = \sigma_{zo}^2 + [\sigma_{z*} / T_z]^2 \qquad \sigma_{ye}^2 = \sigma_{yo} + [\sigma_{y*} / T_y]^2 \qquad (2\text{-}119)$$

The subscript o denotes a value obtained at $t = t_o$ and the subscript * denotes

$$\sigma_{x*}^2 = \sigma_x^2(t_R) - \sigma_x^2(t_o) \qquad (for\ x = y\ or\ z) \qquad (2\text{-}120)$$

T_z and T_y are factors that contain the effects of the distortion of the flow over the hill on the rates of vertical and lateral diffusion.

In the case of a puff, the sampling function allows us to rewrite the concentration estimate for a receptor on the surface (Equation 2-118) as

$$GLC = \frac{Q}{t_2 - t_1} \frac{F_y(t_R)\, F_z(t_R)}{4\,\pi\, u\, \sigma_{ze}\, \sigma_{ye}} \left\{ erf\left(\frac{t_2 - t_R}{\sqrt{2}\ \sigma_{ye} / u} \right) - erf\left(\frac{t_1 - t_R}{\sqrt{2}\ \sigma_{ye} / u} \right) \right\} \qquad (2\text{-}121)$$

for the period t_1 to t_2 where Q is now the total mass of material (g) in the puff.

The distribution functions are given by

$$F_y = \exp\left(-.5\left[y_{Re} - y_p\right]^2 / \sigma_{ye}^2\right)$$

$$F_z = \exp\left(-.5\left[z_p - H_d\right]^2 / \sigma_{ze}^2\right) erfc\left(\sigma_z * \left[H_d - z_p\right] / \left[2T_L\, \sigma_{ze}\, \sigma_{ze}\right]\right) \qquad (2\text{-}122)$$

$$+ \exp\left(-.5\left[z_p + H_d\right]^2 / \sigma_{ze}^2\right) erfc\left(\sigma_z * \left[H_d + z_p\right] / \left[2T_L\, \sigma_{ze}\, \sigma_{ze}\right]\right)$$

F_y contains information on the deflection in the trajectory over the hill as well as information on changes in the diffusivity. The effective lateral position of the receptor relative to the centerline of the plume is altered by the deformation in streamlines over the hill, and the effective rate of growth of the plume is altered as well. Hence, an effective receptor location (y_{Re}) and an effective lateral plume size (σ_{ye}) are used to compute the horizontal distribution function. F_z also contains the change in diffusivity in the effective vertical plume size, σ_{ze}, and it includes complete reflection from the surface of the hill (marked by H_d) for only that material which lay above H_d at $t = t_o$. "Cutting" the puff at $z = H_d$ and allowing reflection from this surface gives rise to the combination of exponential and error function products in Eqn. (2-122). A full discussion of the development of these equations is contained in Strimaitis et al. (1988).

These expressions do not include the effect of an elevated inversion on the vertical distribution of the puff. When a mixing lid is present, the F_z function contains many more terms to simulate multiple reflections. The derivation of F_z with a mixing lid is an extension to the formulation found in CTDMPLUS, because the lid is not treated for the stable boundary layer, and it is explicitly included in the PDF representation of dispersion in the mixed layer. It is required in the puff implementation because puffs with a Gaussian distribution of mass in the vertical can be released below either a mechanical or convective mixing lid, a may remain Gaussian in the vertical (not well-mixed) during subsequent sampling steps.

For a mixing lid of height z_L, the vertical distribution function in a puff just upwind of the hill is given by

$$F_{zo} = \exp\left(-.5\left[z_p - z\right]^2 / \sigma_{zo}^2\right) + \exp\left(-.5\left[z_p + z\right]^2 / \sigma_{zo}^2\right)$$

$$+ \sum_i^{\infty} \left\{\exp\left(-.5\left[2iz_L - z_p - z\right]^2 / \sigma_{zo}^2\right) + \exp\left(-.5\left[2iz_L - z_p + z\right]^2 / \sigma_{zo}^2\right)\right\} \qquad (2\text{-}123)$$

$$+ \sum_i^{\infty} \left\{\exp\left(-.5\left[2iz_L - z_p - z\right]^2 / \sigma_{zo}^2\right) + \exp\left(-.5\left[2iz_L\, z_p + z\right]^2 / \sigma_{zo}^2\right)\right\}$$

Over the hill, the vertical distribution function (evaluated for a receptor at the surface of the hill--H_d) due to a point source located at a height "z" just upwind of the hill is given by

$$F_{zh} = 2\left\{\exp\left(-.5\left[z - H_d\right]^2 / \sigma_z{}^{*2} / T_z^2\right)\right.$$
$$+ \sum_{i}^{\infty} \exp\left(-.5\left[2i\left(z_L - H_d\right) - \left(z - H_d\right)\right]^2 / \sigma_{z*}^2 / T{-}z^2\right) \qquad (2\text{-}124)$$
$$\left. + \sum_{i}^{\infty} \exp\left(-.5\left[2i\left(z_L - H_d\right) + \left(z - H_d\right)\right]^2 / \sigma_{z*}^2 / T_z^2\right)\right\}$$

Therefore, the total influence of the vertical distribution of puff material just upwind of the hill on the concentration at a receptor on the surface of the hill is obtained by integrating the product of these two distributions from $z = H_d$ to $z = z_L$. The resulting F_z is given by

$$F_z = .5\left\{\sum_{i=1}^{\infty}\sum_{j=1}^{\infty} A_j B\left(E_j, E_{oi}^{+}\right) + \sum_{i=2}^{\infty}\sum_{j=1}^{\infty} A_j B\left(E_j, E_{oi}^{-}\right)\right\} \qquad (2\text{-}125)$$

where

$$A_j = MIN\,(2, j)$$
$$E_J = 2\,[j - 1]\,[z_L - H_d] \qquad (2\text{-}126)$$
$$E_{oi}^{+} = 2\,z_L\,[i - 1] + z_p \qquad E_{oi}^{-} = 2\,z_L\,[i - 1] - z_p$$

and

$$B(E,E_o) = \exp\left(-.5[E - E_o + H_d]^2/\sigma_{ze}^2\right)\left\{erf\left(K\left[\sigma_{ze}^2[z_L - H_d] - D1\right]\right) + erf(K\,D1)\right\}$$
$$+ \exp\left(-.5[E + E_o - H_d]^2/\sigma_{ze}^2\right)\left\{erf\left(K\left[\sigma_{ze}^2[z_L - H_d] - D2\right]\right) + erf(K\,D2)\right\}$$
$$+ \exp\left(-.5[E + E_o + H_d]^2/\sigma_{ze}^2\right)\left\{erf\left(K\left[\sigma_{ze}^2[z_L - H_d] + D3\right]\right) - erf(K\,D3)\right\} \qquad (2\text{-}127)$$
$$+ \exp\left(-.5[E - E_o - H_d]^2/\sigma_{ze}^2\right)\left\{erf\left(K\left[\sigma_{ze}^2[z_L - H_d] + D4\right]\right) - erf(K\,D4)\right\}$$

where

$$K = T_z/\left[\sqrt{2}\;\sigma_{ze}\;\sigma_{zo}\;\sigma_{z*}\right]$$
$$D1 = \sigma_{z*}^2\left[E_o - H_d\right]/T_z^2 + \sigma_{zo}^2\,E$$
$$D2 = \sigma_{z*}^2\left[E_o - H_d\right]/T_z^2 - \sigma_{zo}^2\,E \qquad (2\text{-}128)$$
$$D3 = \sigma_{z*}^2\left[E_o + H_d\right]/T_z^2 - \sigma_{zo}^2\,E$$
$$D4 = \sigma_{z*}^2\left[E_o + H_d\right]/T_z^2 + \sigma_{zo}^2\,E$$

Each term in the sum in Eqn. (2-125) is a product of the exponential function and error functions as in Eqn. (2-122), representing the multiple reflections at H_d and z_L. Clearly, not all of the terms in the sum are needed. The inner sum over index j represents reflections between H_d and z_L once the puff moves over the hill, whereas the outer sum over index i represents reflections between 0 and z_L before the puff reaches the hill. The algorithm that evaluates these sums continues to include greater values of the index until the fractional change in F_z is reduced to less than 1%. The distribution of material in the vertical becomes well-mixed when σ_z reaches 1.6 z_L. At this point, F_z in Eqn. (2-125) reduces to

$$F_z = \sqrt{2\pi}\sigma_z/z_L \qquad (2\text{-}129)$$

These equations take on a more familiar form when H_d is zero and when z_L is infinite. In that limit D1 = D4, D2 = D3, and inspection of the exponential factors reveals that the indices (i,j) must be equal to obtain non-zero terms. Further inspection of the error functions shows that the only non-zero term is that for i = j = 1, so that

$$F_z(H_d = 0, z_L = \infty) = 2\ \exp\left(-.5[z_p/\sigma_{ze}]^2\right) \qquad (2\text{-}130)$$

which is the form commonly used for flat terrain.

Evaluation of the F_z and F_y distribution functions requires the use of a flow model that provides streamlines for stratified flow over a hill. The effective lateral receptor location, y_{Re}, and the effective puff dimensions, σ_{ze} and σ_{ye}, depend on the properties of the flow. These properties are provided by the flow algorithm contained in CTDM. This algorithm incorporates an approximate solution to the linearized equation of motion for steady-state Boussinesq flow over a Gaussian-shaped hill. It is formulated as a "backwards-looking" solution in which the deflection of a streamline that passes through a given point over a hill is provided. Hence, the algorithm answers the question: "Where did the streamline that passes through the point (x,y,z) come from?" rather than the question: "Where does the streamline that passes through the point (x,y,z) in the flow upwind of a hill go as the flow is deflected by the presence of the hill?" As such, the relationship between the lateral position of the center of the puff in the absence of terrain-deflections (y_p), and the "original" lateral position (y_{Re}) of the streamline that passes through the receptor is directly obtained from the flow algorithm because the receptor position on the hill (x_R,y_R,z_R) is known. The description of the algorithm is contained in the CTDMPLUS user's guide (Perry et al. 1989), as modified by Strimaitis and Yamartino (1992).

Evaluation of σ_{ze} and σ_{ye} is more complicated. As indicated in Eqn. (2-119), these effective puff dimensions require the quantities σ_{z*}/T_z and σ_{y*}/T_y, which depend on the rate of puff growth in the absence of the hill and on the amount of distortion to the flow induced by the

hill. These are estimated on the basis of the theory for a narrow plume embedded in a flow with axisymmetric strain developed by Hunt and Mulhearn (1973). Their results show that the spread of material in a straining flow is approximately equal to

$$\sigma_{zd}^2(t) = \frac{1}{S_z^2(t)} \int_0^t S_z^2(t') 2K_z(t')\, dt'$$
$$\sigma_{yd}^2(t) = \frac{1}{S_y^2(t)} \int_0^t S_y^2(t') 2K_y(t')\, dt' \qquad (2\text{-}131)$$

where K_z and K_y are the diffusivities, S_z and S_y are functions of the strain in the flow, and σ_{yd} and σ_{zd} describe the size of a deformed plume. Because we assume that the strain is negligible away from the hill, Eqn. (2-131) can be rewritten as

$$\sigma_z^2(t) = \frac{1}{S_z^2(t)} \left[\sigma_{zo}^2 + \int_{t_o}^t S_z^2(t') 2K_z(t')\, dt' \right]$$
$$\sigma_y^2(t) = \frac{1}{S_y^2(t)} \left[\sigma_{yo}^2 + \int_{t_o}^t S_y^2(t') 2K_y(t')\, dt' \right] \qquad (2\text{-}132)$$

The expressions in brackets are equivalent to the quantities σ_{ze}^2 and σ_{ye}^2 defined by Eqn. (2-119), so that

$$\frac{\sigma_{z*}^2}{T_z^2} = \frac{\sigma_z^2(t) - \sigma_{zo}^2}{T_z^2} = \int_{t_o}^t S_z^2(t') 2K_z(t')\, dt'$$
$$\frac{\sigma_{y*}^2}{T_y^2} = \frac{\sigma_y^2(t) - \sigma_{yo}^2}{T_y^2} = \int_{t_o}^t S_y^2(t') 2K_y(t')\, dt' \qquad (2\text{-}133)$$

The strain functions are given by

$$S_z(t) = \exp(-Th(t)) \qquad S_y(t) = \exp(1 - Tl(t)) \qquad (2\text{-}134)$$

where Th and Tl are deformation factors. Th is the ratio of streamline spacing in the vertical in the deformed flow to that in the undistorted flow. Tl is the corresponding ratio for streamline spacing in the lateral direction (normal to the flow). The inverse of the product of these two factors at any point in the flow equals the speed up factor, Tu. These factors are computed

from the flow model contained in CTDM. The integrals in Eqn. (2-133) are evaluated numerically along the trajectory of the center of the puff. Vertical and lateral diffusivities (m^2/s) in the absence of the terrain are found from the dispersion coefficients as

$$2K(t) = d(\sigma^2)/dt \tag{2-135}$$

where σ denotes either σ_y or σ_z. The effect of the terrain on the diffusivity is assumed to be restricted to the change in the vertical turbulence over the hill. We write the dispersion coefficient as the product of the turbulence and a function of time (in the absence of terrain). Over the hill, the vertical turbulence velocity is assumed to increase with wind speed as in the "inner layer" theory, and the lateral turbulence velocity is assumed constant as in the "rapid distortion" theory (e.g., see Britter et al. (1981) for a discussion of these theories). These assumptions tend to accentuate the effect of the hill in the diffusion calculation. Substituting Eqns. (2-134) and (2-135) and augmenting the the vertical turbulence intensity by the speed-up factor Tu, the integrands of Eqn. (2-133) become

$$\begin{aligned} S_z^2\, 2K_z &= exp2(1 - Th)\, Tu^2\, \frac{d\left(\sigma_z^2\right)}{dt} \\ S_y^2\, 2K_y &= exp2(1 - Tl)\, \frac{d\left(\sigma_y^2\right)}{dt} \end{aligned} \tag{2-136}$$

Due to the computations required to obtain Th, Tl, and Tu, these factors are evaluated at no more than 25 points along the streamline that passes through the center of the puff. Linear interpolation between these points is then used in the numerical integration required to evaluate Eqn. (2-133) for each receptor. The range of points is centered at the midpoint of the intersections of the puff trajectory (without deflection) and the ellipse that marks the boundary of the portion of the hill below H_d, and cover a distance equal to one and one-half times the distance between points of intersection of the line y = 0 (the centerplane of the flow over the hill) and the ellipse. If the undeflected trajectory of the puff does not intersect the ellipse, then the distortion factors are set to unity and the hill has no effect on σ_z and σ_y. Note that the hill also has no effect on σ_z or σ_y when the growth rate of the puff is virtually zero. This is not to say that the hill has no effect on concentrations, however, because the flow distortion over the hill results in $y_{Re} \neq y_R$, and the dividing-streamline height still allows puff material at $z = H_d$ to contact the surface of the hill.

2.6.1.4 Lower Layer

The equation for estimating the concentration (g/m^3) at a receptor at the surface of a hill in region 2, due to a plume whose initial position is (z_r, y_r), is given by

$$C(t_r, Y_d, z_R, t_e) = q\, F_z\, F_y / [2\, \pi\, u\, \sigma_z\, \sigma_y] \tag{2-137}$$

where Y_d is the cross-wind location (m) of the lateral dividing-streamline which coincides with the side of the hill, z_R is the elevation of the receptor on the surface of the hill, F_z and F_y are the vertical and horizontal distribution functions, u is the mean wind speed (m/s) at the elevation of the center of the plume, and σ_z and σ_y are the dispersion parameters (m) at t_R. Note that unlike Eqn. (2-118) for the upper layer, changes to the rate of diffusion that are induced by the hill in the lower layer are considered small.

In the case of a puff, the sampling function allows us to rewrite the concentration estimate for a receptor on the surface (Eqn. (2-137)) as

$$GLC = \frac{Q}{t_2 - t_1} \frac{F_y(t_R)\, F_z(t_R)}{4\, \pi\, u\, \sigma_z\, \sigma_y} \left\{ erf\left\{\frac{t_2 - t_R}{\sqrt{2}\sigma_y/u}\right\} - erf\left(\frac{t_1 - t_R}{\sqrt{2}\sigma_y/u}\right)\right\} \tag{2-138}$$

The distribution functions are given by

$$\begin{aligned} F_y &= \exp\left(-.5[Y_d - y_p]^2 / \sigma_y^2\right) \left[1 \pm erf\left([Y_d - y_p]\, \sigma_{y*} / [\sqrt{2}\, \sigma_{yo}\, \sigma_y]\right)\right] \\ F_z &= .5 \exp\left(-.5[z_p - z_R]^2 / \sigma_z^2\right) [erf([b1 - b2 - b3]*K) + erf([b1 + b2 + b3]*K)] \\ &\quad + .5 \exp\left(-.5[z_p + z_R]^2 / \sigma_z^2\right) [erf([b1 - b2 + b3]*K) + erf([b1 + b2 - b3]*K)] \end{aligned} \tag{2-139}$$

where

$$\begin{aligned} K &= \frac{1}{\sqrt{2}\, \sigma_z\, \sigma_{zo}\, \sigma_{z*}} & b1 &= H_d\, \sigma_z^2 \\ b2 &= z_R\, \sigma_{zo}^2 & b3 &= z_p\, \sigma_{z*}^2 \end{aligned} \tag{2-140}$$

The notation is the same as that in section 2.6.1.3. The only new quantity introduced in these equations is Y_d, the lateral position of the stagnation streamline upwind of any flow distortion. As in CTDM, it is found by solving for the two-dimensional streamline pattern about an ellipse.

F_y contains information about the amount of material on each side of the hill and about how the puff is sampled in the lateral direction. The lateral offset is the distance from the centerline to Y_d, reflecting the notion that all receptors lie along the side of a hill, coincident with the lateral dividing-streamline position. Furthermore, material may be split on either side, and complete reflection of material is allowed along this surface, giving rise to the form of the product of the exponential and error functions in Eqn. (2-139). Note that the sign of the error function (taking the sign of its argument into account) is positive when both the receptor and the trajectory of the center of the puff lie on the same side of Y_d. If all of the material were to reside on one side of Y_d at t_o, then F_y would equal either 2 or 0, depending on whether the receptor were on the same side or on the other side of Y_d as the puff.

F_z contains information about the amount of material below H_d at t_o, and about how this material is sampled in the vertical. The form is a product of an exponential function and error functions in which the sampling height z_R is most evident in the exponential function, and the effects of splitting the plume at H_d are contained in the error functions. A full discussion of the development of these equations is contained in Strimaitis et al. (1988).

These expressions do not include the effect of an elevated inversion on the vertical distribution of the puff. When a mixing lid is present, the F_z function contains many more terms to simulate multiple reflections and the result is similar to that discussed in 2.6.1.3:

$$F_z = .5\left\{\sum_{i=1}^{\infty}\sum_{j=1}^{\infty} B\left(E_j^+, E_{oi}^+\right) + \sum_{i=1}^{\infty}\sum_{j=2}^{\infty} B\left(E_j^-, E_{oi}^+\right) + \sum_{i=2}^{\infty}\sum_{j=1}^{\infty} B\left(E_j^+, E_{oi}^-\right) + \sum_{i=2}^{\infty}\sum_{j=2}^{\infty} B\left(E_j^-, E_{oi}^-\right)\right\} \quad (2\text{-}141)$$

where

$$\begin{aligned} E_j^+ &= 2(j-1)z_L + z_R \\ E_j^- &= 2(j-1)z_L - z_R \\ E_{oi}^+ &= 2(i-1)z_L + z_p \\ E_{oi}^- &= 2(i-1)z_L - z_p \end{aligned} \quad (2\text{-}142)$$

and

$$B(E,E_o) = \exp\left(-.5[E_o - E]^2 / \sigma_z^2\right)\{erf(K[b1 - b2 - b3]) + erf(K[b1 + b2 + b3])\}$$
$$+ \exp\left(-.5[E_o + E]^2 / \sigma_z^2\right)\{erf(K[b1 + b2 - b3]) + erf(K[b1 - b2 + b3])\} \quad (2\text{-}143)$$

where

$$K = \frac{1}{\sqrt{2}\ \sigma_z\ \sigma_{zw}\ \sigma_{z*}} \qquad b1 = H_d\ \sigma_z^2$$
$$b2 = E\ \sigma_{zw}^2 \qquad b3 = E_o\ \sigma_{z*}^2 \quad (2\text{-}144)$$

The form of the "B-function" is identical to F_z (Eqn. (2-139)) for the case of no limit to vertical mixing. Differences arise in the use of (E,E_o) rather than (z_R,z_p), so that the presence of the mixing lid is manifest in Eqn. (2-142).

The outer sum over the index i accounts for reflections between the mixing lid and the surface before the puff reaches the hill. The inner sum over the index j accounts for reflections that may occur as material diffuses above H_d when the puff passes the hill. The inner summation will generally produce non-zero terms only for j = 1, unless a mixing height only slightly greater than H_d is found. This circumstance may not occur at all, given the definition of H_d and z_L. In evaluating the sums, terms are included for greater values of each index until the fractional change in F_z is reduced to less than 1%. The distribution of material in the vertical becomes well-mixed when σ_z reaches 1.6 z_L. At this point, F_z in Eqn. (2-138) reduces to

$$F_z = \sqrt{2\pi}\ \sigma_z / z_L \quad (2\text{-}145)$$

2.6.1.5 Operational Characteristics

The best way to illustrate the behavior of CTSG is to present concentrations obtained for a specific application, and to compare these with what would have been obtained if the terrain feature had been ignored. We take this approach in this section by simulating ground-level concentration patterns at receptors on a hill for the situation in which a single puff moves across the hill along a curved trajectory.

The hill chosen for this exercise is twice as long as it is wide, with its major dimension oriented north-south. The relief height of the hill is set to 100 m, and its dimensions at its base

are 2264 m by 1132 m. The polynomial function describing its shape is characterized by the following parameters:

relief (m)	100
expo (1,2)	2, 2
scale (1,2) (m)	800, 400
axmax (1,2) (m)	1132, 566
xc, yc (m)	0, 0
thetah (deg)	0
zgrid (m)	25

Note that (xc,yc) are the coordinates of the center of the hill, thetah is the angle (CW) from north to the major axis of the hill, and zgrid is the elevation of the grid-plane above sea level.

The incident flow for this hill consists of a height-profile in which wind speeds are constant at 1.5 m/s, and the temperature gradient is constant with a Brunt-Vaisala frequency of 0.0167 s^{-1}. For the 100 m tall hill, this profile produces a dividing-streamline height of 10.18 m. The mixing height is set at 2000 m.

For this demonstration, the following formulas were used to specify the dispersion parameters:

$$\sigma_z = \sqrt{\sigma_{zi}^2 + (i_z t \mathcal{F}_z)^2}$$

$$\mathcal{F}_z = 1/(1 + .945(t/100)^{.806})$$

where σ_{zi} = 5 m and i_z = 0.1; and

$$\sigma_y = \sqrt{\sigma_{yi}^2 + (i_y t \mathcal{F}_y)^2}$$

$$\mathcal{F}_y = 1/(1 + .9\sqrt{t/1200})$$

where σ_{yi} = 50 m and i_y = 0.25.

These equations result in a puff size that produces significant concentrations on the ground in the absence of the hill, since the puff height is set at 45 m (MSL), or 20 m above the local grid elevation. Hence, the center of the puff is approximately 10 m above H_d for this demonstration.

The puff initially lies to the southwest of the hill. Its movement is tracked in timesteps of 5 minutes, so that it takes several timesteps to move across the hill. The wind direction shifts by 10 degrees each time-step, from an initial direction of 270 degrees. The puff contains 600 g of material.

The 1-hour average "foot-print" of concentrations produced by the movement of this puff is shown in Figure 2-18. The left panel illustrates simulated concentrations in the absence of the hill, and the right panel illustrates concentrations simulated by CTSG when terrain is present. The base of the hill function is outlined as an ellipse in each of these panels. Major features of CTSG are immediately apparent in these concentration patterns. Peak concentrations over the crest of the hill are larger by almost a factor of two, and puff material below H_d travels around the hill on either side. Note that some detail in the contours arises from discrete receptor locations. Even though 325 receptors were used (one at each intersection of the 100 m tic-marks), there is not enough coverage to produce smooth contours everywhere.

The "foot-prints" of the puff during each of the time-steps in which the puff was over the hill are shown in Figures 2-19 (a-f) corresponding to time-steps 3 through 8. These figures illustrate how CTSG partitions the puff during each step according to the relative position of the center of the puff, the dividing streamline height (H_d), and the position of the stagnation streamline. It is important to note that this partition does not increase the number of puffs in the model. Although the distribution becomes fragmented in the mathematics, all information remains referenced to a circular puff of a prescribed size. When a variable such as the flow direction changes between steps as it does in this example, the concentrations are obtained as if the current properties of the flow existed for all time, and the puff is partitioned according to those properties. Hence, the stagnation streamline in this demonstration differs from one step to another, and so the separation distance between the trajectory of the center of the puff and the stagnation streamline also differs from one step to another.

2.6.2 "Simple" Terrain Adjustments

Terrain adjustments other than those provided by the wind field model and the CTSG subroutine are needed in CALPUFF. Because CALPUFF is designed to emulate ISC in the limit of steady winds and a constant emission rate, it must also contain the terrain treatment used in ISC. This is described in Section 2.6.2.1. Furthermore, general applications typically involve terrain variations on many spatial scales which are impractical to address with CTSG. The wind field transports a puff along the surface of the terrain, but never causes its height above the surface to change. Hence, puffs in the flow may be channeled or deflected by the terrain, but they do not "impinge" or otherwise strongly interact with the terrain without a

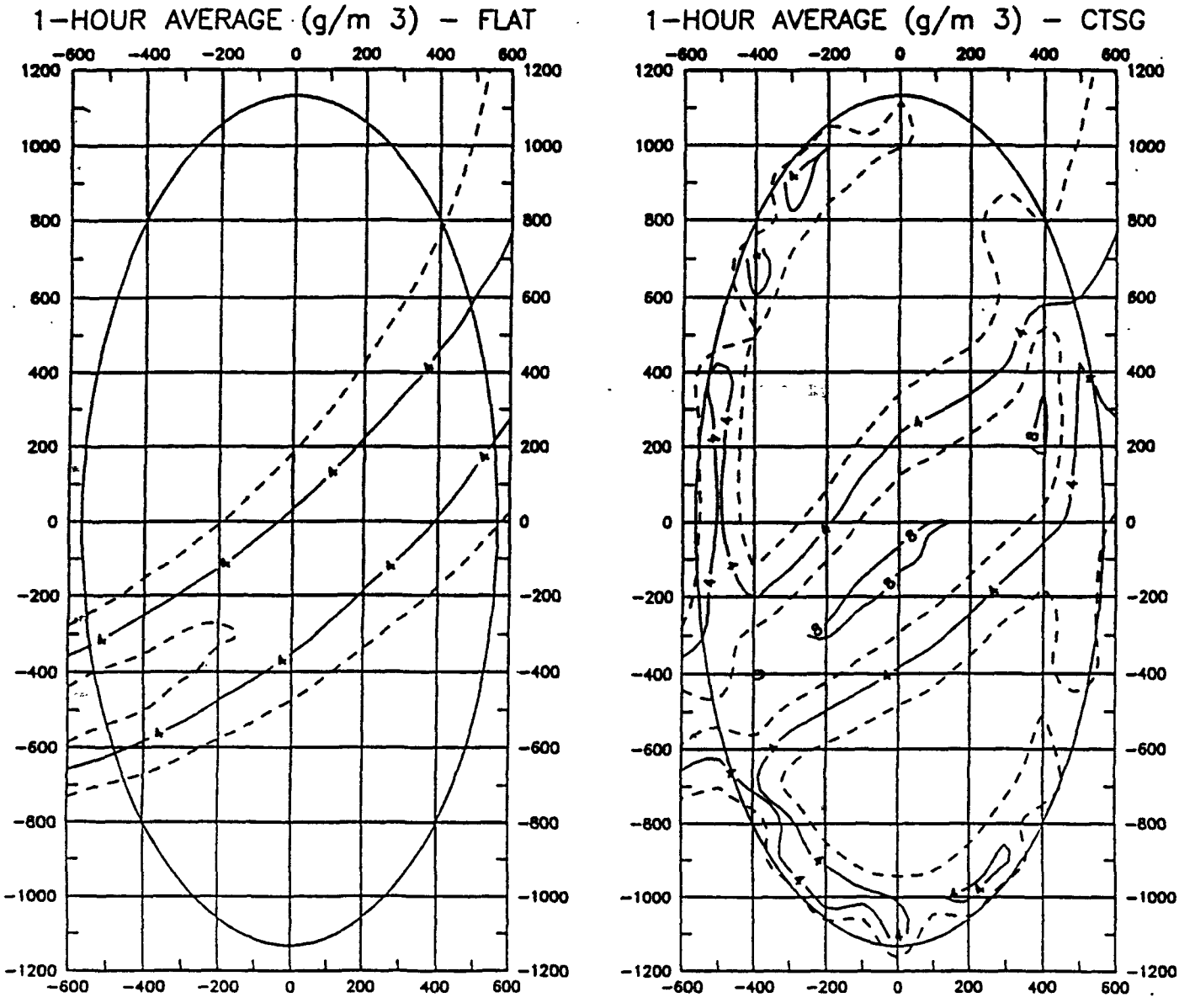


Figure 2-18. Concentrations (g/m^3) produced by CTSG (both with and without the hill), averaged over a period of one hour. The single puff that was simulated traveled over the hill in approximately 25 minutes during the hour.
(Contour interval = 2 g/m^3; grid units = m).

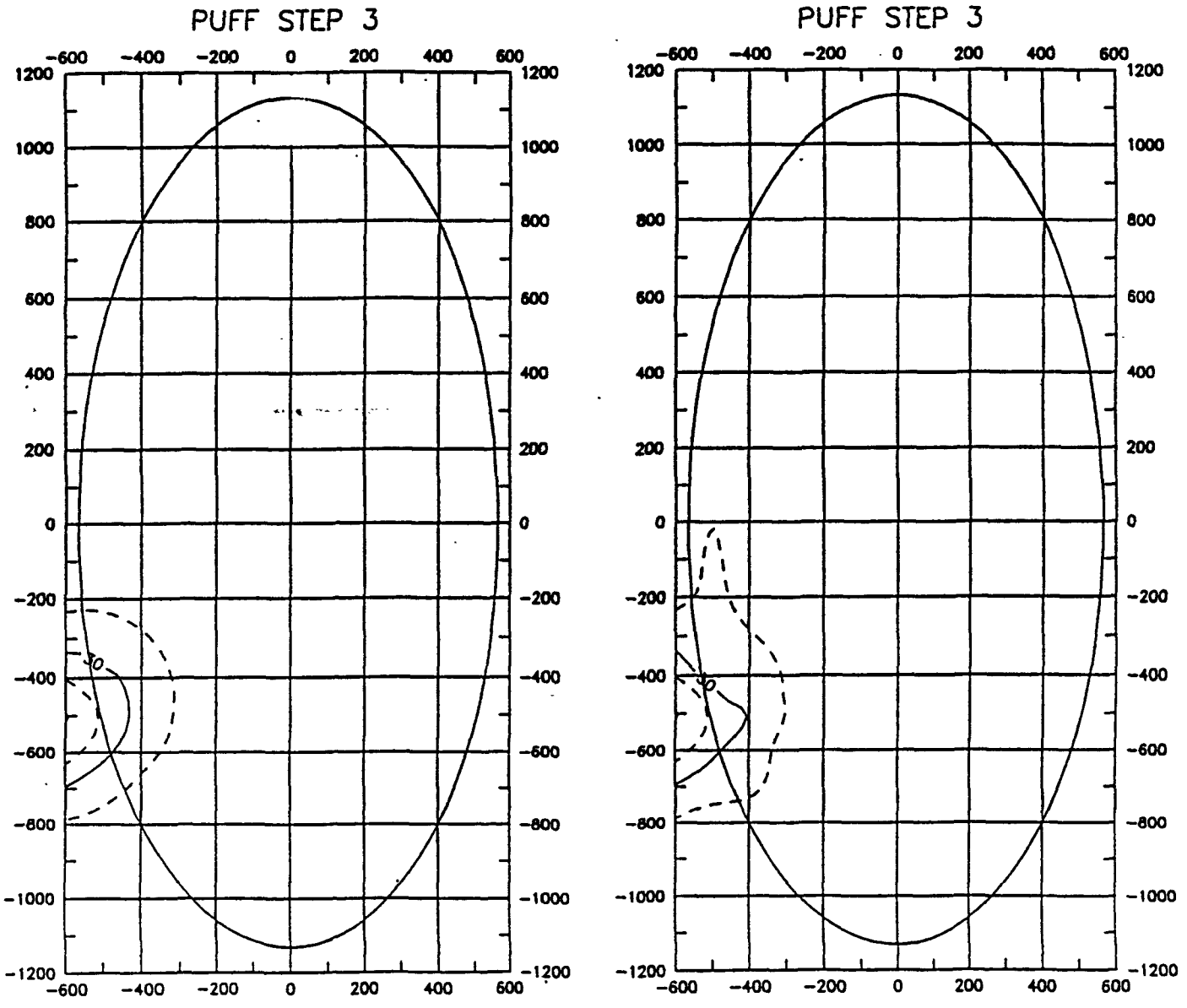


Figure 2-19a. Concentrations (g/m^3) produced by CTSG (both with and without the hill) during 5-minute time-step number 3.
(Contour interval = 20 g/m^3; grid units = m).

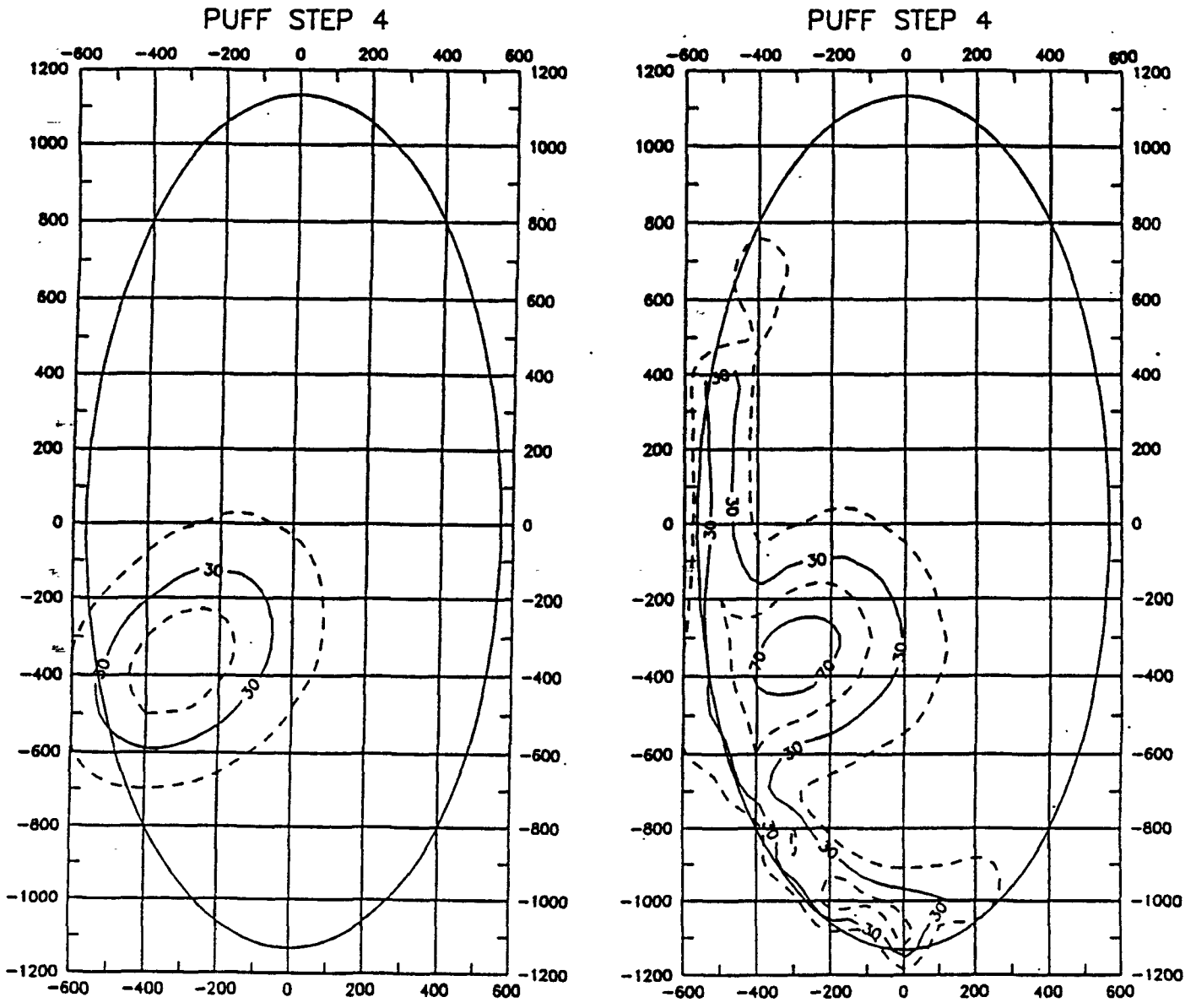


Figure 2-19b. Concentrations (g/m^3) produced by CTSG (both with and without the hill) during 5-minute time-step number 4.
(Contour interval = 20 g/m^3; grid units = m).

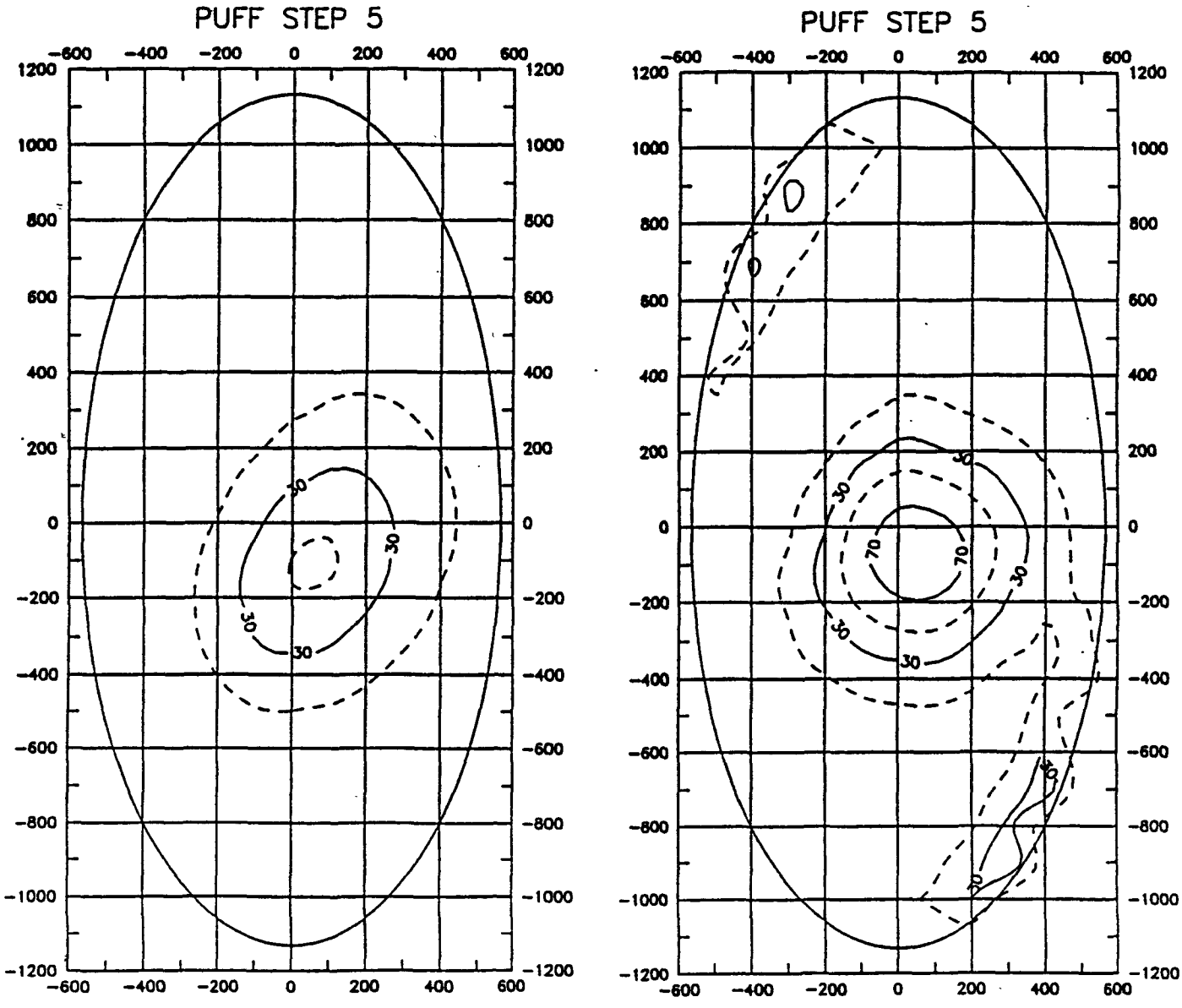


Figure 2-19c. Concentrations (g/m^3) produced by CTSG (both with and without the hill) during 5-minute time-step number 5.
(Contour interval = 20 g/m^3; grid units = m).

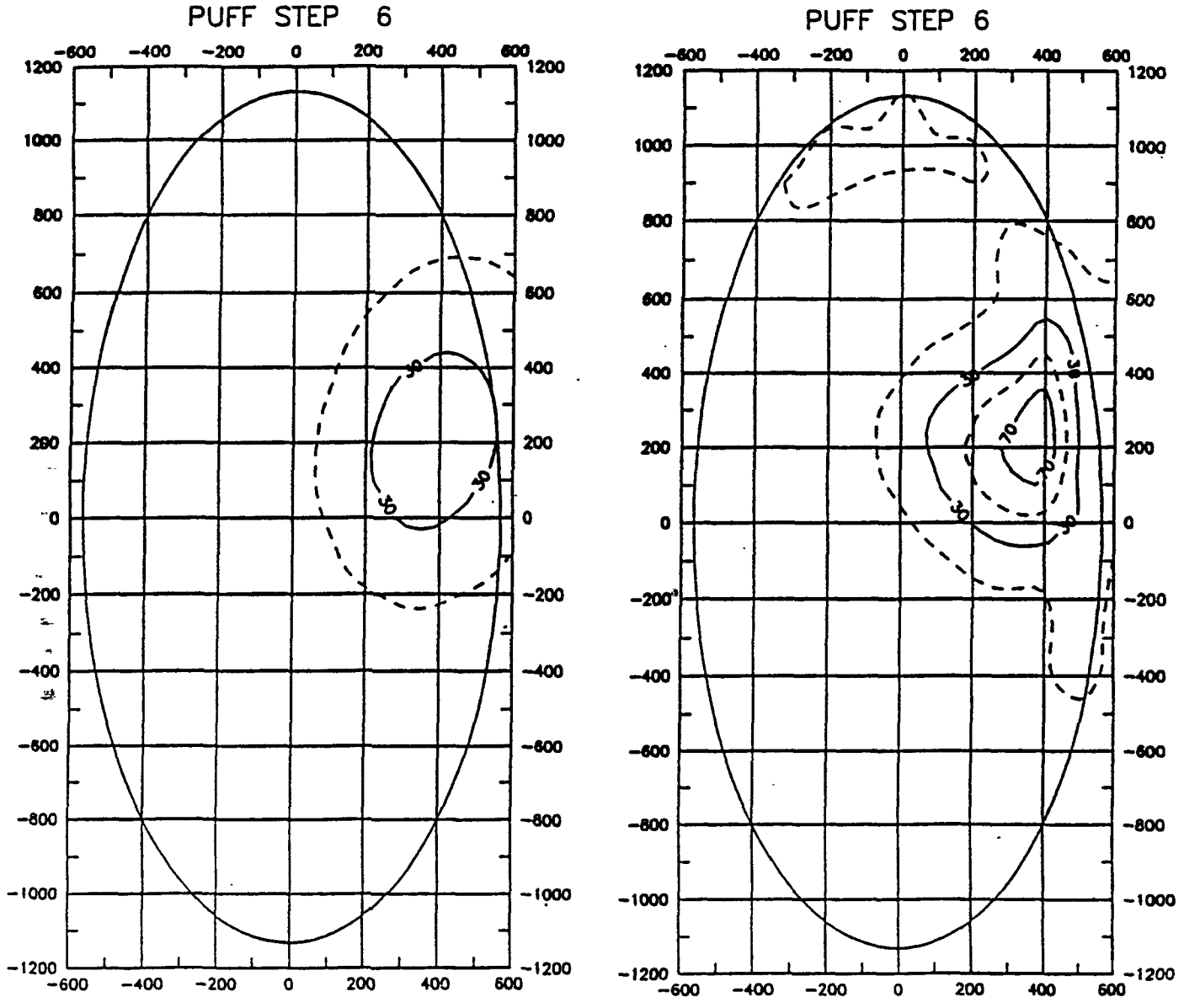


Figure 2-19d. Concentrations (g/m^3) produced by CTSG (both with and without the hill) during 5-minute time-step number 6.
(Contour interval = 20 g/m^3; grid units = m).

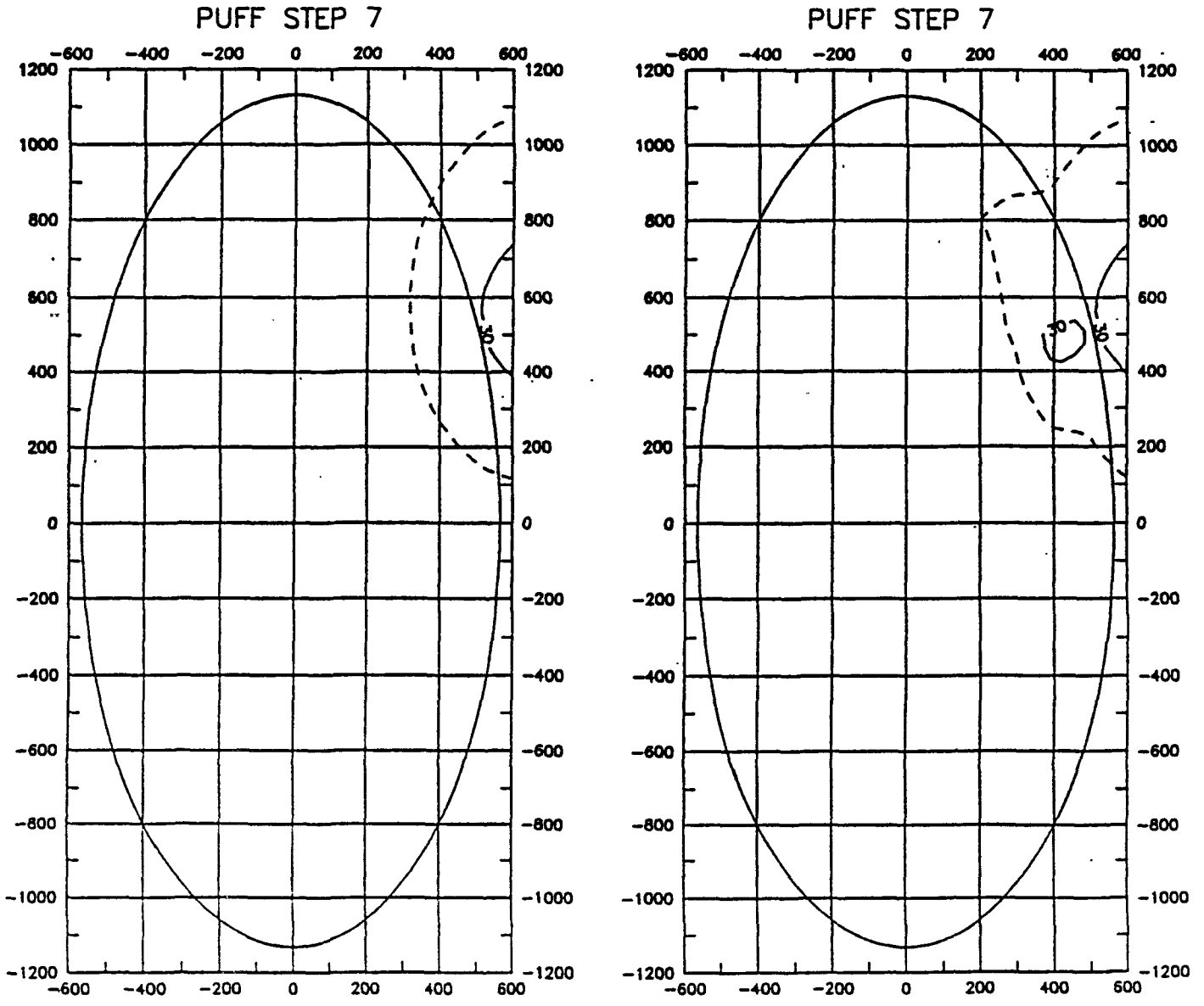


Figure 2-19e. Concentrations (g/m^3) produced by CTSG (both with and without the hill) during 5-minute time-step number 7.
(Contour interval = 20 g/m^3; grid units = m).

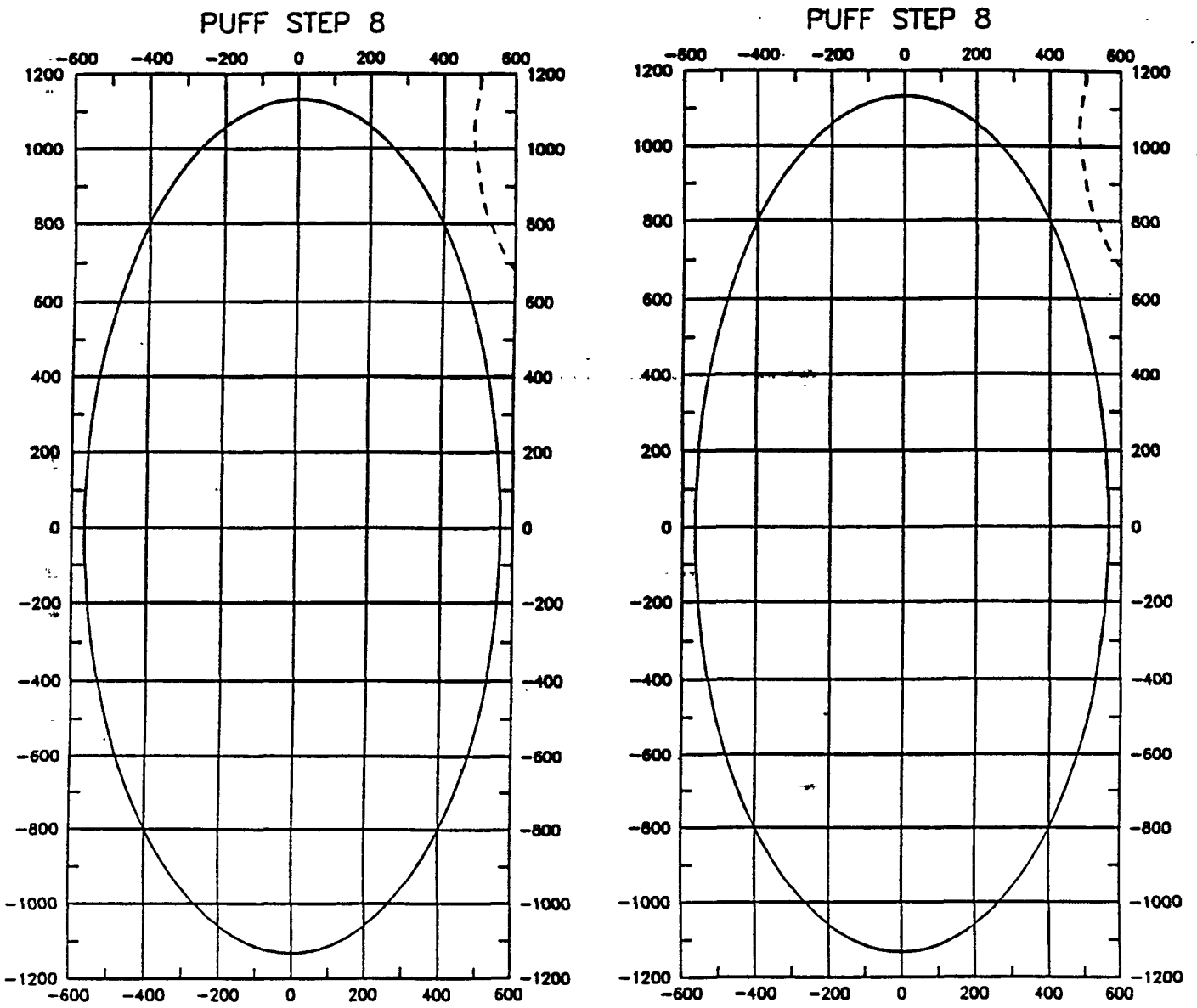


Figure 2-19f. Concentrations (g/m^3) produced by CTSG (both with and without the hill) during 5-minute time-step number 8.
(Contour interval = 20 g/m^3; grid units = m).

simple terrain treatment.

A simple terrain adjustment such as the plume path correction factor (e.g., the half-height adjustment found in plume models such as COMPLEX I) could be used for such general terrain, but this technique has several drawbacks. A new treatment has been developed that avoids such drawbacks. It is derived from concepts that lie behind the basic CTSG treatment, but employs sufficient simplifications that it is readily applied to any array of terrain. We review simple terrain adjustments that are used in other models, and identify drawbacks that are particularly troubling in the context of a puff model, in Section 2.6.2.2; and we develop the rationale for a new "simple" treatment that is based on the same theory used in CTSG in Section 2.6.2.3.

2.6.2.1 ISC Terrain Treatment

ISC is not intended for use in situations in which receptors are placed on terrain that exceeds the height of the "stack". Any receptors that are found above this height are lowered to a height that is 0.005 m below the height of the stack. This is done hourly for each source in the simulation, and is therefore source-specific. The mixing height is not adjusted for the presence of any terrain feature, and the result of any downwash calculations does not modify the stack height used to determine the height of the receptor. Once the receptor height is determined, the vertical distribution factor contains the difference in elevation between the centerline of the plume and the receptor. In effect, the centerline of the plume is lowered by an amount equal to the modified elevation of the receptor above the base of the stack.

This treatment has been implemented in CALPUFF, but the dependence of the effective puff height above a receptor on the elevation at which puffs are initially released (prior to any buoyant rise) can lead to troubling inconsistencies. If two sources with different stack heights are being modeled, consider a situation in which plume rise differs for the two in such a way that the puffs reach identical elevations. Why should the difference in elevation between the puff and a receptor depend upon the stack heights? We believe that they should be treated alike in this regard, so we have sought alternate formulations.

2.6.2.2 Simple Terrain Adjustments in Existing Complex Terrain Plume Models

COMPLEX I/II

COMPLEX I is a screening model for use in complex terrain. It differs from COMPLEX II only in its use of 22.5° sector-averaging rather than the traditional Gaussian

lateral distribution function. Within the context of puff-modeling, we are only interested in the treatment of the vertical distribution, which is the same in both variants, so we shall refer to the models as one -- named COMPLEX. COMPLEX employs the partial height correction method to simulate the effect of terrain. The height of the plume at a receptor depends on the height of the plume over level terrain (which is taken to be the height of the plume above the elevation at the base of the stack from which the plume was released), the receptor height (above the base of the stack), and the plume path coefficient (which depends on the stability class). Values for the plume path coefficient are typically C=0.0 for stable (classes E and F), and C=0.5 for the rest (classes A, B, C, and D). The "half-height" correction model is equivalent to C=0.5.

Let H_s be the elevation of the base of the stack above sea level, and H_r be the elevation of the receptor above sea level. Furthermore, let ΔH_s be the height of the plume at the source, and ΔH_r be the height of the plume at the receptor. If the elevation of the receptor exceeds the elevation of the centerline of the plume at the source,

$$\Delta H_r = \Delta H_s * C \qquad (2\text{-}146)$$

If the elevation of the receptor lies below the centerline of the plume at the source,

$$\Delta H_r = \Delta H_s - (H_r - H_s)*(1 - C) \qquad (2\text{-}147)$$

In either case, ΔH_r is not allowed to be less than some minimum value, which is typically set at 10 m. Note that $H_r \geq H_s$ is assumed in the above equation, so that the terrain-following plume result is obtained (C = 1) if the terrain on which the receptor sits lies below the elevation of the base of the stack. The mixing height is not altered unless C = 0.0, in which case the mixing height is reset to 5000 m to simulate unlimited mixing.

When C = 0.0, the full difference between the plume height and the receptor height is obtained, subject to the specified minimum. This gives the appearance of keeping the plume level, and is therefore known as the level-plume treatment. It also results in sending the plume over all terrain greater than plume height, which is not consistent with the behavior of plumes in stably-stratified flows. Therefore, the "400 m correction" factor originally used in the Valley model is applied. This factor varies linearly from 1.0 at the plume centerline height to 0.0 at 400 m above the plume centerline height.

Application of the partial height correction to receptors that lie below the height of the plume centerline is illustrated in Figure 2-20 which depicts the situation for C = 0.5. Panel A shows the relationship between the initial plume height and five receptors located on a single

hill. Panel B shows how the model treats receptors 1 and 5 which are located at the base of the hill, panel C shows how the model treats receptors 2 and 4 which are located halfway up the hill, and panel D shows how the model treats receptor 3 which is located at the top of the hill. The central feature seen in the figure is that a different plume height is used for each receptor elevation, and concentrations are estimated as if the terrain were flat for each plume. That is, the entire "history" of reflection of plume material from both the ground and the mixing lid (if present) differs for receptors located at different heights. The partial height correction treatment is not a unified, local adjustment, as is sometimes assumed.

In addition to the treatment of reflection, the basic notion of "plume height over level terrain" poses a real problem for modeling puffs. When sources are distributed throughout a modeling region of complex terrain, the elevation at the base of each stack can vary considerably. Suppose puffs from two stacks reach the same height above ground after buoyant rise, and suppose that they both are of identical size when they reach a receptor or high terrain. Should both puffs contribute equally to the concentration at that receptor? Eqn. (2-147) indicates that the terrain adjustment for each puff could be different, as H_r, the height of the receptor above the base of the stack, depends on the elevation of the terrain at the location of the stack. Qualitatively, we see that the receptor would appear "higher" to one source location than the other, and so some difference in the effect of terrain on each puff might appear reasonable. But if we take the height-adjustment seriously, these two puffs should not be treated differently at the receptor, since they coincide (after terrain adjustment) at some points upwind of the terrain.

All puffs might be treated similarly at receptors on elevated terrain if H_r were defined relative to a base-plane elevation, rather than stack-base elevation. This would require terrain adjustments at the sources as well as at receptors. In effect, streamlines would be defined on the basis of the height-correction rules and plumes or puffs would follow streamlines. But there are two problems with this approach: (1) a base-plane elevation will not be obvious in many applications; and (2) terrain adjustments to streamlines of the type listed in Eqn. (2-146) reduce to a single height, which would lead to some plumes following a streamline that remains a fixed height above the surface as it travels across higher elevations. The latter situation would produce a "flat terrain" calculation for all receptors located at such higher elevations.

RTDM

RTDM adds several features to the partial height correction treatment described above, including a reflection coefficient, the concept of the critical dividing-streamline height, and alterations to the mixing height. The reflection coefficient seeks to present a more unified

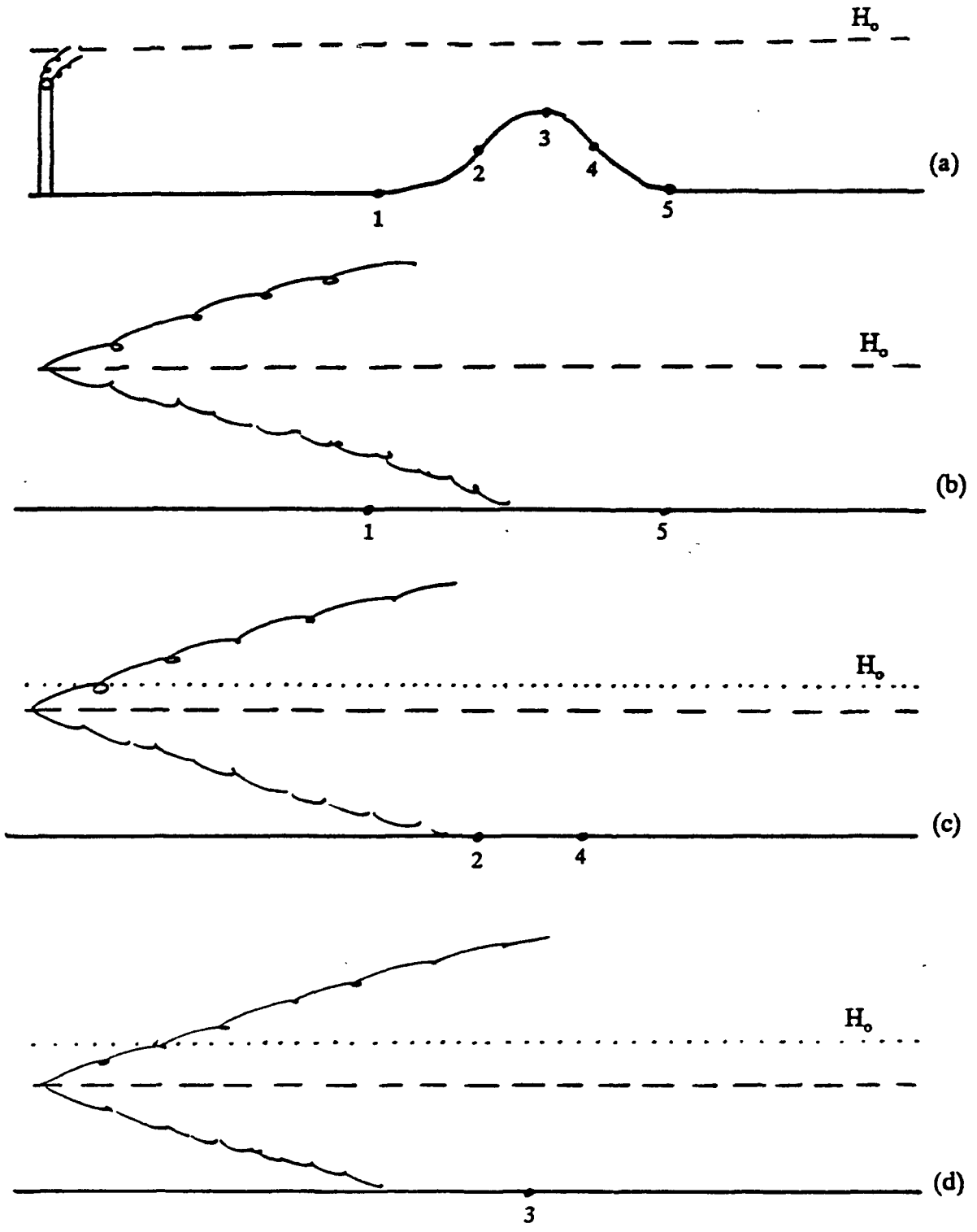


Figure 2-20. Partial height correction method used in COMPLEX for non-stable periods in which receptors lie below the centerline of the plume. (C = 0.5)

treatment of receptors located on the same feature by adding the restriction that peak crosswind-integrated concentrations not increase with distance from the source. Such an increase can be produced in a model if the effective plume height is reduced rapidly in going from one receptor to the next (from receptor 2 to 3 in Figure 2-20, for example) because of the change in the history of the reflection from the lower boundary.

The critical dividing-streamline (H_d) is used to separate the flow into two layers when it is stably-stratified. Plumes below H_d are modeled with a plume path coefficient C = 0.0, while those above are modeled with C = 0.5. Equations similar to those in COMPLEX for the adjusted plume height are revised by subtracting H_d from the plume and receptor elevations. If the elevation of the receptor exceeds the elevation of the centerline of the plume, the effective plume height (ΔH_r) becomes:

$$\Delta H_r = (\Delta H_s - H_d + H_s) * C \qquad (2\text{-}148)$$

If the elevation of the receptor lies below the centerline of the plume,

$$\Delta H_r = (\Delta H_s - H_d + H_s) - (H_r - H_d) * (1 - C) \qquad (2\text{-}149)$$

Furthermore, C = 0.0 if the receptor lies below H_d. There is no minimum limit to the size of ΔH_r so that the plume becomes a ground-level release for receptors located at or above the elevation of the plume. The mixing height above the ground (ΔH_m) is adjusted in exactly the same way, so that ΔH_s and ΔH_r in the equations above are replaced by ΔH_m and ΔH_{mr}.

This use of H_d results in the use of the level plume treatment only when H_d is non-zero. Otherwise, a value of C = 0.5 is used. Furthermore, plumes above H_d treat H_d as the lower surface for reflection when receptors lie at the same elevation as H_d, and the partial height correction for higher receptors is based on heights above H_d, so that the adjustments are effectively more severe than the standard half-height (C = 0.5) correction.

Because of its reliance on the base of each stack (independently) to define the terrain adjustment, the same problems noted for COMPLEX also plague the use of the RTDM procedures in the context of a puff model.

2.6.2.3 Alternate Approach to Terrain Adjustment in a Puff Model

The method of adjusting properties of a puff to simulate the effects of dispersion over terrain should include the following attributes:

(1) Adjustment should be analytic functions of readily-available physical properties of the flow, dispersion, and terrain.

(2) Problems associated with "reflections" should be minimized.

(3) Adjustments should be based on local properties of the terrain, so that heights relative to particular "stack-base" elevations or "base-plume" elevations are not required.

(4) Adjustments should be related to concepts used in the CTSG (CTDM) routine.

(5) Puffs from different sources that happen to coincide at some point should be treated alike as they interact with subsequent terrain features.

In the method outlined below, the properties of a puff are adjusted on the basis of the local strain to the flow imparted by the underlying terrain, using a simplification of the theory on which CTDM is based. The local strain is estimated from the slope of the underlying terrain. Terrain slopes are obtained from a gridded field of terrain elevations, and apply to the segment of the trajectory over which a puff travels during one time-step.

For very stable conditions (Froude number less than 1), we assume that the wind field model will force much of the flow to be parallel to contours of terrain-height, so that puffs will directly encounter relatively minor terrain. For such minor terrain, the strain-induced adjustments described above will also apply. But in addition, we allow the lateral distribution of the puff to remain level, by placing receptors on "poles" whose heights are relative to the elevation of the terrain beneath the center of the puff. This allows the "edges" of a puff to brush against the side-walls of a valley or channel, producing "impingement" concentrations. An explicit calculation and use of the dividing-streamline height (H_d) is not included in this approach.

Figure 2-21 depicts this treatment. The puff is travelling into the plane of the figure, and its size is denoted by the extent of the dotted lines (equal to σ_y, σ_z). The elevation of the terrain under the puff is denoted by the horizontal dashed line, and the actual terrain is denoted in the cross-section by the solid lines. Three receptors are marked. Receptors 1 and 3 lie above the terrain elevation at the puff location, while receptor 2 lies below it. When the Froude number is small, receptors 1 and 3 are placed on "poles", so that they intercept concentrations within the puff. When the Froude number is large, receptors 1 and 3 are placed at the elevation of terrain beneath the center of the puff. Because receptor 2 lies below this terrain elevation, it

is always moved up to the dashed line in the figure. Receptor heights that are modeled along the dashed line produce familiar "flat terrain" results.

In the absence of a dividing-streamline, the LIFT component of CTDMPLUS essentially computes an effective σ_y and σ_z from which terrain-altered concentrations are obtained using the "standard" Gaussian plume equation. The effective σ_y and σ_z are given in the notation of CTSG by Eqn. (2-132). For the "simplified" approach described below, we will focus solely on changes induced on the vertical spread of the puff. Following the implementation for σ_z in CTSG, we define a strain factor $T_z = \eta/z_f$, where η is the spacing between streamlines in the strained flow, and z_f is the spacing between the same streamlines in the unstrained flow over "flat" terrain. The notion of an effective size of the cloud is introduced to allow concentrations to be calculated in the flat-terrain frame of reference. It is assumed that the primary effect of strain in the flow is to alter the rate of exchange of material across streamlines in the flow. Hence, the ratio of σ_z/η in the straining flow can be larger than the corresponding ratio σ_{zf}/z_f. Therefore, the effective size of the cloud in the flat-terrain frame of reference (σ_{ze}) is defined by:

$$\frac{z_f}{\sigma_{ze}} = \frac{\eta}{\sigma_z} \tag{2-150}$$

or

$$\sigma_{ze}^2 = \frac{1}{T_z^2}\,\sigma_z^2 \tag{2-151}$$

This allows σ_{ze} to be calculated as

$$\sigma_{ze}^2(t) = \frac{1}{T_z^2(t)\; S_z^2(t)} \int_o^t 2K(t')\; S_z^2(t')\; dt' \tag{2-152}$$

The integral is evaluated over the life of a cloud, thereby incorporating the history of all of the strain experienced by the cloud.

The strain function S_z depends on the local value of the strain factor, T_z:

$$S_z(t) = e^{(1\,-\,T_z(t))} \tag{2-153}$$

For weak strain, we can approximate the strain function as

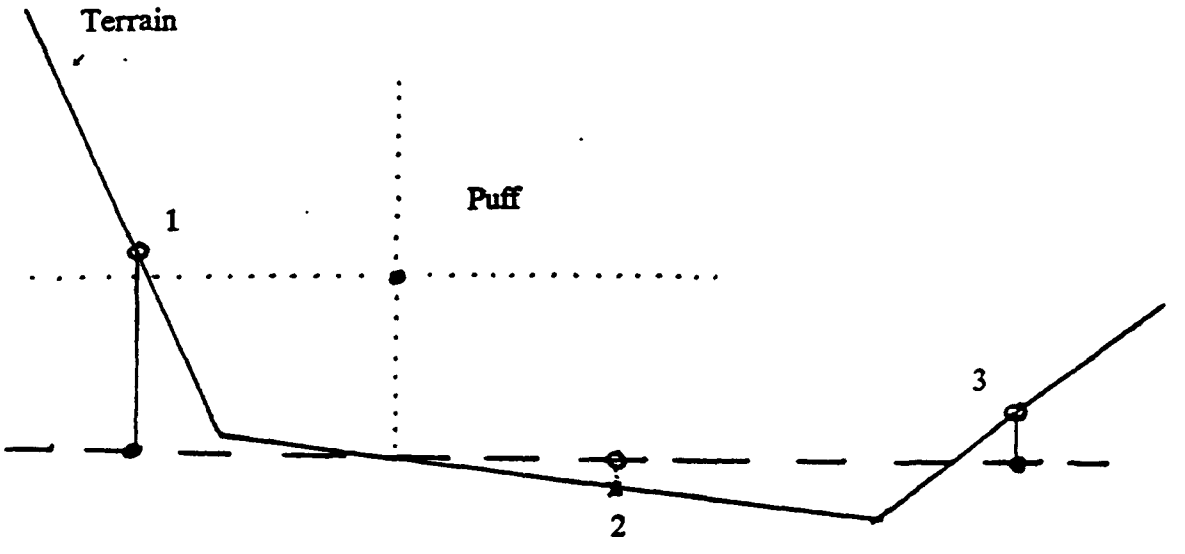


Figure 2-21. Depiction of treatment of puff interaction with a "side-wall" for strongly stratified (stable) conditions. The flow is into the page.

$$S_z(t) = 1 / T_z(t) \tag{2-154}$$

so that the product $S_z(t)\ T_z$ is unity. Although the strain likely to be encountered will not be entirely weak, we adopt the equivalence stated in Eqn. (2-154) as an approximation to simplify the leading factor in Eqn. (2-152).

With this assumption,

$$\sigma_{zc}^2(t) = \int_o^t 2K(t')\ e^{2(1 - T_z(t'))}\ dt' \tag{2-155}$$

which can be expressed for an incremental timestep Δt as

$$\sigma_{zc}^2(t + \Delta t) = \sigma_{zc}^2(t) + \int_o^{\Delta t} 2K(t + t')\ e^{2(1 - T_z(t + t'))}\ dt' \tag{2-156}$$

Over a short timestep in a puff model, Eqn. (2-156) can be approximated by replacing $2K\ (t + t')$ with its mean value during the timestep:

$$2\ \overline{K}\ (t, \Delta t) = \frac{\sigma_z^2\ (t + \Delta t) - \sigma_z^2\ (t)}{\Delta t} \tag{2-157}$$

Furthermore, we assume that the strain factor T_z varies linearly over the timestep, so that

$$T_z(t + t') = T_z(t) + \frac{dT_z}{dt}\ t' \tag{2-158}$$

and Eqn. (2-156) becomes

$$\sigma_{zc}^2\ (t + \Delta t) = \sigma_{zc}^2(t) + 2\overline{K}(t, \Delta t) \int_o^{\Delta t} e^{2\left(1 - T_z(t) - \frac{dT_z}{dt} t'\right)}\ dt' \tag{2-159}$$

Evaluating the integral in Eqn. (2-159),

$$\sigma_{zc}^2(t + \Delta t) = \sigma_{zc}^2(t) + 2\overline{K}(t, \Delta t)\ e^{2(1 - T_z(t))} \left[\frac{1 - e^{-2\Delta t\ dT_z/dt}}{2\ dT_z/dt}\right] \tag{2-160}$$

we have the new expression for the growth in σ_{zc} during one timestep. In the limit that the strain factor is constant over the timestep, Eqn. (2-160) reduces to

$$\text{Lim}\ \frac{dT_z}{dt} \to o: \qquad \sigma_w^2(t + \Delta t)\ \sigma_w^2(t) + e^{2(1 - T_z(t))}\left(\sigma_z^2(t + \Delta t) - \sigma_z^2(t)\right) \tag{2-161}$$

Implementation of Eqn. (2-160) requires a model for the strain $T_z(t)$ in the flow field. In CTSG, we have a description of the length scales and position of a terrain feature, and a flow model within CTSG provides information about the strain in the flow over the feature. Here, we use a surrogate to obtain the strain--we infer the scale of a two-dimensional terrain feature (lying across the flow) from the slope of the underlying surface along the flow (Figure 2-22). The slope $|\alpha|$ of the terrain is identified with a surrogate hill of height h_o, and half-length L, so that

$$|\alpha| = \frac{h_o}{2L} \tag{2-162}$$

The flow model used in CTSG provides the following equation for the deflection of a streamline (δ) over a two-dimensional ridge in stratified flow:

$$\delta(x,\eta) = h(x)\ e^{-\eta/L}\left(\cos \ell\eta - \frac{x}{L}\sin \ell\eta\right) \tag{2-163}$$

where the hill height function has the form

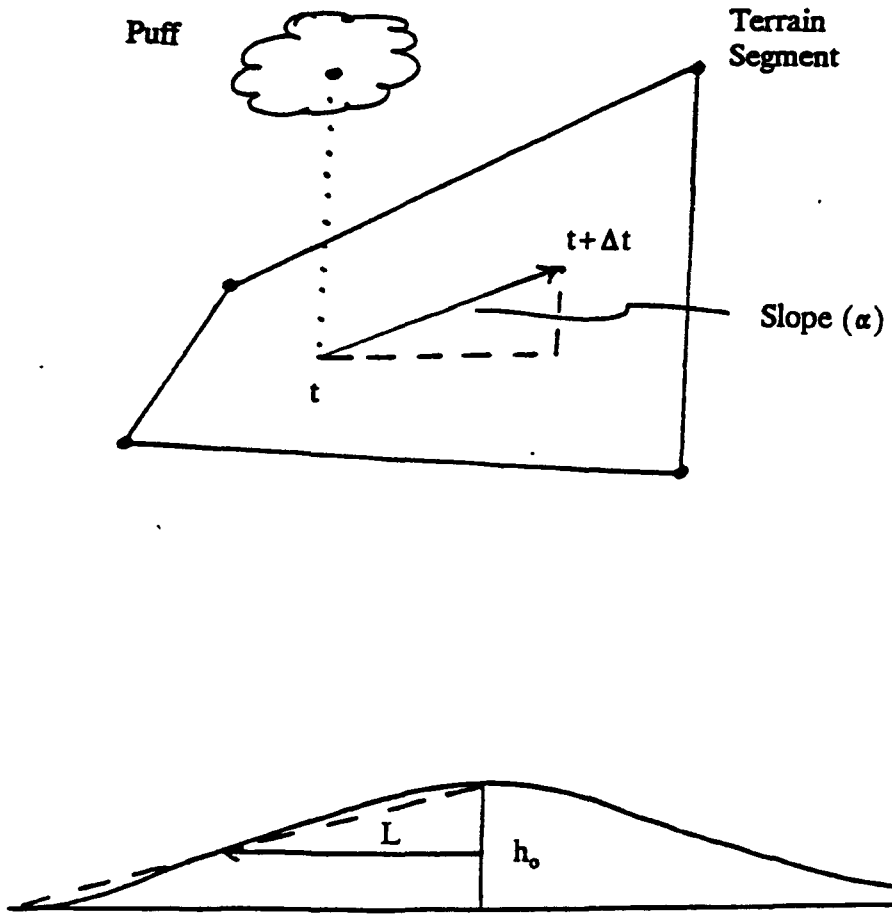
$$h(x) = \frac{h_o}{1 + \left(\frac{x}{L}\right)^2} \tag{2-164}$$

The stratification factor is $\ell = N/u$, x is directed downwind, with origin at the center of the "hill", and η is the height of the streamline above the surface at the position x.

Because we wish to associate a strain with the local slope along the puff trajectory and not a complete hill feature, we must assign representative values of T_z and dT_z/dt from somewhere over our surrogate hill. The location chosen to evaluate T_z and dT_z/dt is the point at which dT_z/dx is an extreme value. The strain factor is defined by the local streamline height divided by the streamline height far upwind (Figure 2-23):

$$T_z(x) = \frac{\eta(x)}{\eta_\infty} = \frac{\eta(x)}{h(x) + \eta(x) - \delta(x,\eta)} \tag{2-165}$$

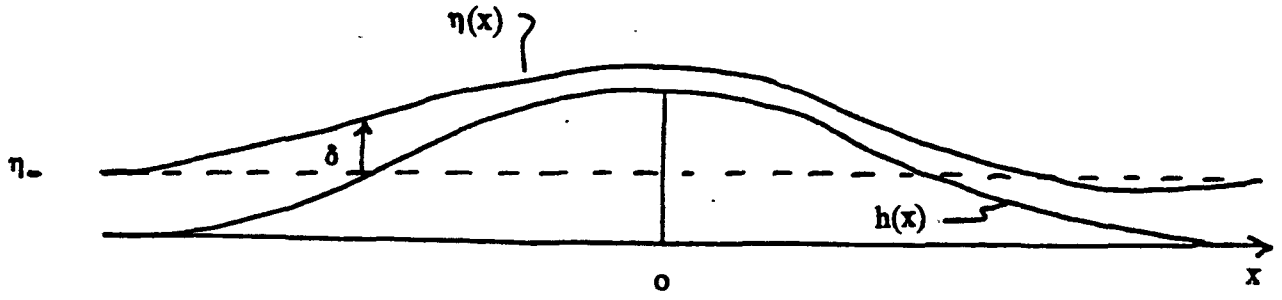
The position x/L at which dT_z/dx reaches an extreme value is approximately:



Surrogate Hill

$|\alpha| = h_o/2L$

Figure 2-22. Identification of a surrogate 2-D hill of the same overall slope (α) as the terrain directly beneath the puff.



$$\eta = \eta_\infty + \delta - h$$

$$T_z \sim \eta/\eta_\infty$$

Figure 2-23. Depiction of streamline height (η), streamline deflection (δ), and strain factor (T_z) nomenclature.

$$(x/L)_u = -\sqrt{\frac{1 + \frac{2\,|\alpha|}{\eta/L}\left(1 - e^{-\eta/L}\right)}{3}} + \frac{1}{2}\,\frac{1 - \sqrt{1 + \left(\frac{\sin \ell\eta}{\cos \ell\eta - e^{\eta/L}}\right)^2}}{\left(\frac{\sin \ell\eta}{\cos \ell\eta - e^{\eta/L}}\right)} \qquad (2\text{-}166)$$

for the upwind "face", and:

$$(x/L)_d = \sqrt{\frac{1 + \frac{2\,|\alpha|}{\eta/L}\left(1 - e^{-\eta/L}\right)}{3}} + \frac{1 - \sqrt{1 + \left(\frac{\sin \ell\eta}{\cos \ell\eta - e^{\eta/L}}\right)^2}}{\left(\frac{\sin \ell\eta}{\cos \ell\eta - e^{\eta/L}}\right)} \qquad (2\text{-}167)$$

for the downwind "face". The "face" is determined by the sign of the slope. For example, if α is less than zero, then we assume that the puff is travelling down the lee-side of the terrain, and $(x/L)_d$ is selected.

The strain factor at (x/L) is given by

$$T_z^{-1}(x/L) = 1 + \frac{2|\alpha|}{\eta/L\,(1 + (x/L)^2)}\left[1 - e^{-\eta/L}\left(\cos \ell\eta - \frac{x}{L}\sin \ell\eta\right)\right] \qquad (2\text{-}168)$$

and the change in T_z with distance at (x/L) is

$$\frac{dT_z}{dx}(x/L) = \frac{-2\,|\alpha|\,T_z^2}{\eta\,(1 + (x/L)^2)}\left[-2(x/L) + e^{-\eta/L}\left(2(x/L)\cos \ell\eta + (1 - (x/L)^2)\sin \ell\eta\right)\right] \qquad (2\text{-}169)$$

We assign dT_z/dt by using the puff speed and dT_z/dx.

The streamline height η, and its ratio to the horizontal length scale of the surrogate hill L remain to be assigned. We set η equal to the centroid height of the puff, because the strain over the scale of the puff will determine its modified growth. As for L, its minimum value is of the same order as the size of one grid cell used to define the terrain. For large features, L can be several kilometers. Therefore, we shall fix the ratio $\eta/L = 0.1$. While this cannot be representative of all puff heights and terrain features, it fixes our focus on the lower part of the flow over terrain in which the strain is most pronounced.

In summary, this simplified implementation of the principles embodied in CTSG involve the following steps:

1) The slope $|\alpha|$ of the terrain beneath the puff, taken along the transport direction, provides the single piece of information used to estimate the influence of the terrain on the growth of the puff on the vertical during one timestep.

2) A surrogate, two-dimensional hill of the same overall slope is used to represent the scale of the terrain.

3) The strain factor T_z is found from the streamline deflection equation used in CTSG, for the surrogate hill.

4) Both T_z and its derivative dT_z/dt are evaluated at the location on the surrogate hill at which dT_z/dt is an extreme value (upwind face of hill if the terrain slope is positive, downwind face if slope is negative).

5) The strain factor is assumed to be a linear function over the timestep, and σ_{ze} is computed from T_z, dT_z/dt, and the ambient rate of growth (the diffusivity).

This formulation conforms to all five attributes stated at the beginning of this subsection. However, several assignments have been made without the benefit of an evaluation study. Because of this, this terrain adjustment procedure should be used with caution at this time.

2.7 Dry Deposition

Many complex processes are involved in the transfer and deposition of pollutants at the surface. Sehmel (1980) compiled a list (Table 2-9) of some of the most important factors that are known to influence dry deposition rates. The variables listed include the properties of the depositing material (e.g., particle size, shape, and density; gas diffusivity, solubility, and reactivity), the characteristics of the surface (e.g., surface roughness, vegetation type, amount, and physiological state), and atmospheric variables (e.g., stability, turbulence intensity). Hicks (1982) noted the important differences controlling the deposition of large particles (e.g., gravitational settling, inertial impaction) and those controlling gases (e.g., turbulence, molecular diffusion). Deposition of small particles is complicated by the fact that they may be influenced by the processes affecting both gases and large particles.

A commonly used measure of deposition is the deposition velocity, v_d, defined as:

Table 2-9

Factors Influencing Dry Deposition Rates

Micrometeorological Variables	Depositing Material	Surface Variables
Aerodynamic roughness	Particles	Accommodation
- Mass transfer		- Exudates
(a) Particles	Agglomeration	- Trichomes
(b) Gases	Diameter	- Pubescence
- Heat	Density	- Wax
- Momentum	Diffusion	Biotic surfaces
Atmospheric stability	- Brownian	Canopy growth:
Diffusion, effect of:	- Eddy equal to	- Dormant
- Canopy	(a) Particle	- Expanding
- Diurnal variation	(b) Momentum	Senescent
- Fetch	(c) Heat	Canopy structure:
Flow separation:	- Effect of canopy on	- Areal density
- Above canopy	Diffusiophoresis	- Bark
- Below canopy	Electrostatic effects	- Bole
Friction velocity	- Attraction	- Leaves
Inversion layer	- Repulsion	- Porosity
Pollutant concentration	Gravitational settling	- Reproductive structure
Relative humidity	Hygroscopicity	- Soils
Seasonal variation	Impaction	- Stem
Solar radiation	Interception	- Type
Surface heating	Momentum	Electrostatic properties
Temperature	Physical properties	Leaf-vegetation:
Terrain	Resuspension	- Boundary layer
- Uniform	Shape	- Change at high winds
- Nonuniform	Size	- Flutter
Turbulence	Solubility	- Stomatal resistance
Wind velocity	Thermophoresis	Non-biotic surfaces
Zero-plane displacements		pH effects on:
- Mass transfer	Gases	- Reaction
(a) Particles		- Solubility
(b) Gases	Chemical activity	Pollutant penetration and distribution in canopy
- Heat	Diffusion:	Prior deposition loading
- Momentum	- Brownian	Water
	- Eddy	
	Partial pressure in equilibrium with surface	
	Solubility	

From: Sehmel (1980)

$$v_d = F / \chi_s \qquad (2\text{-}170)$$

where, v_d is the deposition velocity (m/s),

F is the pollutant deposition flux ($g/m^2/s$), and,

χ_s is the pollutant concentration (g/m^3).

Due to the number and variability of the factors influencing dry deposition rates, reported deposition velocities exhibit considerable variability. For example, SO_2 deposition velocity measurements summarized by Sehmel (1980) range over two orders of magnitude (Figure 2-24). Particle deposition velocities (Slinn et al., 1978) show an even greater variability (Figure 2-25). Although it is not practical to include in the deposition model the effects of all of the variables listed in Table 2-9, it is possible, based on the atmospheric, surface, and pollutant properties to parameterize many of the most important effects. The CALPUFF deposition module provides three options reflecting different levels of detail in the treatment of dry deposition.

- Full treatment of spatially and temporally varying gas/particle deposition rates predicted by a resistance deposition model.

- User-specified 24-hour cycles of deposition velocities for each pollutant. This option allows a "typical" time dependence of deposition to be incorporated, but does not include any spatial dependencies.

- No dry deposition. A switch is incorporated into the model to by-pass all the dry deposition calculations. This option will provide for faster model execution for screening runs or pollutants not experiencing significant deposition.

The user specifies a flag in the control file for each pollutant which determines if dry deposition is treated and the specific method used to compute the deposition velocities (see Input Group 2, Section 4.2.1).

If the resistance deposition model is used, the user must input values for several parameters describing the characteristics of the pollutant (e.g., solubility, reactivity, diffusivity for gases, the size distribution for particles) (see Input Group 7 and 8) which are used in the computation of the resistances. In addition, several reference parameters and a flag indicating the state of unirrigated vegetation (i.e., stressed, unstressed, or inactive) are required (see Input Group 9).

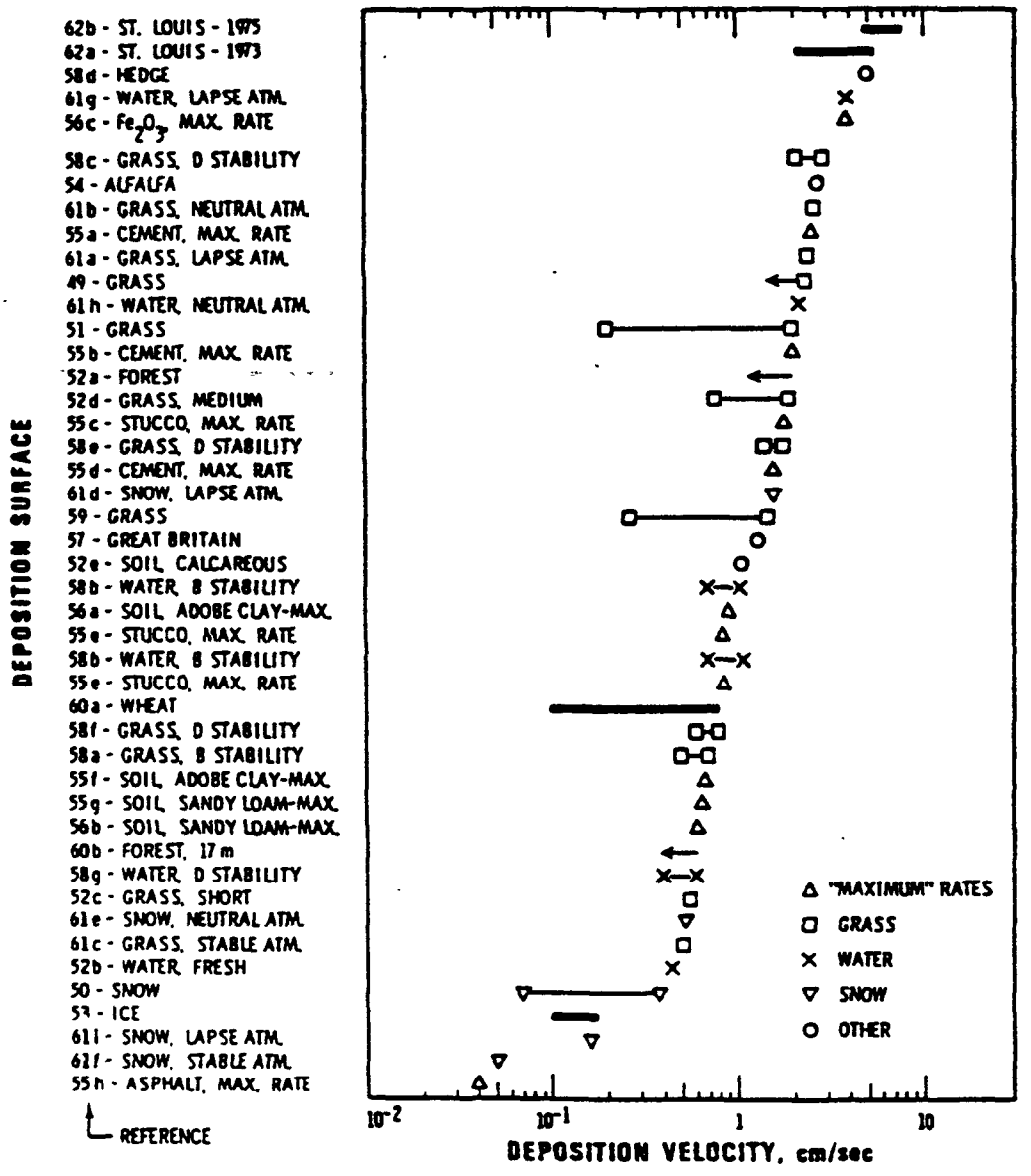


Figure 2-24. Summary of observed SO_2 deposition velocities (from Sehmel (1980)).

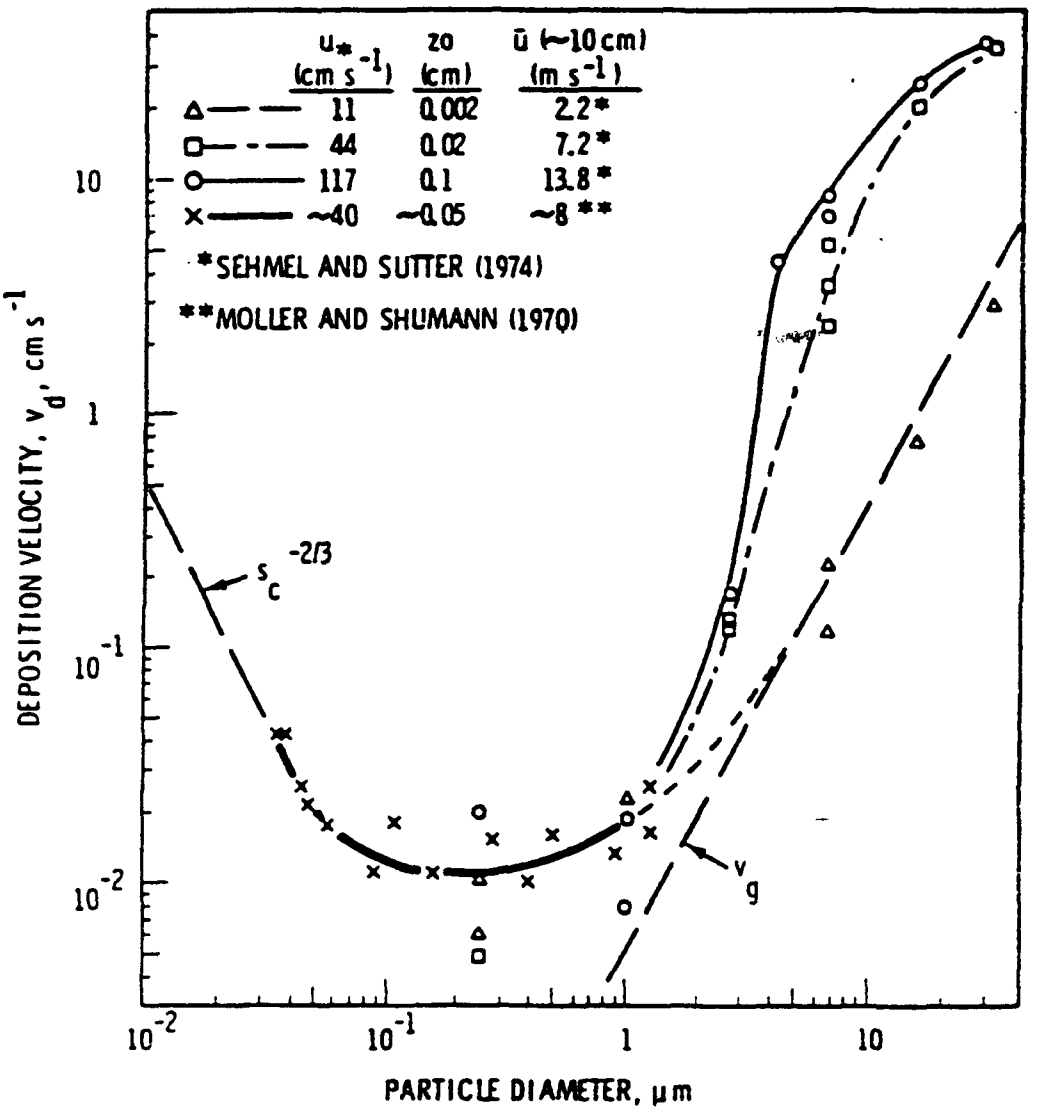


Figure 2-25. Observed deposition velocities as a function of particle size for 1.5 g/cm density particles. Measured by Sehmel and Sutter (1974) and Moller and Schumann (1970). Figure from Slinn et al. (1978).

If any pollutant is flagged as using "user-specified" deposition velocities, the user must prepare a data file with a 24-hour diurnal cycle of deposition velocities for each flagged species (see Section 4.2.5).

2.7.1 Vertical Structure and Mass Depletion

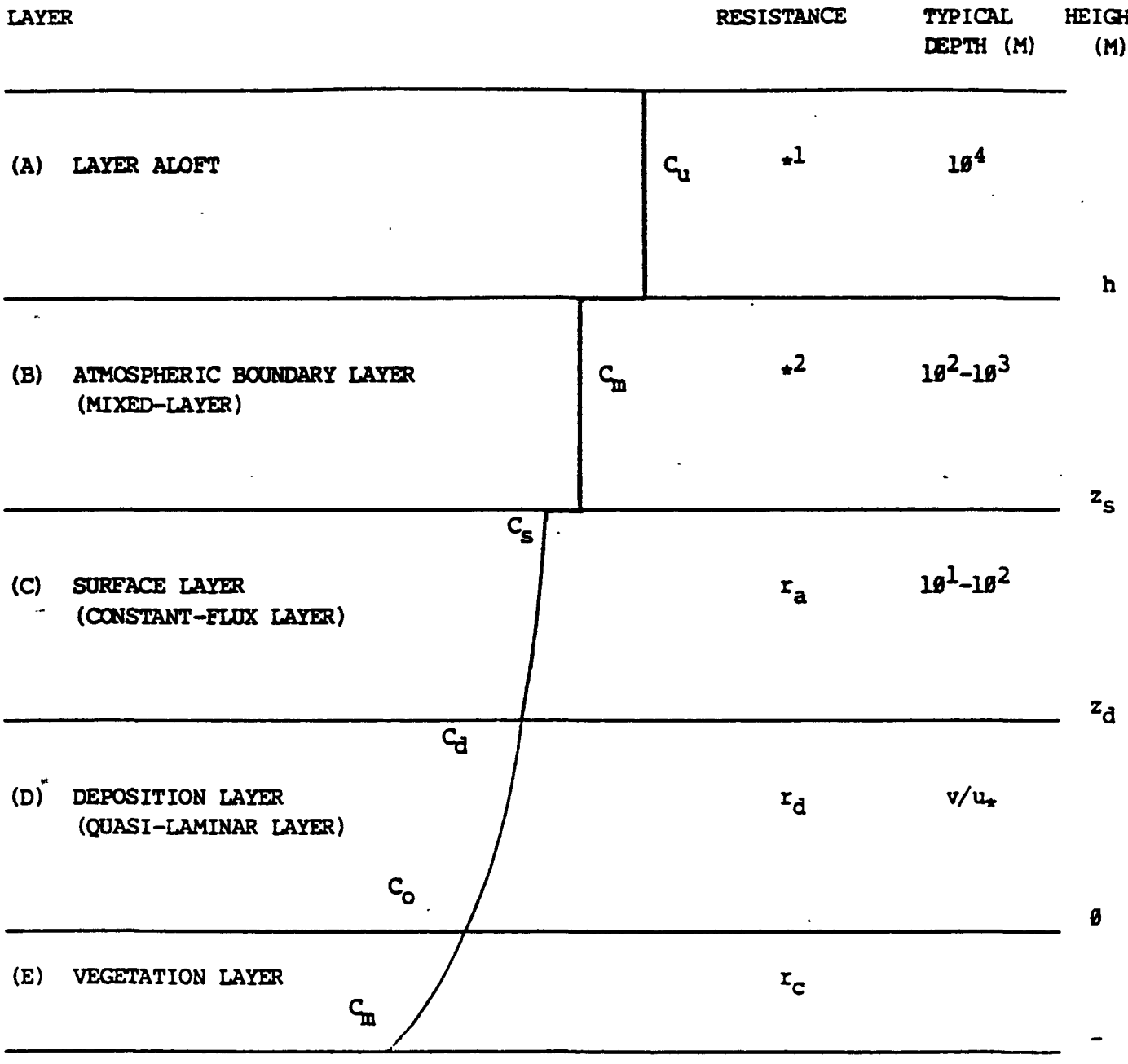
The CALPUFF dry deposition model is based on an approach which expresses the deposition velocity as the inverse of a sum of "resistances" plus, for particles, gravitational settling terms. The resistances represent the opposition to transport of the pollutant through the atmosphere to the surface. Slinn et al. (1978) describe a multilayer resistance model for dry deposition. As illustrated in Figure 2-26, the atmosphere can be divided into four layers for purposes of computing dry deposition rates. For gases, an additional (vegetation) layer is included.

(A) Layer Aloft. The top layer is the region above the current mixing height. It contains pollutant material either injected directly from tall stacks, or dispersed upward during previous turbulent activity. Due to the low rate of turbulent mixing in this layer, its pollutant is essentially cutoff from the surface. Therefore, this material is not subject to dry deposition until it becomes entrained into the mixed-layer.

(B) Mixed-Layer. The top of the mixed-layer defines the depth of the turbulent boundary layer. Layer B extends down to a reference height within the atmospheric surface layer. Pollutant mixing is dominated by turbulent processes. During convective conditions, pollutants in this layer quickly become uniformly mixed in the vertical. The resistance to pollutant transfer during these conditions is very small compared to the resistances in layers C, D, and E. However, during stable conditions, the mixed-layer resistance may be substantial (Wesely and Hicks, 1977). The treatment of the mixed-layer resistance is based on the overall boundary layer diffusivity parameterized in terms of micrometeorological scaling variables.

(C) Surface Layer. The surface layer is a shallow layer (~10 m) next to the ground that rapidly adjusts to changes in surface conditions. Because vertical fluxes are nearly constant, this layer is also called the constant-flux layer. The atmospheric resistance, r_a, is used to parameterize the rate of pollutant transfer in Layer C.

(D) Deposition Layer. Over very smooth surfaces, a thin non-turbulent layer (the deposition layer) develops just above the surface. For typically rough surfaces, this layer is constantly changing and is likely to be intermittently turbulent. For this reason, Hicks



*1 Material in the top layer is not available for deposition at the surface until entrained into the mixed-layer.

*2 Overall mixed-layer resistance included in Eqn. (2.7-5)

Figure 2-26. Multilayer structure used in the dry deposition resistance model (adapted from Slinn et al., 1978).

(1982) calls this layer the "quasi-laminar" layer. The primary transfer mechanisms across the laminar deposition layer are molecular diffusion for gases, and Brownian diffusion and inertial impaction for particles. However, surface roughness elements (e.g., leaf hairs) can sometimes penetrate the deposition layer, providing an alternate route for the pollutant transfer (Hicks, 1982). Under conditions of low atmospheric resistance, the deposition layer resistance, r_b, can be the dominant resistance controlling the rate of deposition for particles and some soluble, high molecular weight gases.

(E) Vegetation Layer. Vegetation is a major sink for many soluble or reactive gaseous pollutants. After passing through the stomata, soluble pollutants dissolve in the moist mesophyll cells in the interior of the leaves. Reactive pollutants may also interact with the exterior (cuticle) of the leaves. Due to the response of the stomata to external factors such as moisture stress, temperature, and solar radiation, the resistance in the vegetation layer (i.e., the canopy resistance, r_c) can show significant diurnal and seasonal variability. An alternate pathway that is potentially important in sparsely vegetated areas or overwater is deposition directly to the ground/water surface. Although not involving vegetation, it is convenient to include the ground/water surface resistance as a component of r_c because, like the vegetation resistances, it is a resistance in a layer below the laminar deposition layer.

In the CALPUFF model, the fraction of the pollutant mass above and below the current mixed layer is tracked. At any point in time, only pollutant material below the mixing height can be deposited at the surface. However, each time step as the mixing height changes, pollutant mass is transferred between Layers A and B. Typically, in the morning, as the boundary layer grows in response to solar heating of the land surface, material in the top layer is entrained into the mixed-layer and becomes available for dry deposition at the surface. In the evening, convective activity ceases, and material above the shallow nocturnal boundary layer height is isolated until the next diurnal cycle.

Once puffs have become uniformly mixed through the boundary layer, a surface depletion method (Scire et al., 1984b) can be used to account for the mixed-layer (Layer B) resistance. The pollutant flux, F, at the reference height within the surface layer can be written as:

$$F = D_{bl}\,(\chi_m - \chi_s)/(h - z_s) = v_d \chi_s \qquad (2\text{-}171)$$

where, χ_m is the pollutant concentration (g/m^3) within the mixed-layer,

χ_s is the pollutant concentration (g/m^3) at the top of the surface layer,

h is the mixed-layer height (m),

z_s is the surface layer height (m), and,

D_{bl} is an overall boundary layer eddy diffusivity (m^2/s).

The boundary layer eddy diffusivities during stable conditions (Brost and Wyngaard, 1978) can be expressed as:

$$D_{bl} = k_1 u_* h \tag{2-172}$$

and during neutral or unstable conditions as:

$$D_{bl} = Maximum\ [k_1 u_* h\ ,\ k_2 w_* h] \tag{2-173}$$

where k_1 and k_2 are constants with default values of 0.01 and 0.1, respectively.

The term $v_d \chi_s$ can be written as $v_d' \chi_m$, where v_d' is an effective deposition velocity taking into account boundary layer mass transfer. From Eqn. (2-171), v_d' is:

$$v_d' = D_{bl} v_d / [D_{bl} + v_d (h - z_s)] \tag{2-174}$$

When turbulent mixing within Layer B is rapid compared to the rate of deposition at the surface, the atmosphere quickly replaces material that is deposited. During these conditions, D_{bl} is large, and $v_d' \sim v_d$. However, under other conditions the rate of deposition can sometimes be limited by the rate of pollutant transfer through Layer B to the vicinity of the surface. During stable conditions, D_{bl} may be small compared to $v_d(h-z_s)$, and v_d' may be substantially smaller than v_d. In the near-field of a source, before the plume has spread through the boundary layer, it is assumed that $v_d' \sim v_d$. This allows the near-field vertical Gaussian distribution to be maintained.

The resistances in the layers below the reference height in the surface constant-flux layer determine v_d. The parameterization of these resistances is discussed separately for gases and particles in Sections 2.7.2 and 2.7.3, respectively. Once v_d is determined, v_d' is computed from Eqn. (2-174). Each time step, the mass of the pollutant in the puff is adjusted to account for the dry removal:

$$Q_m(t + \Delta t) = Q_m(t)\ \exp\left[-\left(v_d' dt / \Delta s\right) \int_s^{s+\Delta s} g(s')ds'\right] \tag{2-175}$$

where, Q_m is the mass (g) of the pollutant in the puff below the mixing height (h) at time t and $t+\Delta t$,

Δt is the time step (s),

$s, s+\Delta s$ are the positions of the puff at the beginning and end of the time step, and,

$g(s)$ is the vertical term of the Gaussian puff equation. For a puff uniformly mixed in the vertical, $g(s) = 1/h$.

If user-specified deposition velocities are used for any of the pollutants, the effective deposition velocity, v_d', is set equal to the user specified value read from the VD.DAT file.

2.7.2 Resistance Deposition Model For Gases

At the reference height, z_s, the deposition velocity for gases is expressed (Wesely and Hicks, 1977; Hicks, 1982) as the inverse of a sum of three resistances.

$$v_d = (r_a + r_d + r_c)^{-1} \tag{2-176}$$

where, r_a is the atmospheric resistance (s/m) through the surface layer,

r_d is the deposition layer resistance (s/m), and,

r_c is the canopy (vegetation layer) resistance (s/m).

Atmospheric Resistance

The atmospheric resistance is obtained by integration of the micrometeorological flux-gradient relationships (Wesely and Hicks, 1977):

$$r_a = \frac{1}{k\, u_*} \left[\ln(z_s / z_o) - \phi_H\right] \tag{2-177}$$

where, z_s is the reference height (m),

z_o is the surface roughness length (m),

k is the von Karman constant (~ 0.4),

u_* is the friction velocity (m/s),

ϕ_H is a stability correction term, and,

L is the Monin-Obukhov length (m).

The stability correction term accounts for the effects of buoyancy on the eddy diffusivity of the pollutant. It is assumed that the pollutant transfer is similar to that for heat (Wesely and Hicks, 1977). A gridded field of surface roughness lengths is passed to the model in the output file of the meteorological model, CALMET. In CALMET, the surface roughness length is either estimated from the predominant land use of each grid cell, or, if available, based on

actual values entered by the user. Over water, due to the effect of the wind on wave height, the surface roughness length varies as a function of wind speed, and is computed internally within CALPUFF using the parameterization of Hosker (1974).

$$z_0 = 2.0 \times 10^{-6} u^{2.5} \quad (2\text{-}178)$$

where u is the wind speed (m/s) at 10 m.

Deposition Layer Resistance

Due to the importance of molecular diffusion to the transport through the laminar deposition layer, the deposition layer resistance for gaseous pollutants is parameterized in terms of the Schmidt number:

$$r_d = d_1 S_c^{d_2} / (k\, u_*) \quad (2\text{-}179)$$

where, S_c is the Schmidt number (υ/D),
υ is the kinematic viscosity of air (0.15×10^{-4} m^2/s),
D is the molecular diffusivity of the pollutant (m^2/s), and,
d_1, d_2 are empirical parameters.

Experimental studies summarized by Hicks (1982) suggest a range of values for the empirical variables of 1.6 to 16.7 for d_1/k and 0.4 to 0.8 for d_2. Intermediate values of $d_1 = 2$ (or d_1/k of 5), and $d_2 = 2/3$ are recommended based on Shepherd (1974), Slinn et al. (1978), and Hicks (1982).

Canopy Resistance

The canopy resistance is the resistance for gases in the vegetation layer. There are three main pathways for uptake/reaction of the pollutant within the vegetation or surface:

(1) Transfer through the stomatal pore and dissolution or reaction in the mesophyll cells.
(2) Reaction with or transfer through the leaf cuticle.
(3) Transfer into the ground/water surface.

In the resistance model, these pathways are treated as three resistances in parallel.

$$r_c = [LAI/r_f + LAI/r_{cut} + 1/r_g]^{-1} \quad (2\text{-}180)$$

where, r_f is the internal foliage resistance (s/m) (Pathway 1),
r_{cut} is the cuticle resistance (s/m), (Pathway 2),
r_g is the ground or water surface resistance (s/m), (Pathway 3), and,
LAI is the leaf area index (ratio of leaf surface area divided by ground surface area). The LAI is specified in the model as a function of land use type.

The first pathway is usually the most important for uptake of soluble pollutants in vegetated areas. The internal foliage resistance consists of two components:

$$r_f = r_s + r_m \quad (2\text{-}181)$$

where, r_s is the resistance (s/m) to transport through the stomatal pore, and,
r_m is the resistance (s/m) to dissolution or reaction of the pollutant in the mesophyll (spongy parenchyma) cells.

Stomatal action imposes a strong diurnal cycle on the stomatal resistance, and, due to its important role in determining deposition rates for gaseous soluble pollutants such as SO_2, on the deposition velocity, as well. Stomatal opening/closing is a response to the plant's competing needs for uptake of CO_2 and prevention of water loss from the leaves. The stomatal resistance can be written (O'Dell et al., 1977) as:

$$r_s = p/(bD) \quad (2\text{-}182)$$

where, p is a stomatal constant ($\sim 2.3 \times 10^{-8}$ m^2),
b is the width of the stomatal opening (m), and,
D is the molecular diffusivity of the pollutant (m^2/s).

The width of the stomatal opening is a function of the radiation intensity, moisture availability, and temperature. The variation of b during periods when vegetation is active can be represented (Pleim et al., 1984) as:

$$b = b_{max}[S/S_{max}] + b_{min} \quad (2\text{-}183)$$

where, b_{max} is the maximum width (m) of the stomatal opening ($\sim 2.5 \times 10^{-6}$ m) (Padro et al., 1991),
b_{min} is the minimum width (m) of the stomatal opening ($\sim 0.1 \times 10^{-6}$ m),
S is the solar radiation (W/m^2) received at the ground, and,

S_{max} is the solar radiation (W/m^2) at which full opening of the stomata occur.

However, during periods of moisture stress, the need to prevent moisture loss becomes critical, and the stomata close. It can be assumed that $b = b_{min}$ for unirrigated vegetation under moisture stress conditions. When vegetation is inactive (e.g., during the seasonal dry periods in much of California), the internal foliage resistance becomes very large, essentially cutting off Pathway 1. In CALGRID, the state of the unirrigated vegetation is specified as one of these states (A) active and unstressed, (B) active and stressed, or (C) inactive.

The effect of temperature on stomatal activity has been reviewed by Pleim et al. (1984). The most significant effects are due to temperature extremes. During cold periods ($T < 10°$ C), metabolic activity slows, and b is set equal to b_{min}. During hot weather conditions ($T > \sim 35°$ C), the stomata are fully open ($b = b_{max}$) to allow evaporative cooling of the plant (assuming the vegetation is in state A - active and unstressed). These temperature effects provide additional bounds on the value of r_s given by Eqn. (2-182).

Mesophyll Resistance

The mesophyll resistance depends on the solubility and reactivity of the pollutant. It is an input parameter supplied to the deposition model for each gaseous species. O'Dell et al. (1977) estimate the mesophyll resistance for several pollutants. For soluble pollutants such as HF, SO_2, Cl_2 and NH_3, $r_m \sim 0.0$. The mesophyll resistance can be large for less soluble pollutants such as NO_2 ($\sim$ 500 s/cm) and NO (9400 s/cm). For other pollutants, r_m can be estimated based on the solubility and reactivity characteristics of the pollutant.

Cuticle Resistance

The second pathway for deposition of gases in the vegetation layer is via the leaf cuticle. This includes potential direct passage through the cuticle or reaction of the pollutant on the cuticle surface. Hicks (1982) notes that measurements of SO_2 deposition to wheat (Fowler and Unsworth, 1979) show significant cuticle deposition. However, Hosker and Lindberg (1982) suggest that passage of gases through the cuticle is negligible. Therefore, the cuticle deposition is likely to be controlled by the pollutant reactivity. Pleim et al. (1984) parameterize r_{cut} as a function of the pollutant reactivity of the depositing gas relative to the reference values for SO_2.

$$r_{cut} = (A_{ref}/A) r_{cut}(ref) \qquad (2\text{-}184)$$

where, A is the reactivity parameter for the depositing gas,

A_{ref} is the reference reactivity of SO_2 (~ 8.0), and,

$r_{cut}(ref)$ is the empirically determined reference cuticle resistance (s/m) of SO_2.

Padro et al. (1991) suggest $r_{cut}(ref)$ is about 30 s/cm. Reactivity values for other pollutants are estimated at 8.0 (NO_2), 15.0 (O_3), 18.0 (HNO_3), and 4.0 (PAN).

Ground/Water Resistance

The third pathway through the "vegetation layer" involves deposition directly to the ground or water surface. In moderately or heavily vegetated areas, the internal foliage and cuticle resistances usually control the total canopy resistance. However, in sparsely vegetated areas, deposition directly to the surface may be an important pathway. Over water, deposition of soluble pollutants can be quite rapid.

The ground resistance, r_g, over land surfaces can be expressed (Pleim et al., 1984) relative to a reference value for SO_2:

$$r_g = (A_{ref}/A) r_g(ref) \qquad (2\text{-}185)$$

where, $r_g(ref)$ is the reference ground resistance of SO_2 (~ 10 s/cm) (Padro et al., 1991).

Slinn et al. (1978) parameterize the liquid phase resistance of the depositing pollutant as a function of its solubility and reactivity characteristics. Their results can be expressed as:

$$r_g = H/(\alpha_* d_3 u_*) \qquad (2\text{-}186)$$

where, H is the Henry's law constant, which is the ratio of gas to liquid phase concentration of the pollutant, (H ~ 4×10^{-2} (SO_2), 4×10^{-7} (H_2O_2), 8×10^{-8} (HNO_3), 2×10^{0} (O_3), 3.5×10^{0} (NO_2), 1×10^{-2} (PAN), and 4×10^{-6} (HCHO)),

α_* is a solubility enhancement factor due to the aqueous phase dissociation of the pollutant (α_* ~ 10^3 for SO_2, ~ 1 for CO_2), and

d_3 is a constant (~ 4.8×10^{-4}).

2.7.3 Resistances for Particulate Matter

Because particulate matter does not interact with vegetation in the same way as gaseous pollutants, particle deposition velocities are commonly expressed only in terms of r_a, r_d and a gravitational settling term. The atmospheric resistance, r_a, for a particle is the same as for a gas

(Eqn. 2-177). The resistance in the vegetation layer (r_c) is not a factor because once penetrating the deposition layer, particles are usually assumed to stick to the surface (e.g., Voldner et al., 1986). Therefore, their behavior is similar to highly soluble/reactive gases with $r_c \sim 0$. Based on an assumption of steady-state conditions, the deposition velocity for particles can be expressed (Slinn and Slinn, 1980; Pleim et al., 1984) as:

$$v = (r_a + r_d + r_a r_d v_g)^{-1} + v_g \qquad (2\text{-}187)$$

where v_g is the gravitational settling speed (m/s) of the particle.

In CALPUFF, the puff centerline height at each receptor is adjusted to account for the cumulative effects of gravitational settling. The puff centerline height is assumed to decrease by an amount given by:

$$\Delta h_g = -v_g \cdot t_{tot}$$

where, Δh is the change in puff height (m) due to settling effects,
v_g is the gravitational settling velocity (m/s), and
t_{tot} is the total travel time (s) from the source to the receptor.

There are three major mechanisms for transport of particles across the deposition layer. Small particles (< 0.1 μm diameter) are transported through the laminar deposition layer primarily by Brownian diffusion. This process becomes less efficient as the particle diameter increases. Particles in the 2-20 μm diameter range tend to penetrate the deposition layer by inertial impaction. The stopping time, t, defined as the settling velocity divided by the acceleration due to gravity, is a measure of tendency of a particle to impact. Inertial impaction is most effective in the 2-20 μm diameter range. Larger particles are dominated by gravitational settling effects. The effect of the terms involving v_g in Eqn. (2-187) always is to increase the deposition velocity. Particles in the range of 0.1-2 μm diameter range, such as sulfate, have very small settling velocities and are not efficiently transported across the deposition layer by either the Brownian diffusion or the inertial impaction mechanism. As a result, these particles have the lowest deposition velocities.

The deposition layer resistance can be parameterized (e.g., Pleim et al., 1984) in terms of the Schmidt number (Sc = υ/D, where υ is the viscosity of air, and, for particles, D is the Brownian diffusivity of the pollutant in air) and the Stokes number (St = $(v_g/g)(u_*^2/\upsilon)$, where v_g is the gravitational settling velocity and g is the acceleration due to gravity).

$$r_d = (Sc^{-2/3} + 10^{-3/St})^{-1} u_*^{-1} \qquad (2\text{-}188)$$

The diffusivity of a particle in air, D, is a function of the particle size. Smaller particles tend to be more efficiently transported by Brownian motion, and therefore have higher diffusivities. The Stokes number is a measure of the likelihood of impaction of the particle. It increases with increasing particle size.

The gravitational settling velocity is a function of the particle size, shape, and density. For spheres, the settling velocity is given by the Stokes equation:

$$v_g = \left[(d_p)^2 g(\rho_p - \rho_g)C\right]/(18\ \upsilon) \quad (2\text{-}189)$$

where, d_p is the particle diameter (m)
ρ_p is the particle density (g/m^3),
ρ_g is the air density (g/m^3), and,
C is the Cunningham correction for small particles.

This correction given by:

$$C = 1 + (2\ \lambda / d_p)\left[a_1 + a_2 \exp\left(-a_3 d_p / \lambda\right)\right] \quad (2\text{-}190)$$

where, λ is the mean free path of air molecules (6.53×10^{-6} cm), and
a_1, a_2, a_3 are constants (1.257, 0.40, 0.55, respectively).

Because of the sensitivity of the deposition velocity to particle size, the effective deposition velocity is computed for a number of individual size categories, and then weighted by the actual size distribution. The particle size distribution is specified in terms of the geometric mass mean diameter and geometric standard deviation of the distribution. For sulfate, the geometric mass mean diameter is approximately 0.5 μm with a geometric standard deviation of approximately 2 μm.

2.8 Chemical Transformation

One of the design criteria of the CALPUFF model required the capability of modeling linear chemical transformation effects in a manner consistent with the puff formulation of the model. The CALPUFF chemical module contains three options for dealing with chemical processes:

- A pseudo-first-order chemical reaction mechanism for the conversion of SO_2 to $SO_4^=$ and NO_x (NO + NO_2) to NO_3^-. This mechanism is based on the chemical transformation scheme used in the MESOPUFF II model (Scire et al., 1984b)

and incorporates the most significant dependencies of spatially and temporally varying environmental conditions on the transformation rates.

- User-specified 24-hour cycles of transformation rates. This option allows simulation of the diurnal, time-dependent behavior of the transformation rates. However, the transformation rates with this option are spatially uniform.

- No chemical transformation. An option is provided to completely by-pass the chemical transformation calculations. This will reduce computer requirements for situations or pollutants for which chemical transformation effects are not significant.

The user selects one of the above options by specifying a mechanism flag in the CALPUFF control flag (see Section 4.2.1). The MESOPUFF II mechanism (Option 1) uses ozone concentrations (along with radiation intensity) as surrogates for the OH concentration during the day when gas phase free radical chemistry is active. With Option 1, hourly observations of ozone concentrations at one or more monitoring stations can be read from a data file (OZONE.DAT) to provide the necessary estimates of ozone concentrations (see Section 4.2.6).

If "user-specified" transformation rates are used (Option 2), the user must prepare a data file (CHEM.DAT) with a 24-hour diurnal cycle of typical transformation rates for each species (see Section 4.2.7).

2.8.1 Description of the MESOPUFF II Chemical Mechanism

The chemical processes included in the MESOPUFF II mechanism (Option 1) are the conversion of sulfur dioxide to sulfate and the conversion of nitrogen oxides to nitrate aerosol. Figures 2-26 and 2-27 illustrate the chemical pathways for SO_2 and NO_x oxidation and aerosol formation. Oxidation may occur by gas and aqueous phase reactions. The gas phase reactions for both SO_x and NO_x involve free radical photochemistry and, therefore, are coupled to the oxidation of reactive organic gases (ROG). Homogeneous gas phase reaction is the dominant SO_2 oxidation pathway during clear, dry conditions (Calvert et al., 1978). Ozone and hydrogen peroxide are believed to be the principal oxidants for aqueous-phase oxidation of SO_2.

The oxidation of NO_x is dependent on gas phase $ROG/NO_x/O_3$ photochemistry. It is generally more rapid than SO_2 oxidation. As shown in Figure 2-27, NO_x can be oxidized to nitric acid (HNO_3) and organic nitrates (RNO_3) such as peroxyacetylnitrate (PAN). Nitric acid

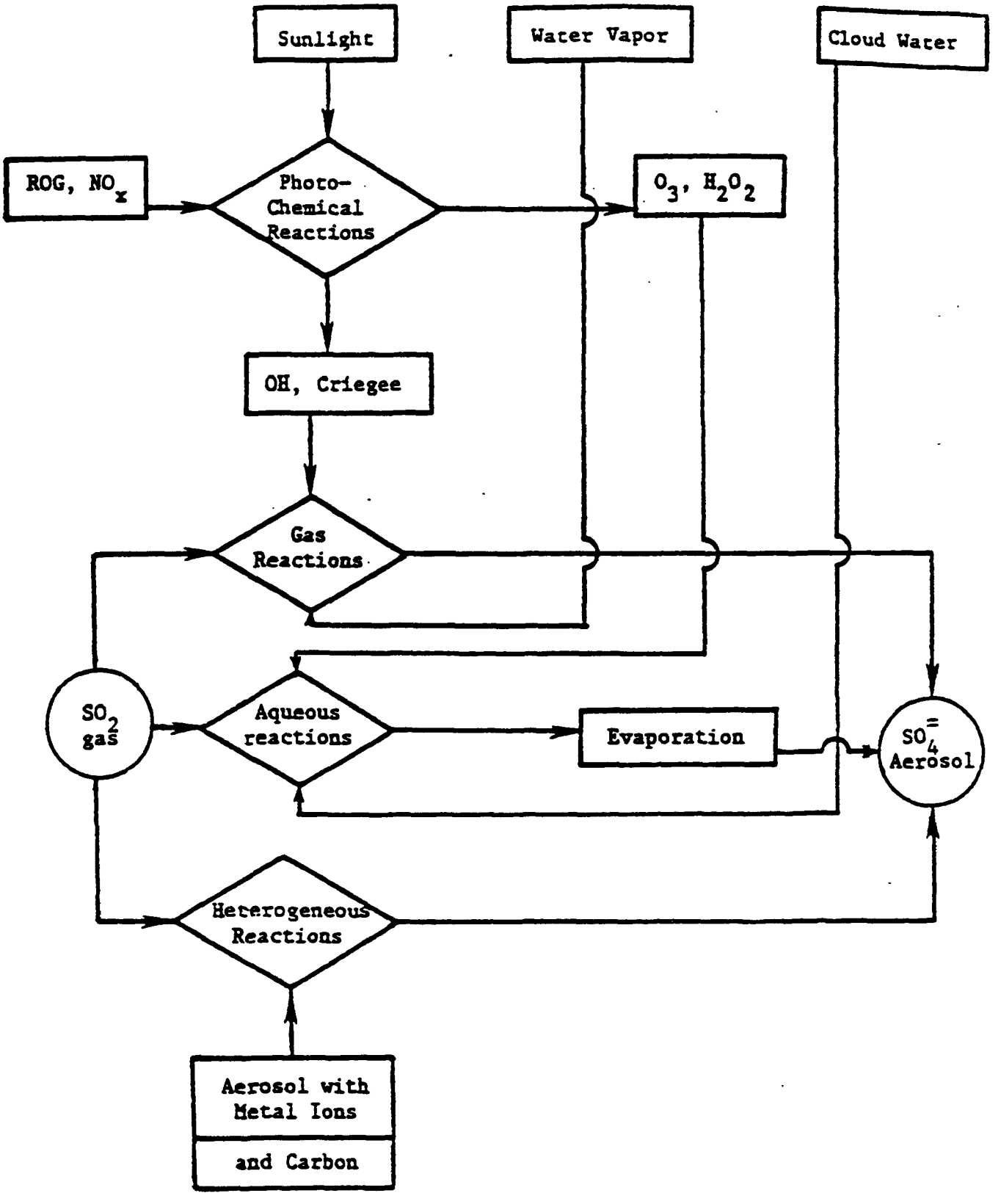


Figure 2-26. SO_2 oxidation pathways (from Scire et al., (1984b)).

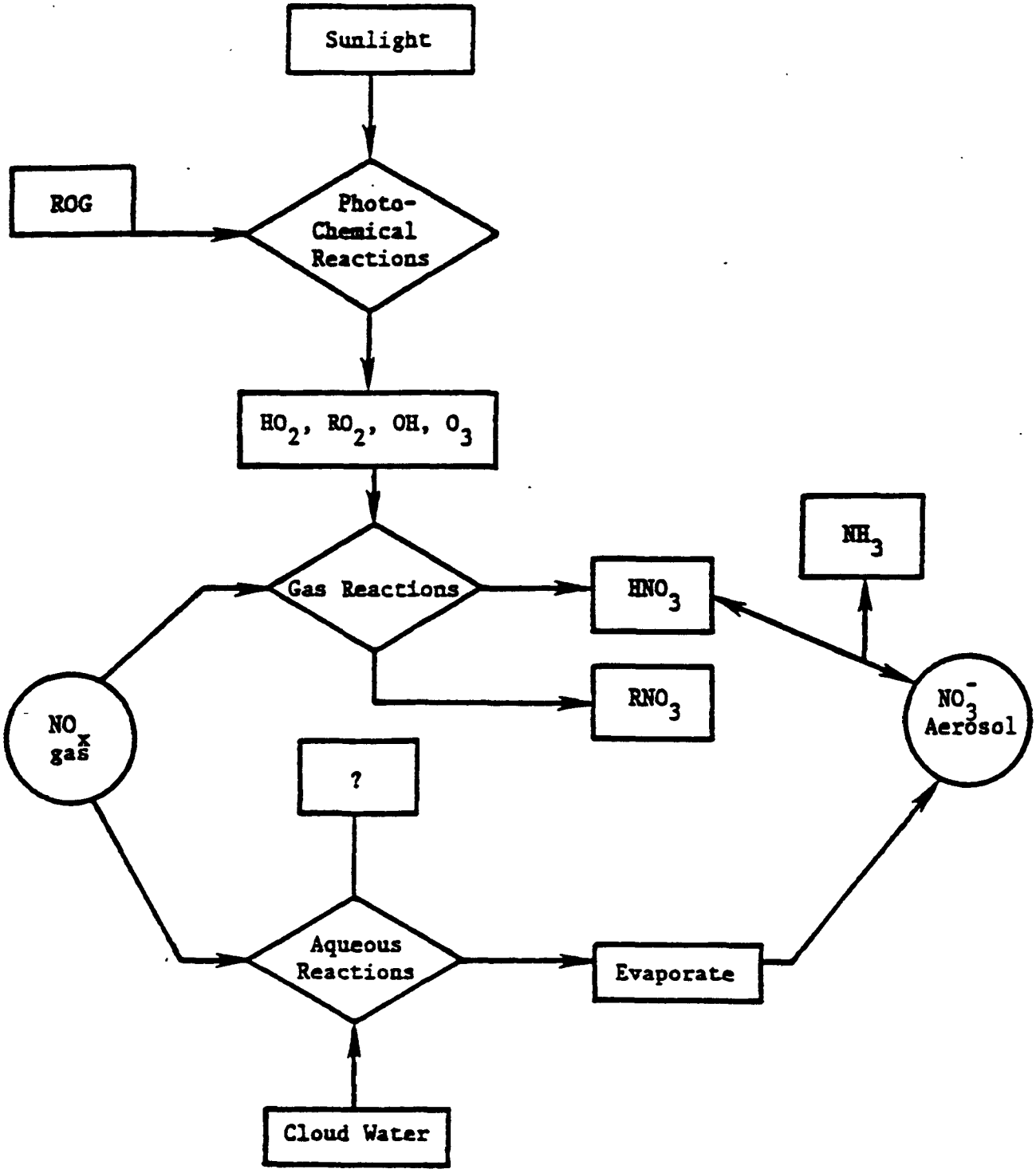


Figure 2-27. NO_x oxidation pathways (from Scire et al., (1984b)).

combines with ammonia gas to form solid or aqueous ammonium nitrate (NH_4NO_3). Unlike sulfate formation, the nitrate process is reversible. Equilibrium is established between nitric acid, ammonia, and ammonium nitrate:

$$NH_4NO_3 \leftrightarrow HNO_3\,(g) + NH_3\,(g) \tag{2-191}$$

The equilibrium constant for this reaction ($K = [NH_3][HNO_3]/[NH_4NO_3]$) is a nonlinear function of temperature and relative humidity as shown in Figure 2-28 (Stelson and Seinfeld, 1982). The equilibrium constant can vary several orders of magnitude over a typical diurnal cycle. Given fixed amounts of total nitrate, ammonia, and water vapor, higher NH_4NO_3 concentrations are expected at night due to lower nighttime temperatures and higher relative humidities. Thus, the nitrate aerosol cannot be considered a stable product like sulfate. Also, unlike sulfate, the ambient concentration of nitrate is limited by the availability of ammonia which is preferentially scavenged by sulfate (Stelson et al., 1983).

The transformation pathways for the five active pollutants (SO_2, $SO_4^=$, NO_x, HNO_3, and NO_3^-) included in the MESOPUFF II scheme are shown in Figure 2-29. Transformation rate expressions were developed by statistically analyzing hourly transformation rates produced by a photochemical model. The photochemical model employed the $RHC/NO_x/SO_x$ chemical mechanism of Atkinson et al. (1982). Plume SO_x/NO_x dispersing into background air containing ozone and reactive hydrocarbons was simulated over a wide range of conditions representing different solar radiation intensities, temperatures, dispersion conditions, background ozone and RHC concentrations, plume NO_x concentrations and emission times. The following transformation rate expressions, representing curve fits to the daytime hourly conversion rates predicted by the photochemical model, were determined:

$$k_1 = 36\, R^{0.55} [O_3]^{0.71}\, S^{-1.29} + k_{1(aq)} \tag{2-192}$$

$$k_2 = 1206\, [O_3]^{1.5}\, S^{-1.41}\, [NO_x]^{-0.33} \tag{2-193}$$

$$k_3 = 1261\, [O_3]^{1.45}\, S^{-1.34}\, [NO_x]^{-0.12} \tag{2-194}$$

where, k_1 is the SO_2 to SO_4 transformation rate (percent/hour),

k_2 is the NO_x to $HNO_3 + RNO_3$ transformation rate (percent/hour),

k_3 is the NO_x to HNO_3 (only) transformation rate (percent/hour),

R is the total solar radiation intensity (kw/m^2),

S is a stability index ranging from 2 to 6 (PGT class A and B=2, C=3, D=4, E=5, F=6),

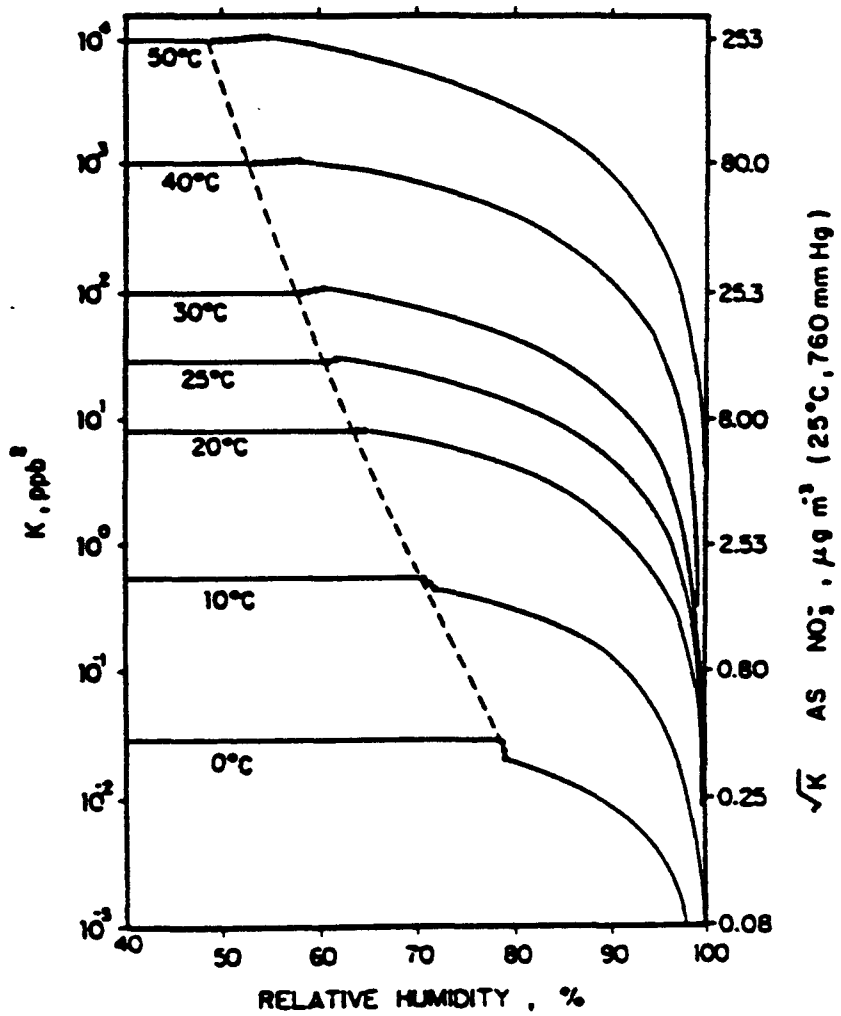


Figure 2-28. NH_4NO_3 dissociation constant as a function of temperature and relative humidity (from Stelson and Seinfeld, (1982)).

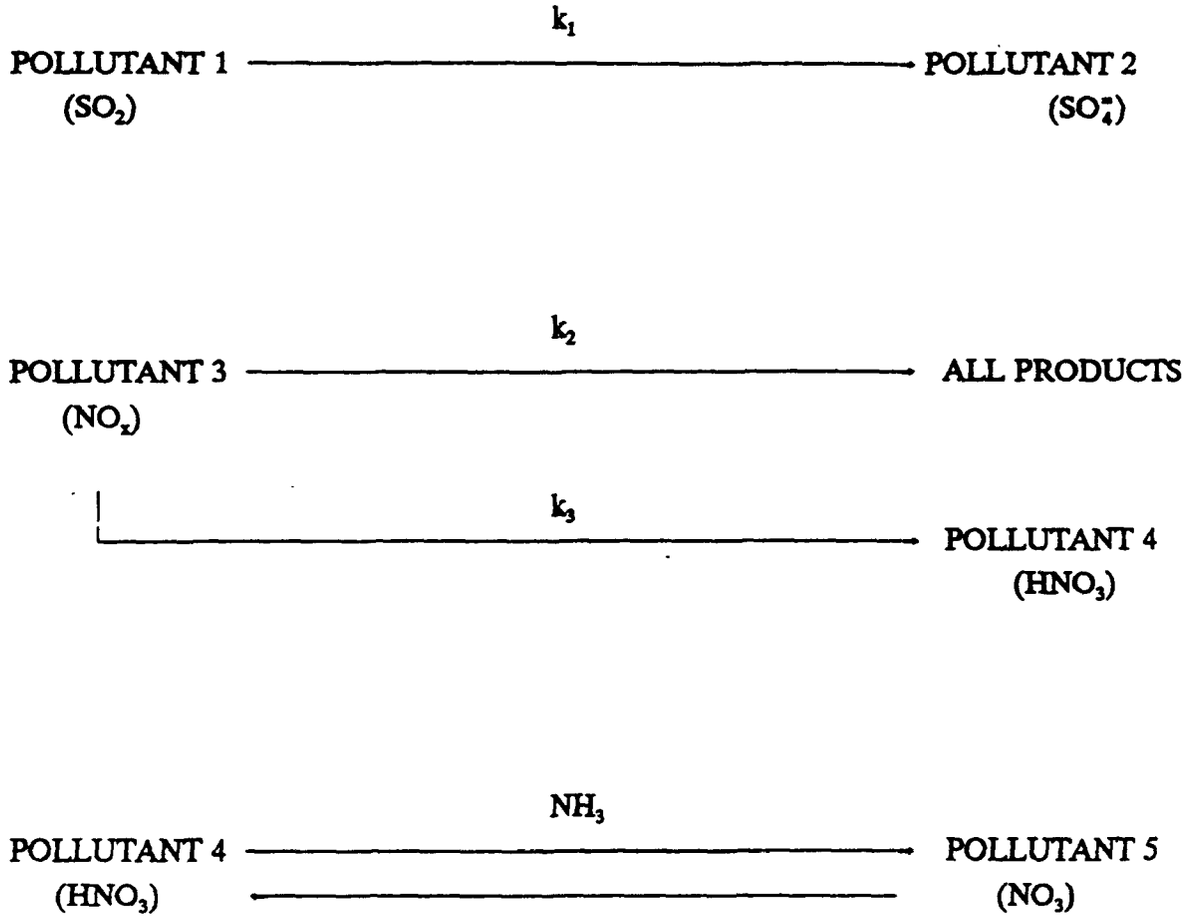


Figure 2-29. Schematic representation of chemical pathways in the five-pollutant system assumed with the MESOPUFF II chemical mechanism.

RH is the relative humidity (percent),
$[O_3]$ is the background ozone concentration (ppm),
$[NO_x]$ is the plume NO_x concentration (ppm), and,
$k_{1(aq)}$ is the aqueous phase SO_2 oxidation term (percent/hour).

The aqueous phase component of the SO_2 conversion rate was parameterized as:

$$k_{1(aq)} = 3 \times 10^{-5} RH^4 \qquad (2\text{-}195)$$

Equations (2.192) to (2.194) apply only during daytime periods when gas phase free radical chemistry is active. The use of the ozone concentration and the radiation intensity as surrogates for the OH concentration, as in the above equations, is appropriate only during the day. At night, SO_2 and NO_x oxidation rates resulting from heterogeneous reactions, are generally much lower than typical daytime rates (Wilson, 1981; Forrest et al., 1981). Nighttime oxidation rates of 0.2% and 2.0% for SO_2 and NO_x, respectively, are used as default values in the model.

Two options are provided for the specification of ozone concentrations: (1) hourly ozone data from a network of stations (OZONE.DAT, see Section 4.2.6), or, (2) a single, user-specified background ozone value may be used. The background ammonia concentration required for the HNO_3/NH_4NO_3 equilibrium calculation can be user-specified or a default value will be assumed.

The parameterized NO_x oxidation rate depends on the NO_x concentration. In situations where puffs overlap, it is necessary to estimate the total NO_x concentration at a particular point to properly determine k_2 and k_3. Similarly, the nitrate equilibrium relationship requires knowledge of the total (local average) SO_4, NO_x, and total nitrate (HNO_3 + NO_x) concentrations. Because of the preferential scavenging of ammonia by sulfate, the available ammonia is computed as total ammonia minus sulfate. The local average concentrations within a puff are estimated as the sum of contributions from the puff's own pollutants plus those of nearby puffs. Local average concentrations are separately computed for puffs within and above the mixed-layer.

2.9 Wet Removal

Many studies have shown that during rain events, wet scavenging of soluble or reactive pollutants can be of the order of tens of percent per hour (Barrie, 1981; Slinn et al., 1978;

Levine and Schwartz, 1982; Scire and Venkatram, 1985). Gaseous pollutants are scavenged by dissolution into cloud droplets and precipitation. For SO_2, aqueous-phase oxidation can be an important removal pathway. Particulate pollutants are removed by both in-cloud scavenging (rainout) and below-cloud scavenging (washout). Over source-receptor distances of tens to hundreds of kilometers, wet scavenging can deplete a substantial fraction of the pollutant material from the puff.

A simple approach that has been shown (e.g., Maul, 1980) to yield realistic long-term estimates of wet removal is the empirically-based scavenging coefficient method. The depletion of a pollutant is represented as:

$$\chi_{t+dt} = \chi_t \exp[-\Lambda \Delta t] \tag{2-196}$$

where, χ is the concentration (g/m^3) at time t and t + Δt, and,
Λ is the scavenging ratio.

The scavenging ratio can be expressed as:

$$\Lambda = \lambda (R/R_1) \tag{2-197}$$

where, λ is the scavenging coefficient (s^{-1}),
R is the precipitation rate (mm/hr), and,
R_1 is a reference precipitation rate of 1 mm/hr.

The scavenging coefficient depends on the characteristics of the pollutant (e.g., solubility and reactivity) as well as the nature of the precipitation. Table 2-10 contains the default values of the scavenging coefficient for SO_2, $SO_4^=$, NO_x, HNO_3, and NO_3^-. A precipitation code determined from the hourly surface meteorological observations of precipitation type (CD144 data) is used to determine if the value of λ for liquid or frozen precipitation is most appropriate. The reported precipitation code is related to precipitation type as shown in Table 2-11. The liquid precipitation values of λ are used for precipitation codes 1-18. The frozen precipitation values are used for precipitation codes 19-45.

The user can override the default values of the scavenging coefficient by entering new values in the CALPUFF control file (see Section 4.2.1). An option is provided in the model to completely by-pass the wet removal calculation for pollutants or time periods for which it is not of importance.

Table 2-10
Default Values of the Scavenging Coefficient, $\lambda(s^{-1})$

Pollutant	Liquid Precipitation	Frozen Precipitation
SO_2	3×10^{-5}	0.0
$SO_4^=$	1×10^{-4}	3×10^{-5}
NO_x	0.0	0.0
HNO_3	6×10^{-5}	0.0
NO_3^-	1×10^{-4}	3×10^{-5}

Table 2-11
Conversion of Reported Precipitation Type/Intensity To Precipitation Codes

Precipitation Code	Type	Intensity
Liquid Precipitation		
1	Rain	Light
2	Rain	Moderate
3	Rain	Heavy
4	Rain Showers	Light
5	Rain Showers	Moderate
6	Rain Showers	Heavy
7	Freezing Rain	Light
8	Freezing Rain	Moderate
9	Freezing Rain	Heavy
10	Not Used	-
11	Not Used	-
12	Not Used	-
13	Drizzle	Light
14	Drizzle	Moderate
15	Drizzle	Heavy
16	Freezing Drizzle	Light
17	Freezing Drizzle	Moderate
18	Freezing Drizzle	Heavy
Frozen Precipitation		
19	Snow	Light
20	Snow	Moderate
21	Snow	Heavy
22	Snow Pellets	Light
23	Snow Pellets	Moderate
24	Snow Pellets	Heavy
25	Not Used	-
26	Ice Crystals	*
27	Not Used	-
28	Snow Showers	Light
29	Snow Showers	Moderate
30	Snow Showers	Heavy
31	Not Used	-
32	Not Used	-
33	Not Used	-
34	Snow Grains	Light
35	Snow Grains	Moderate
36	Snow Grains	Heavy
37	Ice Pellets	Light
38	Ice Pellets	Moderate
39	Ice Pellets	Heavy
40	Not Used	-
41	Hail	*
42	Not Used	-
43	Not Used	-
44	Small Hail	*
45	Not Used	-

* Intensity not currently reported for ice crystals, hail and small hail.

2.10 Odor Modeling

CALPUFF uses a simple averaging-time scaling factor to estimate short-term peak concentration for assessing the perception of odor. Such adjustments to the mean concentration are necessary because the averaging time associated with the dispersion curves are 3 to 60 minutes, while odors are perceived on time scales of a few seconds.

The scaling factor (Turner, 1970) for averaging time in AUSPLUME is:

$$f(t,t_o) = (t_o/t)^{0.2} \qquad (2\text{-}198)$$

where (t) is the averaging time (min.) of interest, and (t_o) is the averaging time consistent with the dispersion rates used to obtain the mean concentration (assumed to be 60 minutes in CALPUFF). The concentration averaging time is specified by the variable AVET in Input Group 1 of the control file.

3. CALPUFF MODEL STRUCTURE

3.1 Memory Management

A flexible memory management system is used in CALPUFF which facilitates the user's ability to alter the dimension of the major arrays within the code. Arrays dealing with the number of horizontal or vertical grid cells, meteorological stations, chemical species, puffs, sources, and several other internal variables are dimensioned throughout the code with parameter statements. The declaration of the values of the parameters are stored in a file called "PARAMS.PUF." This file is automatically inserted into any CALPUFF subroutine or function requiring one of its parameters via FORTRAN "include" statements. Thus, a global redimensioning of all of the model arrays dealing with the number of vertical layers, for example, can be accomplished simply by modifying the PARAMS.PUF file and recompiling the program.

The parameter file contains variables which set the array dimensions or the maximum allowed number of vertical layers, or horizontal grid cells, etc. The actual value of the variables for a particular run is set within the user input file (i.e., the control file), and can be less than the maximum value set in the parameter file.

A sample parameter file is shown in Table 3-1. In addition to the parameters specifying the maximum array dimensions of the major model arrays, the parameter file also contains variables determining the Fortran I/O unit numbers associated with each input and output file. For example, the input control file (IO5) and output list file (IO6) are normally associated with unit numbers 5 and 6. However, if these units are reserved on a particular computer system, these files can be redirected to other non-reserved units by setting IO5 and IO6 equal to 1 and 2, for example, as in the sample PARAMS.PUF file.

3.2 Structure of the CALPUFF Modules

Execution of the CALPUFF model is divided into three major phases: setup, computational, and termination (see Figure 3-1). In the setup phase of the model execution, a variety of initialization and one-time I/O and computational operations are performed, including the following:

- Processing of the command line argument.
- Opening of input and output files.

Table 3-1
Sample CALPUFF Parameter File

```
c------------------------------------------------------------------------
c --- PARAMETER statements                                        CALPUFF
c------------------------------------------------------------------------
c --- Specify model version
      character*8 mver, mlevel, mmodel
      parameter(mver='3.0',mlevel='950715')
      parameter(mmodel='CALPUFF')
c
c --- Specify parameters
      parameter(mxpuff=5000,mxspec=5)
      parameter(mxnx=90,mxny=90,mxnz=12)
      parameter(mxnxg=90,mxnyg=90,mxrec=2000)
      parameter(mxss=150,mxus=20,mxps=60)
      parameter(mxpt1=20,mxpt2=20,mxarea=20,mxvert=5)
      parameter(mxlines=10,mxvol=20)
      parameter(mxpdep=2,mxint=9)
      parameter(mxoz=20)
      parameter(mxhill=5,mxtpts=25,mxrect=180,mxcntr=21)
      parameter(mxsg=30,mxvar=60,mxcol=132)
      parameter(io5=1,io6=2,io7=7,io8=8,io9=9,io10=10,io11=11)
      parameter(io14=14,io16=16)
      parameter(io17=17,io18=18,io20=20,io22=22,io24=24,io26=26,io28=28)
      parameter(io30=30,iomesg=0)
c
c --- Compute derived parameters
      parameter(mxnzp1=mxnz+1)
      parameter(mxvertp1=mxvert+1)
      parameter(mxnxy=mxnx*mxny)
      parameter(mxgsp=mxnxg*mxnyg*mxspec)
      parameter(mxrsp=mxrec*mxspec)
      parameter(mxcsp=mxrect*mxspec)
      parameter(mx2=2*mxspec,mx5=5*mxspec,mx6=6*mxspec)
      parameter(mxp3=3+mxspec,mxp6=6+mxspec)
      parameter(mxp7=7+mxspec,mxp8=8+mxspec)
      parameter(mxpuf6=6*mxpuff)
      parameter(mxlev=mxnz)
c
c --- GENERAL PARAMETER definitions:
c        MXPUFF - Maximum number of active puffs allowed on the
c                 computational grid at one time
c        MXSLUG - Maximum number of active slugs allowed on the
c                 computational grid at one time (can be set to
c                 one if the slug option is not used)
c        MXSPEC - Maximum number of chemical species
c          MXNX - Maximum number of METEOROLOGICAL grid cells in
c                 the X direction
c          MXNY - Maximum number of METEOROLOGICAL grid cells in
c                 the Y direction
c          MXNZ - Maximum number of vertical layers in
c                 the METEOROLOGICAL grid
c         MXNXG - Maximum number of SAMPLING grid cells in
c                 the X direction
c         MXNYG - Maximum number of SAMPLING grid cells in
c                 the Y direction
c         MXREC - Maximum number of non-gridded receptors
c          MXSS - Maximum number of surface meteorological stations
c                 in the CALMET data
c          MXUS - Maximum number of upper air stations in the CALMET
c                 data
c          MXPS - Maximum number of precipitation stations in the
c                 CALMET data
```

Table 3-1

Sample CALPUFF Parameter File (Continued)

```
c         MXPT1 - Maximum number of point sources with constant
c                 emission parameters
c         MXPT2 - Maximum number of point sources with time-varying
c                 emission parameters
c        MXAREA - Maximum number of polygon area sources with constant
c                 emission parameters (i.e., non-gridded area sources)
c        MXVERT - Maximum number of vertices in polygon area source
c        MXLINES- Maximum number of line sources with constant
c                 emission parameters
c         MXVOL - Maximum number of volume sources
c        MXRISE - Maximum number of points in computed plume rise
c                 tabulation for buoyant area and line sources
c        MXPDEP - Maximum number of particle species dry deposited
c         MXINT - Maximum number of particle size intervals used
c                 in defining mass-weighted deposition velocities
c           MXOZ - Maximum number of ozone data stations (for use in the
c                 chemistry module)
c        MXHILL - Maximum number of subgrid-scale (CTSG) terrain
c                 features
c        MXTPTS - Maximum number of points used to obtain flow
c                 factors along the trajectory of a puff over the hill
c        MXRECT - Maximum number of complex terrain (CTSG) receptors
c        MXCNTR - Maximum number of hill height contours (CTDM ellipses)
c         MXLEV - Maximum number of vertical levels of met. data
c                 allowed in the CTSG module (set to MXNZ in the
c                 current implementation of CALPUFF)
c
c --- CONTROL FILE READER definitions:
c          MXSG - Maximum number of input groups in control file
c         MXVAR - Maximum number of variables in each input group
c         MXCOL - Maximum length (bytes) of a control file input record
c
c --- FORTRAN I/O unit numbers:
c           I05 - Control file (CALPUFF.INP)     - input  - formatted
c           I06 - List file (CALPUFF.LST)        - output - formatted
c
c           I07 - Meteorological data file       - input  - unformatted,
c                 (CALMET.DAT), or                          formatted,
c                 ISCMET.DAT, or                            formatted
c                 PLMMET.DAT
c
c           I08 - Concentration output file      - output - unformatted
c                 (CONC.DAT)
c           I09 - Dry flux output file           - output - unformatted
c                 (DFLX.DAT)
c          I010 - Wet flux output file           - output - unformatted
c                 (WFLX.DAT)
c          I011 - Visibility output file         - output - unformatted
c                 (VISB.DAT)
c          I014 - I/O file name file             - input  - formatted
c                 (PUFFILES.DAT)
c          I016 - Pt. source emissions file      - input  - unformatted
c                 (PTEMARB.DAT) with arbitrarily
c                 varying point source emissions
c          I017 - Buoyant area sources file      - input  - formatted
c                 (BAEMARB.DAT) with arbitrarily-
c                 varying location & emissions
c          I018 - Gridded volume source          - input  - unformatted
c                 emissions file (VOLEM.DAT)
c          I020 - User-specified deposition      - input  - formatted
c                 velocities (VD.DAT)
```

Table 3-1
Sample CALPUFF Parameter File (Concluded)

```
c          IO22 - Hourly ozone monitoring data  - input  - formatted
c                 (OZONE.DAT)
c          IO24 - User-specified chemical       - input  - formatted
c                 transformation rates
c                 (CHEM.DAT)
c          IO26 - Hourly turbulence measurements- input  - formatted
c                 sigma v, sigma w
c                 (SIGMA.DAT)
c          IO28 - CTSG hill specifications from - input  - formatted
c                 CTDM terrain processor
c                 (HILL.DAT)
c          IO30 - Tracking puff/slug data       - output - formatted
c                 (DEBUG.DAT)
c        IOMESG - Fortran unit number for screen- output - formatted
c                 output (NOTE: This unit is NOT
c                 opened -- it must be a
c                 preconnected unit to the screen.
c                 Screen output can be suppressed by
c                 the variable "IMESG" in the control
c                 file)
```

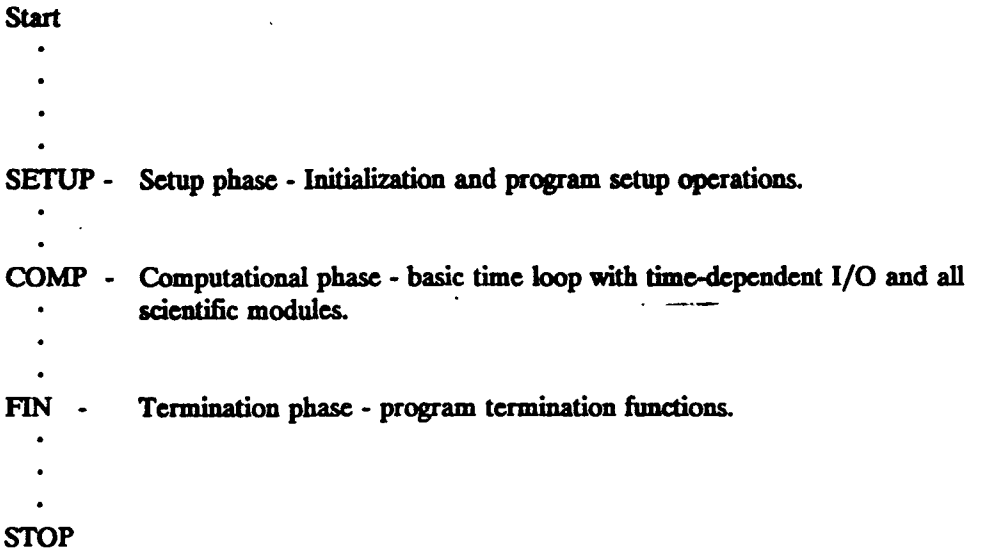


Figure 3-1. Flow diagram showing the calling sequence of major routines in the CALPUFF MAIN program.

- Reading and processing the control file inputs which includes model option flags and run control variables.

- Reading and processing the time-invariant data records of the model's input data bases (i.e., meteorological data file, optional emissions files, ozone data files, and user-specified deposition velocities and transformation rate files).

- Performing consistency checks of the input data base information versus the control file inputs.

- Performing initialization and setup operations for the chemistry, dry deposition, dispersion coefficient, and sampling modules.

- Writing the header records to the model's output concentration and dry/wet deposition files.

The computational phase of the model includes the basic time loop within which the hourly concentrations and deposition fluxes are computed and, if appropriate, time averaged. The functions performed in the computation phase include the following:

- Retrieving and processing time-averaging data from the meteorological, emissions, and ozone data files.

- Emitting, transporting, and removals puffs from the computation grid.

- Evaluating the effects of dispersion, chemical transformation, wet removal, dry deposition, and subgrid scale complex terrain.

- Sampling the puffs to determine concentrations and deposition fluxes at gridded and discrete receptors.

- Time-averaging and storing concentrations and deposition flux results to the appropriate output files.

The final phase of the model execution deals with run termination functions. The termination phase includes the closing of any active data files, computation of model run time, and printing of summary or normal termination messages.

A flow diagram for the setup module is provided in Figure 3-2. The flow diagram contains the name of each subroutine or function called by the setup module along with a brief description of the routine's purpose. A flow diagram for the main computational routine, subroutine COMP, is shown in Figure 3-3. As illustrated in the figure, COMP contains the basic time loop and calls to all of the technical modules.

At the beginning of the hour loop, the data files containing meteorological fields, time-varying emissions, and ozone observations are read. Then, a loop over puffs is entered which computes plume rise, determines puff-independent complex terrain parameters, and determines advective winds for the hour. Plume dispersion, advection, chemical transformation, wet deposition, dry deposition, terrain effects, and puff/slug sampling are performed within the innermost loop over sampling steps.

Enter SETUP

DATETM - Get date and time from the system clock.

COMLINE - Get the I/O file name from the command line

READFN - Get the control file name and the list file name from the I/O file

OPENFL - Open control file (input) and list file (output).

READCF - Read the control file inputs.

WRFILES - Write the file names used in this run to the list file

SETCOM - Set miscellaneous common block parameters (grid parameters, etc.)

OPENOT - Open all other input and output files.

RDHDEM2 - Read header records for the PTEMARB.DAT emission file (arbitrarily-varying point source emissions).

RDHDEM3 - Read header records for the BAEMARB.DAT emission file (arbitrarily-varying buoyant area source emissions).

RDHDEM4 - Read header records for the VOLEM.DAT emissions file (gridded volume source emissions).

CHEMI - Perform setup operations for the chemistry module.

EMQA - Perform QA checks on emission header record data, set up cross-referencing arrays.

RDTIEM2 - Read the time-invariant data from the PTEMARB.DAT file (arbitrarily-varying point source emissions).

RDTIEM3 - Read the time-invariant data from the BAEMARB.DAT file (arbitrarily-varying area source emissions).

(Continued)

Figure 3-2. Flow diagram showing the calling sequence of major routines in subroutine SETUP (Setup Phase).

```
  .
  .
  .
MET1      -  Read the header records for the meteorological data file
MET2         MET1 for CALMET.DAT, MET2 for ISCMET.DAT, MET3 for PLMMET.DAT).
MET3
  .
  .
ELEVI     -  Interpolate the elevations from the meteorological grid to the gridded
  .            receptor points
  .
  .
RDHDTVW   -  Read the header record from the turbulence data file (SIGMA.DAT)
  .
  .
SIGSET    -  Perform setup operations for the dispersion coefficient module.
  .
  .
SLUGI     -  Perform setup operations for the slug sampling function.
  .
  .
DRYI      -  Perform setup operations for the dry deposition module.
  .
  .
CTINIT    -   Perform setup computations for the subgrid-scale complex terrain module (CTSG)
  .
  .
WROUT1    -  Write the header records to the CONC.DAT (concentrations), DFLX.DAT
  .            (dry deposition flux), and WFLX.DAT (wet deposition flux) output files.
  .
  .
Return to MAIN PROGRAM
```

Figure 3-2. Flow diagram showing the calling sequence of major routines in subroutine SETUP (Setup Phase). (Concluded).

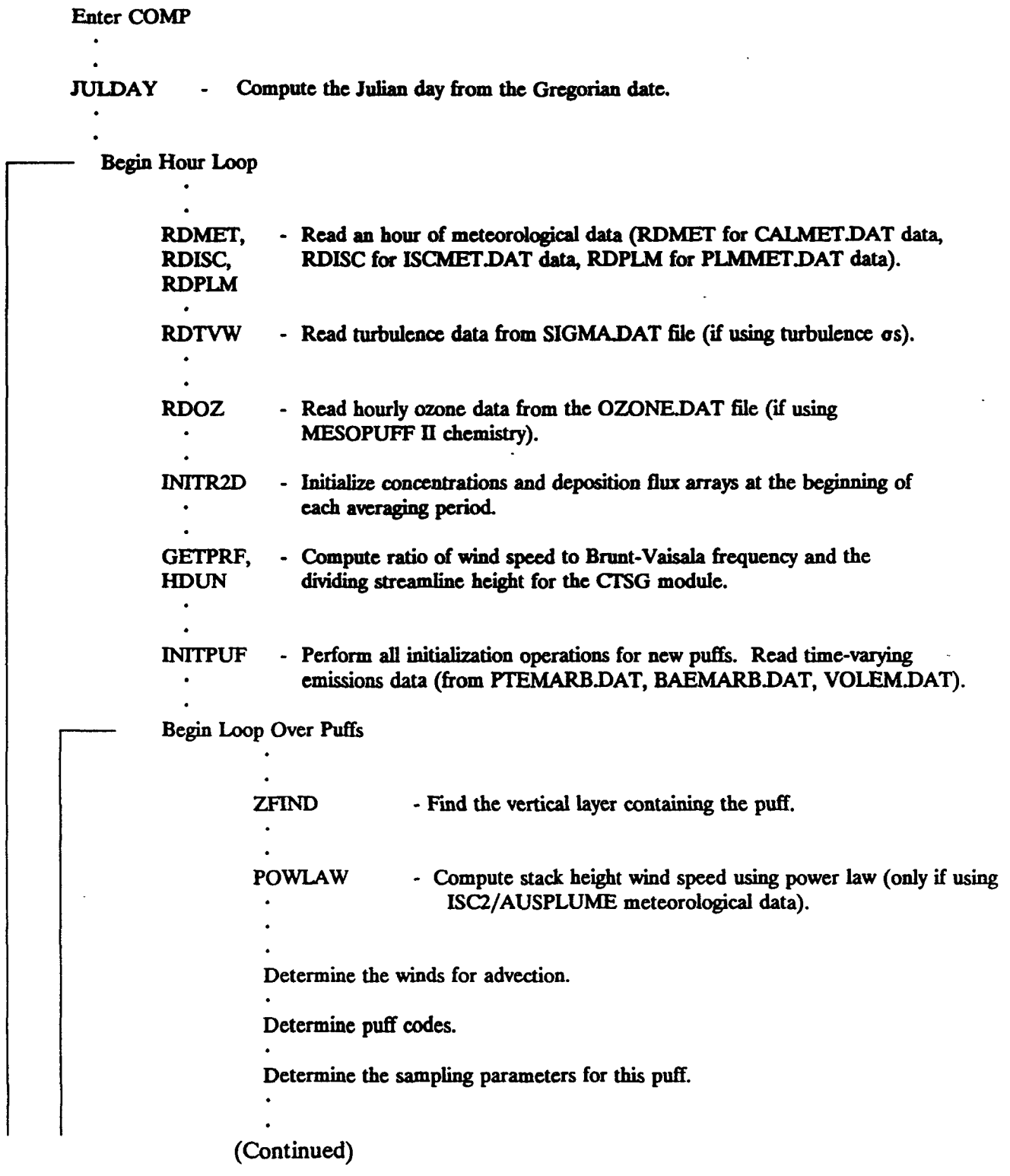


Figure 3-3. Flow diagram showing the calling sequence of major routines in Subroutine COMP (Computational Phase).

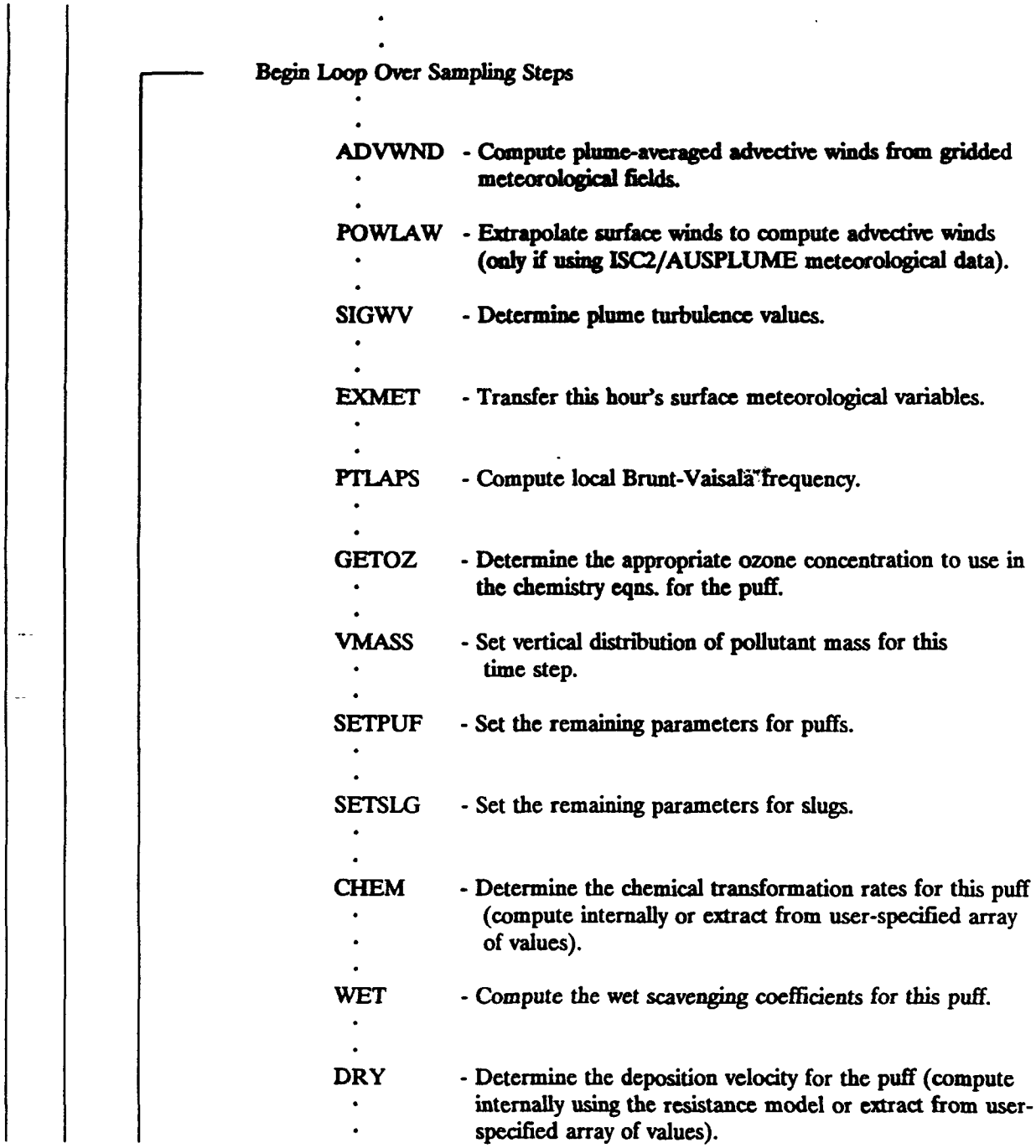


Figure 3-3. Flow diagram showing the calling sequence of major routines in Subroutine COMP (Computational Phase).

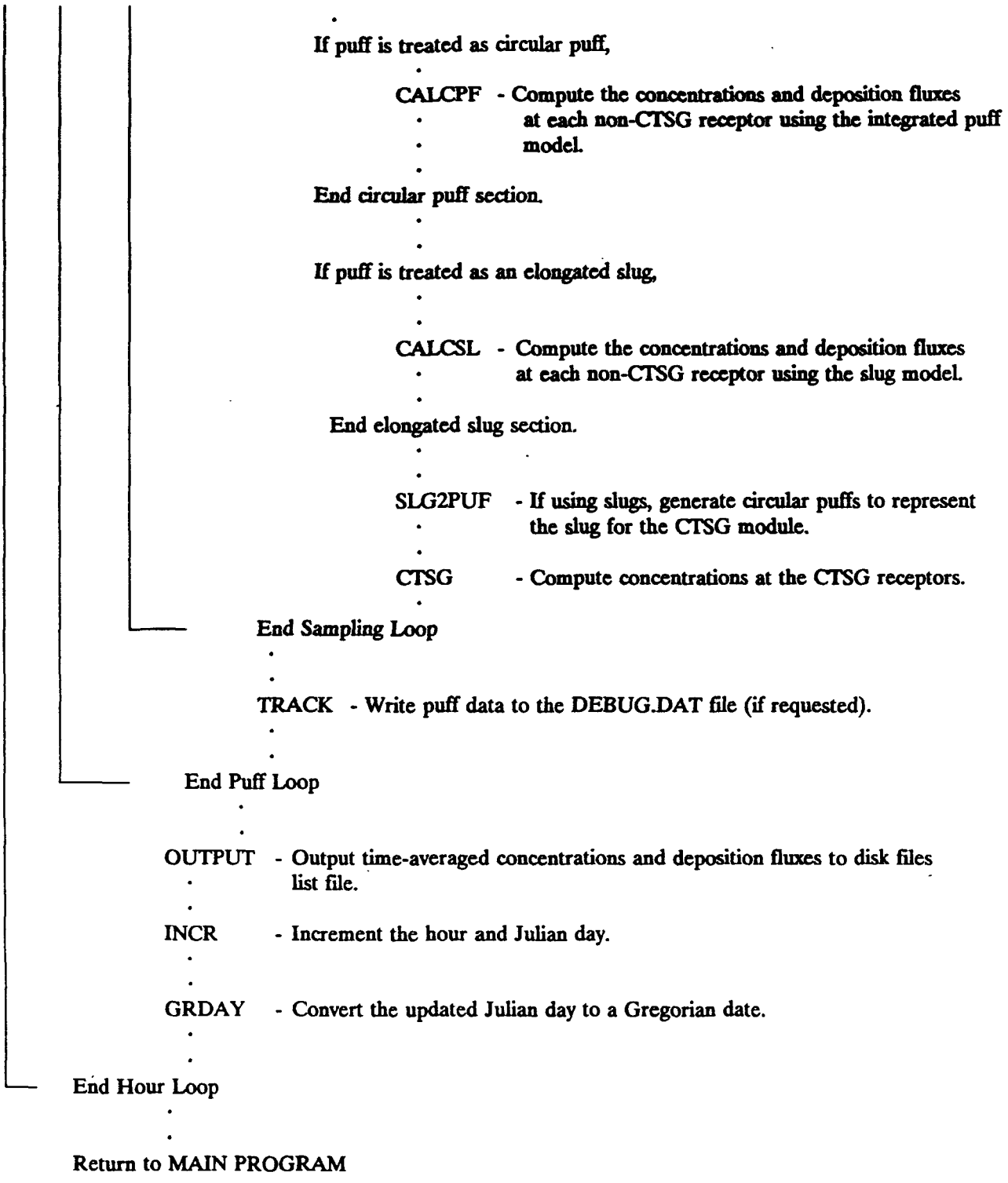


Figure 3-3. Flow diagram showing the calling sequence of major routines in Subroutine COMP (Computational Phase). (Concluded).

4. USER'S INSTRUCTIONS

4.1 OPTHILL

When the subgrid scale complex terrain (CTSG) option of the CALPUFF model is invoked, two groups of additional data must be prepared by the user and entered into the CALPUFF control file: non-gridded receptor information and sub-grid scale terrain information. The purpose of the optimizer program OPTHILL is to provide the user with the means for calculating the set of terrain data that best characterizes each feature.

4.1.1 CTSG Terrain Information

CTSG requires information on the location, orientation, size, and shape of each terrain feature being modeled (see Section 4.2.2). The variables that contain this information are:

xc,yc	coordinates (km) of the center of the hill
thetah	orientation (deg) of major axis of hill (clockwise from north)
zgrid	height (m) of "grid-plane" of grid above mean sea level
relief	height (m) of crest of hill above the "grid-plane" elevation
expo (1)	hill-shape exponent for major axis
expo (2)	hill-shape exponent for minor axis
scale(1)	horizontal length scale (m) along major axis
scale(2)	horizontal length scale (m) along minor axis
axmax(1)	maximum allowed axis length (m) for major axis
axmax(2)	maximum allowed axis length (m) for minor axis

The profile of the terrain along each axis of the feature is prescribed by the following equation:

$$ht(x) = \left[\frac{1 - (x/axmax)^{expo}}{1 + (x/scale)^{expo}}\right] * relief \qquad (4\text{-}1)$$

where ht is the height of the profile above the base of the feature, at a distance x from the peak (Figure 4-1).

The terrain profile-optimizing program (OPTHILL) computes the hill shape exponent (EXPO) and horizontal terrain length scale (SCALE) parameters from a user-entered terrain profile along each of two axes. This terrain profile defines the height of the surface of the hill at a number of distances from the center of the hill, along each axis. The OPTHILL program

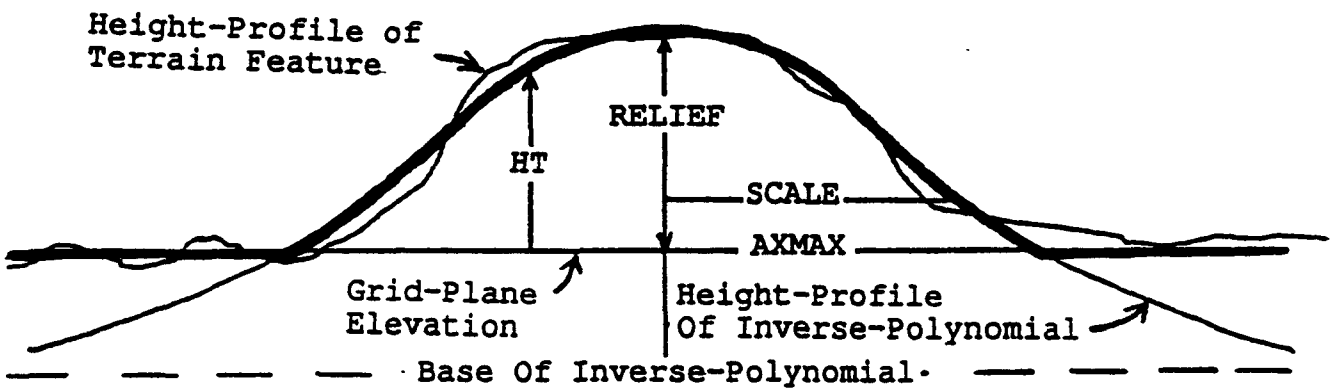


Figure 4-1. Profile of a terrain feature along one of its two axes. A best-fit inverse polynomial function describes this profile to CTSG.

performs computations for one axis (i.e., major or minor axis) of the terrain feature at a time. Therefore, two runs of OPTHILL are necessary for each subgrid scale terrain feature.

The following procedure is recommended to determine the terrain inputs for the CALPUFF CTSG algorithm from a topographic map.

a. Identify the sub-grid terrain features to be modeled.

Such features will generally be small enough that they could be contained within one grid-square. This does not mean that they cannot straddle two or more squares. The features should be prominent, and possibly lie near source regions so that the additional computations required by CTSG are warranted in resolving important pollutant impact areas.

b. Decide on the orientation of the feature.

The orientation of the feature is generally evident if the feature is longer in one direction than another. If there is no dominant direction to the feature, model it as a symmetric feature, and choose an orientation of north.

c. Obtain height-profiles along each axis of the feature.

Choose an approximate center for the feature and draw axes through it (one axis should lie along the direction of orientation). Along each axis, measure the distance between approximate intersections of the axis with marked contours. The distances so measured should extend from the contour furthest to the south to the same contour furthest to the north (for a north-south axis). Divide each of these distances by two, and tabulate the results.

d. Identify the maximum elevation of the feature.

Take the peak elevation directly from the map.

e. Identify the elevation at the base of the feature.

Generally, the base of the feature will be that point at which the feature becomes indistinguishable from terrain variations around it.

f. Convert all elevations that were tabulated to heights above the base of the feature.

g. Use optimizer program (OPTHILL) to obtain shape parameters.

The "relief" parameter is just the peak elevation less the base elevation. The "axmax" value for each axis should be representative of the maximum extent of the feature along each axis at the elevation of the base of the feature. With these two variables fixed for each axis, the height-profile data from step c. can be put through OPTHILL to obtain "expo" and "scale" for each axis.

OPTHILL requires a single input file (OPTHILL.INP) which contains the user's inputs describing the terrain profile, each height, and maximum axis length. The computed volumes of EXPO and SCALE for one axis of the hill are listed in the output list file (OPTHILL.LST). Table 4-1 summarizes the OPTHILL input and output file contents. The format and contents of the OPTHILL control file are variables explained in Table 4-2.

4.1.2 Example OPTHILL Application

The OPTHILL program is an optimization that takes a value of "relief" and "axmax," and a sequence of pairs of (x,ht) values along an axis, and returns a value of "expo" and "scale" that prescribes the profile function that best matches the (x,ht) pairs. Its use is illustrated by the following example.

Figure 4-2 shows the terrain surrounding the site of EPA's "Full-Scale Plume Study" (FSPS) that was performed in the Truckee River Valley near Reno, NV (Strimaitis et al., 1985), as part of the Complex Terrain Model Development Program. Nocturnal flow in this valley is frequently channeled by the high terrain to the north and south of the Tracy power plant. Elevations typical of nocturnal plume heights (4600-4800 ft. MSL) are emphasized on the figure. Given the predominant flow to the east during stable conditions, there is potential for plume impact on the feature just northeast of the plant. This feature, marked by axes in Figure 4-2, was named "Beacon Hill" during the study.

Following the procedures outlined above, axes were drawn over the feature and distances between fixed contour elevations were tabulated. After subtracting the elevation above sea level of the base of the feature (the floor of the river valley), these data were entered into two files. Figure 4-3 displays the contents of both files. The files (names axis1.inp and axis2.inp) contain "relief" and the value for "axmax" for each axis of the hill, followed by five pairs of (x,ht) values. The first record of each file is reserved for comments to identify the data. Values for "relief"

Table 4-1
OPTHILL Input and Output Files

Unit	File Name	Type	Format	Description
5	OPTHILL.INP	input	formatted	Control file containing user inputs
6	OPTHILL.LST	output	formatted	List file (line printer output file

Table 4-2
OPTHILL Control File Inputs (OPTHILL.INP)

Record	Variable No.	Variable Name	Columns	Type of Format	Description
1	1	TITLE(15)	1-60	15A4	60 character title
2	1	RELIEF	*	real	Height (m) of the crest of the hill above the grid elevation
3	1	AXMAX	*	real	Maximum allowed axis length (m) for the axis (major or minor) being evaluated
4	1	-	*	-	This record is skipped by the program. May contain optional text data (see example)
5	1	DIST	*	real	Distance-height pairs describing the profile of the terrain. Units: m
5	2	HGT	*	real	Distance-height pairs describing the profile of the terrain. Units: m

* Entered in FORTRAN free format.

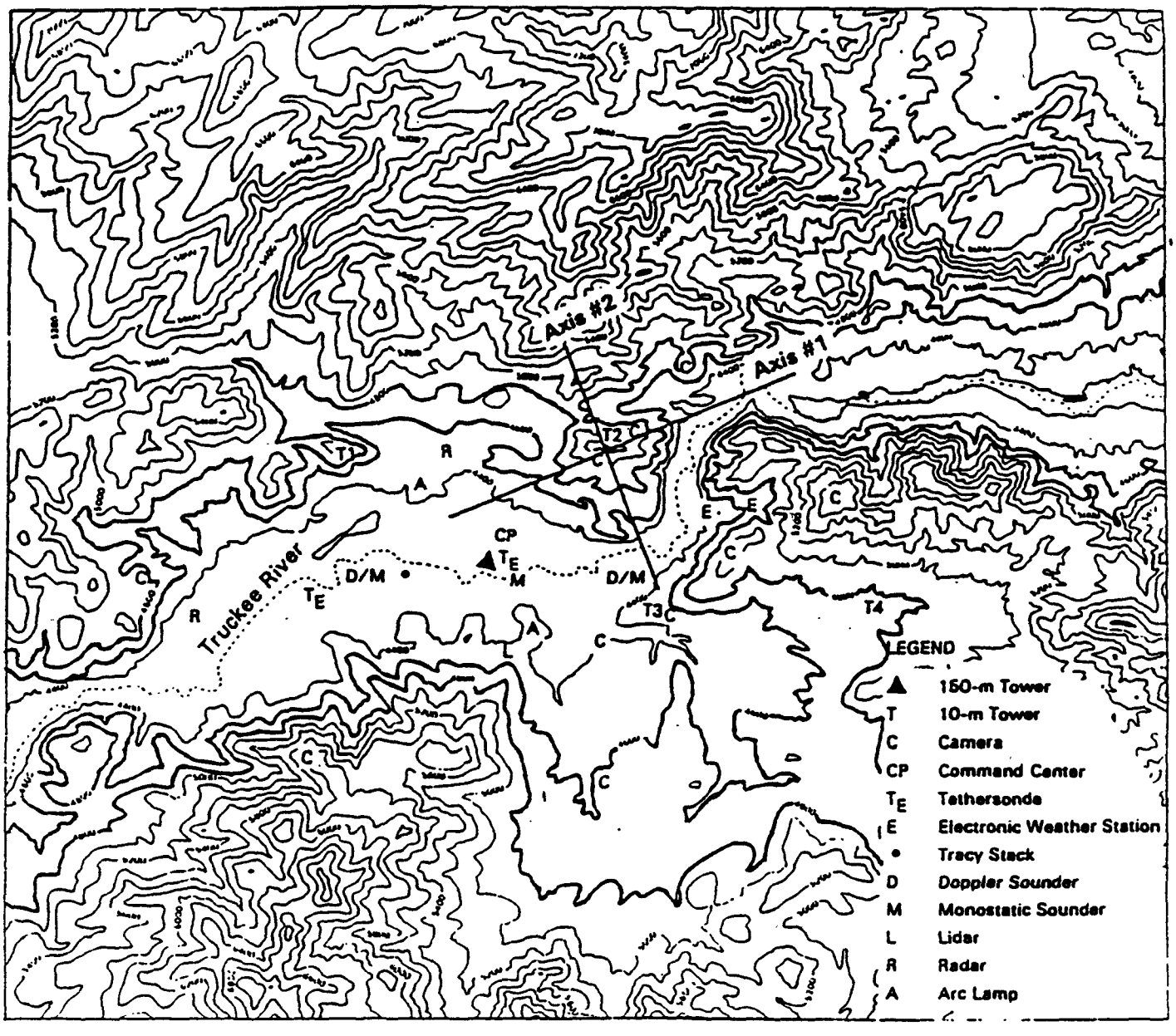


Figure 4-2. Map of terrain surrounding the site of the FSPS, illustrating the selection and characterization of a terrain feature for CTSG modeling.

```
Optimal SCALE and EXPO factors -- Axis #1 of example problem
300.- Height (m) of hill crest above "zero-plane" elevation (RELIEF)
2000.- Maximum allowed length (m) for this axis (AXMAX)
---------- Distance-height pairs describing hill profile ----------
564.,239.- Dist.(m) from crest, terrain ht (m) above "zero-plane" elev.
826.,  178.      (Repeated for each dist.-height pair)
1062.,  150.
1193.,  117.
1508.,   56.
```

(a) OPTHILL.INP for Axis #1 of the hill.

```
Optimal SCALE and EXPO factors -- Axis #2 of example problem
300.                          - Height (m) of hill crest above "zero-plane" elevation (RELIEF)
1500.                         - Maximum allowed length (m) for this axis (AXMAX)
----------                    - Distance-height pairs describing hill profile ----------
302.,  239.                   - Dist.(m) from crest, terrain ht (m) above "zero-plane" elev.
551.,  178.                     (Repeated for each dist.-height pair)
708.,  150.
970.,  117.
1311.,  56.
```

(b) OPTHILL.INP for Axis #2 of the hill.

Figure 4-3. Sample OPTHILL input files for (a) Axis #1 and (b) Axis #2 of the hill is in the example.

and "axmax" are free-format, and should be entered anywhere in the open space provided on the next two lines. Pairs of (x,ht) should be entered right after the next comment record.

OPTHILL must be invoked separately for each of the two axes of the hill. This is accomplished by renaming one input file (e.g., axis1.inp) to the OPTHILL input control file name (OPTHILL.INP), executing the program, renaming the output file (OPTHILL.LST) to a new name (e.g., axis1.lst), and then repeating these steps for the second axis of the hill. The output files produced by OPTHILL for the current example are presented in Figure 4-4 and 4-5. The output file lists the final values of the profile parameters, and it also lists the profile data provided by the user along with the corresponding data computed from the profile parameters.

With these results, hill information that is independent of the choice of coordinate system and the modeling grid for the wind model can be specified:

xc,yc (m)	(depends on choice of coordinates)
thetah (deg)	69°
zgrid (m)	(depends on grid for wind model)
relief (m)	300.
expo (1)	1.91
expo (2)	1.24
scale (1) (m)	1523.
scale (2) (m)	2896.
axmax (1) (m)	2000.
axmax (2) (m)	1500.

Note that scale(2) is almost twice scale(1), even though axis 1 corresponds to the longer axis of the hill. This can occur because the "scale" parameter is a property of the entire inverse-polynomial function (Equation 4-1), rather than just the portion of the function that is fit to the profile of the terrain. In Figure 4-1, the shape of the terrain might best conform to the upper 10% of the polynomial function, in which case the "scale" parameter would exceed "axmax." In this example application of the OPTHILL program, we see that axmax(2) is substantially less than axmax(1), whereas scale(2) exceeds scale(1), indicating that a comparatively smaller portion of the polynomial function represents the terrain profile along the minor axis.

*** Optimal SCALE and EXPO factors – Axis #1 of example problem ***

EVOL TIME LIMIT = 60. SECONDS SKIP = 10

NUMBER OF PARAMETERS FOR THIS STUDY : 4

PARAMETER		START VALUE	STEP CONTROL	LOWER LIMIT	UPPER LIMIT
1 RELIEF	0.3000E+03	0.0000E+00	0.3000E+03	0.3000E+03	
2 AXMAX	0.2000E+04	0.0000E+00	0.2000E+04	0.2000E+04	
3 EXPO	0.2000E+01	0.2000E+01	0.1000E+00	0.1000E+02	
4 SCALE	0.2000E+04	0.1000E+04	0.2000E+02	0.2000E+06	

CALCULATIONS STARTED

RETURN VALUE: 2 NORMAL RETURN FUNCTION VALUE: 0.50303

PARAMETER VALUES:

RELIEF	=	300.00000
AXMAX	=	2000.00000
EXPO	=	1.90651
SCALE	=	1522.94500

Distance	Height	Fitted Value
564.0	239.0	237.4
826.0	178.0	186.4
1062.0	150.0	139.9
1193.0	117.0	115.5
1508.0	56.0	63.0

Figure 4-4. Content of output file produced by OPTHILL in processing axis #1 of sample hill.

*** Optimal SCALE and EXPO factors -- Axis #2 of example problem ***

EVOL TIME LIMIT = 60. SECONDS SKIP = 10

NUMBER OF PARAMETERS FOR THIS STUDY : 4

PARAMETER		START VALUE	STEP CONTROL	LOWER LIMIT	UPPER LIMIT
1 RELIEF	0.3000E+03	0.0000E+00	0.3000E+03	0.3000E+03	
2 AXMAX	0.1500E+04	0.0000E+00	0.1500E+04	0.1500E+04	
3 EXPO	0.2000E+01	0.2000E+01	0.1000E+00	0.1000E+02	
4 SCALE	0.1500E+04	0.7500E+03	0.1500E+02	0.1500E+06	

CALCULATIONS STARTED

RETURN VALUE: 2 NORMAL RETURN FUNCTION VALUE: 2.17504

PARAMETER VALUES:

RELIEF = 300.00000
AXMAX = 1500.00000
EXPO = 1.23912
SCALE = 2895.90200

Distance	Height	Fitted Value
302.0	239.0	244.4
551.0	178.0	189.1
708.0	150.0	154.7
970.0	117.0	99.5
1311.0	56.0	33.0

Figure 4-5. Content of output file produced by OPTHILL in processing axis #2 of sample hill.

4.2 CALPUFF Model Input Files

The CALPUFF model obtains the necessary information concerning sources, receptors, meteorological data, geophysical data, and model control parameters from a series of input files. These files are listed in Table 1-2. The model creates several output files, which are listed in Table 1-4. In this section, detailed information on the structure and content of each of the input and output files is provided.

Tables 1-2 and 1-4 show the Fortran unit numbers associated with each file. As indicated in Section 3.1, these unit numbers are specified in the parameter file (PARAMS.PUF). They can be easily modified to accommodate system-dependent restrictions on allowable unit numbers. Any changes to variables in the parameter file are automatically modified throughout the CALPUFF Fortran code. The code must be re-compiled for changes in the parameter file to take effect, since the parameter values are set at the program compilation stage rather than at program execution.

The name and full path of each CALPUFF file (except one) is assigned in an I/O file. The exception, the I/O filename itself, is assigned on the command line. For example, on a DOS system,

```
CALPUF3  d:\CALPUFF\PUFFILES.DAT
```

will execute the CALPUFF code (CALPUF3.EXE), and read the input and output filenames for the current run from the file PUFFILES.DAT in the directory d:\CALPUFF. If the I/O filename is not specified on the command line, the default I/O filename (i.e., PUFFILES.DAT in the current working directory) will be used. The I/O path and filename can be up to 70 characters long.

The utility routine that delivers a command line argument is system dependent. The function that provides the system clock time and system CPU time are also system or compiler-specific. All system-dependent or compiler-specific routines in CALPUFF are isolated into a file called DATETM.xxx, where the file extension (.xxx) indicates the system for which the code is designed. For example, DATETM.HP contains code for Hewlett-Packard Unix systems, DATETM.SUN is for Sun Unix systems, DATETM.LAH is for Lahey-compiled PC-applications, and DATETM.MS is for Microsoft-compiled PC applications. By appending the correct system-dependent DATETM file onto the main CALPUFF code, the code should run without any modifications.

A sample I/O file is shown in Table 4-3. Each CALPUFF input and output file has a default name and path (i.e., the current working directory). If the filename is not specified in the I/O file, the default name will be assumed. Each filename must be less than or equal to 70 characters long.

The I/O file is read by the CALPUFF control file reader module. Therefore, the same syntax rules that apply to the control file (explained in Section 4.2.1) also apply to the I/O file. Basically, all text except that between the delimiters (i.e., ! characters) is treated as user comments, and is ignored by the input module. Between the delimiters, the character filename variables (e.g., PUFINP, METDAT, PUFLST, etc.) must be entered as shown in the sample file. The control file reader is case insensitive. The filename is placed between the equals sign and the right delimiter character (!). Files that are not used or are not to be changed from their default names can be omitted from the I/O file. For example, by replacing the delimiter characters ("!"s) with "*"s, the line becomes a comment, and will not be interpreted by the program as data:

! PUFINP = calpuff.inp !	- this line sets the control file name
* PUFINP = calpuff.old *	- this line is a comment that does nothing
* PUFLST = *	- this line is OK (interpreted as a comment)
! PUFLST = !	- this is not OK (delimiters present, so file must be specified)

Blanks within the delimiters are ignored, and all delimiters must appear in pairs. If the optional CALPUFF GUI is being used, the I/O file will automatically be correctly formatted and written to disk for used by CALPUFF.

4.2.1 User Control File (CALPUFF.INP)

The selection and control of CALPUFF options are determined by user-specified inputs contained in a file called the control file. This file, CALPUFF.INP, contains all the information necessary to define a model run (e.g., starting date, run length, grid specifications, technical options, output options, etc.).

Table 4-3
Sample CALPUFF I/O File (PUFFILES.DAT)

```
                        CALPUFF file names
                        ==================

Common input and output files
-----------------------------
Default Name  Type          File Name
------------  ----          ---------
CALPUFF.INP   input    ! PUFINP =d:\calpuff\testcase\CALPUFF.INP    !
CALMET.DAT    input    ! METDAT =d:\calpuff\testcase\CALMET.DAT     !
    or
ISCMET.DAT    input    ! iscdat =test.met      !
    or
PLMMET.DAT    input    ! plmdat =austest.met   !
-------------------------------------------------------------------------------
CALPUFF.LST   output   ! PUFLST =CALPUFF2.LST  !
CONC.DAT      output   ! CONDAT =CONC2.DAT     !
DFLX.DAT      output   ! DFDAT  =DFLX2.DAT     !
WFLX.DAT      output   ! WFDAT  =WFLX2.DAT     !
VISB.DAT      output   ! VISDAT =VISB2.DAT     !
-------------------------------------------------------------------------------
Emission files
--------------
PTEMARB.DAT   input    ! ptdat  =ptemarb.dat   !
VOLEM.DAT     input    ! voldat =volem.dat     !
BAEMARB.DAT   input    ! ardat  =baemdat.dat   !
-------------------------------------------------------------------------------
Other Files
-----------
OZONE.DAT     input    ! OZDAT  =OZONE.DAT     !
SIGMA.DAT     input    ! sigdat =sigma.dat     !
VD.DAT        input    ! vddat  =vd.dat        !
CHEM.DAT      input    ! chemdat=chem.dat      !
HILL.DAT      input    ! hildat =hill.dat      !
DEBUG.LST     output   ! debug  =debug.lst     !
-------------------------------------------------------------------------------
All filenames will be converted to lower case if LCFILES = T
Otherwise, if LCFILES = F, file names will be converted to UPPER CASE
         T = lower case      ! LCFILES = T !
         F = UPPER CASE
!END!
-------------------------------------------------------------------------------
NOTE: (1) file/path names can be up to 70 characters in length
```

CALPUFF has a PC-based, Windows-compatible Graphical User Interface (GUI) that can be used to prepare the CALPUFF control file (CALPUFF.INP), execute the model, or conduct file management functions. The user interface contains an extensive help system that makes much of the information in this manual available to the user on-line.

The source data and receptor information required for a CALPUFF run can be entered through the edit screens or read from external ASCII files (spreadsheet-compatible). Each source type (points, areas, volumes, and lines) contains an external ASCII file format description and sample file in the help system.

Although the model can be set up and run entirely within the user interface system, the interface is designed to always create an ASCII CALPUFF.INP file. This allows runs to be set up on PC-based systems and the control file transferred to workstation or mainframe computer for computational intensive applications. The ASCII CALPUFF.INP file should be directly transportable to virtually any non-PC system. Also, the model can be setup and run entirely on a non-PC system by using a conventional editor directly on the CALPUFF.INP file, which itself contains extensive self-documenting statements.

The control file is organized into 17 major Input Groups and a variable number of subgroups within several of the major Input Groups. The first three lines of the input file consist of a run title. As shown in Table 4-4, the major Input Groups are defined along functional lines (e.g., technical options, output options, subgrid scale, complex terrain inputs, etc.). Each subgroup contains a set of data such as source variables, subgrid scale hill descriptions, or discrete receptor information. The number of subgroups varies with the number of sources, hills, etc., in the model run.

A sample control file is shown in Table 4-5. The control file is read by a set of Fortran text processing routines contained within CALPUFF which allow the user considerable flexibility in designing and customizing the input file. An unlimited amount of optional descriptive text can be inserted within the control file to make it self-documenting. For example, the definition, allowed values, units, and default value of each input variable can be included within the control file.

The control file processor searches for pairs of special delimiter characters (!). All text outside the delimiters is assumed to be user comment information and is echoed back but otherwise ignored by the input module. Only data within the delimiter characters is processed. The input data consists of a leading delimiter followed by the variable name, equals sign, input

value or values, and a terminating delimiter (e.g., !XX = 12.5 !). The variable name can be lower or upper case, or a mixture of both (i.e., XX, xx, Xx are all equivalent). The variable type can be real, integer, logical, or character and it can be an array or a scalar. The use of repetition factors for arrays is allowed (e.g., ! XARRAY = 3 * 1.5 ! instead of ! XARRAY = 1.5, 1.5, 1.5 !). Different values must be separated by commas. Spaces within the delimiter pair are ignored. Exponential notation (E format) for real numbers is allowed. However, the optional plus sign should be omitted (e.g., enter +1.5E+10 as 1.5E10). The data may be extended over more than one line (except for character variables, which must be entirely on one line). The line being continued must end with a comma. Each leading delimiter must be paired with a terminating delimiter. All text between the delimiters is assumed to be data, so no user comment information is allowed to appear within the delimiters. The inclusion in the control file of any variable that is being assigned its default value is optional. The control file reader expects that logical variables will be assigned using only a one character representation (i.e., 'T' or 'F').

The major Input Groups must appear in order, i.e., Input Group 1 followed by Input Group 2, etc. However, the variables within an Input Group may appear in any order. The variable names in each Input Group are independent, so that the same name can be repeated in different Input Groups (e.g., as shown in the sample control file, species names (SO2, SO4) are use in several Input Groups). Each Input Group and subgroup must end with an Input Group terminator consisting of the word END between two delimiters (i.e., !END!). Every major Input Group, even blank Input Groups (i.e., one in which no variables are included) must end with an Input Group terminator in order to signal the end of that Input Group and the beginning of another.

The control file module has a list of variable names and array dimensions for each Input Group. Checks are performed to ensure that the proper variable names are used in each Input Group, and that no array dimensions are exceeded. Error messages result if an unrecognized variable name is encountered or too many values are entered for a variable.

Table 4-4
Input Groups in the CALPUFF Control File

Input Group	Description
*	**Run title** First three lines of control file (up to 80 characters/line)
1	General run control parameters Starting date and hour, run length, time step. Number of species.
2	Technical options Control variables determining methods for treating chemistry, wet deposition, dry deposition, dispersion, plume rise, complex terrain, and near-field puff sampling methods
3	Species list Species names, flags for determining which species are modeled, advected, emitted, and dry deposited
4	Grid control parameters Specification of meteorological, computational, and sampling grids, number of cells, vertical layers, and reference coordinates.
5	Output options Printer control variables, disk output control variables
6a,b,c	Subgrid scale complex terrain (CTSG) inputs Information describing subgrid scale hill location, shape and height. Complex terrain receptor locations and elevations.
7	Dry deposition parameters - Gases Pollutant diffusivity, dissociation constant, reactivity, mesophyll resistance, Henry's law coefficient
8	Dry deposition parameters - Particles Geometric mass mean diameter, geometric standard deviation

Table 4-4 (Concluded)
Input Groups in the CALPUFF Control File

Input Group	Description
9	Miscellaneous dry deposition parameters Reference cuticle and ground resistances, reference pollutant reactivity, vegetation state
10	Wet deposition parameters Scavenging coefficients for each pollutant and precipitation type (liquid and frozen precipitation)
11	Chemistry parameters Control variables for input of ozone data, background ozone and ammonia concentrations, nighttime transformation rates
12	Miscellaneous dispersion parameters and computational parameters Vertical dispersion constants, dispersion rate above the boundary layer, crossover distance to time-dependent dispersion coefficients, land use associated with urban dispersion
13a,b,c	Point source parameters Point source data including source location, stack parameters and emissions, and building dimensions
14a,b	Area source parameters Area source data including source location, effective height, elevation, initial sigmas and emission rates
15a,b	Line source parameters Buoyant line source data including source location, line length, buoyancy parameters, release height, and emission rates
16a,b	Volume source parameters Volume source data including source location, effective height, initial size data
17a,b	Non-gridded (discrete) receptor information Receptor coordinates and ground elevation

Table 4-5
Sample CALPUFF Control File (CALPUFF.INP)
Input Groups 1 and 2

```
CALPUFF test run -- 3 hour simulation
10 x 10 meteorological grid
1 point source and CTSG hill set up to compare with INPUFF_3 test
---------------- Run title (3 lines) ------------------------------------------

                  CALPUFF MODEL CONTROL FILE
                  --------------------------

------------------------------------------------------------------------------

INPUT GROUP: 1 -- General run control parameters
--------------

     Starting date:   Year (IBYR) -- No default       ! IBYR=  94  !
                     Month (IBMO) -- No default       ! IBMO=  11  !
                       Day (IBDY) -- No default       ! IBDY=  1   !
                      Hour (IBHR) -- No default       ! IBHR=  10  !

     Length of run (hours) (IRLG) -- No default       ! IRLG=  2   !

     Number of chemical species (NSPEC)
                                  Default: 5          ! NSPEC=  2  !

     Number of chemical species
     to be emitted  (NSE)         Default: 3          ! NSE=  1  !

     Flag to stop run after
     SETUP phase (ITEST)          Default: 2          ! ITEST=  2  !
     (Used to allow checking
     of the model inputs, files, etc.)
          ITEST = 1 - STOPS program after SETUP phase
          ITEST = 2 - Continues with execution of program
                      after SETUP

     Meteorological Data Format (METFM)
                                  Default: 1          ! METFM =  2  !

          METFM = 1 - CALMET binary file (CALMET.DAT)
          METFM = 2 - ISC ASCII file (ISCMET.DAT)
          METFM = 3 - AUSPLUME ASCII file (PLMMET.DAT)

     Averaging Time (minutes) (AVET)
                                  Default: 60.0       ! AVET = 60.0 !
     PG sigma-y is adjusted by the equation
     (AVET/60.0)**0.2


!END!


------------------------------------------------------------------------------

INPUT GROUP: 2 -- Technical options
--------------


     Vertical distribution used in the
     near field (MGAUSS)                 Default: 1     ! MGAUSS =  1  !
        0 = uniform
        1 = Gaussian
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 2

```
Terrain adjustment method
(MCTADJ)                          Default: 1     ! MCTADJ =  0  !
   0 = no adjustment
   1 = ISC-type of terrain adjustment
   2 = simple, CALPUFF-type of terrain
       adjustment *

Subgrid-scale complex terrain
flag (MCTSG)                      Default: 0     ! MCTSG =  0  !
   0 = not modeled
   1 = modeled

Near-field puffs modeled as
elongated 0 (MSLUG)               Default: 1     ! MSLUG =  1  !
   0 = no
   1 = yes (slug model used)

Transitional plume rise modeled ?
(MTRANS)                          Default: 1     ! MTRANS =  0  !
   0 = no  (i.e., final rise only)
   1 = yes (i.e., transitional rise computed)

Stack tip downwash? (MTIP)        Default: 1     ! MTIP =  0 !
   0 = no  (i.e., no stack tip downwash)
   1 = yes (i.e., use stack tip downwash)

Effects on plume rise of vertical wind shear
above stack top modeled ? (MSHEAR)  Default: 0   ! MSHEAR =  0  !
   0 = no  (i.e., shear not modeled)
   1 = yes (i.e., shear modeled)

Puff splitting allowed ? (MSPLIT)   Default: 0   ! MSPLIT = 0  !
   0 = no (i.e., puffs not split)
   1 = yes (i.e., puffs are split)

Chemical mechanism flag (MCHEM)     Default: 1   ! MCHEM =  0  !
   0 = chemical transformation not
       modeled
   1 = transformation rates computed
       internally (MESOPUFF II scheme)
   2 = user-specified transformation
       rates used

Wet removal modeled ? (MWET)        Default: 1   ! MWET =  0  !
   0 = no
   1 = yes

Dry deposition modeled ? (MDRY)     Default: 1   ! MDRY =  0  !
   0 = no
   1 = yes
   (dry deposition method specified
    for each species in Input Group 3)
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 2

```
Method used to compute dispersion
coefficients (MDISP)                Default: 4   ! MDISP =  3  !

   1 = dispersion coefficients computed from values of
       sigma v, sigma w read from SIGMA.DAT file
   2 = dispersion coefficients sigma v, sigma w computed
       internally from micrometeorological variables (u*, w*, L, etc.)
   3 = PG dispersion coefficients for RURAL areas (computed using
       the ISCST multi-segment approximation) and MP coefficients in
       urban areas
   4 = same as 3 except PG coefficients computed using
       the MESOPUFF II eqns.
   5 = CTDM sigmas used for stable and neutral conditions.
       For unstable conditions, sigmas are computed as in
       MDISP = 1, described above.  MDISP = 5 assumes that
       sigma v, sigma w are read from a SIGMA.DAT file

PG sigma-y, z adj. for roughness?       Default: 0    ! MROUGH =  1  !
(MROUGH)
   0 = no
   1 = yes

Partial plume penetration of            Default: 0    ! MPARTL =  1  !
elevated inversion?
(MPARTL)
   0 = no
   1 = yes

Test options specified to see if
they conform to regulatory
values? (MREG)                      Default: 0   ! MREG =  0  !

   0 = NO checks are made
   1 = Technical options must conform to USEPA values for
       short-range modeling ( e.g. ISC-type applications)
   2 = Technical options must conform to USEPA values for
       long-range modeling (e.g. visibility-type applications)
   3 = Environmental Protection Authority of Victoria (EPAV)
       default values

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Groups 3 and 4

```
------------------------------------------------------------------------------

INPUT GROUP: 3 -- Species list
-------------

The following species are modeled:

! CSPEC = SO2 !  !END!
! CSPEC = SO4 !  !END!

                                                 Dry
SPECIES          MODELED          EMITTED      DEPOSITED
 NAME       (0=NO, 1=YES)    (0=NO, 1=YES)  (0=NO,
                                             1=COMPUTED-GAS
                                             2=COMPUTED-PARTICLE
                                             3=USER-SPECIFIED)
! SO2        =     1 ,              1 ,          1            !
! SO4        =     1 ,              0 ,          2            !

!END!

------------------------------------------------------------------------------

INPUT GROUP: 4 -- Grid control parameters
-------------

METEOROLOGICAL grid:

           No. X grid cells (NX)      No default     ! NX =  10  !
           No. Y grid cells (NY)      No default     ! NY =  10  !
         No. vertical layers (NZ)     No default     ! NZ =  2   !

           Grid spacing (DGRIDKM)     No default     ! DGRIDKM = 4.0 !
                                      Units: km

               Cell face heights
                   (ZFACE(nz+1))      No defaults
                                      Units: m
                                                     ! ZFACE = 0.0, 200.0, 1000.0 !
            Reference Coordinates
           of SOUTHWEST corner of
                grid POINT(1, 1):

            X coordinate (XORIGKM)    No default     ! XORIGKM = -4.0 !
            Y coordinate (YORIGKM)    No default     ! YORIGKM = -4.0 !
                                      Units: km

                UTM zone (IUTMZN)     No default     ! IUTMZN =  19  !

   Reference coordinates of CENTER
        of the domain
            Latitude  (deg.) (XLAT)   No default     ! XLAT  = 42.0  !
           Longitude (deg.) (XLONG)   No default     ! XLONG = 75.0  !
             Time zone        (XTZ)   No default     ! XTZ   = 5.0   !
       (PST=8, MST=7, CST=6, EST=5)
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 4

```
Computational grid:

     The computational grid is identical to or a subset of the MET. grid.
     The lower left (LL) corner of the computational grid is at grid point
     (IBCOMP, JBCOMP) of the MET. grid.  The upper right (UR) corner of the
     computational grid is at grid point (IECOMP, JECOMP) of the MET. grid.
     The grid spacing of the computational grid is the same as the MET. grid.

        X index of LL corner (IBCOMP)      No default     ! IBCOMP =  1  !
                  (1 <= IBCOMP <= NX)

        Y index of LL corner (JBCOMP)      No default     ! JBCOMP =  1  !
                  (1 <= JBCOMP <= NY)


        X index of UR corner (IECOMP)      No default     ! IECOMP =  10 !
                  (1 <= IECOMP <= NX)

        Y index of UR corner (JECOMP)      No default     ! JECOMP =  10 !
                  (1 <= JECOMP <= NY)


SAMPLING GRID (GRIDDED RECEPTORS):

     The lower left (LL) corner of the sampling grid is at grid point
     (IBSAMP, JBSAMP) of the MET. grid.  The upper right (UR) corner of the
     sampling grid is at grid point (IESAMP, JESAMP) of the MET. grid.
     The sampling grid must be identical to or a subset of the computational
     grid.  It may be a nested grid inside the computational grid.
     The grid spacing of the sampling grid is DGRIDKM/MESHDN.  The number of sampling
     grid points is NXSAM * NYSAM, where:
                                        NXSAM = MESHDN*(IESAMP-IBSAMP)+1
                                        NYSAM = MESHDN*(JESAMP-JBSAMP)+1

        Logical flag indicating if gridded
        receptors are used (LSAMP)         Default: T     ! LSAMP = T !
        (T=yes, F=no)

        X index of LL corner (IBSAMP)      No default     ! IBSAMP =  1  !
         (IBCOMP <= IBSAMP <= IECOMP)

        Y index of LL corner (JBSAMP)      No default     ! JBSAMP =  1  !
         (JBCOMP <= JBSAMP <= JECOMP)


        X index of UR corner (IESAMP)      No default     ! IESAMP =  10 !
         (IBCOMP <= IESAMP <= IECOMP)

        Y index of UR corner (JESAMP)      No default     ! JESAMP =  10 !
         (JBCOMP <= JESAMP <= JECOMP)

       Nesting factor of the sampling
        grid (MESHDN)                      No default     ! MESHDN =  1  !
        (MESHDN is an integer >= 1)

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 5

```
------------------------------------------------------------------------

INPUT GROUP: 5 -- Output Options
--------------

                                        *                       *
     FILE                          DEFAULT VALUE           VALUE THIS RUN
     ----                          -------------           --------------

   Concentrations (ICON)               1                  !   ICON =  1  !
   Dry Fluxes (IDRY)                   1                  !   IDRY =  0  !
   Wet Fluxes (IWET)                   1                  !   IWET =  0  !
   Relative Humidity (IVIS)            1                  !   IVIS =  0  !
    (relative humidity file is
     required for visibility
     analysis)

   *
    0 = Do not create file, 1 = create file


    LINE PRINTER OUTPUT OPTIONS:

       Print concentrations (ICPRT)    Default: 0          ! ICPRT =  1  !
       Print dry fluxes (IDPRT)        Default: 0          ! IDPRT =  0  !
       Print wet fluxes (IWPRT)        Default: 0          ! IWPRT =  0  !
       (0 = Do not print, 1 = Print)

       Concentration print interval
       (ICFRQ) in hours                Default: 1          !  ICFRQ =  1  !
       Dry flux print interval
       (IDFRQ) in hours                Default: 1          !  IDFRQ =  1  !
       Wet flux print interval
       (IWFRQ) in hours                Default: 1          !  IWFRQ =  1  !

       Messages tracking progress of   Default: 1          !  IMESG =  1  !
       run written to the screen ?
       (IMESG) -- 0=no, 1=yes


     SPECIES LIST FOR OUTPUT OPTIONS

              -------- CONCENTRATIONS ---------   ---------- DRY FLUXES ----------   --------- WET FLUXES ----------
SPECIES
 NAME          PRINTED ?       SAVED ON DISK ?     PRINTED ?       SAVED ON DISK ?    PRINTED ?      SAVED ON DISK ?
-------      ----------------------------------   ----------------------------------  ---------------------------------

! SO2         =   1 ,             1 ,               0 ,             0 ,              0 ,            0 ,  !
! SO4         =   1 ,             1 ,               0 ,             0 ,              0 ,            0 ,  !


     OPTIONS FOR PRINTING "DEBUG" QUANTITIES (much output)

       Logical for debug output
       (LDEBUG)                              Default: F     !  LDEBUG = F !

       Number of puffs to track
       (NPFDEB)                              Default: 1     !  NPFDEB =  1  !

       Time step to start debug output
       (NN1)                                 Default: 1     !  NN1 =  1  !

       Time step to end debug output
       (NN2)                                 Default: 10    !  NN2 =  10  !

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 6

```
------------------------------------------------------------------------------

INPUT GROUP: 6a, 6b, & 6c -- Subgrid scale complex terrain inputs
-------------------------

--------------
Subgroup (6a)
--------------
      Number of terrain features (NHILL)      Default: 0     ! NHILL =  1  !

      Number of special complex terrain
      receptors  (NCTREC)                     Default: 0     ! NCTREC =  9  !

      Terrain data for CTSG hills input in
      CTDM format ? (MHILL)                   No Default     ! MHILL =  2  !
      1 = Hill data created by CTDM
          processors & read from HILL.DAT
          file
      2 = Hill data created by OPTHILL &
          input below in Subgroup (6b)

      Factor to convert horizontal dimensions Default: 1.0   !XHILL2M = 1.0 !
      to meters (MHILL = 1)

      Factor to convert vertical dimensions   Default: 1.0   !ZHILL2M = 1.0 !
      to meters (MHILL = 1)

!END!

--------------
Subgroup (6b)
--------------

                    1 **
    HILL information

HILL              XC     YC    THETAH    ZGRID    RELIEF    EXPO 1    EXPO 2    SCALE 1    SCALE 2    AMAX1    AMAX2
 NO.             (km)   (km)   (deg.)     (m)       (m)       (m)       (m)       (m)        (m)       (m)      (m)
----             ----   ----   ------    -----    ------    ------    ------    -------    -------    -----    -----
  1  ! HILL =     0.0,   0.0,    0.0,     25.0,    100.0,     2.0,      2.0,      800.0,     400.0,    1132.0, 566.0 !
!END!


--------------
Subgroup (6c)
--------------

                                      1  **
   COMPLEX TERRAIN RECEPTOR INFORMATION

             XRCT       YRCT       ZRCT         XHH
             (km)       (km)        (m)
            ------     -----      ------       ----
! CTREC =    -0.2,       0.0,      95.0,        1.0       !  !END!
! CTREC =    -0.2,      -0.1,      93.5,        1.0       !  !END!
! CTREC =    -0.2,      -0.2,      89.3,        1.0       !  !END!
! CTREC =    -0.2,      -0.3,      82.9,        1.0       !  !END!
! CTREC =    -0.2,      -0.4,      75.0,        1.0       !  !END!
! CTREC =    -0.2,      -0.5,      66.4,        1.0       !  !END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 6

```
! CTREC =     -0.2,      -0.6,      57.8,        1.0      !  !END!
! CTREC =     -0.2,      -0.7,      49.4,        1.0      !  !END!
! CTREC =     -0.2,      -0.8,      41.7,        1.0      !  !END!

------------------
1
     Description of Complex Terrain Variables:
          XC, YC  = Coordinates of center of hill
          THETAH  = Orientation of major axis of hill (clockwise from
                    North)
          ZGRID   = Height of the  0  of the grid above mean sea
                    level
          RELIEF  = Height of the crest of the hill above the grid elevation
          EXPO 1  = Hill-shape exponent for the major axis
          EXPO 2  = Hill-shape exponent for the major axis
          SCALE 1 = Horizontal length scale along the major axis
          SCALE 2 = Horizontal length scale along the minor axis
          AMAX    = Maximum allowed axis length for the major axis
          BMAX    = Maximum allowed axis length for the major axis

          XRCT, YRCT = Coordinates of the complex terrain receptors
          ZRCT    = Height of the ground (MSL) at the complex terrain
                    Receptor
          XHH     = Hill number associated with each complex terrain receptor
                    (NOTE: MUST BE ENTERED AS A REAL NUMBER)

     **
       NOTE: DATA for each hill and CTSG receptor are treated as a separate
             input subgroup and therefore must end with an input group terminator.
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Groups 7, 8, and 9

```
------------------------------------------------------------------------------

INPUT GROUP: 7 -- Chemical parameters for dry deposition of gases
--------------

SPECIES      DIFFUSIVITY      ALPHA STAR      REACTIVITY    MESOPHYLL RESISTANCE     HENRY'S LAW COEFFICIENT
 NAME        (cm**2/s)                                            (s/cm)              (dimensionless)
-------      ----------       ----------      ----------    --------------------     ----------------------

! SO2         = 0.1509,         1000.0,         8.0,              0.0,                    0.0             !

!END!

------------------------------------------------------------------------------

INPUT GROUP: 8 -- Size parameters for dry deposition of particles
--------------

SPECIES       GEOMETRIC MASS MEAN        GEOMETRIC STANDARD
 NAME              DIAMETER                   DEVIATION
                   (microns)                  (microns)
-------       ------------------         -----------------
! SO4     =         0.48                       2.0        !

!END!

------------------------------------------------------------------------------

INPUT GROUP: 9 -- Miscellaneous dry deposition parameters
--------------

     Reference cuticle resistance   (RCUTR)  (s/cm)   !  RCUTR = 30.0 !
     Reference ground resistance    (RGR)    (s/cm)   !    RGR = 10.0 !
     Reference pollutant reactivity (REACTR)          ! REACTR = 8.0 !

     Vegetation state in unirrigated areas (IVEG)     !   IVEG =  1  !
        IVEG=1 for active and unstressed vegetation
        IVEG=2 for active and stressed vegetation
        IVEG=3 for inactive vegetation

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Groups 10 and 11

```
------------------------------------------------------------------------------

INPUT GROUP: 10 -- Wet Deposition Parameters
--------------

                                                        -1
                  Scavenging Coefficient -- Units: (sec)

     Pollutant       Liquid Precip.       Frozen Precip.
     ---------       --------------       --------------
! SO2           =      3.0E-05,              0.0          !
! SO4           =     10.0E-05,             3.0E-5        !

!END!

------------------------------------------------------------------------------

INPUT GROUP: 11 -- Chemistry Parameters
--------------

     Ozone data input option (MOZ)     Default: 1          ! MOZ =  0  !
     (Used only if MCHEM = 1)
        0 = use a constant background ozone value
        1 = read hourly ozone concentrations from
            the OZONE.DAT data file

     Background ozone concentration
     (BCKO3) in ppb                    Default: 80.        ! BCKO3 = 80 !
     (Used only if MCHEM = 1 and
      MOZ = 0 or (MOZ = 1 and all hourly
      O3 data missing)

     Background ammonia concentration
     (BCKNH3) in ppb                   Default: 10.        ! BCKNH3 = 10 !

     Nighttime SO2 loss rate (RNITE1)
     in percent/hour                   Default: 0.2        ! RNITE1 = .2 !

     Nighttime NOx loss rate (RNITE2)
     in percent/hour                   Default: 2.0        ! RNITE2 = 2. !

     Nighttime HNO3 formation rate (RNITE3)
     in percent/hour                   Default: 2.0        ! RNITE3 = 2. !

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 12

```
------------------------------------------------------------------------------

INPUT GROUP: 12 -- Misc. Dispersion and Computational Parameters
--------------

     Horizontal size of puff (m) beyond which
     time-dependent dispersion equations (Heffter)
     are used to determine sigma-y and
     sigma-z (SYTDEP)                    Default: 550.   ! SYTDEP = 9999 !

     Switch for using Heffter equation for
     sigma-z as above. (0=Do NOT use Heffter
     1=Use Heffter for sigma-z)
     (MHFTSZ)                            Default: 1      ! MHFTSZ = 1 !

     Stability class used to determine plume
     growth rates for puffs above the boundary
     layer (JSUP)                        Default: 5      ! JSUP = 5 !

     Vertical dispersion constant for stable
     conditions (k1 in Eqn. 2-173)  (CONK1)  Default: 0.01   ! CONK1 = 0.01 !

     Vertical dispersion constant for neutral/
     unstable conditions (k2 in Eqn. 2-173)
     (CONK2)                             Default: 0.1    ! CONK2 = 0.1 !

     Range of land use categories for which
     urban dispersion is assumed
     (IURB1, IURB2)                      Default: 10,    ! IURB1 =  10  !
                                                  19     ! IURB2 =  19  !

     Maximum length of a slug (met. grid units)
     (XMXLEN)                            Default: 1.0    ! XMXLEN = 1.0 !

     Maximum travel distance of a puff/slug (in
     met. grid units) during one sampling step
     (XSAMLEN)                           Default: 5.0    ! XSAMLEN = 10. !

     Maximum number of puffs or slugs released
     from one source during one time step
     (serves as a cap if XMXLEN is specified
     too small)
     (MXNEW)                             Default:  99    ! MXNEW = 99 !

     Maximum number of sampling steps during
     one time step for a puff/slug
     (serves as a cap if XSAMLEN is specified
     as too small)
     (MXSAM)                             Default:  5     ! MXSAM = 5  !

     Slug-to-puff transition criterion factor.
     When the ratio of the slug's sigma-y to its
     length exceeds SL2PF, it will be converted
     to a circular puff.
     (SL2PF)                             Default: 100    ! sl2pf = 100 !
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 12

```
Minimum sigma-y for a new puff/slug
(SYMIN)                                  Default: 0.01   ! SYMIN = 0.01 !
                                         Units: m
Minimum sigma-z for a new puff/slug
(SZMIN)                                  Default: 0.01   ! SZMIN = 0.01 !
                                         Units: m

Minimum turbulence sigma-v
(SVMIN)                                  Default: 0.50   ! SVMIN = 0.50 !
                                         Units: m/s

Minimum turbulence sigma-z
(SZMIN)                                  Default: 0.016  ! SWMIN = 0.016 !
                                         Units: m/s

Minimum wind speed allowed for
non-calm conditions.  Wind speeds
less than WSCALM will be considered
as "calm" by the model.  Also used
as the minimum speed returned when
using power-law extrapolation            Default: 1.0    ! WSCALM  = 1.0 !
toward the surface                       Units: m/s
(WSCALM)

Maximum mixing height
(XMAXZI)                                 Default: 3000.  ! XMAXZI = 3000.  !
                                         Units: m

Minimum mixing height                    Default:  20.   ! XMINZI = 20.    !
(XMINZI)                                 Units: m

Default wind speed profile power-law
exponents for stabilities 1-6
(PLXO(6))                    Default ISC values used if ALL are ZERO
                             ISC RURAL : .07, .07, .10, .15, .35, .55
                             ISC URBAN : .15, .15, .20, .25, .30, .30

                          Stability Class :  A     B     C     D     E     F
                                             ---   ---   ---   ---   ---   ---
                                  ! PLXO = 0.07, 0.07, 0.1, 0.15, 0.35, 0.55 !


Default potential temperature gradient
for stable classes E, F
(PTGO(2))              Default:  0.020, 0.035          ! PTGO = 0.02, 0.035 !
                       Units: deg. K/m

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 13

```
------------------------------------------------------------------------

INPUT GROUPS: 13a, 13b, 13c -- Point source parameters
--------------------------

--------------
Subgroup (13a)
--------------

     Number of point sources with
     constant emission parameters   (NPT1)  No default  !  NPT1 =  1  !

     Number of point sources with
     variable emission parameters   (NPT2)  No default  !  NPT2 =  0  !

     (If NPT2 > 0, the variable point
     source emissions are read from
     the file: PTEMARB.DAT)

!END!


--------------
Subgroup (13b)
--------------
                                                                    a
          POINT SOURCE DATA FOR SOURCES WITH CONSTANT EMISSION PARAMETERS
          --------------------------------------------------------------
                                                                                  b          c
Source      X UTM       Y UTM       Stack      Base       Stack      Exit       Exit      Bldg.    Emission
 No.     Coordinate  Coordinate   Height   Elevation   Diameter   Velocity    Temp.    Downwash    Rates
           (km)        (km)         (m)        (m)        (m)       (m/s)   (deg. K)                (g/s)
------   ----------  ----------   ------     ------     --------   --------  --------  --------  ------------
   1  ! X =  0.1,       -3.0,       40.,       25.,       2.2,       10.,      450.,     1.,       1.7, 0.0 !
!END!

--------

    a
     Data for each source receptor are treated as a separate
     input subgroup and therefore must end with an input group terminator.

    b
     0. = No building downwash modeled, 1. = downwash modeled

    c
      Emission rates must be entered for every pollutant ("NSPEC" values).
      Enter emission rate of zero for secondary pollutants.

--------------
Subgroup (13c)
--------------

          BUILDING DIMENSION DATA FOR SOURCES SUBJECT TO DOWNWASH
          -------------------------------------------------------
Source
 No.      Effective building width and height (in meters) every 10 degrees
------    ---------------------------------------------------------------
  1       ! WIDTH  = 9 * 12.5, 9 * 0.0, 9 * 12.5, 9 * 0.0                !
  1       ! HEIGHT = 9 * 45.0, 9 * 0.0, 9 * 45.0, 9 * 0.0                !
!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 14

```
------------------------------------------------------------------------

INPUT GROUPS: 14a, 14b & 14c -- Area source parameters
----------------------

--------------
Subgroup (14a)
--------------

    Number of polygon area sources with
    constant emission parameters (NAR1)     No default  !  NAR1 =  2  !

!END!

--------------
Subgroup (14b)
--------------
                                                                      a
          AREA SOURCE DATA FOR SOURCES WITH CONSTANT EMISSION PARAMETERS
          ------------------------------------------------------------
                                                        b
Source          Effect.    Base      Initial    Emission
 No.            Height   Elevation  Sigma z     Rates
                  (m)       (m)       (m)      (g/s/m^2)
-------         ------    ------    --------   ---------

  1      ! X =     1.0,      0.0,      2.5,       0.85, 0.0 !  !END!
  2      ! X =     1.5,      0.0,      3.0,       1.15, 0.0 !  !END!

--------
    a
     Data for each source are treated as a separate input subgroup
     and therefore must end with an input group terminator.
    b
      Emission rates must be entered for every pollutant ("NSPEC" values).
      Enter emission rate of zero for secondary pollutants.


--------------
Subgroup (14c)
--------------

          COORDINATES (UTM-km) FOR EACH VERTEX(4) OF EACH POLYGON
          ------------------------------------------------------
Source                                                              a
 No.      Ordered list of X followed by list of Y, grouped by source
-------   ------------------------------------------------------

  1   !   X = 0.500, 0.510, 0.510, 0.500  !
  1   !   Y = 1.600, 1.600, 1.610, 1.610  !
!END!
  2   !   X = 0.750, 0.760, 0.760, 0.750  !
  2   !   Y = 1.800, 1.800, 1.810, 1.810  !
!END!
--------
    a
     Data for each source are treated as a separate input subgroup
     and therefore must end with an input group terminator.
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 2

```
    Method used to compute dispersion
    coefficients (MDISP)                Default: 4   ! MDISP =  3  !

       1 = dispersion coefficients computed from values of
           sigma v, sigma w read from SIGMA.DAT file
       2 = dispersion coefficients sigma v, sigma w computed
           internally from micrometeorological variables (u*, w*, L, etc.)
       3 = PG dispersion coefficients for RURAL areas (computed using
           the ISCST multi-segment approximation) and MP coefficients in
           urban areas
       4 = same as 3 except PG coefficients computed using
           the MESOPUFF II eqns.
       5 = CTDM sigmas used for stable and neutral conditions.
           For unstable conditions, sigmas are computed as in
           MDISP = 1, described above.  MDISP = 5 assumes that
           sigma v, sigma w are read from a SIGMA.DAT file

    PG sigma-y, z adj. for roughness?       Default: 0    ! MROUGH =  1  !
    (MROUGH)
       0 = no
       1 = yes

    Partial plume penetration of            Default: 0    ! MPARTL =  1  !
    elevated inversion?
    (MPARTL)
       0 = no
       1 = yes

    Test options specified to see if
    they conform to regulatory
    values? (MREG)                      Default: 0   ! MREG =  0  !

       0 = NO checks are made
       1 = Technical options must conform to USEPA values for
           short-range modeling ( e.g. ISC-type applications)
       2 = Technical options must conform to USEPA values for
           long-range modeling (e.g. visibility-type applications)
       3 = Environmental Protection Authority of Victoria (EPAV)
           default values

!END!
```

Table 4-5 (Continued)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 16

```
------------------------------------------------------------------------------

INPUT GROUPS: 16a & 16b -- Volume source parameters
----------------------

--------------
Subgroup (16a)
--------------

     Number of volume sources with
     constant emission parameters (NVL1)     No default  !  NVL1 =  1  !

     Gridded volume source data
     used ? (GRIDVL)                         No default  !  GRIDVL =  0  !
        0 = no
        1 = yes (gridded volume source
            emissions read from the file:
            VOLEM.DAT)

     The following parameters apply to the data in the
     gridded volume source emissions file (VOLEM.DAT)

       -  Effective height of emissions
          (VEFFHT) in meters                 No default  ! VEFFHT = 10 !

       -  Initial sigma y (VSIGYI) in
          meters                             No default  ! VSIGYI = 3000 !

       -  Initial sigma z (VSIGZI) in
          meters                             No default  ! VSIGZI = 10 !

!END!


--------------
Subgroup (16b)
--------------
                                                                        a
          VOLUME SOURCE DATA FOR SOURCES WITH CONSTANT EMISSION PARAMETERS
          ---------------------------------------------------------------
                                                                                b
      X UTM       Y UTM       Effect.    Base      Initial     Initial     Emission
    Coordinate  Coordinate    Height   Elevation  Sigma y     Sigma z      Rates
      (km)        (km)          (m)      (m)        (m)         (m)       (g/s)
    ----------  ----------    ------   ------    --------    --------    --------

! X =  -5.6,        -1.2,       10.,      0.0,      6.2,        6.2,        2.2, 0.0, !  !END!
--------
    a
     Data for each source are treated as a separate input subgroup
     and therefore must end with an input group terminator.
    b
      Emission rates must be entered for every pollutant ("NSPEC" values).
      Enter emission rate of zero for secondary pollutants.
```

Table 4-5 (Concluded)
Sample CALPUFF Control File (CALPUFF.INP)
Input Group 17

```
------------------------------------------------------------------------------

INPUT GROUPS: 17a & 17b -- Non-gridded (discrete) receptor information
-----------------------

--------------
Subgroup (17a)
--------------

     Number of non-gridded receptors (NREC)  No default  !  NREC =  3  !

!END!


--------------
Subgroup (17b)
--------------
                                                    a
           NON-GRIDDED (DISCRETE) RECEPTOR DATA
           -----------------------------------

                 X UTM       Y UTM       Ground
Receptor      Coordinate  Coordinate  Elevation
  No.            (km)        (km)        (m)
--------      ----------  ----------  ---------

  1    !  X =    1.0,         1.0,        12.5 !  !END!
  2    !  X =    2.5,         4.2,        28.1 !  !END!
  3    !  X =    2.89,        3.2,        39.6 !  !END!

-------------
    a
     Data for each receptor are treated as a separate input subgroup
     and therefore must end with an input group terminator.
```

Table 4-6
CALPUFF Control File Inputs - Input Group 1
General Run Control Parameters

Variable	Type	Description	Default Value
IBYR	integer	Starting year of the CALPUFF run (two digits)	-
IBMO	integer	Starting month	-
IBDY	integer	Starting day	-
IBHR	integer	Starting hour (00-23)	-
IRLG	integer	Length of the run (hours)	-
NSPEC	integer	Total number of species modeled	5
NSE	integer	Number of species emitted	3
ITEST	integer	Flag to stop run after the setup phase (1 = stops the program, 2 = continues with execution after setup)	2
METFM	integer	Meteorological data format 1 = CALMET unformatted file (CALMET.DAT) 2 = ISC2 ASCII file (ISCMET.DAT) 3 = AUSPLUME ASCII file (PLMMET.DAT)	1
AVET	real	Averaging time (minutes) (PG - σ_y is adjusted by the equation $(AVET/60.0)^{0.2}$	60.0

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 2
Technical Options

Variable	Type	Description	Default Value
MGAUSS	integer	Control variable determining the vertical distribution used in the near field (See Section 2.1.1). (0 = uniform, 1 = Gaussian)	1
MCTADJ	integer	Terrain adjustment method (See Section 2.6.2). 0 = no adjustment 1 = ISC-type of terrain adjustment 2 = simple, CALPUFF-type of terrain adjustment	1
MCTSG	integer	CALPUFF subgrid scale complex terrain module (CTSG) flag (See Section 2.6.1). (0 = CTSG not modeled, 1 = CTSG modeled)	0
MSLUG	integer	Near-field puffs are modeled as elongated "slugs" ? (0 = no, 1 = yes) (See Section 2.1).	1
MTRANS	integer	Transitional plume rise modeled ? (see Section 2.4.1). (0 = only final rise computed, 1 = transitional rise computed) Note: Transitional plume rise is always computed for sources subject to building downwash effects.	1
MTIP	integer	Stack tip downwash modeled ? (See Section 2.4.2). 0 = no (i.e., no stack tip downwash) 1 = yes (i.e., use stack tip downwash)	1
MSHEAR	integer	Vertical wind shear above stack top modeled in plume rise ? (See Section 2.4.5). (0 = no, 1 = yes)	1
MSPLIT	integer	Puff splitting allowed ? (See Section 2.2.4). (0 = no, 1 = yes)	0
MCHEM	integer	Chemical mechanism flag (See Section 2.8). 0 = chemical transformation not modeled 1 = transformation rates computed internally (MESOPUFF II scheme) 2 = user specified transformation rates used (If MCHEM = 2, the user must prepare a file (CHEM.DAT) with a diurnal cycle of transformation rates)	1
MWET	integer	Wet removal modeled ? (See Section 2.9). (0 = no, 1 = yes)	1

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 2
Technical Options

Variable	Type	Description	Default Value
MDRY	integer	Dry deposition modeled ? (See Section 2.7). (0 = no, 1 = yes) Note: The method used to determine dry deposition velocities is specified by the user on a species-by-species basis in Input Group 3.	1
MDISP	integer	Method used to compute the horizontal and vertical dispersion coefficients (See Section 2.2). 1 = computed from values of σ_v and σ_w from the SIGMA.DAT file 2 = computed from σ_v and σ_w which are calculated internally from the micrometeorological variables (u_*, w_*, L, etc.) 3 = PG dispersion coefficients used in RURAL areas (computed using the ISCST multi-segment approximation) and MP coefficients used in URBAN areas 4 = same as 3 except PG coefficients computed using the MESOPUFF II equations 5 = CTDM sigmas used for stable and neutral conditions for unstable conditions, sigmas are computed as in MDISP = 1. MDISP = 5 assumes that σ_v and σ_w are read from SIGMA.DAT file.	3
MROUGH	integer	PG σ_y and σ_z adjusted for surface roughness ? (0 = no, 1 = yes) (See Eqns.(2-73) to (2-75)).	0
MPARTL	integer	Partial plume penetration of elevated inversion? (0 = no, 1 = yes) (See Section 2.4.3).	0
MREG	integer	Test options in control file to see if they conform to regulatory values? (0 = no, 1 = yes (US EPA), 2 = yes (USA visibility application), 3 = yes (Victorian EPA)	0

Table 4-6 (Continued)
Control File Inputs - Input Group 3
Species List

Input Group 3 consists of two parts. The first part is a list of the species names and the second part contains a table with three integer flags for each species. These flags indicate if a pollutant is modeled (0=no, 1=yes), emitted (0=no, 1=yes), and dry deposited (0=no, 1=yes, treated as a gas with the resistance model, 2=yes, treated as a particle with the resistance model, or 3=yes, user-specified deposition velocities used).

However, the user must first specify the species names to be modeled. Each species is entered on a separate line with ! CSPEC = XXX ! !END!, where XXX is a species name (up to 12 characters in length), and the variable delimiter and group delimiter (!END!) appears on the line. For example, a five-species SO_x, NO_x run would be:

```
INPUT GROUP: 3 - Species List

    ! CSPEC = SO2  !      !END!
    ! CSPEC = SO4  !      !END!
    ! CSPEC = NOX  !      !END!
    ! CSPEC = HNO3 !      !END!
    ! CSPEC = NO3  !      !END!
```

The chemical transformation scheme in CALPUFF is designed to simulate the conversion of $SO_2 \rightarrow SO_4^=$ and $NO_x \rightarrow HNO_3 \rightarrow NO_3^-$. Therefore, the five pollutants in CALPUFF are labeled as SO_2, $SO_4^=$, NO_x, HNO_3, and NO_3^-. However, by setting the appropriate flags controlling the various technical options (chemical transformation, deposition, etc.), other reactive or non-reactive pollutants can be simulated.

The user has control over which species are to be emitted and dry deposited in a particular run. If the dry deposition flag is set equal to 3 for any pollutant, a file called VD.DAT must be made available to the model. This file contains a diurnal cycle of 24 user-specified deposition velocities for each pollutant flagged (see Section 4.2.5).

Table 4-6 (Continued)

The format of the species list table is:

INPUT GROUP: 3 – Species list

SPECIES NAME	MODELED (0=NO, 1=YES)	EMITTED (0=NO, 1=YES)	DRY DEPOSITED (0=NO, 1=COMPUTED-GAS 2=COMPUTED-PARTICLE 3=USER-SPECIFIED)
! SO2	= 1 ,	1 ,	1 !
! SO4	= 1 ,	1 ,	2 !
! NOX	= 1 ,	1 ,	1 !
! HNO3	= 1 ,	0 ,	1 !
! NO3	= 1 ,	0 ,	1 !

!END!

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 4
Grid Control Parameters

Variable	Type	Description	Default Value
NX	integer	Number of grid cells in the X direction of the meteorological grid	-
NY	integer	Number of grid cells in the Y direction of the meteorological grid	-
DGRIDKM	real	Grid spacing (km) of the meteorological grid	-
XORIGKM	real	Reference X coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid	-
YORIGKM	real	Reference Y coordinate (km) of the southwest corner of grid cell (1,1) of the meteorological grid	-
IUTMZN	integer	Zone of coordinates	-
XLAT	real	Reference latitude (deg.) of the center of the modeling domain (used in solar elevation angle calculations)	-
XLONG	real	Reference longitude (deg.) of the center of the modeling domain	-
XTZ	real	Reference time zone of the center of the modeling domain (PST=8, MST=7, CST=6, EST=5)	-
NZ	integer	Number of vertical layers	-
ZFACE	real array	Cell face heights (m) for the meteorological grid (NX + 1 values must be entered). Note: Cell center (grid point) height of layer "i" is ((ZFACE(i+1) + (ZFACE(i))/2).	-
IBCOMP	integer	X index of lower left corner of the computational grid ($1 \leq$ IBCOMP $\leq$ NX)	-
JBCOMP	integer	Y index of lower left corner of the computational grid ($1 \leq$ JBCOMP $\leq$ NY)	-

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 4
Grid Control Parameters

Variable	Type	Description	Default Value
IECOMP	integer	X index of upper right corner of the computational grid (1 ≤ IECOMP ≤ NX)	-
JECOMP	integer	Y index of upper right corner of computational grid (1 ≤ JECOMP ≤ NY)	-
LSAMP	integer	Flag indicating if an array of gridded receptors (i.e., sampling grid) is used (T = yes, F = no)	-
IBSAMP	integer	X index of lower left corner of the sampling grid (IBCOMP ≤ IBSAMP ≤ IECOMP)	-
JBSAMP	integer	Y index of lower left corner of the sampling grid (JBCOMP ≤ JBSAMP ≤ JECOMP)	-
IESAMP	integer	X index of upper right corner of the sampling grid (IBCOMP ≤ IESAMP ≤ IECOMP)	-
JESAMP	integer	Y index of upper right corner of the sampling gird (JBCOMP ≤ JESAMP ≤ JECOMP)	-
MESHDN	integer	Nesting factor of the sampling grid (MESHDN ≥ 1). The grid spacing of the sampling grid is DGRIDKM/MESHDN. The number of sampling grid points is NXSAM * NYSAM, where NXSAM = MESHDN * (IESAMP - IBSAMP) + 1 NYSAM = MESHDN * (JESAMP - JBSAMP) + 1	-

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 5
Output Options

Variable	Type	Description	Default Value
ICON	integer	Control variable for creation of an output disk file (CONC.DAT) containing concentration fields (species stored in this file are controlled by the output species table described below). (0 = do not create CONC.DAT, 1 = create CONC.DAT)	1
IDRY	integer	Control variable for creation of an output disk file (DFLX.DAT) containing dry flux fields. (The species stored in this file are controlled by the output species table in Input Group 5 described below.) (0 = do not create DFLX.DAT, 1 = create DFLX.DAT)	1
IWET	integer	Control variable for creation of an output disk file (WFLX.DAT) containing wet flux fields. (The species stored in this file are controlled by the output species table in Input Group 5 described below.) (0 = do not create WFLX.DAT, 1 = create WFLX.DAT)	1
IVIS	integer	Control variable for creation of an output disk file containing relative humidity data required for visibility applications	0
ICPRT	integer	Control variable for printing of concentration fields to the output list file (CALPUFF.LST). (0 = do not print any dry fluxes, 1 = print dry fluxes indicated in output species table)	0
IDPRT	integer	Control variable for printing of dry flux fields to the output list file (CALPUFF.LST). (0 = do not print any dry fluxes, 1 = print dry fluxes indicated in output species table)	0
IWPRT	integer	Control variable for printing of wet flux fields to the output list file (CALPUFF.LST). (0 = do not print any wet fluxes, 1 = print wet fluxes indicated in output species table)	0

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 5
Output Options

Variable	Type	Description	Default Value
ICFRQ	integer	Printing interval for the concentration fields. Concentrations are printed every "ICFRQ" hours. (Used only if ICPRT = 1.)	1
IDFRQ	integer	Printing interval for the dry flux fields. Dry fluxes are printed every "IDFRQ" hours. (Used only if IDPRT = 1.)	1
IWFRQ	integer	Printing interval for the wet flux fields. Wet fluxes are printed every "IWFRQ" hours. (Used only if IWPRT = 1.)	1
IMESG	integer	Control variable determining if messages tracking the progress of the run are written to the screen (0 = not written, 1 = written).	1
LDEBUG	logical	Control variable for activation of "debug" write statements	F
NPFDEB	integer	Number of puffs to write in debug option (used only if LDEBUG = T)	1
NN1	integer	Time period (hour) to begin debug output (used only if LDEBUG = T)	1
NN2	integer	Time period (hour) to stop debug output (used only if LDEBUG = T)	10

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 5
Output Options

In addition to the variable described above, Input Group 5 also contains a table of species with a series of flags indicating if the pollutant's concentration and wet/dry flux fields are to be printed to the output list file (CALPUFF.LST) and/or stored in the output disk files (CONC.DAT, DFLX.DAT, and WFLX.DAT).

The format of the species output table is shown below. A value of 0 indicates "no", and a value of 1 indicates "yes".

```
SPECIES LIST FOR OUTPUT OPTIONS

                ------ CONCENTRATIONS ------    -------- DRY FLUXES ---------    ---------- WET FLUXES ----------
SPECIES
NAME            PRINTED ?   SAVED ON DISK ?    PRINTED ?   SAVED ON DISK ?    PRINTED ?   SAVED ON DISK ?
--------        ---------   ---------------    ---------   ---------------    ---------   ---------------

! SO2    =      1     ,     1     ,            0     ,     0     ,            0     ,     0     !
! SO4    =      0     ,     0     ,            0     ,     0     ,            0     ,     0     !
! NOX    =      0     ,     0     ,            0     ,     0     ,            0     ,     0     !
! HNO3   =      0     ,     0     ,            0     ,     0     ,            0     ,     0     !
! NO3    =      0     ,     0     ,            0     ,     0     ,            0     ,     0     !

!END!
```

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 6
Subgrid Scale Complex Terrain (CTSG) Inputs

Variable	Type	Description	Default Value
		(Input Group 6a - General CTSG Parameters)	
NHILL	integer	Number of subgrid scale terrain features	0
NCTREC	integer	Number of special subgrid scale complex terrain receptors	0
MHILL	integer	Terrain data for CTSG hills input in CTDM format ? (0 = hill data created by CTDM processors and read from a HILL.DAT file; 1 = hill data created by OPTHILL & input below in Subgroup (6b)).	-
XHILL2M	real	Factor to convert horizontal dimensions to meters (used only if MHILL = 1)	1.0
ZHILL2M	real	Factor to convert vertical dimensions to meters (used only if MHILL = 1)	1.0
		(Input Group 6b - Hill Information)	
XC	real	UTM X coordinate (km) of the center of the hill on the meteorological grid	-
YC	real	UTM Y coordinate (km) of the center of the hill on the meteorological grid	-
THETAH	real	Orientation of the major axis of the hill (in degrees) clockwise from north	-
ZGRID	real	Height (m) of the "zero-plane" of the grid above mean sea level	-
RELIEF	real	Height (m) of the crest of the hill above the grid elevation	-
EXPO1	real	Hill shape exponent for the major axis of the hill	-
EXPO2	real	Hill shape exponent for the minor axis of the hill	-
SCALE1	real	Horizontal length scale of the hill along the major axis	-
SCALE2	real	Horizontal length scale of the hill along the minor axis	-
AMAX1	real	Maximum allowed axis length of the major axis of the hill	-
AMAX2	real	Maximum allowed axis length of the minor axis of the hill	-

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 6
Subgrid Scale Complex Terrain (CTSG) Inputs

The variables in Input Group 6b are entered for each of the "NHILL" subgrid scale hills treated in the model run. The data for each hill is treated as a separate input subgroup, and therefore must end with an input group terminator (i.e., !END!). The format of Input Group 6b is shown below.

```
------------
Subgroup (6b)
------------

                                1 **
   HILL INFORMATION

HILL       XC    YC    THETAH  ZGRID  RELIEF   EXPO 1   EXPO 2   SCALE 1   SCALE 2   AMAX1    AMAX2
NO.        (km)  (km)  (deg.)  (m)    (m)      (m)      (m)      (m)       (m)       (m)      (m)
------     ----  ----  ------  -----  -------  -------  -------  --------  --------  -------  -------
1 ! HILL = 170.5, 3841.0, 69. ,  1310. , 300. ,  1.91 ,  1.24 ,  1523. ,  2896. ,  2000.,  1500.! !END!
2 ! HILL = 173.0, 3839.0, 49. ,  1310. , 230. ,  1.50 ,  1.50 ,  3000. ,  1000. ,  4000.,  2000.! !END!
```

Note that the hill number is an optional user comment which is outside of the delimiters containing the required data. The data for each hill must follow the opening delimiter and "HILL=". The data for each hill is followed by a closing delimiter and an input group terminator (i.e., !END!).

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 6
Subgrid Scale Complex Terrain (CTSG) Inputs

Variable	Type	Description	Default Value
		(Input Group 6c - CTSG Receptor Data)	
XRCT	real	UTM X coordinate (km) on the meteorological grid system of a CTSG receptor	-
YRCT	real	UTM Y coordinate (km) on the meteorological grid system of a CTSG receptor	-
ZRCT	real	Height (m) of the ground above mean sea level at the CTSG receptor	-
XHH	real	Hill number associated with this CTSG receptor	-

The variables in Input Group 6c are entered for each of the "NCTREC" complex terrain receptors in the model run. The data for each receptor is treated as a separate input subgroup, and therefore must end with an input group terminator (i.e., !END!). The format of Input Group 6c is shown below.

Subgroup (6c)

```
                                                        1 **
   COMPLEX TERRAIN RECEPTOR INFORMATION

                XRCT     YRCT     ZRCT     XHH
                (km)     (km)     (m)
               ------   ------   -------   -----
! CTREC =  170.5,   3840.0 ,  1430.  ,  1.  !  !END!
! CTREC =  169.0,   3840.5 ,  1430.  ,  1.  !  !END!
! CTREC =  170.5,   3841.0 ,  1580.  ,  1.  !  !END!
! CTREC =  173.5,   3840.0 ,  1525.  ,  2.  !  !END!
! CTREC =  172.5,   3840.0 ,  1430.  ,  2.  !  !END!
```

** The data for each CTSG receptor must follow an opening delimiter and "CTREC=". The data for each receptor is followed by a closing delimiter and an input group terminator (i.e., !END!).

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 7
Dry Deposition Parameters - Gases

Input Group 7 consists of a table containing the following five parameters which are required by the resistance deposition model for computing deposition velocities for gases:

- Pollutant diffusivity (cm^2/s) (see Eqn. 2-182)
- Aqueous phase dissociation constant, α^* (see Eqn. 2-186)
- Pollutant reactivity (see Eqn. 2-184)
- Mesophyll resistance, r_m (s/cm) (see Eqn. 2-181)
- Henry's Law coefficient, H (dimensionless) (see Eqn. 2-186)

These parameters must be specified for each pollutant with a dry deposition flag of "1" in the species list (Input Group 3) indicating the use of the resistance model for a gas.

The format of the input table is shown below:

INPUT GROUP: 7 -- Chemical parameters for dry deposition of gases

SPECIES NAME	DIFFUSIVITY (cm**2/s)	ALPHA STAR	REACTIVITY	MESOPHYLL RESISTANCE (s/cm)	HENRY'S LAW COEFFICIENT (dimensionless)
! SO2 =	0.1509 ,	1.00E3 ,	8.0 ,	0.0 ,	4.e-2 !
! NOX =	0.1656 ,	1.00 ,	8.0 ,	5.0 ,	3.5 !
! HNO3 =	0.1628 ,	1.00 ,	18.0 ,	0.0 ,	8.e-8 !

!END!

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 8
Dry Deposition Parameters - Particles

Input Group 8 consists of a table containing the geometric mass mean diameter (microns) and the geometric standard deviation (microns) required by the resistance deposition model for computing deposition velocities for particulate matter.

These parameters must be specified for each pollutant with a dry deposition flag of "2" in the species list (Input Group 3) indicating the use of the resistance model for a pollutant deposited as particulate matter.

The format of the input table is shown below:

INPUT GROUP: 8 -- Size parameters for dry deposition of particles

SPECIES NAME		GEOMETRIC MASS MEAN DIAMETER (microns)		GEOMETRIC STANDARD DEVIATION (microns)	
! SO4	=	0.48	,	2.00	!
! NO3	=	0.48	,	2.00	!

!END!

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 9
Miscellaneous Dry Deposition Parameters

Variable	Type	Description	Default Value
RCUTR	real	Reference cuticle resistance (s/cm) (see Eqn. 2-184)	30.
RGR	real	Reference ground resistance (s/cm) (see Eqn. 2-185)	10.
REACTR	real	Reference pollutant reactivity (see Eqn. 2-184)	8.
IVEG	integer	Flag specifying the state of vegetation in unirrigated areas 1 = vegetation is active and unstressed 2 = vegetation is active and stressed 3 = vegetation is inactive	1

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 10
Wet Deposition Parameters

Input Group 10 consists of a table containing pollutant-dependent values of the scavenging coefficient, λ, defined by Equation (2-197), for both liquid and frozen precipitation types. The format of the input table is shown below.

```
INPUT GROUP: 10 -- Wet Deposition Parameters
-------------------

                    Scavenging Coefficient -- Units: (sec)-1

     Pollutant          Liquid Precip.        Frozen Precip.
     ----------         --------------        --------------
     ! SO2    =          3.0e-5       ,          0.0        !
     ! SO4    =          10.0e-5      ,          3.0e-5     !
     ! NOX    =          0.0          ,          0.0        !
     ! HNO3   =          6.0e-5       ,          0.0        !
     ! NO3    =          10.0e-5      ,          3.0e-5     !

!END!
```

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 11
Chemistry Parameters

Variable	Type	Description	Default Value
MOZ	integer	Control variable for the input of hourly ozone data used in the chemical transformation module (Used only if MCHEM = 1) 0 = use a constant background ozone value in chemistry calculation 1 = use hourly ozone concentrations from the OZONE.DAT data file	1
BCKO3	real	Background ozone concentration in ppb (Used only if MCHEM=1 and MOZ = 0 or if (MOZ=1 and all hourly ozone data are missing))	80.
BCKNH3	real	Background ammonia concentration in ppb	10.
RNITE1	real	Nighttime SO_2 loss rate in percent/hour (k_1 in Eqn. 2-192)	0.2
RNITE2	real	Nighttime NO_x loss rate in percent/hour (k_2 in Eqn. 2-193)	2.0
RNITE3	real	Nighttime HNO_3 formation rate in percent/hour (k_3 in Eqn. 2-194)	2.0

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 12
Dispersion Parameters

Variable	Type	Description	Default Value
SYTDEP	real	Horizontal size of a puff (m) beyond which the time-dependent dispersion equation of Heffter (1965)	550
MHFTRZ	integer	Use Heffter formulas for σ_z ? (0 = no; 1 = yes). If yes, the distance at which the Heffter formula will be applied for σ_z is determined by when σ_y switches to Heffter's eqn. (see SYTDEP).	1
JSUP	integer	Stability class used to determine dispersion rates for puffs above the boundary layer (e.g., 6 = F stability)	6
CONK1	real	Vertical dispersion constant for stable conditions (k_1 in Eqn. 2-173)	0.01
CONK2	real	Vertical dispersion constant for neutral/unstable conditions (k_2 in Eqn. 2-173)	0.10
IURB1, IURB2	integer	Land use categories associated with urban areas. If MDISP = 3 or 4, MP dispersion coefficients are used when puff is over land use type IURB1 through IURB2	10,19
XMXLEN	real	Maximum length of an emitted slug (in met. grid units)	1.0
XSAMLEN	real	Maximum travel distance of a slug or puff (in met. grid units) during one sampling step	5.0
MXNEW	integer	Maximum number of puffs or slugs released from one source during one time step (serves as a cap if XMXLEN is specified too small)	99
MXSAM	integer	Maximum number of sampling steps during one time step for a puff or slug (serves as a cap if XSAMLEN is specified too small)	5
SL2PF	real	Slug-to-puff transition criterion factor (max. σ_y/slug length before transition to puff)	100.
PLX0(6)	real array	Wind speed profile power-law exponents for stabilities A-F	0.07, 0.07, 0.10, 0.15, 0.35, 0.55

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 12
Dispersion Parameters

Variable	Type	Description	Default Value
PTG0(2)	real array	Potential temperature gradient (deg. k/m) for stability classes E and F	.020, .035
SYMIN	real	Minimum σ_y (m) a new puff or slug	0.01
SZMIN	real	Minimum σ_z (m) a new puff or slug	0.01
SVMIN	real	Minimum turbulence σ_v (m/s)	0.50
SWMIN	real	Minimum turbulence σ_w (m/s)	0.016
WSCALM	real	Minimum wind speed allowed for non-calm conditions. Wind speeds less than WSCALM will be considered as "calm" by the model. WSCALM is also used as the minimum speed returned from the power law extrapolation of the wind speed toward the surface.	1.0
XMAXZI	real	Maximum mixing height (m)	3000.
XMINZI	real	Minimum mixing height (m)	20.

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 13
Point Source Parameters

Variable	Type	Description	Default Value
Input Group 13a - General Data			
NPT1	integer	Number of point sources with constant stack and emission parameters	-
NPT2	integer	Number of point sources with arbitrarily-varying emission parameters (If NPT2 > 0, the point source emissions file PTEMARB.DAT must be provided)	-
Input Group 13b - Point Source Data for Sources with Constant Stack and Emissions Parameters			-
XUTM	real	X coordinate (km) of the stack on the meteorological grid	-
YUTM	real	Y coordinate (km) of the stack on the meteorological grid	-
HSTAK	real	Stack height (m)	-
SELEV	real	Stack base elevation (m) above mean sea level	-
DIAM	real	Stack diameter (m)	-
EXITW	real	Stack gas exit velocity (m/s)	-
EXITT	real	Stack gas exit temperature (deg. K)	-
BDOWN	real	Building downwash flag 0. = building downwash not modeled, 1. = building downwash modeled	-
EMS	real array	Emission rate (g/s) of each modeled species Note: "NSPEC" values must be entered	-

The variables in Input Group 13b are entered for each of the "NPT1" point sources with constant emission parameters. The data for each source is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!). The format of Input Group 13b is shown below.

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 13
Point Source Parameters

Subgroup (13a)

Number of point sources with constant emission parameters	**(NPT1)**	**No default**	**! NPT1 = 1 !**
Number of point sources with variable emission parameters	**(NPT2)**	**No default**	**! NPT2 = 0 !**

(If NPT2 > 0, the variable point source emissions are read from the file: PTEMARB.DAT)

!END!

Subgroup (13b)

POINT SOURCE DATA FOR SOURCES WITH CONSTANT EMISSION PARAMETERS[a]

Source No.	X Coordinate (km)	Y Coordinate (km)	Stack Height (m)	Base Elevation (m)	Stack Diameter (m)	Exit Velocity (m/s)	Exit Temp. (deg. K)	Bldg. Downwash[b]	Emission Rates[c] (g/s)	
1	! X = 168.1,	3839.0,	40.,	25.0,	1.0,	0.001,	250.,	0. ,	1.667	! !END!
2	! X = 172.1,	3861.0,	20.5	0.0,	2.2,	3.5,	283.,	1. ,	0.9	! !END!
3	! X = 180,1,	3869,2,	85.0	0.0,	4.5,	12.0,	350.,	1. ,	22.9	! !END!

a
Data for each source receptor are treated as a separate input subgroup and therefore must end with an input group terminator.

b
0. = No building downwash modeled, 1. = downwash modeled
NOTE: must be entered as a REAL number (i.e., with decimal point)

c
"NSPEC" emission rates must be entered (one for every pollutant).
Enter emission rate of zero for secondary pollutants.

Note that the source number is an optional user comment which is outside of the delimiter containing the required source data. The data for each source must follow an opening delimiter and "X=". The data for each source is followed by a closing delimiter and an input group terminator.

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 13
Point Source Parameters

Variable	Type	Description	Default Value
		(Input Group 13c - Building Dimension Data)	
WIDTH	real array	Array of 36 direction-specific building widths (m) for flow vectors from 10°-360° in 10° increments	-
HEIGHT	real array	Array of 36-direction-specific building heights (m) for flow vectors from 10°-360° in 10° increments	-

The variables in Input Group 13c are entered for each point source for which IDOWN=1 in Input Group 13b. The data for each point source (i.e., 36 widths and 36 heights) is treated as a separate input subgroup and therefore must end with an input group terminator (i.e., !END!). The format of Input Group 13c is shown below.

```
----------
Subgroup (13c)
----------

          BUILDING DIMENSION DATA FOR SOURCES SUBJECT TO DOWNWASH
          ------------------------------------------------------
Source
 No.      Effective building width and height (in meters) every 10 degrees
-------   ---------------------------------------------------------------------

  2       ! WIDTH  = 36 * 12.0 !
  2       ! HEIGHT = 36 * 22.5 !
!END!


  3       ! WIDTH  = 20 * 0.0, 45.5, 48.5, 52.5, 13 * 0.0 !
  3       ! HEIGHT = 20 * 0.0, 78.0, 78.0, 78.0, 13 * 0.0 !
!END!
```

Note that the source number is an optional user comment which is outside of the delimiters. The data for each source must follow an opening delimiter and either "WIDTH=" or "HEIGHT=". The data for each source is followed by a closing delimiter and an input group terminator (i.e., !END!).

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 14
Area Source Parameters

Variable	Type	Description	Default Value
(Input Group 14a - General Area Source Data)			
NAR1	integer	Number of area sources with constant emission parameters	-
NAR2	integer	Number of buoyant area sources with arbitrary varying emission parameters	-
(Input Group 14b - Area Source Data for Sources with Constant Emissions)			
XUTM	real	X coordinates (km) of each vertex of the area source on the meteorological grid	-
YUTM	real	Y coordinate (km) of each vertex of the area source on the meteorological grid	-
HTEFF	real	Effective height (m) of the area source	-
AELEV	real	Base elevation (m) above mean sea level	-
SIGZI	real	Initial vertical dispersion coefficient (σ_z), in meters, of the area source	-
EMIS	real array	Emission rate (g/s) of each modeled species Note: "NSPEC" values must be entered	-

The variables in Input Group 14b are entered for each of the "NAR1" area sources with constant emissions. The data for each source is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!). The format of Input Group 14 is shown below.

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 14
Area Source Parameters

Subgroup (14a)

Number of polygon area sources with constant emission parameters (NAR1) **No default** **! NAR1 = 0 !**

!END!

Subgroup (14b)

AREA SOURCE DATA FOR SOURCES WITH CONSTANT EMISSION PARAMETERS[a]

Source No.	Effect. Height (m)	Base Elevation (m)	Initial Sigma z (m)	Emission Rates[b] (g/s/m^2)	
1	! X = 1.0,	0.0,	2.5,	0.85, 0.0 !	!END!
2	! X = 1.5,	0.0,	3.0,	1.15, 0.0 !	!END!

---

[a] Data for each source are treated as a separate input subgroup and therefore must end with an input group terminator.

[b] Emission rates must be entered for every pollutant ("NSPEC" values). Enter emission rate of zero for secondary pollutants.

Subgroup (14c)

COORDINATES (UTM-km) FOR EACH VERTEX(4) OF EACH POLYGON

Source No.	Ordered list of X followed by list of Y, grouped by source[a]
1	! X = 0.500, 0.510, 0.510, 0.500 !
1	! Y = 1.600, 1.600, 1.610, 1.610 !
!END!	
2	! X = 0.750, 0.760, 0.760, 0.750 !
2	! Y = 1.800, 1.800, 1.810, 1.810 !
!END!	

---

[a] Data for each source are treated as a separate input subgroup and therefore must end with an input group terminator.

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 15
Line Source Parameters

Variable	Type	Description	Default Value
(Input Group 15a - General Line Source Data)			
NLINES	integer	Number of buoyant line sources	-
MXNSEG	integer	Maximum number of line segments into which each line may be divided (if MSLUG=1); Actual number of virtual points which will be used to represent each line (if MSLUG=0)	7
XL	real	Average line source length (m)	-
HBL	real	Average height of line source (m)	-
WBL	real	Average building width (m)	-
WML	real	Average line source width (m)	-
DXL	real	Average deviation between building (m)	
FPRIMEL	real	Average buoyancy parameter (m^4/s^3)	-
(Input Group 15b - Buoyant Line Source Data) - repeated for each line source			
XBEGL	real	Beginning X coordinate (km)	-
YBEGL	real	Beginning Y coordinate (km)	-
XENDL	real	Ending X coordinate (km)	-
YENDL	real	Ending Y coordinate (km)	-
HTL	real	Release height (m)	-
ELEVL	real	Base elevation (m)	-
QL	real	Emissions rate (g/s) of each pollutant	-

Table 4-6 (Continued)
CALPUFF Control File Inputs - Input Group 16
Volume Source Parameters

Variable	Type	Description	Default Value
(Input Group 16a - General Volume Source Data)			
NVL1	integer	Number of volume sources with constant emission parameters	-
GRIDVL	integer	Gridded volume source data used? (0 = no, 1 = yes - read from file VOLEM.DAT)	-
VEFFHT	real	Effective height (m) of emissions in gridded volume source file	-
VSIGYI	real	Initial σ_y (m) of emissions in gridded volume source file	-
VSIGZI	real	Initial σ_z (m) of emissions in gridded volume source file	-
Input Group 16b - Volume Source Data for Sources with Constant Emissions data (repeated for each volume source (NVL1))			
XVOL	real	X coordinate (km) of center of volume source	-
YVOL	real	Y coordinate (km) of center of volume source	-
HTVOL	real	Effective height (m) of volume source	-
ELEVOL	real	Base elevation (m) of volume source	-
SYVOL	real	Initial σ_y (m) of volume source	-
SZVOL	real	Initial σ_z (m) of volume source	-
QVOL	real	Emission rates (g/s) of each pollutant from volume source	-

Table 4-6 (Concluded)
CALPUFF Control File Inputs - Input Group 17
Non-Gridded (Discrete) Receptor Data

Variable	Type	Description	Default Value
(Input Group 17a - General Discrete Receptor Data)			
NREC	integer	Number of non-gridded receptors	-
(Input Group 17b - Discrete Receptor Data)			
XUTM	real	X coordinate (km) of the discrete receptor on the meteorological grid	-
YUTM	real	Y coordinate (km) of the discrete receptor on the meteorological grid	-
ELEV	real	Ground elevation (m) above mean sea level of the receptor	-

The variables in Input Group 17b are entered for each of the "NREC" discrete receptors. The data for each receptor is treated as a separate input subgroup, and therefore, must end with an input group terminator (i.e., !END!). The format of Input Group 17b is shown below.

Subgroup (17b)

NON-GRIDDED (DISCRETE) RECEPTOR DATA[a]

Receptor No.		X Coordinate (km)	Y Coordinate (km)	Ground Elevation (m)	
1	! X =	180.1,	3859.2,	22.0	! !END!
2	! X =	195.1,	3862.2,	65.0	! !END!
3	! X =	212.5,	3877.2,	105.0	! !END!

---

[a] Data for each receptor are treated as a separate input subgroup and therefore must end with an input group terminator.

Note that the receptor number is an optional user comment which is outside of the delimiter. The data for each receptor must follow an opening delimiter and "X=". The data for each receptor is followed by a closing delimiter and an input group terminator (i.e., !END!).

4.2.2 Meteorological Data Files

Three types of meteorological data files can be used to drive the CALPUFF model. In order to take full advantage of the capabilities of the model to simulate the effects spatially-varying meteorological fields, gridded fields of winds, temperatures, mixing heights, and other meteorological variables can be input into CALPUFF through the CALMET.DAT file. The format and contants of this file is described in Section 4.2.2.1.

Alternatively, CALPUFF will also accept single station meteorological data in the ISC2 format or AUSPLUME data. The ISC2 meteorological data file (ISCMET.DAT) is described in Section 4.2.2.2, and the AUSPLUME file (PLMMET.DAT) is described in Section 4.2.2.3. It should be noted that three header records must be added to the standard ISC2 or AUSPLUME files for use with CALPUFF.

4.2.2.1 CALMET.DAT

The CALMET.DAT file contains gridded meteorological data fields required to drive the CALPUFF model. It also contains certain geophysical fields, such as terrain elevations, surface roughness lengths, and land use types, used by both the CALMET meteorological model and CALPUFF. Although the input requirements of CALPUFF are designed to be directly compatible with CALMET, meteorological fields produced by other meteorological models can be substituted for the CALMET output as long as the required variables are produced and the output is reformatted to be consistent with the CALMET.DAT file specifications described in this section.

CALMET.DAT File - Header Records

The CALMET.DAT file consists of a set of up to fourteen header records, followed by a set of hourly data records. The header records contains a descriptive title of the meteorological run, information including the horizontal and vertical grid systems of the meteorological grid, the number, type, and coordinates of the meteorological stations included in the CALMET run, gridded fields of surface roughness lengths, land use, terrain elevations, leaf area indexes, and a pre-compute field of the closest surface meteorological station number to each grid point.

The actual number of header records may vary because, as explained below, records containing surface, upper air, and precipitation station coordinates are not included if these

stations were not included in the run. A description of each variable in the header records is provided in Table 4-7.

The following variables stored in the CALMET.DAT header records are checked in the setup phase of the CALPUFF model run to ensure compatibility with variables specified in the CALPUFF control file: number of grid cells in the X and Y directions, grid size, reference UTM or Lambert conformal coordinates of the grid origin, and UTM zone of the grid origin.

Sample FORTRAN write statements for the CALMET.DAT header records are:

```
c ---   Header record 1 -- Run title
        write(iunit)TITLE

c ---   Header record 2 -- General run and grid information
        write(iunit)VER,LEVEL,IBYR,IBMO,IBDY,IBHR,IBTZ,IRLG,IRTYPE,
      1 NX,NY,NZ,DGRID,XORIGR,YORIGR,IUTMZN,IWFCOD,NSSTA,
      2 NUSTA,NPSTA,NOWSTA,NLU,IWAT1,IWAT2,LCALGRD

c ---   Header record 3 -- Vertical cell face heights (nz+1 values)
        write(iunit)CLAB1,IDUM,ZFACEM

c ---   Header records 4 and 5 -- Surface station coordinates
        if(nssta.ge.1)then
          write(iunit)CLAB2,IDUM,XSSTA
          write(iunit)CLAB3,IDUM,YSSTA
        endif

c ---   Header records 6 and 7 -- Upper air station coordinates
        if(nusta.ge.1)then
          write(iunit)CLAB4,IDUM,XUSTA
          write(iunit)CLAB5,IDUM,YUSTA
        endif

c ---   Header records 8 and 9 -- Precipitation station coordinates
        if(npsta.ge.1)then
          write(iunit)CLAB6,IDUM,XPSTA
          write(iunit)CLAB7,IDUM,YPSTA
        endif

c ---   Header record 10 -- Surface roughness lengths
        write(iunit)CLAB8,IDUM,Z0

c ---   Header record 11 -- Land use categories
        write(iunit)CLAB9,IDUM,ILANDU

c ---   Header record 12 -- Terrain elevations
        write(iunit)CLAB10,IDUM,ELEV
```

```
c ---   Header record 13 - Leaf area indexes
        write(iunit)CLAB11,IDUM,XLAI

c ---   Header record 14 - Nearest surface station to each grid point
        write(iunit)CLAB12,IDUM,NEARS
```

where the following declarations apply:

```
real ZFACEM(nz+1),XSSTA(nssta),YSSTA(nssta),XUSTA(nusta),YUSTA(nusta)
real XPSTA(npsta),YPSTA(npsta)
real Z0(nx,ny),ELEV(nx,ny),XLAI(nx,ny)
integer ILANDU(nx,ny),NEARS(nx,ny)
character*80 TITLE(3)
character*8 VER,LEVEL,CLAB1,CLAB2,CLAB3,CLAB4,CLAB5,CLAB6
character*8 CLAB7,CLAB8,CLAB9,CLAB10,CLAB11,CLAB12
logical LCALGRD
```

Table 4-7
CALMET.DAT file - Header Records

Header Record No.	Variable No.	Variable	Type*	Description
1	1	TITLE	char*80 array	Array with three 80-character lines of the user's title of the CALMET run
2	1	VER	char*8	CALMET model version number
2	2	LEVEL	char*8	CALMET model level number
2	3	IBYR	integer	Starting year of CALMET run
2	4	IBMO	integer	Starting month
2	5	IBDY	integer	Starting day
2	6	IBHR	integer	Starting hour
2	7	IBTZ	integer	Base time zone (e.g., 05=EST, 06=CST, 07=MST, 08=PST)
2	8	IRLG	integer	Run length (hours)
2	9	IRTYPE	integer	Run type (0=wind fields only, 1=wind and micrometeorological fields). IRTYPE must be run type 1 to drive CALGRID or the CTSG option of CALPUFF
2	10	NX	integer	Number of grid cells in the X direction
2	11	NY	integer	Number of grid cells in the Y direction
2	12	NZ	integer	Number of vertical layers
2	13	DGRID	real	Grid spacing (m)
2	14	XORIGR	real	X coordinate (m) of southwest corner of grid cell (1,1)
2	15	YORIGR	real	Y coordinate (m) of southwest corner of grid cell (1,1)
2	16	IUTMZN	integer	UTM zone of coordinates (0 if using a Lambert conformal projection)

*char*80 = Character*80
char*8 = Character*8

Table 4-7 (Continued)
CALMET.DAT file - Header Records

Header Record No.	Variable No.	Variable	Type[a]	Description
2	17	IWFCOD	integer	Wind field module used (0=objective analysis, 1=diagnostic model)
2	18	NSSTA	integer	Number of surface meteorological stations
2	19	NUSTA	integer	Number of upper air stations
2	20	NPSTA	integer	Number of precipitation stations
2	21	NOWSTA	integer	Number of over water stations
2	22	NLU	integer	Number of land use categories
2	23	IWAT1	integer	Range of land use categories
2	24	IWAT2	integer	Corresponding to water surfaces (IWAT1 or IWAT2, inclusive)
2	25	LCALGRD	logical	Flag indicating if special meteorological parameters required by CALGRID are contained in the file (LCALGRD must be TRUE to drive CALGRID or the CTSG option of CALPUFF)
3	1	CLAB1	char*8	Variable label ('ZFACE')
3	2	IDUM	integer	Variable not used
3	3	ZFACEM	real array	Heights (m) of cell faces (NZ + 1 values)
4[b]	1	CLAB2	char*8	Variable label ('XSSTA')
4[b]	2	IDUM	integer	Variable not used
4[b]	3	XSSTA	real array	X coordinates (m) of each surface met. station

[a] char*8 = Character*8
[b] Included only if NSSTA > 0

Table 4-7 (Continued)
CALMET.DAT file - Header Records

Header Record No.	Variable No.	Variable	Type[a]	Description
5[b]	1	CLAB3	char*8	Variable label ('YSSTA')
5[b]	2	IDUM	integer	Variable not used
5[b]	3	YSSTA	real array	Y coordinates (m) of each surface met. station
6[c]	1	CLAB4	char*8	Variable label ('XUSTA')
6[c]	2	IDUM	integer	Variable not used
6[c]	3	XUSTA	real array	X coordinates (m) of each upper air met. station
7[c]	1	CLAB5	char*8	Variable label ('YUSTA')
7[c]	2	IDUM	integer	Variable not used
7[c]	3	YUSTA	real array	Y coordinate (m) of each upper air met. station
8[d]	1	CLAB6	char*8	Variable label ('XPSTA')
8[d]	2	IDUM	integer	Variable not used
8[d]	3	XPSTA	real array	X coordinate (m) of each precipitation station
9[d]	1	CLAB7	char*8	Variable label ('YPSTA')
9[d]	2	IDUM	integer	Variable not used
9[d]	3	YPSTA	real array	Y coordinate (m) of each precipitation station
10	1	CLAB8	char*8	Variable label ('Z0')
10	2	IDUM	integer	Variable not used
10	3	Z0	real array	Gridded field of surface roughness lengths (m) for each grid cell

[a] char*8 = Character*8
[b] Included only if NSSTA > 0
[c] Included only if NUSTA > 0
[d] Included only if NPSTA > 0

Table 4-7 (Concluded)
CALMET.DAT file - Header Records

Header Record No.	Variable No.	Variable	Type[a]	Description
11	1	CLAB9	char*8	Variable label ('ILANDU')
11	2	IDUM	integer	Variable not used
11	3	ILANDU	integer array	Gridded field of land use category for each grid cell
12	1	CLAB10	char*8	Variable label ('ELEV')
12	2	IDUM	integer	Variable not used
12	3	ELEV	real array	Gridded field of terrain elevations for each grid cell
13	1	CLAB11	char*8	Variable label ('XLAI')
13	2	IDUM	integer	Variable not used
13	3	XLAI	real array	Gridded field of leaf area index for each grid cell
14	1	CLAB12	char*8	Variable label ('NEARS')
14	2	IDUM	integer	Variable not used
14	3	NEARS	integer array	Nearest surface meteorological station to each grid point

[a]char*8 = Character*8

CALMET.DAT File - Data Records

The CALMET.DAT data records include hourly fields of winds and meteorological variables. In addition to the regular CALMET output variables, CALGRID and the subgrid scale complex terrain (CTSG) module of CALPUFF require additional three-dimensional fields (air temperature and/or vertical velocity). The presence of these fields in the CALMET output file is flagged by the header record logical variable, LCALGRD, having a value of TRUE.

The data records contain three-dimensional gridded fields of U, V, and W wind components and air temperature, two-dimensional fields of PGT stability class, surface friction velocity, mixing height, Monin-Obukhov length, convective velocity scale, and precipitation rate (not used by CALGRID), and values of the temperature, air density, short-wave solar radiation, relative humidity, and precipitation type codes (not used by CALGRID) defined at the surface meteorological stations. A description of each variable in the data records is provided in Table 4-8.

Sample FORTRAN write statements for the CALMET.DAT data records are:

```
c ---   Write U, V, W wind components
        Loop over vertical layers, k

          write(iunit)CLABU,NDATHR((U(i,j,k),i=1,nx),j=1,ny)
          write(iunit)CLABV,NDATHR((V(i,j,k),i=1,nx),j=1,ny)
          if(LCALGRD)write(iunit)CLABW,NDATHR((W(i,j,k+1),i=1,nx),j=1,ny)

        End loop over vertical layers

c ---   Write 3-D temperature field
        if(LCALGRD.and.irtype.eq.1) then
          Loop over vertical layers, k

            write(iunit)CLABT,NDATHR((ZTEMP(i,j,k),i=1,nxm),j=1,nym)

          End loop over vertical layers
        endif
```

```
c ---   Write 2-D meteorological fields
        if(irtype.eq.1) then

              write(iunit)CLABSC,NDATHR,IPGT
              write(iunit)CLABUS,NDATHR,USTAR
              write(iunit)CLABZI,NDATHR,ZI
              write(iunit)CLABL,NDATHR,EL
              write(iunit)CLABWS,NDATHR,WSTAR
              write(iunit)CLABRMM,NDATHR,RMM

        endif

c ---   Write 1-D variables defined at surface met. stations
        if(irtype.eq.1) then

              write(iunit)CLABTK,NDATHR,TEMPK
              write(iunit)CLABD,NDATHR,RHO
              write(iunit)CLABQ,NDATHR,QSW
              write(iunit)CLABRH,NDATHR,IRH
              write(iunit)CLABPC,NDATHR,IPCODE

        endif
```

where the following declarations apply:

```
real U(nx,ny,nz),V(nx,ny,nz),W(nx,ny,nz)
real ZTEMP(nx,ny,nz)
real USTAR(nx,ny),ZI(nx,ny),EL(nx,ny)
real WSTAR(nx,ny),RMM(nx,ny)
real TEMPK(nssta),RHO(nssta),QSW(nssta)
integer IPGT(nx,ny)
integer IRH(nssta),IPCODE(nssta)
character*8 CLABU, CLABV, CLABW, CLABT, CLABSC, CLABUS, CLABZI
character*8 CLABL, CLABWS, CLABRMM, CLABTK, CLABD, CLABQ, CLABRH
character*8 CLABPC
```

Table 4-8
CALMET.DAT file - Data Records

Record Type	Variable No.	Variable Name	Type[a]	Description
1	1	CLABU	char*8	Variable label ('U-LEVxxx', where xxx indicates the layer number)
1	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
1	3	U	real array	U-component (m/s) of the winds at each grid point
2	1	CLABV	char*8	Variable label ('V-LEVxxx', where xxx indicates the layer number)
2	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
2	3	V	real array	V-component (m/s) of the winds at each grid point
3[b]	1	CLABW	char*8	Variable label ('WFACExxx"), where xxx indicates the layer number)
3[b]	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
3[b]	3	W	real array	W-component (m/s) of the winds at each grid point
(Record types 1,2,3 repeated NZ times (once per layer) as a set)				
4[b]	1	CLABT	char*8	Variable label ('T-LEVxxx', where xxx indicates the layer number)
4[b]	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
4[b]	3	ZTEMP	real array	Air temperature (deg. K) at each grid point
(Record type 4 repeated NZM times (once per layer))				

[a] char*8 = Character*8
[b] Record types 3 and 4 are included only if LCALGRD is TRUE

Table 4-8 (Continued)
CALMET.DAT file - Data Records

Record Type	Variable No.	Variable Name	Type[a]	Description
5	1	CLABSC	char*8	Variable label ('IPGT')
5	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
5	3	IPGT	integer array	PGT stability class at each grid point
6	1	CLABUS	char*8	Variable label ('USTAR')
6	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
6	3	USTAR	real array	Surface friction velocity (m/s)
7	1	CLABZI	char*8	Variable label ('ZI')
7	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
7	3	ZI	real array	Mixing height (m)
8	1	CLABL	char*8	Variable label ('EL')
8	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
8	3	EL	real array	Monin-Obukhov length (m)
9	1	CLABWS	char*8	Variable label ('WSTAR')
9	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
9	3	WSTAR	real array	Convective velocity scale (m/s)
10	1	CLABRMM	char*8	Variable label ('RMM')
10	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
10	3	RMM	real array	Precipitation rate (mm/hr). Not used by CALGRID.

[a] char*8 = Character*8

Table 4-8 (Concluded)
CALMET.DAT file - Data Records

Record Type	Variable No.	Variable Name	Type[a]	Description
11	1	CLABTK	char*8	Variable label ('TEMPK')
11	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
11	3	TEMPK	real array	Temperature (deg. K) at each surface met. station
12	1	CLABD	char*8	Variable label ('RHO')
12	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
12	3	RHO	real array	Air density (kg/m^3) at each surface met. station
13	1	CLABQ	char*8	Variable label ('QSW')
13	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
13	3	QSW	real array	Short-wave solar radiation (W/m^2) at each surface met. station
14	1	CLABRH	char*8	Variable label ('IRH')
14	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
14	3	IRH	integer array	Relative humidity (percent) at each surface met. station
15	1	CLABPC	char*8	Variable label ('IPCODE')
15	2	NDATHR	integer	Year, Julian day and hour in the form YYJJJHH
15	3	IPCODE	integer array	Precipitation type code (not used by CALGRID)

[a] char*8 = Character*8

4.2.2.2 ISCMET.DAT

CALPUFF can be driven by a single-station ISC2-type of meteorological file. However, the header records of the standard ISC2 data file must be modified to provide some additional information required by CALPUFF. In addition, the ISCMET.DAT file used by CALPUFF can accommodate an extended data record, provding variables not found in a standard ISC2 data record.

CALPUFF is normally run with a full three-dimensional wind field and temperature field, as well as two-dimensional fields of mixing heights and other meteorological variables (see CALMET.DAT in Section 4.2.2.1). However, in some near-field applications, when spatial variability of the meteorological fields may not be significant, the single-station data file may be used. The model uses the data in the ISCMET.DAT file to fill the 2-D or 3-D arrays with the scalar values read from the file. For example, the ISCMET.DAT header records contain a single value of land use, and the hourly data records contain single values of mixing height and temperature. In single-station mode, CALPUFF assigns the single value of each variable read from the ISCMET.DAT file to all grid points, resulting in a spatially uniform gridded field. However, the model does not assume the meteorological conditions are steady-state, which allows the important effects of causality to be simulated even with the single-station meteorological data. For example, the time required for plume material to reach a receptor is accounted for in the puff formulation, and curved trajectories and variable dispersion and stability conditions over multiple hours of transport will result even when using the single-station meteorological data. However, in general, the preferred mode for most applications of CALPUFF is to use the spatially variable fields generated by CALMET.

The minimum data required in the ISCMET.DAT file includes hourly values of the vector flow direction, wind speed, temperature, stability class, and mixing height (urban or rural). In addition, if dry or wet deposition are being modeled, or if turbulence-based dispersion coefficients are to be computed based on micrometeorological parameters, hourly values of the surface friction velocity (u_*), Monin-Obukhov length (L), a time-varying surface roughness length (z_o), displacement height, precipitation rate, and precipitation type code can be entered on an extended record. If chemical transformation is being modeled, hourly values of short-wave solar radiation and relative humidity can also be included. In addition, hourly values of the potential temperature lapse rate ($d\theta/dz$) and power law profile exponent (p) can be entered. Non-missing values of the basic meteorological variables (i.e., vector wind direction, wind speed, temperature, stability class, and mixing height) must be provided for all applications. The data fields for the extended record variables (u_*, L, etc.) may be left blank if the CALPUFF options are set so that they are not needed (e.g., no wet or dry deposition, no chemical transformation, no computation of turbulence-based dispersion coefficients). However, if the CALPUFF model

options are set to require them, the model assumes that valid values of the extended record variables will be provided for every hour. The only exceptions are $d\theta/dz$ and p, which can be entered for some hours and not others. If values of $d\theta/dz$ or p are missing (i.e., blank) for a given hour, the model will use its default or user-specified stability-dependent values (see the PLX0 and PTG0 variables in Input Group 12 of the control file).

Sample ISCMET.DAT files are shown in Tables 4-7(a) and 4-7(b). Part (a) of the table shows the "base" data record (i.e., an ISC2 meteorological data record). The extended data record is shown in Part (b) of the table. Table 4-8 lists the contents of the ISCMET.DAT header records, and Table 4-9 describes the data records.

The ISCMET.DAT header records are not part of the standard ISC2 ASCII meteorological data file, so they must be added to an existing ISC2 data file before running CALPUFF. The header records contain: (1) an 80-character title of the data set; (2) the starting date and hour of the data in the file; and (3) the anemometer height, surface roughness length, land use type, elevation, and leaf area index of the modeling region. The starting date and time in the header record allows checks in the setup phase of the model to be conducted to verify that the model starting date is at or after the start of the data in the file. The anemometer height is required in the vertical power law extrapolation of the wind speed. The roughness length is used if turbulence-based dispersion coefficients are selected, and in the calculation of dry deposition velocities. The land use category is used to determine if urban or rural dispersion coefficients are appropriate when the Pasquill-Gifford/McElroy-Pooler dispersion coefficients are used. Also see the variables IURB1 and IURB2 in Input Group 12 of the control file. They define the range of land use categories that are to be considered urban (i.e., if the value of the land use category in the ISCMET.DAT file is between IURB1 and IURB2, inclusive, the modeling domain will be consider urban). Otherwise, it will be considered rural. The leaf area index is only used by the model if dry deposition velocities are being computed (see Section 2.7). However, all of the header record variables must be present in the ISCMET.DAT file, even if the model options will result in them not being used.

The elevation on the ISCMET.DAT header record is used to fill the 2-D terrain elevation array in CALPUFF. This array is used to determine, through interpolation, the elevation of the *gridded* receptors generated by the model as an option. Because a single value is available in the ISCMET.DAT file, all of the gridded receptors will be assigned this elevation. Receptor-specific elevations are assigned to each *discrete* receptor by the user in the CALPUFF control file (see Input Group 17).

Table 4-7
Sample ISCMET.DAT files

(a) Base Data Records

```
Austin ,TX meteorological data - 10 hrs - Base ISC2 data only
90  1 1  1                              : iyr,imo,iday,ihr(1-24)   (begin)
10.06 0.25  2  0.0  3.0                  : anemht(m),z0(m),ilandu,elev(m),xlai
90 1 1 1  81.0000   3.0866 280.9 5  881.5   53.0
90 1 1 2  98.0000   1.5433 279.8 6  904.6   53.0
90 1 1 3 114.0000   2.5722 279.8 5  927.8   53.0
90 1 1 4 113.0000   4.1155 280.4 4  951.0  951.0
90 1 1 5 103.0000   3.0866 279.8 5  974.2   53.0
90 1 1 6 102.0000   5.1444 280.4 4  997.4  997.4
90 1 1 7 105.0000   4.6300 280.4 4 1020.6 1020.6
90 1 1 8  73.0000   2.5722 280.4 4 1043.8 1043.8
90 1 1 9 117.0000   4.1155 280.9 4 1067.0 1067.0
90 1 110 141.0000   3.6011 283.7 3 1090.2 1090.2
 ↑ ↑ ↑ ↑       ↑       ↑     ↑ ↑      ↑      ↑
yr  dy    WD vect     WS  Temp    rural  urban
  mo  hr                    stab    zi     zi
```

(b) Extended Data Records

```
Austin ,TX meteorological data - 10 hrs - Extended data records
90  1 1  1                              : iyr,imo,iday,ihr(1-24)   (begin)
10.06 0.25  2  0.0  3.0                  : anemht(m),z0(m),ilandu,elev(m),xlai
90 1 1 1  81.0000   3.0866 280.9 5  881.5   53.0     0.33     355.   0.25  0.0  0    0.0     .020  .35     0. 77
90 1 1 2  98.0000   1.5433 279.8 6  904.6   53.0     0.17     122.   0.25  0.0  0    0.0     .035  .55     0. 68
90 1 1 3 114.0000   2.5722 279.8 5  927.8   53.0     0.28     259.   0.25  0.0  0    0.0           .30     0. 72
90 1 1 4 113.0000   4.1155 280.4 4  951.0  951.0     0.45     655.   0.25  0.0  0    0.0           .15     0. 74
90 1 1 5 103.0000   3.0866 279.8 5  974.2   53.0     0.33     355.   0.25  0.0  0    0.0     .022          0. 75
90 1 1 6 102.0000   5.1444 280.4 4  997.4  997.4     0.56    1025.   0.25  0.0  1    .25           .18     0. 73
90 1 1 7 105.0000   4.6300 280.4 4 1020.6 1020.6     0.50   -1005.   0.25  0.0  0    0.0           .17    70. 71
90 1 1 8  73.0000   2.5722 280.4 4 1043.8 1043.8     0.28    -355.   0.25  0.0  1    .75                  120. 65
90 1 1 9 117.0000   4.1155 280.9 4 1067.0 1067.0     0.45    -395.   0.25  0.0  2   2.64           .22    180. 68
90 1 110 141.0000   3.6011 283.7 3 1090.2 1090.2     0.39    -148.   0.25  0.0  0    0.0           .12    240. 62
 ↑ ↑ ↑ ↑       ↑       ↑     ↑ ↑      ↑      ↑       ↑       ↑      ↑    ↑    ↑    ↑      ↑     ↑   ↑      ↑  ↑
yr  dy    WD vect     WS  Temp    rural  urban      u*       L      zo    zd   p  precip.  dθ/dz   p     SW  rh
  mo  hr                    stab    zi     zi                                code   amt.                rad.  %
```

Table 4-8
ISCMET.DAT File - Header Records

Records 1-3. Title, starting date, geophysical data.

Record	Columns	Variable	Type	Description
1	1-80	TITLE	character*80	Title of file.
2	*	IBYR	integer	Begining year of data.
2	*	IBMO	integer	Beginning month.
2	*	IBHR	integer	Beginning day.
2	*	IBHY	integer	Beginning hour (1-24).
3	*	ANEMHT	integer	Anemometer height (m).
3	*	Z0IN	real	Roughness length (m).
3	*	ILANDUIN	integer	Land use category.
3	*	ELEVIN	real	Elevation (m).
3	*	XLAIIN	real	Leaf area index (LAI)

* Free formatted input

Table 4-9
ISCMET.DAT File - Data Records
(One record per hour)

Records 4,5,6,... Hourly meteorological data.

Columns	Variable	Type	Description
	Base Data		
1-2	IY	integer	Year of data in record
3-4	IM	integer	Month
5-6	ID	integer	Day
7-8	IH	integer	Hour (ISC2 convention (1-24))
9-17	FVEC	real	Flow vector (deg.)
18-26	WSPD	real	Wind speed (m/s)
27-32	TMPK	real	Temperature (deg. K)
33-34	KST	integer	Stability class (1-6)
35-41	RMIX	real	Rural mixing height (m)
42-48	UMIX	real	Urban mixing height (m)
	Extended data		
49-57	USTR	real	Friction velocity (m/s)
58-67	XMON	real	Monin-Obukhov length (m)
68-75	Z0M	real	Surface roughness length (m)
76-80	ZDISP	real	Displacement height (m)
81-84	IPC	integer	Precipitation type code (see Table 2-11)
85-91	PMMHR	real	Precipitation rate (mm/hr)
92-101	DTHTD	real	Potential temperature lapse rate (deg. K/m)
102-106	PLAW	real	Wind speed power law exponent
107-115	QSWRAD	real	Short-wave solar radiation (W/m^2)
116-118	IRH	integer	Relative humidity (%)

4.2.2.3 PLMMET.DAT

In addition to the capability to use three-dimensional wind fields generated by CALMET, a single-station meteorological file can also be used by CALPUFF as its source of meteorological data. The single station data can be in the form of the ISC2 meteorological data file (see Section 4.2.2.2) or the AUSPLUME (Lorimer, 1976) type of data file. The standard AUSPLUME data file must be modified by adding three header records at the beginning of the file to provide additional information required by CALPUFF.

CALPUFF is normally run with a full three-dimensional wind field and temperature field, as well as two-dimensional fields of mixing heights and other meteorological variables (see CALMET.DAT in Section 4.2.2.1). However, in some near-field applications, when spatial variability of the meteorological fields may not be significant, the single-station data file may be used. The model uses the data in the PLMMET.DAT file to fill the 2-D or 3-D arrays with the scalar values read from the file. For example, the PLMMET.DAT header records contain a single value of land use, and the hourly data records contain single values of mixing height and temperature. In single station mode, CALPUFF assigns the single value of each variable read from the PLMMET.DAT file to all grid points, resulting in a spatially uniform gridded field. However, the model does not assume the meteorological conditions are steady-state, which allows the important effects of causality to be simulated even with the single-station meteorological data. For example, the time required for plume material to reach a receptor is accounted for in the puff formulation, and curved trajectories and variable dispersion and stability conditions over multiple hours of transport will result even when using the single-station meteorological data. However, in general, the preferred mode for most applications of CALPUFF is to use the spatially variable fields generated by CALMET.

The PLMMET.DAT file includes the basic hourly data required by CALPUFF, including the wind direction, wind speed, temperature, stability class, and mixing height. Note that PLMMET.DAT uses *wind direction* in the usual meteorological convention (i.e., winds from the west blowing toward the east has a value of 270°), while ISCMET.DAT uses *flow vector* (i.e., winds from the west toward the east have a vector direction of 90°). The PLMMET.DAT format contains two data fields that are not used by CALPUFF (σ_θ and a chemical decay constant). If turbulence data are available, they should be entered through the use of the SIGMA.DAT data file (see Section 4.2.9). Also, CALPUFF contains several options for modeling chemical transformation that do not involve the use of a decay constant (see section 2.8).

The PLMMET.DAT format does not allow for micrometeorological variables, such as the surface friction velocity and Monin-Obukhov length, or precipitation data to be entered. The

CALMET.DAT or ISCMET.DAT formats should be used if the selected CALPUFF options require these parameters.

A sample PLMMET.DAT file is shown in Table 4-10. A description of the contents of the header records is provided in Table 4-11, and the data records are described in Table 4-12. The header records are not part of the standard AUSPLUME meteorological data file, and must be added by the user. The data record format is identical to the standard AUSPLUME format.

The header records contain: (1) an 80-character title of the data set; (2) the starting date and hour (1-24) of the data in the file; and (3) the anemometer height, surface roughness length, land use type, elevation, and leaf area index of the modeling region. The starting date and time in the header record allows checks in the setup phase of the model to be conducted to verify that the model starting date is at or after the start of the data in the file. The anemometer height is required in the vertical power law extrapolation of the wind speed. The roughness length is used if turbulence-based dispersion coefficients are selected, and in the calculation of dry deposition velocities. The land use category is used to determine if urban or rural dispersion coefficients are appropriate when the Pasquill-Gifford/McElroy-Pooler dispersion coefficients are used. Also see the variables IURB1 and IURB2 in Input Group 12 of the control file. They define the range of land use categories that are to be considered urban (i.e., if the value of the land use category in the PLMMET.DAT file is between IURB1 and IURB2, inclusive, the modeling domain will be consider urban). Otherwise, it will be considered rural. The leaf area index is only used by the model if dry deposition velocities are being computed (see Section 2.7). However, all of the header record variables must be present in the PLMET.DAT file, even if the model options will result in them not being used.

The elevation on the PLMMET.DAT header record is used to fill the 2-D terrain elevation array in CALPUFF. This array is used to determine, through interpolation, the elevation of the *gridded* receptors generated by the model as an option. Because a single value is available in the PLMMET.DAT file, all of the gridded receptors will be assigned this elevation. Receptor-specific elevations are assigned to each *discrete* receptor by the user in the CALPUFF control file (see Input Group 17).

Table 4-10
Sample PLMMET.DAT file

```
Sample PLMMET.DAT data file.  Min. ws=1.0 m/s
94 1 1  1                                  : iyr,imo,iday,ihr(1-24)   (begin)
10.  0.25  2  0.0   3.                     : anemht(m),z0(m),ilandu,elev(m),xlai
94010101 19  1.0 270 F  100  17. 0.55 .035        0.
94010102 19  1.2 270 F  122  22.      .030        0.
94010103 20  1.5 270 F  132  18.                  0.
94010104 19  3.2 270 E  256      0.35             0.
94010105 20  1.8 270 F  103      0.45 .031        0.
94010106 20  3.3 270 E  201      0.32 .024        0.
94010107 21  5.0 270 D  284      0.25             0.
94010108 21  4.6 270 D  301  12.                  0.
94010109 22  3.5 270 D  525  11.                  0.
94010110 22  3.9 270 C  658  16. 0.19             0.
94010111 22  3.5 270 C  881      0.17             0.
94010112 23  2.7 270 B  905      0.12             0.
94010113 23  4.1 270 C 1194      0.15             0.
94010114 24  2.8 270 C 1254      0.14             0.
94010115 25  6.1 270 D 1289      0.18             0.
94010116 25  5.3 270 D 1305                       0.
94010117 24  5.2 270 D 1211                       0.
94010118 24  4.9 270 D 1032      0.25             0.
94010119 23  5.1 270 D  995      0.25             0.
94010120 21  3.1 270 E  255      0.37 .027        0.
94010121 20  2.8 270 E  305      0.39 .019        0.
94010122 19  1.5 270 E  239      0.29 .023        0.
94010123 18  4.5 270 D  367  17. 0.30             0.
94010124 18  2.2 270 F  305  11. 0.21 .022        0.
 ↑ ↑ ↑ ↑  ↑    ↑   ↑ ↑    ↑    ↑    ↑    ↑         ↑
yr  dy   Temp WS  WD     zi   σθ    p  dθ/dz   decay
  mo  hr          stab
```

Table 4-11
PLMMET.DAT File - Header Records

Records 1-3. Title, starting date, geophysical data.

Record	Columns	Variable	Type	Description
1	1-80	TITLE	character*80	Title of file.
2	*	IBYR	integer	Begining year of data.
2	*	IBMO	integer	Beginning month.
2	*	IBHR	integer	Beginning day.
2	*	IBHY	integer	Beginning hour.
3	*	ANEMHT	integer	Anemometer height (m).
3	*	Z0IN	real	Roughness length (m).
3	*	ILANDUIN	integer	Land use category.
3	*	ELEVIN	real	Elevation (m).
3	*	XLAIIN	real	Leaf area index (LAI)

* Free formatted input

Table 4-12
PLMMET.DAT File - Data Records
(One record per hour)

Records 4,5,6,... Hourly meteorological data.

Columns	Variable	Type	Description
1-2	IY	integer	Year of data in record
3-4	IM	integer	Month
5-6	ID	integer	Day
7-8	IH	integer	Hour (1-24 hour clock)
9-11	TMPC	real	Temperature (deg. C)
12-16	WSPD	real	Wind speed (m/s)
17-20	IWD	integer	Wind direction (deg.)
21-22	KST	integer	Stability class
23-27	ZMIX	real	Mixing height (m)
28-32	SIGTHA	real	σ_θ (deg.). Not used by CALPUFF. Use SIGMA.DAT file for turbulence measurements. See Section 4.2.9.
33-37	PLEXP	real	Wind speed power law exponent
38-42	PTGDF	real	Potential temperature gradient (deg. K/m)
43-52	DECAY	real	Decay constant (s^{-1}). Not used by CALPUFF. See Section 2.8 for chemical transformation options.

4.2.3 Point Source Emissions File With Arbitrarily Varying Emissions (PTEMARB.DAT)

The PTEMARB.DAT file contains point source emissions data for sources with detailed, arbitrarily varying emissions parameters. In the PTEMARB.DAT file, values for the stack parameters and emission rates can be specified for each time step in the run. Plume rise is computed within the CALPUFF model for each source.

PTEMARB.DAT is a sequential, unformatted data file consisting of three header records (see Table 4-13), followed by a set of data records containing time-invariant source information. The time-invariant records contain the stack height, diameter, coordinates, and optional descriptive codes for each source. The time varying emissions and stack parameter data follow in subsequent records. One data record per source is required for each time period (e.g.,usually at hourly intervals).

The data in the PTEMARB.DAT file is independent of the horizontal and vertical grid systems being used in the model. The horizontal coordinates are specified in terms of the meteorological grid projection (UTM or Lambert conformal coordinates). The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model. However, the PTEMARB.DAT file does contain time-dependent data specifying the emission parameters for a particular time period.

PTEMARB.DAT File - Header Records

The header records of the PTEMARB.DAT file contain the number of sources, starting and ending time periods of data in the file, and a list of the emitted species. Sample Fortran read statements are:

```
READ(iunit)FNAME2,NSRC2,NSE2,IUTMZ2,IBDAT2,IBTIM2,IEDAT2,
1 IETIM2,VRS2,LABEL2

READ(iunit)CSLST2
READ(iunit)XMWEM2
```

where the following declarations apply:

```
CHARACTER*12 FNAME2,VRS2,LABEL2,CSLST2(nse2)
REAL XMWEM2(nse2)
```

Table 4-13
PTEMARB.DAT - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
1	FNAME2	C*12	Data set name	PTEMARB
2	NSRC2	integer	Number of sources in the file	10
3	NSE2	integer	Number of species emitted	3
4	IUTMZ2	integer	UTM zone in which source coordinates are specified (enter 0 if using Lambert conformal coordinates)	11
5	IBDAT2	integer	Date of beginning of data in the file (YYJJJ, where YY=year, JJJ=Julian day)	84220
6	IBTIM2	integer	Hour of beginning of data in the file (00-23, LST)	00
7	IEDAT2	integer	Date of end of data in the file (YYJJJ, where YY=year, JJJ=Julian day)	84224
8	IETIM2	integer	Hour of end of data in the file (00-23, LST)	23
9	VRS2	C*12	Data set version	Base Case
10	LABEL2	C*12	Data set label	Major pts.

[a] C*12 = Character*12

Table 4-13 (Continued)
PTEMARB.DAT - Header Record 2 - Species List

No.*	Type[a]	Description	Sample Values
1	C*12	Species identifier for species 1	SO2
2	C*12	Species identifier for species 2	SO4
.	.	.	.
.	.	.	.
.	.	.	.
NSE2	C*12	Species identifier for species "NSE2"	NOX

* "NSE2" elements of CSLST2 array
[a] C*12 = Character*12

Table 4-13 (Concluded)
PTEMARB.DAT - Header Record 3 - Molecular Weights

No.*	Type[a]	Description	Sample Values
1	real	Molecular weight for species 1	64. SO2
2	real	Molecular weight for species 2	96. SO4
.	.	.	.
.	.	.	.
.	.	.	.
NSE2	real	Molecular weight for species "NSE2"	30. (NOX as NO)

* "NSE2" elements of XMWEM2 array

PTEMARB.DAT File - Data Records

The PTEMARB.DAT file contains two types of data records. A set of time-invariant records (see Table 4-14) are read after the header records. These records specify the time-invariant source parameters, including the source coordinates, stack height, and diameter. A set of time-varying data follows (see Table 4-15). The time-varying records contain the stack temperature, exit velocity, flow rate, and emission rate for each species.

Sample Fortran read statements for time-invariant data records are:

```
Loop over sources
READ(iunit)CID,TIDATA
End loop over sources
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL TIDATA(7)
```

Sample Fortran read statements for time-varying data records are:

```
Loop over time periods
READ(iunit)IBDAT,IBTIM,IEDAT,IETIM
    Loop over sources
        READ(iunit)CID,TEMPK,VEXIT,VOLFLOW,QEMIT
    End loop over sources
End loop over time periods
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL QEMIT(nse2)
```

Table 4-14
PTEMARB.DAT - Time-Invariant Data Record Contents
(Repeated for each source)

No.	Variable	Type[a]	Description
1	CID	C*16	Source identifier (16 characters = 4 words)
2	TIDATA(1)	real	Easting UTM or Lambert conformal coordinate (km) of the source
3	TIDATA(2)	real	Northing UTM or Lambert conformal coordinate (km) of the source
4	TIDATA(3)	real	Stack height (m)
5	TIDATA(4)	real	Stack diameter (m)
6	TIDATA(5)	real	Stack base elevation (m)
7	TIDATA(6)	real	User defined flag (e.g., industry code)
8	TIDATA(7)	real	User defined flag (e.g., fuel code)

[a] C*16 = Character*16

Table 4-15
PTEMARB.DAT - Time-Varying Data Record Contents
(First record of "NSRC2" + 1 records required for each time period)

No.	Variable	Type[a]	Description
1	IBDAT	integer	Beginning date for which data in this set is valid (YYJJJ, where YY = year, JJJ = Julian day)
2	IBTIM	integer	Beginning hour for which data in this set is valid (00-23, LST)
3	IEDAT	integer	Ending date for which data in this set is valid (YYJJJ, where YY = year, JJJ = Julian day)
4	IETIM	integer	Ending hour for which data in this set is valid (00-23, LST)

Example:

Data Valid for 1 hour:

IBDAT = 89183,IBTIM = 00,IEDAT = 89183,IETIM = 00
IBDAT = 89183,IBTIM = 01,IEDAT = 89183,IETIM = 01
IBDAT = 89183,IBTIM = 02,IEDAT = 89183,IETIM = 02

Data Valid for 3 hours:

IBDAT = 89183,IBTIM = 00,IEDAT = 89183,IETIM = 02
IBDAT = 89183,IBTIM = 03,IEDAT = 89183,IETIM = 05
IBDAT = 89183,IBTIM = 06,IEDAT = 89183,IETIM = 08

Table 4-15 (Concluded)
PTEMARB.DAT - Time-Varying Data Record Contents
(Next "NSRC2" records)

No.	Variable	Type[a]	Description
1	CID	C*16	Source identifier (must match values in time-invariant records)
2	TEMPK	real	Exit temperature (deg. K)
3	VEXIT	real	Exit velocity (m/s)
4	VOLFLOW	real	Volumetric flow rate (m^3/s)
Next NSE2	QEMIT	real array	Emission rates (g/s) for each species in the order specified in Header Record 2

[a]C*16 = Character*16

4.2.4 Buoyant Area Source Emissions File With Arbitrarily Varying Emissions (BAEMARB.DAT)

The BAEMARB.DAT file contains buoyant area source emissions data for sources with detailed, arbitrarily varying emissions parameters. This file can be generated from the output of the Forest Service's Emissions Production Model (EPM) using a reformatting and preprocessing program provided with CALPUFF. In the BAEMARB.DAT file, values for the source parameters and emission rates can be specified for each time step in the run. Plume rise is computed within the CALPUFF model for each source using the numerical plume rise algorithm described in Section 2.4.6.

BAEMARB.DAT is a free-formatted ASCII data file consisting of three header records (see Table 4-16), followed by a set of data records containing source information. The time-invariant data records contain character source identifiers. The time varying emissions and source parameter data follow in subsequent records. One data record per source is required for each time period (e.g.,usually at hourly intervals).

The data in the BAEMARB.DAT file are independent of the horizontal and vertical grid systems being used in the model. The horizontal coordinates are specified in terms of UTM or Lambert conformal coordinates. The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model. However, the BAEMARB.DAT file does contain time-dependent data specifying the emission parameters for a particular time period.

BAEMARB.DAT File - Header Records

The header records of the BAEMARB.DAT file contain the number of sources, starting and ending time periods of data in the file, and a list of the emitted species. Sample Fortran read statements are:

```
READ(iunit,*)FNAME3,NSRC3,NSE3,IUTMZ3,IBDAT3,IBTIM3,IEDAT3,
1 IETIM3,VRS3,LABEL3

READ(iunit,*)CSLST3
READ(iunit,*)XMWEM3
```

where the following declarations apply:

```
CHARACTER*12 FNAME3,VRS3,LABEL3,CSLST3(nse3)
REAL XMWEM3(nse3)
```

Table 4-16
BAEMARB.DAT - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
1	FNAME3	C*12	Data set name	BAEMARB
2	NSRC3	integer	Number of sources in the file	10
3	NSE3	integer	Number of species emitted	3
4	IUTMZ3	integer	UTM zone in which source coordinates are specified (enter 0 is using Lambert conformal coordinates)	11
5	IBDAT3	integer	Date of beginning of data in the file (YYJJJ, where YY=year, JJJ=Julian day)	84220
6	IBTIM3	integer	Hour of beginning of data in the file (00-23, LST)	00
7	IEDAT3	integer	Date of end of data in the file (YYJJJ, where YY=year, JJJ=Julian day)	84224
8	IETIM3	integer	Hour of end of data in the file (00-23, LST)	23
9	VRS3	C*12	Data set version	Base Case
10	LABEL3	C*12	Data set label	Burn #1

[a] C*12 = Character*12

Table 4-16 (Continued)
BAEMARB.DAT - Header Record 2 - Species List

No.*	Type[a]	Description	Sample Values
1	C*12	Species identifier for species 1	PM
2	C*12	Species identifier for species 2	PM10
.	.	.	.
.	.	.	.
.	.	.	.
NSE3	C*12	Species identifier for species "NSE3"	PM25

* "NSE3" elements of CSLST3 array
[a] C*12 = Character*12

Table 4-16 (Concluded)
BAEMARB.DAT - Header Record 3 - Molecular Weights

No.*	Type*	Description	Sample Values
1	real	Molecular weight for species 1	200.
2	real	Molecular weight for species 2	200.
.	.	.	.
.	.	.	.
.	.	.	.
NSE3	real	Molecular weight for species "NSE3"	200.

* "NSE3" elements of XMWEM3 array

BAEMARB.DAT File - Data Records

The BAEMARB.DAT file contains two types of data records. A set of time-invariant records (see Table 4-17) are read after the header records. These records specify the time-invariant source names. A set of time-varying data follows (see Table 4-18). The time-varying records contain the coordinates of four vertices that define the perimeter of the source, effective release heights, temperature, heat flux, and an emission rate for each species. Note that the four vertices must be centered in sequence around the perimeter; all four "x" coordinates followed by all four "y" coordinates.

Sample Fortran read statements for time-invariant data records are:

```
Loop over sources
READ(iunit,*)CID
End loop over sources
```

where the following declarations apply:

```
CHARACTER*16 CID
```

Sample Fortran read statements for time-varying data records are:

```
Loop over time periods
  READ(iunit,*)IBDAT,IBTIM,IEDAT,IETIM
    Loop over sources
      READ(iunit,*)CID,VERTX,VERTY,HT,TEMPK,QHFLX,QEMIT
    End loop over sources
End loop over time periods
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL VERTX(4),VERTY(4)
REAL QEMIT(nse3)
```

Table 4-17
BAEMARB.DAT - Time-Invariant Data Record Contents
(Repeated for each source)

No.	Variable	Type[a]	Description
1	CID	C*16	Source identifier (16 characters = 4 words)

[a] C*16 = Character*16

Table 4-18

BAEMARB.DAT - Time-Varying Data Record Contents

(First record of "NSRC3"+1 records required for each time period)

No.	Variable	Type[a]	Description
1	IBDAT	integer	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	integer	Beginning hour for which data in this set is valid (00-23, LST)
3	IEDAT	integer	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	integer	Ending hour for which data in this set is valid (00-23, LST)

Example:

Data Valid for 1 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hours:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

Table 4-18 (Concluded)
BAEMARB.DAT - Time-Varying Data Record Contents
(Next "NSRC3" records)

No.	Variable	Type*	Description
1	CID	C*16	Source identifier (must match values in time-invariant records)
2–5	VERTX	real array	X-coordinate (km) of each of the four vertices defining the perimeter of the area source
6–9	VERTY	real array	Y-coordinate (km) of each of the four vertices defining the perimeter of the area source
10	HT	real	Effective height (m) of the emissions above the ground
11	TEMPK	real	Temperature (deg. K)
12	QHFLX	real	Total heat flux (kW)
Next NSE3	QEMIT	real array	Emission rates (g/s) for each species in the order specified in Header Record 2

*C*16 = Character*16

4.2.5 Volume Source Emissions File (VOLEM.DAT) with Arbitrarily Varying Emissions

Time independent volume source data are contained in the CALPUFF control file (CALPUFF.INP). The VOLEM.DAT emissions file contains time-dependent volume source emissions data. VOLEM.DAT is a sequential, unformatted data file containing one two-dimensional grid for each emitted species modeled by CALPUFF for each time step. There are three header records with information describing the grid system, dates and time of data in the file, species names, and molecular weights.

The total emission rate for each pollutant is specified for the grid column. Individual source information is not stored in the file, so plume rise is not computed by CALPUFF for the VOLEM.DAT emissions. The effective height and initial vertical and horizontal plume dimensions (σ_y, σ_z) are specified by the user in the control file (CALPUFF.INP) for the gridded area source inventory.

VOLEM File - Header Records

The header records contain information regarding the horizontal grid system, species emitted, molecular weights, and dates of the data contained in the file (see Table 4-19). These data are checked by CALPUFF in the setup phase of the model run to ensure the parameters are compatible with those specified in the CALPUFF control file. Any mismatch in the specifications results in an error message and termination of the run.

Sample Fortran read statements for the header records are:

```
READ(iunit)FNAME4,IGTYP4,NX4,NY4,DELX4,DELY4,XORIG4,YORIG4,IUTMZ4,
 1 NSE4,IBDAT4,IBTIM4,IEDAT4,IETIM4,VRS4,LABEL4

READ(iunit)CSLST4
READ(iunit)XMWEM4
```

where the following declarations apply:

```
CHARACTER*12 FNAME4,VRS4,LABEL4,CSLST4(nse4)
REAL XMWEM4(nse4)
```

Table 4-19

VOLEM - Header Record 1 - General Grid, Species, and Date Data

No.	Variable	Type[a]	Description	Sample Values
1	FNAME4	C*12	Data set name	VOLEM
2	IGTYP4	integer	Horizontal grid type (always = 1 for CALPUFF runs)	1
3	NX4	integer	Number of grid cells in the X direction	30
4	NY4	integer	Number of grid cells in the Y direction	30
5	DELX4	real	Grid spacing (km) in the X direction	5.
6	DELY4	real	Grid spacing (km) in the Y direction	5.
7	XORIG4	real	Reference X coordinate (km) of the southwest corner of grid cell (1,1)	168.000
8	YORIG4	real	Reference Y coordinate (km) of the southwest corner of grid cell (1,1)	3930.000
9	IUTMZ4	integer	UTM zone of horizontal coordinates (enter 0 if using Lambert conformal coordinates)	11
10	NSE4	integer	Number of species emitted	3
11	IBDAT4	integer	Date of beginning of data in file (YYJJJ, where YY=year, JJJ=Julian day)	84220
12	IBTIM4	integer	Hour of beginning of data in file (00-23, LST)	00
13	IEDAT4	integer	Date of end of data in file (YYJJJ, where YY=year, JJJ=Julian day)	84224
14	IETIM4	integer	Hour of end of data in file (00-23, LST)	23
15	VRS4	C*12	Data set version	Base Case
16	LABEL4	C*12	Data set label	'84 - KERN

[a]C*12 = Character*12

Table 4-19 (Continued)
VOLEM - Header Record 2 - Species List

No.	Type[a]	Description	Sample Values
1	C*12	Species identifier for species 1	SO2
2	C*12	Species identifier for species 2	SO4
.	.	.	.
.	.	.	.
.	.	.	.
NSE4	C*12	Species identifier for species "NSE4"	NOX

* "NSE4" elements of CSLST4 array
[a]C*12 = Character*12

Table 4-19 (Concluded)
VOLEM - Header Record 3 - Molecular Weights

No.	Type*	Description	Sample Values
1	real	Molecular weight for species 1	64. (SO2)
2	real	Molecular weight for species 2	96. (SO4)
.	.	.	.
.	.	.	.
.	.	.	.
NSE4	real	Molecular weight for species "NSE4"	30. (NOX)

* "NSE4" elements of XMWEM1 array

VOLEM.DAT File - Data Records

The VOLEM.DAT file contains a set of "NSE4"+1 records for each time period (e.g., hour). The first data record of each set defines the time period over which the emissions data in the following records are valid. The next "NSE4" records each contain a species identifier and a two-dimensional gridded field of emissions. See Table 4-20 for a description of the variables in the VOLEM.DAT data records.

Sample Fortran read statements for a set of data records are:

```
Loop over time periods (e.g., Hours)
READ(iunit)IBDAT,IBTIM,IEDAT,IETIM
    Loop over species
    READ(iunit)CSPEC,QEMIT
    End loop over species
End loop over time periods
```

where the following declarations apply:

```
CHARACTER*12 CSPEC
REAL QEMIT(nx4,ny4)
```

Table 4-20
VOLEM - Data Record Contents
(Record 1 of each set)

No.	Variable	Type[a]	Description
1	IBDAT	integer	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	integer	Beginning time for which data in this set is valid (00-23, LST)
3	IEDAT	integer	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	integer	Ending time for which data in this set is valid (00-23, LST)

Example:

Data Valid for 1 hour:
IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hours:
IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

Table 4-20 (Concluded)
VOLEM - Data Record Contents
(Records 2, 3, ... "NSE4"+1 of each set)

No.	Variable	Type*	Description
1	CSPEC	C*12	Species identifier (up to 12 characters)
Next NX4*NY4	QEMIT	real array	Volume source emission rate (g/s) of species CSPEC" for each grid column (QEMIT (nx4,ny4)

*C*12 = Character*12

4.2.6 User-Specified Deposition Velocity Data File (VD.DAT)

The CALPUFF model requires that the user specify the method for determining dry deposition velocities for each species. In Input Group 3 of the control file, one of the following flags must be specified for each pollutant.

0 = no dry deposition (deposition velocities set to zero)
1 = resistance model used - pollutant deposited as a gas
2 = resistance model used - pollutant deposited as a particle
3 = user-specified deposition velocities used

Note that different methods can be used for different pollutants in the same CALPUFF run.

If any species are flagged as using "user-specified" deposition velocities, CALPUFF reads a formatted user-prepared data file with a 24-hour diurnal cycle of deposition velocities for each species flagged. The 24 values correspond to hours 01-24 (LST) of the simulated day. Twenty-four values must be entered for each flagged pollutant, even if the model run is for less than a full diurnal cycle. The units of the deposition velocities are m/s.

An example of a user-specified VD.DAT file is shown in Table 4-21. The VD.DAT file uses a control file format (see Section 4.2.2). All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module. Each data line consists of a delimiter followed by the species name, 24 deposition velocities, and a terminating delimiter. The data may extend over more than one line. The line being continued must end with a comma. The control file format allows the use of repetition factors (e.g., 3 * 1.0 instead of 1.0, 1.0, 1.0). The order in which the species are entered in the file is not important. However, the file must end with an input group terminator (i.e., !END!).

The model checks that values have been entered for each species flagged as using user-specified deposition velocities. An error message is printed and execution of the run is terminated if any values are missing. The run will also terminate with an error message from the input routine if too many values are entered (i.e., more than 24 values for a particular pollutant). The species names must match those used in the chemical mechanism of the model.

Table 4-21
Sample User-Specified Deposition Velocity File for Two Species

```
                DEPOSITION VELOCITY FILE (VD.DAT)
                ---------------------------------

VD.DAT contains 24-hour diurnal cycle of deposition velocities for each species flagged as using user-specified
values in the control file (CALPUFF.INP).

The first value correspond to the period from 0:00 to 1:00, and the 24th value corresponds to 23:00-0:00.

NOTE: Units are in m/s.
----------------------

SPECIES
 NAME                  Deposition Velocities (m/s)
-------                ---------------------------

!  HNO3        =       5*1.5e-2, 4*1.7e-2, 3*1.8e-2, 3*1.9e-2, 3*1.7e-2, 6*1.5e-2        !
!  SO2         =       5*0.8e-2, 13*1.0e-2, 6*0.8e-2                                     !


!END!
```

4.2.7 Hourly Ozone Data File (OZONE.DAT)

If the MESOPUFF II chemical mechanism is used to simulate the chemical transformation of $SO_2 \rightarrow SO_4^=$ and $NO_x \rightarrow HNO_3 \rightarrow NO_3^-$, estimates of background ambient ozone concentration levels are required to compute the hourly conversion rates. CALPUFF provides two options for the user to provide these data: (1) a single, typical background value appropriate for the modeling region, or (2) hourly ozone data from one or more ozone monitoring stations. The selection of Option 2 requires that a file called OZONE.DAT be created with the necessary data.

OZONE.DAT is a sequential, formatted data file containing three types of records: single header record, time-invariant data records, and hourly ozone data records. A sample OZONE.DAT file is shown in Table 4-22. The header record contains information on the number of stations in the data set, the time period of the data, and descriptive information regarding the file. The time-invariant records contain the coordinates of each of the ozone stations. The time-varying data consists of hourly ozone concentrations at each of the ozone stations.

Table 4-22
Sample Hourly Ozone Data File (OZONE.DAT)

```
'OZONE', 3, 11, 80001, 0, 80002, 0, 'TEST DATA', 'V1.0'
'STATION 1',      168.000,      3840.000
'STATION 2',      200.000,      3880.000
'STATION 3',      180.000,      3860.000
80,  001,  0,  9999.,    62.,    50.
80,  001,  1,  9999.,  9999.,  9999.
80,  001,  2,    68.,    61.,  9999.
80,  001,  3,    66.,  9999.,  9999.
80,  001,  4,  9999.,  9999.,    53.
80,  001,  5,  9999.,  9999.,  9999.
80,  001,  6,  9999.,  9999.,  9999.
80,  001,  7,  9999.,  9999.,  9999.
80,  001,  8,    69.,    68.,    60.
80,  001,  9,    72.,    75.,    65.
80,  001, 10,    74.,    78.,    69.
80,  001, 11,    87.,    85.,    74.
80,  001, 12,   102.,    99.,    84.
80,  001, 13,   109.,   105.,    92.
80,  001, 14,   120.,   118.,   102.
80,  001, 15,   116.,   116.,    95.
80,  001, 16,   103.,   100.,    97.
80,  001, 17,    98.,    90.,    88.
80,  001, 18,    89.,    82.,    83.
80,  001, 19,  9999.,  9999.,    80.
80,  001, 20,  9999.,  9999.,    78.
80,  001, 21,  9999.,  9999.,    74.
80,  001, 22,  9999.,  9999.,    69.
80,  001, 23,  9999.,  9999.,    69.
80,  002, 00,  9999.,  9999.,    68.
```

OZONE.DAT File - Header Record

The header records of the OZONE.DAT file contain the name, version, and label of the data set, the number of ozone stations, and starting and ending time periods of data in the file (see Table 4-23). A sample Fortran read statement for the header record is:

```
READ(iunit,*)FNAMEO,NOZSTA,IUTMOZ,IBDATO,IBTIMO,IEDATO,
1 IETIMO,VRSOZ,LABOZ
```

where the following declaration applies:

```
CHARACTER*12 FNAMEO,VRSOZ,LABOZ.
```

Table 4-23
OZONE.DAT - Header Record - General Data

No.	Variable	Type[a]	Description	Sample Values
1	FNAMEO	C*12	Data set name	OZONE
2	NOZSTA	integer	Number of ozone stations in the file	3
3	ITUMOZ	integer	UTM zone in which ozone station coordinates are specified (enter 0 if using Lambert conformal coordinates)	11
4	IBDATO	integer	Date of beginning of data in the file (YYJJJ, where YY=year, JJJ=Julian day)	80001
5	IBTIMO	integer	Hour of beginning of data in the file (00-23, LST)	00
6	IEDATO	integer	Date of end of data in the file (YYJJJ, where YY=year, JJJ=Julian day)	80002
7	IETIMO	integer	Hour of end of data in the file (00-23, LST)	00
8	VRSOZ	C*12	Data set version	"Test Data"
9	LABOZ	C*12	Data set label	"V1.0"

[a]C*12 = Character*12

OZONE.DAT File - Data Records

The OZONE.DAT file contains two types of data records. A set of time-invariant records are read after the header records. These records specify the coordinates of each ozone station (see Table 4-24). A set of time-varying data follows, which contain the hourly ozone concentration (in ppb) for each station (see Table 4-25).

Sample Fortran read statements for time-invariant data records are:

```
Loop over stations
READ(iunit,*)CID,XOZ,YOZ
End loop over stations
```

where the following declaration applies:

```
CHARACTER*16 CID
```

Sample Fortran read statements for time-varying data records are:

```
Loop over hours
      READ(iunit,*)IYR,IJUL,IHR,OZCONC
End loop over hours
```

where the following declaration applies:

```
REAL OZCONC(nozsta)
```

Table 4-24
OZONE.DAT - Time-Invariant Data Record Contents
(Repeated for each station)

No.	Variable	Type*	Description
1	CID	C*16	Station identifier (16 characters = 4 words)
2	XOZ	real	X coordinate (km) of the ozone station
3	YOZ	real	Y coordinate (km) of the ozone station

*C*16 = Character*16

Table 4-25
OZONE.DAT - Time-Varying Data Record Contents
(One record per hour)

No.	Variable	Type[a]	Description
1	IYR	integer	Year of data (two digits)
2	IJUL	integer	Julian day
3	IRH	integer	Hour of data (00-23 LST)
Next "NOZSTA"	OZCONC	real array	Ozone concentration (ppb) at each ozone station (in the same order as the station coordinates in the time-invariant records)

4.2.8 User-Specified Chemical Transformation Rate Data File (CHEM.DAT)

If chemical conversion is to be considered by CALPUFF, the user must specify a variable in the control file, MCHEM, which determines how chemical transformation rates are computed. The options for MCHEM are:

0 = chemical transformation is not modeled
1 = the MESOPUFF II chemical scheme is used to compute transformation rates
2 = user-specified 24-hour cycles of transformation rates are used

If MCHEM is set equal to 2, CALPUFF reads a formatted user-prepared data file with 24-hour diurnal cycles of transformation rates k_1, k_2, k_3 (described in Section 2.8). The nature of the equilibrium relationship assumed between pollutants 4 and 5 (e.g., HNO_3 and NO_3^-) precludes the use of a user-specified conversion rate between these pollutants. If NO_3 is being modeled, the NH_4NO_3 dissociation constant is determined as a function of temperature and relative humidity as described in Section 2.8.1.

A sample user-specified CHEM.DAT file is shown in Table 4-26. The CHEM.DAT file uses a control file format (see Section 4.2.2). All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module. Each data line consists of a delimiter followed by the species name, 24 conversion rates, and a terminating delimiter. The data may extend over more than one line. The line being continued must end with a comma. The control file format allows the use of repetition factors (e.g., 3 * 1.0 instead of 1.0, 1.0, 1.0). The order in which the species are entered in the file is not important. However, the file must end with an input group terminator (i.e., !END).

The model checks that the proper number of values have been entered for each conversion rate. An error message is printed and execution of the run is terminated if any values are missing. The run will also terminate with an error message from the input routine if too many values are entered (i.e., more than 24 values).

Table 4-26
Sample User-Specified Chemical Transformation Rate Data File (CHEM.DAT)

```
                    CHEMICAL TRANSFORMATION RATE FILE (CHEM.DAT)
                    --------------------------------------------

CHEM.DAT contains a 24-hour diurnal cycle of chemical transformation
rates for the chemical transformation of SO2 to SO4, and NOx to HNO3/PAN.

          k1 = SO2 to SO4 transformation rate(percent/hour)

          k2 = NOx to HNO3 + PAN transformation rate (percent/hour)

          k3 = NOx to HNO3 (only) transformation rate (percent/hour)

The first value correspond to the period from 0:00 to 1:00, and the 24th value corresponds to 23:00-0:00.


                TRANSFORMATION RATE (percent/hour)
                ----------------------------------

! K1          =  7*0.2, 0.4, 0.8, 1.2, 1.6, 3*2.0,   1.6,  1.2, 0.8, 0.4, 6*0.2 !
! K2          =  7*2.0, 4.0, 8.0,12.0,15.0, 3*20.0, 15.0, 12.0, 8.0, 4.0, 6*2.0 !
! K3          =  7*2.0, 3.0, 6.0, 8.0,11.0, 3*15.0, 11.0,  8.0, 6.0, 3.0, 6*2.0 !

!END!
```

4.2.9 Site-Specific Turbulence Data (SIGMA.DAT)

CALPUFF provides several options for computing the dispersion coefficients, σ_y and σ_z. In Input Group 2 of the control file, the user specifies a value for the dispersion method flag, MDISP:

1 = dispersion coefficients computed from values of σ_v and σ_w read from a data file (SIGMA.DAT),

2 = dispersion coefficients determined from internally computed values of σ_v and σ_w based on similarity scaling relationships,

3 = PG coefficients (computed using the ISCST multi-segment approximation) used for rural areas and MP coefficients used in urban areas,

4 = same as 3 except that the PG coefficients are computed using the MESOPUFF II equations.

Section 2.2.1 contains more information on these options. If Option 1 is selected, the user must prepare a data file with hourly values of σ_v and σ_w. This option is intended primarily for application to a single source or facility with onsite measurements of σ_v and σ_w. Therefore, only one set of observations are allowed in the data base and they are assumed to apply over the entire computational region.

SIGMA.DAT is a sequential, formatted data file containing a single time-invariant header record followed by a set of hourly data records. A sample SIGMA.DAT file is shown in Table 4-27. The header record contains some general descriptive information on the file and specifies the time period of the data in the file. The time-varying data records consist of a date and hour followed by values of σ_v and σ_w.

Table 4-27
Sample Site-Specific Turbulence Data File (SIGMA.DAT)

```
'SIGMA', 80001, 0, 80002, 0, 'BASE CASE', 'Onsite10m'
80,    001,    01,    0.52,    0.01
80,    001,    02,    0.54,    0.01
80,    001,    03,    0.57,    0.01
80,    001,    04,    0.61,    0.01
80,    001,    05,    0.64,    0.02
80,    001,    06,    0.64,    0.02
80,    001,    07,    0.65,    0.04
80,    001,    08,    0.68,    0.04
80,    001,    09,    0.70,    0.05
80,    001,    10,    0.72,    0.05
80,    001,    11,    0.73,    0.07
80,    001,    12,    0.93,    0.07
80,    001,    13,    1.03,    0.08
80,    001,    14,    1.18,    0.08
80,    001,    15,    1.23,    0.08
80,    001,    16,    1.12,    0.10
80,    001,    17,    1.12,    0.10
80,    001,    18,    0.99,    0.12
80,    001,    19,    0.93,    0.12
80,    001,    20,    0.89,    0.14
80,    001,    21,    0.87,    0.14
80,    001,    22,    0.76,    0.26
80,    001,    23,    0.71,    0.26
80,    002,    00,    0.63,    0.28
```

SIGMA.DAT File - Header Record

The header record of the SIGMA.DAT file contains the name, version, and label of the data set, and the starting and ending time periods of the data in the file (see Table 4-28). A sample Fortran read statement for the header record is:

```
READ(iunit)FNAMES,IBDATS,IBTIMS,IEDATS,IETIMS,VRSS,LABELS
```

where the following declaration applies:

```
CHARACTER*12 FNAMES, VRSS, LABELS
```

Table 4-28
SIGMA.DAT - Heater Record - General Data

No.	Variable	Type[a]	Description	Sample Values
1	FNAMES	C*12	Data set name	SIGMA
2	IBDATS	integer	Date of beginning of data in the file (YYJJJ, where YY=year and JJJ=Julian day)	80001
3	IBTIMS	integer	Hour of beginning of data in the file (00-23, LST)	00
4	IEDATS	integer	Date of end of data in the file (YYJJJ, where YY=year and JJJ=Julian day)	80002
5	IETIMS	integer	Hour of end of data in the file (00-23, LST)	00
6	VRSS	C*12	Data set version	Base Case
7	LABELS	C*12	Data set label	Onsite10m

[a] C*12 = Character*12

SIGMA.DAT File - Data Records

The SIGMA.DAT file contains one data record per hour. Each record contains values for σ_v and σ_w, in m/s (see Table 4-29). Preferably, the measurement height of σ_v and σ_w should be at or near the height of the stack being modeled. The values of σ_v and σ_w provided in the SIGMA.DAT file are used in Eqns. (2-39) and (2-40) to compute σ_y and σ_z (see Section 2.2.1). A sample read statement for the hourly data records is:

```
Loop over hours
  READ(iunit,*)IYR,IJUL,IHR,SIGV,SIGW
End loop over hours
```

Table 4-29
SIGMA.DAT - Time-Varying Data Record Contents
(One record per hour)

No.	Variable	Type[a]	Description
1	IYR	integer	Year of data (two digits)
2	IJUL	integer	Julian day
3	IHR	integer	Hour of data
4	SIGV	real	Standard deviation (m/s) of the horizontal crosswind component of the wind (σ_v)
5	SIGW	real	Standard deviation (m/s) of the vertical component of the wind (σ_w)

4.2.10 CTDMPLUS Terrain Feature Description - for CTSG (TERRAIN)

CALPUFF allows two ways of specifying the characteristics of terrain features modeled by CTSG. The first is by means of the OPTHILL processor described in Section 4.1. The second approach allows the use of the terrain preprocessing programs provided with CTDMPLUS (Mills et al., 1987). If a user is familiar with the terrain preprocessor, then this may be the preferred option because the standard terrain file used in CTDMPLUS can be used in CALPUFF without modification. CTDMPLUS subroutines that read and process the terrain data have been incorporated in CALPUFF.

Table 4-30 illustrates a typical TERRAIN file for one hill. This one is defined by ellipse/polynomial shapes determined for a range of 10 "critical elevations" from 25 m to 115 m above the base of the hill. After the header record, the first group of 10 records provides the ellipse parameters at each "critical elevation", and the second group of 10 records provides the parameters for the corresponding inverse polynomial shape profile fit to the portion of the hill above it. Refer to Mills et al. (1987) for more detailed information.

Table 4-30
Sample CTDMPLUS Terrain Feature File (TERRAIN)

1	10	125.		CTSG Test Hill			
25.	0.	0.	0.	1132.	566.		
35.	0.	0.	0.	980.	490.		
45.	0.	0.	0.	855.6	427.8		
55.	0.	0.	0.	748.6	374.3		
65.	0.	0.	0.	653.4	326.7		
75.	0.	0.	0.	565.8	282.9		
85.	0.	0.	0.	482.6	241.3		
95.	0.	0.	0.	400.	200.		
105.	0.	0.	0.	313.8	156.9		
115.	0.	0.	0.	213.8	106.9		
25.	0.	0.	0.	2.5	2.5	540.	270.
35.	0.	0.	0.	2.4	2.4	500.	250.
45.	0.	0.	0.	2.6	2.5	460.	230.
55.	0.	0.	0.	2.7	2.6	420.	210.
65.	0.	0.	0.	2.5	2.4	380.	190.
75.	0.	0.	0.	2.8	2.6	340.	170.
85.	0.	0.	0.	2.8	2.5	300.	150.
95.	0.	0.	0.	2.9	2.0	260.	130.
105.	0.	0.	0.	2.0	2.0	107.	53.5
115.	0.	0.	0.	2.0	2.0	53.5	26.8

4.3 CALPUFF Output Files

4.3.1 Concentration File (CONC.DAT)

The CONC.DAT file is an unformatted data file containing gridded fields of time averaged concentrations predicted by CALPUFF. The creation and contents of the CONC.DAT file are controlled by user-specified inputs in Input Group 7 of the control file (see Section 4.2.2). The control file variable ICON must be set equal to one in order to create the CONC.DAT file.

CONC.DAT File - Header Records

The CONC.DAT file consists of five header records followed by a set of data records. The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input title, a list of the species combinations stored in the output file, and receptor information (see Table 4-31).

Sample FORTRAN read statements for the header records are:

```
READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,
1 IRLG,IAVG,NXM,NYM,DXKM,DYKM,IONE,IBCOMP,IECOMP,JBCOMP,JECOMP,
2 IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NDREC,NCTREC,LSGRID,
3 NSPOUT
READ(iunit)TITLE
READ(iunit)CSOUT
READ(iunit)XREC,YREC,ZREC
READ(iunit)XRCT,YRCT,ZRCT,IHILL
```

where the following declarations apply:

```
Character*80 TITLE(3)
Character*15 CSOUT(NSPOUT)
Character*12 CMODEL,VER,LEVEL

Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)

Integer IHILL(NCTREC)
```

Table 4-31
Unformatted CONC.DAT file - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
1	CMODEL	C*12	Model name	CALPUFF
2	VER	C*12	Model version number	3.0
3	LEVEL	C*12	Model level number	950715
4	IBYR	integer	Starting year of the run	80
5	IBJUL	integer	Starting Julian day	183
6	IBHR	integer	Starting hour (00-23)	8
7	IRLG	integer	Length of run (hours)	5
8	IAVG	integer	Averaging time (hours) of output concentrations	1
9	NXM	integer	Number of grid points in meteorological grid (X direction)	20
10	NYM	integer	Number of grid points in meteorological grid (Y direction)	20
11	DXKM	real	Grid spacing (km) in the X direction	5.
12	DYKM	real	Grid spacing (km) in the Y direction	5.
13	IONE	integer	Number of receptor layers (must be equal to one for CALPUFF runs)	1
14	IBCOMP	integer	Start of computational grid in X direction	1
15	IECOMP	integer	End of computational grid in X direction	20
16	JBCOMP	integer	Start of computation grid in the Y direction	1
17	JECOMP	integer	End of computational grid in Y direction	20
18	IBSAMP	integer	Start of sampling grid in X direction	1
19	JBSAMP	integer	End of sampling grid in X direction	20

[a]C*12 = Character*12

Table 4-31 (Continued)
Unformatted CONC.DAT file - Header Record 1 - General Data

No.	Variable	Type*	Description	Sample Values
20	IESAMP	integer	Start of sampling grid in Y direction	1
21	JESAMP	integer	End of sampling grid in Y direction	20
22	MESHDN	integer	Sampling grid spacing factor	1
23	NPTS	integer	Number of point sources	2
24	NAREAS	integer	Number of area sources	0
25	NDREC	integer	number of discrete receptors	0
26	NCTREC	integer	Number of complex terrain receptors	0
27	LSGRID	logical	Sampling grid flag (T = gridded receptors, F = no gridded receptors)	T
28	NSPOUT	integer	Number of output species	5

Table 4-31 (Continued)
Unformatted CONC.DAT file - Header Record 2 - Run Title

No.	Variable	Type[a]	Description
1	TITLE (3)	C*80	User-specified run title (three lines of up to 80 characters/line)

Header Record 3 - List of Species in Output File

No.	Variable	Type[a]	Description
1-NSPEC	CSOUT array	C*15	Species name (characters 1-12) and layer (characters 13-15) of concentrations stored in the output file. For example, "SO2 1" indicates SO_2 concentrations in Layer 1; "DIOXINP 1" indicates dioxin in particulate form in Layer 1. CALPUFF concentrations are always computed at ground-level, so therefore are labeled as Layer 1.

[a]C*80 = Character*80
C*15 = Character*15

Table 4-31 (Concluded)
Header Record 4 - Discrete Receptors
(Included only if NDREC > 0)

No.	Variable	Type	Description
1	XREC	real array	X-coordinate (km) of each discrete receptor
2	YREC	real array	Y-coordinate (km) of each discrete receptor
3	ZREC	real array	Ground level elevation (m) of each discrete receptor

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

No.	Variable	Type	Description
1	XRCT	real array	X-coordinate (km) of each complex terrain receptor
2	YRCT	real array	Y-coordinate (km) of each complex terrain receptor
3	ZRCT	real array	Ground level elevation (m) of each complex terrain receptor
4	IHILL	integer array	Hill number associated with this receptor

CONC.DAT File - Data Records

The CONC.DAT data records consist of a set of "NSPOUT+1" records for each hour of the CALPUFF run (NSPOUT is the number of output species in the CALPUFF run). The first record of each set contains the date and hour of the data in the records which follow it. The next "NSPOUT" records contain the predicted concentrations in g/m^3, for each species, flagged for output in the control file. See Table 4-32 for a description of the variables.

Sample FORTRAN read statements for the data records are:

```
LOOP OVER OUTPUT SPECIES

GRIDDED RECEPTOR CONCENTRATIONS
IF(LSGRID)READ(iunit)CSPECG,CONCG

DISCRETE RECEPTOR CONCENTRATIONS
IF(NDREC.GT.0)READ(iunit)CSPECD,CONCD

COMPLEX TERRAIN RECEPTOR CONCENTRATIONS
IF(NCTREC.GT.0)READ(iunit)CSPECCT,CONCCT

END LOOP OVER OUTPUT SPECIES
```

where the following declarations apply:

```
Character*15 CSPECG,CPSECD,CSPECCT
Real CONCG(nxg,nyg),CONCD(NDREC),CONCCT(NCTREC)
```

and

```
nxg = IESAMP - IBSAMP+1
nyg = JESAMP - JBSAMP+1
```

Table 4-32
Unformatted CONC.DAT File - Data Records
(Record 1 of each set)

No.	Variable	Type	Description
1	NYR	integer	Year of concentration data (two digits)
2	NJUL	integer	Julian day of data
3	NHR	integer	Hour (00-23) of data

(Next Data Record)
(Included only if LSGRID = TRUE)

No.	Variable	Type[a]	Description
1	CSPECG	C*15	Species name (characters 1-12) and layer (characters 13-15) of the concentrations in this record. For example, "SO2 1" indicates SO_2 concentrations in Layer 1; "DIOXINP 1" indicates dioxin in particulate form in Layer 1. (Note: Layer is always " 1" in CALPUFF output, but can be up to NZ in CALGRID.)
Next NXG*NYG	CONCG	real array	"IAVG" - hour averaged concentrations (g/m^3) for each sampling grid point.

[a] C*15 = Character*15

4.3.2 Dry Flux File (DFLX.DAT)

The DFLX.DAT file is an unformatted data file containing gridded fields of time averaged dry deposition fluxes predicted by CALPUFF. The creation and contents of the DFLX.DAT file are controlled by user-specified inputs in Input Group 7 of the control file (see Section 4.2.1).

The control file variable IDRY must be set equal to one in order to create the DFLX.DAT file. The species saved in the output file are also controlled by the user by setting flags in the output species table in Input Group 7 of the control file. The model checks that only deposited species are flagged for output into the DFLX.DAT file. The effects of dry deposition on ambient concentrations can be evaluated without saving the dry fluxes in the output file if the actual values of the deposition fluxes are not of interest.

DFLX.DAT File - Header Records

The DFLX.DAT file consists of five header records followed by a set of data records. The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input run title, and a list of the deposited species stored in the output file, and receptor information (see Table 4-33).

Sample FORTRAN read statements for the header records are:

```
READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,IRLG,
1 IAVG,NXM,NYM,DXKM,DYKM,IONE,IBCOMP,IECOMP,JBCOMP,JECOMP
2 IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NDREC,NCTREC,LSGRID,
3 NDFOUT
READ(iunit)TITLE
READ(iunit)CDFOUT
READ(iunit)XREC,YREC,ZREC
READ(iunit)XRCT,YRCT,ZRCT,IHILL
```

where the following declarations apply:

```
Character*80 TITLE(3)
Character*15 CDFOUT(NDFOUT)
Character*12 CMODEL,VER,LEVEL

Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)
Integer IHILL(NCTREC)
```

Table 4-33

Unformatted DFLX.DAT file - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
1	CMODEL	C*12	Model name	CALPUFF
2	VER	C*12	Model version number	3.0
3	LEVEL	C*12	Model level number	950715
4	IBYR	integer	Starting year of the run	80
5	IBJUL	integer	Starting Julian day	183
6	IBHR	integer	Starting hour (00-23)	8
7	IRLG	integer	Length of run (hours)	5
8	IAVG	integer	Averaging time (hours) of output concentrations	1
9	NXM	integer	Number of grid points in meteorological grid (X direction)	20
10	NYM	integer	Number of grid points in meteorological grid (Y direction)	20
11	DXKM	real	Grid spacing (km) in the X direction	5.
12	DYKM	real	Grid spacing (km) in the Y direction	5.
13	IONE	integer	Layer number (always 1 for deposition fluxes)	1
14	IBCOMP	integer	Start of computational grid in X direction	1
15	IECOMP	integer	End of computational grid in X direction	20
16	JBCOMP	integer	Start of computational grid in Y direction	1
17	JECOMP	integer	End of computational grid in Y direction	20
18	IBSAMP	integer	Start of sampling grid in X direction	1
19	JBSAMP	integer	End of sampling grid in X direction	20

[a] C*12 = Character*12

Table 4-33 (Continued)
Unformatted DFLX.DAT file - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
20	IESAMP	integer	Start of sampling grid in Y direction	1
21	JESAMP	integer	End of sampling grid in Y direction	20
22	MESHON	integer	Sampling grid spacing factor	1
23	NPTS	integer	Number of point sources	2
24	NAREAS	integer	Number of area sources	0
25	NDREC	integer	Number of discrete receptors	0
26	NCTREC	integer	Number of complex terrain receptors	0
27	LSGRID	logical	Sampling grid flag (T = gridded receptors, F = no gridded receptors)	T
28	NDFOUT	integer	Number of dry deposited species stored in the output file	5

Table 4-33 (Continued)
Unformatted DFLX.DAT file - Header Record 2 - Run Title

No.	Variable	Type[a]	Description
1	TITLE(3)	C*80	User-specified run title (three lines of up to 80 characters/line)

Header Record 3 - List of Species-Layers in Output File

No.	Variable	Type	Description
1-NDFOUT	CDFOUT array	C*15	Species name (characters 1-12) and variable flag (characters 13-15) of data stored in the output file. The variable flag for dry fluxes is " DF". For example, "SO2 DF" corresponds to SO_2 dry fluxes.

[a] C*80 = Character*80
C*15 = Character*15

Table 4-33 (Concluded)
Header Record 4 - Discrete Receptors
(Included only if NDREC > 0)

No.	Variable	Type[a]	Description
1	XREC	real array	X-coordinate (km) of each discrete receptor
2	YREC	real array	Y-coordinate (km) of each discrete receptor
3	ZREC	real array	Ground level elevation (m) of each discrete receptor

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

No.	Variable	Type	Description
1	XRCT	real array	X-coordinate (km) of each complex terrain receptor
2	YRCT	real array	Y-coordinate (km) of each complex terrain receptor
3	ZRCT	real array	Ground level elevation (m) of each complex terrain receptor
4	IHILL	integer array	Hill number associated with this receptor

DFLX.DAT File - Data Records

The DFLX.DAT data records consist of a set of "NDFOUT+1" records for each hour of the CALPUFF runs (NDFOUT is the number of species flagged as being stored in the output file). The first record of each set contains the date and hour of the data in the records which follow it. The next "NDFOUT" records contain predicted one-hour averaged dry deposition fluxes in $g/m^2/s$ for each relevant species (see Table 4-34).

Sample FORTRAN read statements for the data records are:

```
LOOP OVER DRY DEPOSITED SPECIES STORED ON DISK

GRIDDED RECEPTOR DRY FLUXES
   IF(LSGRID)READ(iunit)CDFG,DFLXG

DISCRETE RECEPTOR DRY FLUXES
   IF(NDREC.GT.0)READ(iunit)CDFD,DFLXD

COMPLEX TERRAIN RECEPTOR DRY FLUXES
   IF (NCTREC.GT.0)READ(iunit)CDFCT,DFLXCT

AND LOOP OVER DRY DEPOSITED SPECIES STORED ON DISK
```

where the following declarations apply:

```
Character*15 CDFG,CDFD,CDFCT
Real DFLXG(nxg,nyg),DFLXD(NDREC),DFLXCT(NCTREC)
```

and

```
nxg = IESAMP - IBSAMP+1
nyg = JESAMP - JBSAMP+1
```

Table 4-34
Unformatted DFLX.DAT File - Data Records
(Record 1 of each set)

No.	Variable	Type[a]	Description
1	NYR	integer	Year of dry flux data (two digits)
2	NJUL	integer	Julian day of data
3	NHR	integer	Hour (00-23) of data

(Next Data Record)
(Included only if LSGRID = TRUE)

No.	Variable	Type	Description
1	CDFG	C*15	Species name (characters 1-12) and variable flag (characters 13-15) of the data in this record. For example, "SO2 DF" corresponds to SO_2 dry flux.
Next NXG*NYG	DFLXG	real array	"IAVG" - hour averaged dry deposition fluxes ($g/m^2/s$) for each gridded receptor

[a] C*15 = Character*15

4.3.3 Wet Flux File (WFLX.DAT)

The WFLX.DAT file is an unformatted data file containing gridded fields of time averaged wet deposition fluxes predicted by CALPUFF. The creation and contents of the WFLX.DAT file are controlled by user-specified inputs in Input Group 7 of the control file (see Section 4.2.1).

The control file variable IWET must be set equal to one in order to create the WFLX.DAT file. The species saved in the output file are also controlled by the user by setting flags in the output species table in Input Group 7 of the control file. The model checks that only deposited species are flagged for output into the WFLX.DAT file. The effects of wet deposition on ambient concentrations can be evaluated without saving the wet fluxes in the output file if the actual values of the deposition fluxes are not of interest.

WFLX.DAT File - Header Records

The WFLX.DAT file consists of five header records followed by a set of data records. The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input run title, and a list of the deposited species stored in the output file, and receptor information (see Table 4-35).

Sample FORTRAN read statements for the header records are:

```
READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR,IRLG,
1 IAVG,NXM,NYM,DXKM,DYKM,IONE,IBCOMP,IECOMP,JBCOMP,JECOMP
2 IBSAMP,JBSAMP,IESAMP,JESAMP,MESHDN,NPTS,NAREAS,NDREC,NCTREC,LSGRID,
3 NWFOUT
READ(iunit)TITLE
READ(iunit)CWFOUT
READ(iunit)XREC,YREC,ZREC
READ(iunit)XRCT,YRCT,ZRCT,IHILL
```

where the following declarations apply:

```
Character*80 TITLE(3)
Character*15 CWFOUT(NWFOUT)
Character*12 CMODEL,VER,LEVEL

Real XREC(NDREC),YREC(NDREC),ZREC(NDREC)
Real XRCT(NCTREC),YRCT(NCTREC),ZRCT(NCTREC)
Integer IHILL(NCTREC)
```

Table 4-35
Unformatted WFLX.DAT file - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
1	CMODEL	C*12	Model name	CALPUFF
2	VER	C*12	Model version number	3.0
3	LEVEL	C*12	Model level number	950715
4	IBYR	integer	Starting year of the run	80
5	IBJUL	integer	Starting Julian day	183
6	IBHR	integer	Starting hour (00-23)	8
7	IRLG	integer	Length of run (hours)	5
8	IAVG	integer	Averaging time (hours) of output concentrations	1
9	NXM	integer	Number of grid points in meteorological grid (X direction)	20
10	NYM	integer	Number of grid points in meteorological grid (Y direction)	20
11	DXKM	real	Grid spacing (km) in the X direction	5.
12	DYKM	real	Grid spacing (km) in the Y direction	5.
13	IONE	integer	Layer number (always 1 for deposition fluxes)	1
14	IBCOMP	integer	Start of computational grid in X direction	1
15	IECOMP	integer	End of computational grid in X direction	20
16	JBCOMP	integer	Start of computational grid in Y direction	1
17	JECOMP	integer	End of computational grid in Y direction	20
18	IBSAMP	integer	Start of sampling grid in X direction	1

[a] C*12 = Character*12

Table 4-35 (Continued)
Unformatted WFLX.DAT file - Header Record 1 - General Data

No.	Variable	Type[a]	Description	Sample Values
19	JBSAMP	integer	End of sampling grid in X direction	20
20	IESAMP	integer	Start of sampling grid in Y direction	1
21	JESAMP	integer	End of sampling grid in Y direction	20
22	MESHON	integer	Sampling grid spacing factor	1
23	NPTS	integer	Number of point sources	2
24	NAREAS	integer	Number of area sources	0
25	NDREC	integer	Number of discrete receptors	0
26	NCTREC	integer	Number of complex terrain receptors	0
27	LSGRID	logical	Sampling grid flag (T = gridded receptors, F = no gridded receptors)	T
28	NWFOUT	integer	Number of wet deposited species stored in the output file	5

Table 4-35 (Continued)
Unformatted WFLX.DAT file - Header Record 2 - Run Title

No.	Variable	Type[a]	Description
1	TITLE(3)	C*80	User-specified run title (three lines of up to 80 characters/line)

Header Record 3 - List of Species-Layers in Output File

No.	Variable	Type	Description
1-NWFOUT	CWFOUT array	C*15	Species name (characters 1-12) and wet flux flag (characters 13-15) of data stored in the output file. The wet flux flag is " WF". For example, "SO2 WF" corresponds to SO_2 wet fluxes.

[a] C*80 = Character*80
C*15 = Character*15

Table 4-35 (Concluded)
Unformatted WFLX.DAT File

Header Record 4 - Discrete Receptors
(Included only if NDREC > 0)

No.	Variable	Type[a]	Description
1	XREC	real array	X-coordinate (km) of each discrete receptor
2	YREC	real array	Y-coordinate (km) of each discrete receptor
3	ZREC	real array	Ground level elevation (m) of each discrete receptor

Header Record 5 - Complex Terrain Receptors
(Included only if NCTREC > 0)

No.	Variable	Type	Description
1	XRCT	real array	X-coordinate (km) of each complex terrain receptor
2	YRCT	real array	Y-coordinate (km) of each complex terrain receptor
3	ZRCT	real array	Ground level elevation (m) of each complex terrain receptor
4	IHILL	integer array	Hill number associated with this receptor

WFLX.DAT File - Data Records

The WFLX.DAT data records consist of a set of "NWFOUT+1" records for each hour of the CALPUFF runs (NWFOUT is the number of species flagged as being stored in the output file). The first record of each set contains the date and hour of the data in the records which follow it. The next "NWFOUT" records contain predicted one-hour averaged wet deposition fluxes in $g/m^2/s$ for each relevant species (see Table 4-36).

Sample FORTRAN read statements for the data records are:

```
LOOP OVER WET DEPOSITED SPECIES STORED ON DISK

  GRIDDED RECEPTOR WET FLUXES
     IF(LSGRID)READ(iunit)CWFG,WFLXG

  DISCRETE RECEPTOR WET FLUXES
     IF(NDREC.GT.0)READ(iunit)CWFD,WFLXD

  COMPLEX TERRAIN RECEPTOR WET FLUXES
     IF (NCTREC.GT.0)READ(iunit)CWFCT,WFLXCT

END LOOP OVER WET DEPOSITED SPECIES STORED ON DISK
```

where the following declarations apply:

```
Character*15 CWFG,CWFD,CWFCT
Real WFLXG(nxg,nyg),WFLXD(NDREC),WFLXCT(NCTREC)
```

and

```
nxg = IESAMP - IBSAMP+1
nyg = JESAMP - JBSAMP+1
```

Table 4-36
Unformatted WFLX.DAT File - Data Records
(Record 1 of each set)

No.	Variable	Type[a]	Description
1	NYR	integer	Year of wet flux data (two digits)
2	NJUL	integer	Julian day of data
3	NHR	integer	Hour (00-23) of data

(Next Data Record)
(Included only if LSGRID = TRUE)

No.	Variable	Type	Description
1	CWFG	C*15	Species name (characters 1-12) and wet flux flag (characters 13-15) of the data in this record. For example, "SO2 WF" corresponds to SO_2 wet fluxes.
Next NXG*NYG	DWLXG	real array	"IAVG" - hour averaged wet deposition fluxes ($g/m^2/s$) for each gridded receptor

[a] C*15 = Character*15

Table 4-36 (Concluded)
Unformatted WFLX.DAT File - Data Records

(Next Data Record)
(Included only if NDREC > 0)

No.	Variable	Type[a]	Description
1	CWFD	C*15	Species name (characters 1-12) and wet flux flag (characters 13-15) of the data in this record. For example, "SO2 WF" corresponds to SO_2 wet fluxes.
Next NDREC	WFLXD	real array	"IAVG" - hour averaged wet deposition fluxes ($g/m^2/s$) for each discrete receptor

(Next Data Record)
(Included only if NCTREC > 0)

No.	Variable	Type	Description
1	CWFCT	C*15	Species name (characters 1-12) and wet flux flag (characters 13-15) of the data in this record. For example, "SO2 WF" corresponds to SO_2 wet fluxes.
Next NCTREC	WFLXD	real array	"IAVG" - hour averaged wet deposition fluxes ($g/m^3/s$) at each complex terrain (CTSG) receptor

[a] C*15 = Character*15

4.4 CALPOST Postprocessing Program

The CALPOST program is a postprocessor designed to produce ranked tabulations of averages of selected concentration (or wet/dry deposition flux) data obtained from the CALPUFF or CALGRID models. Its capabilities and options include:

- Option to produce tables of the "top-50" average concentration/deposition data (includes time and receptor information) for specified averaging times.
- Option to produce tables of the "top-N" (user specifies the number N) average concentration/deposition data at each receptor for specified averaging times.
- Option to produce a table of the annual (or length-of-run) average concentration/deposition at each receptor.
- Option to print concentration/deposition averages for selected days.
- Option to print tables of the number of exceedances of user-specified threshold values for each averaging time at each receptor.
- Option to produce plot files containing the "top N" concentrations or deposition fluxes at each receptor or the number of exceedances of the user-specified thresholds at each receptor.
- User-selected processing periods.
- User-selected chemical species.
- User-selected layer from which concentration data are obtained.
- Option to include gridded receptors, discrete receptors, and complex terrain receptors in any combination.
- Option to scale all concentration/deposition data by means of a linear function of the form: a*X + b (where X is concentration or deposition, and a,b are user-supplied scaling factors).
- User-specified averaging time.

The user-specified inputs to CALPOST are read from the control file: CALPOST.INP. The program reads the concentration/deposition flux data from an unformatted data file called MODEL.DAT that is generated by the CALPUFF model (or CALGRID). CALPUFF also generates a file containing relative humidity data, called VISB.DAT, which is read by CALPOST if the visibility options in CALPOST are selected.

The CALPOST control file uses the same self-documenting control file format as CALPUFF. See Section 4.2.1 for a description of the control file input conventions. A description of each input variable is shown in Table 4-38. A sample input file is presented in Table 4-39. A sample output list file is shown in Table 4-40.

CALPOST generates an output list file, called CALPOST.LST, and a set of optional plot files containing the "top N" highest concentrations at each receptor. A second set of optional plot files contains the number of exceedances of user-specified threshold values at each receptor and averaging time. The format of the plot files (Receptor X, Y, value1, values2, etc.) is suitable for direct input into many of the popular PC-based graphics packages.

As with CALPUFF and CALMET, CALPOST also contains a parameter file, called PARAMS.PST, in which all of the array dimensions related to the number of gridded, discrete, and complex terrain receptors, the number of "top N" tables allowed, and the Fortran unit numbers associated with each input and output file are specified. If the user needs for a particular application to increase the number of discrete receptors, for example, beyond the current maximum, a change to the value of the discrete receptor parameter in PARAMS.PST will automatically re-size all arrays related to this parameter upon recompilation of the CALPOST code.

Table 4-37
CALPOST Input and Output Files

Unit*	File Name	Type	Format	Description
in2	CALPOST.INP	input	formatted	Control file containing user inputs
in1	MODEL.DAT	input	unformatted	CALPUFF output file containing modeled concentration or deposition flux data
in3	VISB.DAT	input	unformatted	CALPUFF output file containing relative humidity data (required only for visibility applications)
io1	CALPOST.LST	output	formatted	List file containing CALPOST tables and other generated data
	Optional Plot Files - "Top N" concentrations or deposition fluxes at each receptor			
map1	L1TOPN.MAP	output	formatted	1-hour averaged values
map3	L3TOPN.MAP	output	formatted	3-hour averaged values
map24	L24TOPN.MAP	output	formatted	24-hour averaged values
mapn	LNTOPN.MAP	output	formatted	User-specified averaging time
mapr	LRAVG.MAP	output	formatted	Length of run averaged values
	Optional Plot Files - Number of exceedances of user-specified threshold values			
map1x	L1EXC.MAP	output	formatted	1-hour averaged threshold
map3x	L3EXC.MAP	output	formatted	3-hour averaged threshold
map24x	L24EXC.MAP	output	formatted	24-hour averaged threshold
mapnx	LNEXC.MAP	output	formatted	User-specified averaging time threshold

* See the parameter file, PARAMS.PST, for the numerical values of the unit numbers.

Table 4-38
CALPOST Control File Inputs (CALPOST.INP)

Variable	Type	Description	Default
ISYR	integer	Starting year of data to process (two digits)	-
ISMO	integer	Starting month	-
ISDY	integer	Starting day	-
ISHR	integer	Starting hour (0-23). Uses ending hour convention (e.g., Hour 1 refers to the period from 0:00 - 1:00).	-
NHRS	integer	Number of hours to process	-
ASPEC	character*12	Name of "species" to process**	-
ILAYER	integer	Code indicating layer of concentrations (always "1" when processing concentrations from CALPUFF, "-1" for dry deposition fluxes, and "-2" for wet deposition fluxes)	1
A	real	Multiplicative scaling factor (not applied if A = B = 0.0)	0.0
B	real	Additive factor (not applied if A = B = 0.0)	0.0
LG	logical	Gridded receptors processed ?	F
LD	logical	Discrete receptors processed ?	F
LCT	logical	CTSG complex terrain receptors processed ?	F
BEXTBK	real	Background light extinction coefficient (1/mm)	-
RHFRAC	real	Percentage of particles affected by relative humidity	-
RHMAX	real	Maximum relative humidity (%) used in the particle growth equation	-
NAVG	integer	User-specified averaging time (hours)	0
L1T50	logical	Generate top 50 table for 1-hr averages ?	T
L3T50	logical	Generate top 50 table to 3-hr averages ?	T
L24T50	logical	Generate top 50 table for 24-hr averages ?	T
LNT50	logical	Generate top 50 table for NAVG-hr averages ?	F
LRT50	logical	Generate top 50 table for length-of-run averages ?	T

** Sample values of ASPEC: SO2, SO4, NOX, HNO3, NO3, or for visibility calculations: BEXT (light-extinction coefficient), BEXTS (contribution of sulfate to the light-extinction coefficient), BEXTN (contribution of nitrate), BEXTSN (contribution of both sulfate and nitrate), BEXTRH (light-extinction coefficient of the background aerosol at ambient relative humidity.

Table 4-38 (Concluded)
CALPOST Control File Inputs (CALPOST.INP)

Variable	Type	Description	Default
NTOP	integer	Number of "top" values at each receptor (must be ≤ 4)	4
ITOP(4)	integer array	Specific ranks of "top" values reported (e.g., values of 1, 2, 5 and 48 would produce the highest, 2nd highest, 5th highest, and 48th highest concentrations at each receptor)	1,2,3,4
L1TOPN	logical	Produce "top N" table for 1-hr averages ?	F
L3TOPN	logical	Produce "top N" table for 3-hr averages ?	F
L24TOPN	logical	Produce "top N" table for 24-hr averages ?	F
LNTOPN	logical	Produce "top N" table for NAVG-hr averages ?	F
LRAVG	logical	Produce "top N" table for length-of-run averages ?	F
THRESH1	real	Exceedance threshold* for 1-hr averages	-1.0
THRESH3	real	Exceedance threshold* for 3-hr averages	-1.0
THRESH24	real	Exceedance threshold* for 24-hr averages	-1.0
THRESHN	real	Exceedance threshold* for NAVG-hr averages	-1.0
LMAP	logical	Generate PLOT files for each "top N" table and exceedance table selected above ?	T
LECH1	logical	Output 1-hr averages for selected days ?	F
LECH3	logical	Output 3-hr averages for selected days ?	F
LECH24	logical	Output 24-hr averages for selected days ?	F
LECHN	logical	Output NAVG-hr averages for selected days ?	F
LDEBUG	logical	Activate special debug output statements ?	F
IECHO(366)	integer array	Arrays of days selected to print data for averaging times selected with LECH1, LECH3, LECH24, LECHN variables (0= do not print day, 1=print day)	366*0

* Value of -1.0 inactivates threshold exceedance option.

Table 4-39
Sample CALPOST Control File (CALPOST.INP)

```
CALPOST TEST CASE
Pollutant: SO2
Gridded receptor run
------------------------------------------------------------------------------

General run control parameters
------------------------------
  Starting date:   Year  (ISYR) -- No default   ! ISYR  =  87  !
                  Month  (ISMO) -- No default   ! ISMO  =   1  !
                    Day  (ISDY) -- No default   ! ISDY  =   1  !
                   Hour  (ISHR) -- No default   ! ISHR  =   1  !

     Number of hours to process (NHRS) -- No default   ! NHRS  = 8760 !

           Species to process (ASPEC) -- No default   ! ASPEC = SO2  !
 Examples: SO2, SO4, NOX, HNO3, NO3, or for visibility calculations:
           BEXT (light-extinction coefficient),
           BEXTS (contribution of sulfate to the light extinction coefficient)
           BEXTN (contribution of nitrate to the light extinction coefficient)
           BEXTSN (contribution of both sulfate and nitrate)
           BEXTBK (light-extinction coefficient of the background aerosol at
                   the ambient relative humidity)

Concentration and scaling factors
---------------------------------
     Layer/deposition code  (ILAYER) -- Default: 1      ! ILAYER = 1 !
       "1"  for CALPUFF concentrations,
       "-1" for dry deposition fluxes,
       "-2" for wet deposition fluxes.

     Scaling factors of the form:     -- Defaults:      ! A = 0.0    !
          X(new) = X(old) * A + B          A = 0.0      ! B = 0.0    !
       (NOT applied if A = B = 0.0)        B = 0.0

Receptor Information
--------------------
              Gridded receptors processed (LG) ?        ! LG  = T    !
             Discrete receptors processed (LD) ?        ! LD  = F    !
  CTSG Complex terrain receptors processed (LCT) ?      ! LCT = F    !

Visibility Parameters
---------------------
    Background light extinction coefficient (1/mm)
                           (BEXTBK) -- No default  ! BEXTBK = 50.  !
    Percentage of particles affected by relative humidity
                           (RHFRAC) -- No default  ! RHFRAC =  0.  !
    Maximum relative humidity (%) used in particle growth eqn.
                           (RHMAX) -- No default   ! RHMAX  = 98.  !

Averaging time and TOP 50 Table control
---------------------------------------
    User-specified averaging time
                             (NAVG) -- No default    !   NAVG =  1 !
    Top 50 table for  1-hr averages
                           (L1T50) -- No default     !  L1T50 = T  !
    Top 50 table for  3-hr averages
                           (L3T50) -- No default     !  L3T50 = F  !
    Top 50 table for 24-hr averages
                          (L24T50) -- No default     ! L24T50 = F  !
    Top 50 table for NAVG-hr averages
                           (LNT50) -- No default     !  LNT50 = F  !
    Top 50 table for length of run averages
                           (LRT50) -- No default     !  LRT50 = F  !
```

Table 4-39 (Concluded)
Sample CALPOST Control File (CALPOST.INP)

```
TOP "n" Table control
---------------------

    Number of "top" values at each receptor
                          (NTOP) -- No default    ! NTOP = 4    !
              (NTOP must be <= 4)

    Specific ranks of "top" values reported
                 (ITOP(4) array) -- No default ! ITOP = 1, 2, 5, 15 !
               (NTOP values must be entered)

    Top "n" table for  1-hr averages   (L1TOPN)      !  L1TOPN = T    !
    Top "n" table for  3-hr averages   (L3TOPN)      !  L3TOPN = F    !
    Top "n" table for 24-hr averages   (L24TOPN)     ! L24TOPN = T    !
    Top "n" table for NAVG-hr averages (LNTOPN)      !  LNTOPN = F    !
    Top "n" table for length of run averages (LRAVG) !   LRAVG = T    !


Threshold Exceedance control
----------------------------

    Counts will be tabulated for each average that
    exceeds a specified non-negative threshold.

                                Default = -1.0

    Threshold for  1-hr averages   (THRESH1)     !  THRESH1 =  0.1    !
    Threshold for  3-hr averages   (THRESH3)     !  THRESH3 = -1.0    !
    Threshold for 24-hr averages  (THRESH24)     ! THRESH24 =  0.01   !
    Threshold for NAVG-hr averages (THRESHN)     !  THRESHN = -1.0    !

Output Options
--------------

     Special Output (LMAP):
     Plot files can be created for selected Top-n and Exceedance tables.
     They follow a record format of [x,y,val1,val2,...] so that MAPS of
     these values can be produced with little effort.  Each type of
     data is placed in its own file.  The naming convention for these
     files is adopted from the Top-N control variables, so that
        Top 3-hr values are listed in                : L3TOPN.MAP
        Length-of-run averages are in                : LRAVG.MAP
        Exceedances of the 24-hour threshold are in  : L24EXC.MAP
     A MAP-file will be created for each control variable set to "T",
     if LMAP is also "T".

                                          (LMAP)      ! LMAP    = T !

     Standard Output to List File:
     Output 1-hr averages for selected days (LECH1)     ! LECH1   = F !
     Output 3-hr averages for selected days (LECH3)     ! LECH3   = F !
     Output 24-hr averages for selected days (LECH24)   ! LECH24  = F !
     Output NAVG-hr averages for selected days (LECHN)  ! LECHN   = F !
     Output selected information for debugging (LDEBUG) ! LDEBUG  = F !

     Days selected for output IECHO(366)           ! IECHO  = 366 * 0 !
     (366 values must be entered)


     !END!
```

Table 4-40
Sample CALPOST Output File (CALPOST.LST)
(Partial Listing)

```
**********************************************************************************************
                                    CALPOST  Version  3.0  Level  950531
**********************************************************************************************

                    SO2          1

TOP-50    1-HOUR AVERAGE  CONCENTRATION VALUES

YEAR  DAY HOUR(0-23) RECEPTOR  TYPE  CONCENTRATION  COORDINATES (km)

 87   187     7      ( 4,  4)   G    1.9806E+00     -0.150    -0.150
 87   187     6      ( 4,  4)   G    1.9778E+00     -0.150    -0.150
 87   187     5      ( 4,  4)   G    1.8140E+00     -0.150    -0.150
 87   169     5      ( 4,  4)   G    1.7542E+00     -0.150    -0.150
 87   224     7      ( 4,  4)   G    1.7334E+00     -0.150    -0.150
 87   320     5      ( 4,  4)   G    1.7265E+00     -0.150    -0.150
 87   205    20      ( 4,  5)   G    1.7199E+00     -0.150     0.150
 87   187    19      ( 4,  5)   G    1.7129E+00     -0.150     0.150
 87   156     8      ( 4,  5)   G    1.6689E+00     -0.150     0.150
 87   215    18      ( 4,  5)   G    1.6678E+00     -0.150     0.150
 87   230    19      ( 5,  4)   G    1.6647E+00      0.150    -0.150
 87   188     0      ( 5,  4)   G    1.5849E+00      0.150    -0.150
 87   249     3      ( 4,  4)   G    1.5785E+00     -0.150    -0.150
 87   140     3      ( 5,  4)   G    1.5692E+00      0.150    -0.150
 87   187    21      ( 4,  4)   G    1.5644E+00     -0.150    -0.150
 87   151    21      ( 5,  4)   G    1.5362E+00      0.150    -0.150
 87   188     2      ( 3,  4)   G    1.5247E+00      0.150    -0.150
 87   168    22      ( 5,  4)   G    1.5208E+00      0.150    -0.150
 87   218    20      ( 5,  5)   G    1.4695E+00      0.150     0.150
 87   249     4      ( 4,  4)   G    1.4399E+00     -0.150    -0.150
 87   151    20      ( 5,  4)   G    1.4281E+00      0.150    -0.150
 87     4     2      ( 5,  4)   G    1.4143E+00      0.150    -0.150
 87   215    20      ( 5,  5)   G    1.3184E+00      0.150     0.150
 87   344     5      ( 5,  4)   G    1.2570E+00      0.150    -0.150
 87     7     2      ( 4,  5)   G    1.2426E+00     -0.150     0.150
 87   224     6      ( 4,  5)   G    1.2366E+00     -0.150     0.150
 87   103     4      ( 5,  5)   G    1.2134E+00      0.150     0.150
 87   170     6      ( 4,  4)   G    1.2090E+00     -0.150    -0.150
 87   215    21      ( 5,  4)   G    1.1909E+00      0.150    -0.150
 87    70     5      ( 4,  4)   G    1.1847E+00     -0.150    -0.150
 87   224     4      ( 4,  5)   G    1.1840E+00     -0.150     0.150
 87   169     6      ( 4,  4)   G    1.1177E+00     -0.150    -0.150
 87   247    21      ( 5,  4)   G    1.1100E+00      0.150    -0.150
 87     7     4      ( 5,  4)   G    1.1027E+00      0.150    -0.150
 87   121     4      ( 5,  4)   G    1.1024E+00      0.150    -0.150
 87   187     9      ( 4,  4)   G    1.0899E+00     -0.150    -0.150
 87   319     4      ( 4,  4)   G    1.0719E+00     -0.150    -0.150
 87   201     7      ( 5,  5)   G    1.0394E+00      0.150     0.150
 87   312     5      ( 4,  4)   G    1.0023E+00     -0.150    -0.150
 87   313     5      ( 4,  4)   G    1.0023E+00     -0.150    -0.150
 87    93     0      ( 5,  4)   G    9.7395E-01      0.150    -0.150
 87   274    21      ( 4,  5)   G    9.5399E-01     -0.150     0.150
 87    31     0      ( 4,  5)   G    9.5155E-01     -0.150     0.150
 87   263    23      ( 5,  4)   G    9.4756E-01      0.150    -0.150
 87   114     4      ( 4,  5)   G    9.2938E-01     -0.150     0.150
 87   224     5      ( 4,  5)   G    9.0212E-01     -0.150     0.150
 87   103     1      ( 4,  5)   G    8.9583E-01     -0.150     0.150
 .
 .
 .
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Table 4-40 (Continued)
Sample CALPOST Output File (CALPOST.LST)
(Partial Listing)

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**********************************************************************************************
                                CALPOST  Version 3.0  Level  950531
**********************************************************************************************

                                          SO2          1

 4 RANKED     1-HOUR AVERAGE  CONCENTRATION VALUES AT EACH GRIDDED RECEPTOR  (YEAR,DAY,ENDING HOUR)

RECEPTOR   COORDINATES (km)        1 RANK                    2 RANK                    5 RANK
  1, 1      -1.050   -1.050   2.1750E-01 (87,187, 7)   2.1080E-01 (87,187, 6)   1.9975E-01 (87,349, 3)
  1, 2      -1.050   -0.750   2.0779E-01 (87, 86, 6)   1.8950E-01 (87,322, 4)   1.6159E-01 (87,169, 5)
  1, 3      -1.050   -0.450   1.7986E-01 (87,201, 2)   1.4772E-01 (87,157, 9)   1.2141E-01 (87,128,21)
  1, 4      -1.050   -0.150   2.0151E-01 (87,129,22)   1.7698E-01 (87,321,23)   1.6823E-01 (87,201, 0)
  1, 5      -1.050    0.150   2.9357E-01 (87,188,20)   2.0586E-01 (87,136,18)   1.8382E-01 (87, 84, 7)
  1, 6      -1.050    0.450   2.0552E-01 (87,237,19)   1.8076E-01 (87,167, 3)   1.6457E-01 (87, 29, 1)
  1, 7      -1.050    0.750   2.1575E-01 (87,113, 4)   1.9241E-01 (87,113, 5)   1.8279E-01 (87,296, 6)
  1, 8      -1.050    1.050   1.5381E-01 (87,320,22)   1.5232E-01 (87, 30, 2)   1.4789E-01 (87,319, 0)
  2, 1      -0.750   -1.050   1.9331E-01 (87,187, 2)   1.8414E-01 (87,277, 6)   1.8414E-01 (87,276, 6)
  2, 2      -0.750   -0.750   3.1528E-01 (87,187, 7)   3.0914E-01 (87,187, 6)   2.3857E-01 (87,249, 4)
  2, 3      -0.750   -0.450   2.2436E-01 (87,  4, 1)   1.9363E-01 (87, 34, 6)   1.9363E-01 (87, 33, 6)
  2, 4      -0.750   -0.150   3.8320E-01 (87,201, 0)   3.8168E-01 (87,201, 1)   2.7294E-01 (87,201, 4)
  2, 5      -0.750    0.150   3.0530E-01 (87, 84, 7)   2.9440E-01 (87,188,19)   2.7548E-01 (87,188,20)
  2, 6      -0.750    0.450   2.3981E-01 (87,241,20)   2.2757E-01 (87,230,22)   2.2399E-01 (87,348, 6)
  2, 7      -0.750    0.750   1.7584E-01 (87,320,22)   1.7239E-01 (87, 30, 2)   1.6578E-01 (87,248,20)
  2, 8      -0.750    1.050   1.7498E-01 (87, 48, 3)   1.6996E-01 (87,230,17)   1.6243E-01 (87,304, 6)
  3, 1      -0.450   -1.050   2.2715E-01 (87,220, 6)   1.8972E-01 (87,169,20)   1.8794E-01 (87, 76, 2)
  3, 2      -0.450   -0.750   3.3312E-01 (87,187, 4)   2.8007E-01 (87,187, 2)   2.1963E-01 (87,133, 4)
  3, 3      -0.450   -0.450   5.8862E-01 (87,187, 7)   5.[illegible]16E-01 (87,187, 6)   4.3739E-01 (87,249, 4)
  3, 4      -0.450   -0.150   6.4789E-01 (87,201, 1)   5.6173E-01 (87, 77, 4)   4.4302E-01 (87,201, 4)
  3, 5      -0.450    0.150   7.1469E-01 (87,237,19)   5.3013E-01 (87,237,18)   5.1488E-01 (87,181,18)
  3, 6      -0.450    0.450   3.[illegible]E-01 (87,[illegible],20)   3.6824E-01 (87,187,19)   3.5855E-01 (87,215,18)
  3, 7      -0.450    0.750   3.4948E-01 (87, 93, 5)   2.3832E-01 (87,230,20)   2.2332E-01 (87, 93, 4)
  3, 8      -0.450    1.050   2.7368E-01 (87,230,21)   1.7987E-01 (87,232,17)   1.7687E-01 (87,304, 5)
  4, 1      -0.150   -1.050   2.2752E-01 (87,181, 8)   2.1082E-01 (87,193,20)   1.9991E-01 (87,121,19)
  4, 2      -0.150   -0.750   3.0306E-01 (87,156,22)   3.0029E-01 (87,188, 4)   2.6788E-01 (87,181, 8)
  4, 3      -0.150   -0.450   7.7740E-01 (87,220, 6)   7.3071E-01 (87,188, 4)   7.2638E-01 (87,225, 7)
  4, 4      -0.150   -0.150   1.9806E+00 (87,187, 7)   1.9778E+00 (87,187, 6)   1.8140E+00 (87,187, 5)
  4, 5      -0.150    0.150   1.7199E+00 (87,205,20)   1.7129E+00 (87,187,19)   1.6689E+00 (87,156, 8)
  4, 6      -0.150    0.450   7.2047E-01 (87,  5, 5)   6.6343E-01 (87,321, 0)   6.0132E-01 (87,230,21)
  4, 7      -0.150    0.750   2.3062E-01 (87, 48, 5)   1.9711E-01 (87, 13, 2)   1.9400E-01 (87,360, 2)
  4, 8      -0.150    1.050   1.9978E-01 (87,188,16)   1.8139E-01 (87,360, 5)   1.7795E-01 (87,155,18)
  5, 1       0.150   -1.050   1.8967E-01 (87, 64, 4)   1.8704E-01 (87,181, 9)   1.7676E-01 (87,108,19)
  5, 2       0.150   -0.750   3.8662E-01 (87,220, 3)   2.8236E-01 (87,220, 8)   2.7479E-01 (87,205, 6)
  5, 3       0.150   -0.450   8.1056E-01 (87,188,22)   6.7587E-01 (87,205,21)   6.6029E-01 (87,181, 6)
  5, 4       0.150   -0.150   1.6647E+00 (87,230,19)   1.5849E+00 (87,188, 0)   1.5692E+00 (87,140, 3)
  5, 5       0.150    0.150   1.4695E+00 (87,218,20)   1.3184E+00 (87,215,20)   1.2134E+00 (87,103, 4)
  5, 6       0.150    0.450   5.1957E-01 (87, 93, 1)   5.1656E-01 (87,269, 3)   3.6877E-01 (87,103, 2)
  5, 7       0.150    0.750   2.5949E-01 (87,215,19)   2.2813E-01 (87, 51, 3)   2.2109E-01 (87,214,18)
  5, 8       0.150    1.050   2.1733E-01 (87, 85,20)   1.8420E-01 (87,227,23)   1.6752E-01 (87,103, 6)
  6, 1       0.450   -1.050   2.3204E-01 (87,188,22)   2.0613E-01 (87,265, 7)   2.0613E-01 (87,264, 7)
  6, 2       0.450   -0.750   2.2816E-01 (87, 63, 7)   2.2806E-01 (87, 11, 1)   2.1455E-01 (87, 75, 1)
  6, 3       0.450   -0.450   4.2089E-01 (87,140, 3)   4.1321E-01 (87,151,21)   3.4788E-01 (87,188, 0)
  6, 4       0.450   -0.150   7.2577E-01 (87,222, 8)   5.8829E-01 (87,156, 5)   5.2152E-01 (87,218,23)
  6, 5       0.450    0.150   5.8910E-01 (87,299, 6)   3.6436E-01 (87,222, 5)   3.4410E-01 (87,218,22)
  6, 6       0.450    0.450   3.2808E-01 (87,215,20)   2.7795E-01 (87,103, 4)   2.7025E-01 (87,201, 7)
```

Table 4-40 (Continued)
Sample CALPOST Output File (CALPOST.LST)
(Partial Listing)

```
**********************************************************************************************
                                        CALPOST  Version  3.0  Level  950531
**********************************************************************************************

  1 - RANK HIGHEST VALUES FOR PERIOD

 Multiply all values by 10 **  -3

  8 I  154   175   274   200   217   154   182   160
    I    +     +     +     +     +     +     +     +
  7 I  216   176   349   231   259   190   180   175
    I    +     +     +     +     +     +     +     +
  6 I  206   240   370   720   520   328   251   188
    I    +     +     +     +     +     +     +     +
  5 I  294   305   715  1720  1470   589   330   194
    I    +     +     +     +     +     +     +     +
  4 I  202   383   648  1981  1665   726   240   240
    I    +     +     +     +     +     +     +     +
  3 I  180   224   589   777   811   421   336   216
    I    +     +     +     +     +     +     +     +
  2 I  208   315   333   303   387   228   208   190
    I    +     +     +     +     +     +     +     +
  1 I  217   193   227   228   190   232   177   163
    I    +     +     +     +     +     +     +     +
     ----------------------------------------------
         1     2     3     4     5     6     7     8

  2 - RANK HIGHEST VALUES FOR PERIOD

 Multiply all values by 10 **  -3

  8 I  152   170   180   181   184   145   173   121
    I    +     +     +     +     +     +     +     +
  7 I  192   172   238   197   228   176   143   137
    I    +     +     +     +     +     +     +     +
  6 I  181   228   368   663   517   278   249   178
    I    +     +     +     +     +     +     +     +
  5 I  206   294   530  1713  1318   364   293   189
    I    +     +     +     +     +     +     +     +
  4 I  177   382   562  1978  1585   588   211   150
    I    +     +     +     +     +     +     +     +
  3 I  148   194   583   731   676   413   235   188
    I    +     +     +     +     +     +     +     +
  2 I  189   309   280   300   282   228   206   177
    I    +     +     +     +     +     +     +     +
  1 I  211   184   190   211   187   206   175   142
    I    +     +     +     +     +     +     +     +
     ----------------------------------------------
         1     2     3     4     5     6     7     8
```

Table 4-40 (Continued)
Sample CALPOST Output File (CALPOST.LST)
(Partial Listing)

```
**********************************************************************************************
                                    CALPOST Version 3.0 Level 950531
**********************************************************************************************

                                                SO2          1

          COUNTS OF    1-HOUR AVERAGE  CONCENTRATION EXCEEDENCES AT EACH GRIDDED RECEPTOR

 NUMBER OF AVERAGES   >  0.1000E+00

 8 I  24   26   40   21   12   11    8    4
   I   +    +    +    +    +    +    +    +
 7 I  43   55   57   55   38   14   16    9
   I   +    +    +    +    +    +    +    +
 6 I  41   88  106  185  185   37   22   11
   I   +    +    +    +    +    +    +    +
 5 I  20   38   96  556  463  172   33   19
   I   +    +    +    +    +    +    +    +
 4 I  15   24   31  459  596  232   59   21
   I   +    +    +    +    +    +    +    +
 3 I   8   25  106  334  256  112   77   32
   I   +    +    +    +    +    +    +    +
 2 I   8   54  122  153   85   70   59   35
   I   +    +    +    +    +    +    +    +
 1 I  27   59  101   96   53   46   28   20
   I   +    +    +    +    +    +    +    +
     ------------------------------------------
       1    2    3    4    5    6    7    8
```

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16. ABSTRACT

This report describes the CALPUFF dispersion model and associated processing programs. The CALPUFF model described in this report reflect improvements to the model including 1) new modules to treat buoyant rise and dispersion from area sources (such as forest fires), buoyant line sources, and volume sources, 2) an improved treatment of complex terrain, 3) additional model switches to facilitate its use in regulatory applications, 4) an enhanced treatment of wind shear through puff splitting, and 4) an optional PC-based GUI. CALPUFF has been coupled to the Emissions Production Model (EPM) developed by the Forest Service through an interface processor. EPM provides time-dependent emissions and heat release data for use in modeling controlled burns and wildfires.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
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