EPRI

SCICHEM Version 3.3

User's Guide

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Technical Update, December 2021

EPRI Project Manager

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ABSTRACT

SCICHEM, which stands for SCIPUFF with Chemistry, is used to model the transport, dispersion, and chemical reaction of gaseous and aerosol releases in the atmosphere using gas-phase, aqueous-phase, and aerosol chemistry treatments comparable to those in photochemical grid models (PGMs). In SCIPUFF, atmospheric turbulence is modeled using second-order closure, and a collection of three-dimensional Gaussian puffs is used to represent a time-dependent concentration field. SCICHEM can be used to study the impact on air quality from single or multiple sources.

This user's guide describes, in a step-by-step approach, how to use the various executables provided in the SCICHEM distribution package and the format of the input and output files required for running the model.

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PRIMARY AUDIENCE: Users of the SCICHEM air quality model and reviewers of modeling results

KEY RESEARCH QUESTION

This user's guide describes, in a step-by-step approach, how to use the various executables provided in the SCICHEM distribution package and the format of the input and output files required for running the model. Four in-depth tutorials demonstrate the model capabilities while also providing guidance for setting up model runs.

RESEARCH OVERVIEW

- This report provides an overview of the SCICHEM model and includes basic input data requirements, computer hardware requirements, and modeling options.
- Guidance on installing and running SCICHEM and its pre- and post-processors is presented along with various input and output file formats.
- Tutorials for four case studies are included to provide guidance on model setup.

WHY THIS MATTERS

SCICHEM is a Lagrangian photochemical puff model that is an alternative to steady-state Gaussian plume models for the modeling of ambient SO_2 and NO_2 concentrations. SCICHEM also provides an alternative to more resource-intensive photochemical grid models for single-source air quality modeling applications involving the formation of secondary pollutants such as ozone and fine particulate matter.

LEARNING AND ENGAGEMENT OPPORTUNITIES

- Training on SCICHEM will be offered after model releases and may also be offered at air quality modeling conferences.

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1
INTRODUCTION

SCIPUFF is a Lagrangian transport and diffusion model for atmospheric dispersion applications. The acronym *SCIPUFF* stands for Second-order Closure Integrated PUFF and describes two basic aspects of the model. First, the numerical technique employed to solve the dispersion equations is the Gaussian puff method (Bass, 1980) in which a collection of three-dimensional puffs is used to represent an arbitrary time-dependent concentration field. Second, the turbulent diffusion parameterization used in SCIPUFF is based on the second-order turbulence closure theories of Donaldson (1973) and Lewellen (1977), providing a direct connection between measurable velocity statistics and the predicted dispersion rates. SCIPUFF has been expanded under EPRI sponsorship to include the treatment of gas- and aqueous-phase reactions and aerosol thermodynamics. SCIPUFF with chemistry is referred to as *SCICHEM*.

The Lagrangian puff methodology affords several advantages for atmospheric dispersion applications from localized sources. The Lagrangian scheme avoids the artificial diffusion problems inherent in any Eulerian advection scheme and allows an accurate treatment of the wide range of length scales as a plume or cloud grows from a small source size and spreads onto larger atmospheric scales. This range may extend from a few meters up to continental or global scales of thousands of kilometers. In addition, the puff method provides robust prediction under coarse resolution conditions, giving a flexible model for rapid assessment when detailed results are not required. The model is highly efficient for multiscale dispersion problems because puffs can be merged as they grow, and resolution is therefore adapted to each stage of the diffusion process.

SCICHEM implements efficient adaptive time stepping and output grids. Each puff uses a time step appropriate for resolving its local evolution rate so that the multiscale range can be accurately described in the time domain without using a small step for the entire calculation. The output spatial fields are also computed on an adaptive grid, avoiding the need for the user to specify grid information and providing a complete description of the concentration field within the computational constraints under most conditions.

The generality of the turbulence closure model provides a dispersion representation for arbitrary conditions. Empirical models based on specific dispersion data are limited in their range of application, but the fundamental relationship between the turbulent diffusion and the velocity fluctuation statistics is applicable for a much wider range. Our understanding of the daytime planetary boundary layer velocity fluctuations provides reliable input for the second-order closure description of dispersion for these conditions. For larger scales and upper atmosphere stable conditions, the turbulence description is based on climatological information, but the closure framework is in place to accept improvement as our understanding of these regimes improves. The closure model has been applied on local scales up to 50-km range (Sykes et al., 1988) and on continental scales up to 3000-km range (Sykes et al., 1993).

The second-order closure model also provides the probabilistic feature of SCICHEM through the prediction of the concentration fluctuation variance. In addition to giving a mean value for the concentration field, SCICHEM provides a quantitative value for the random variation in the concentration value because of the stochastic nature of the turbulent diffusion process. This uncertainty estimate is used to provide a probabilistic description of the dispersion result and gives a quantitative characterization of the reliability of the prediction. For many dispersion calculations, the prediction is inherently uncertain because of a lack of detailed knowledge of the wind field, and a probabilistic description is the only meaningful approach.

SCICHEM treats the chemistry by using a passive tracer that carries a set of reactive chemical species, which is referred to as a *multicomponent* material. While the attached species are transported and diffused with the conserved tracer, they are also transformed through chemical reaction. The gas-phase chemical mechanism and rate constants are provided by the user. Dry deposition of the reactive species may also be treated. Details of the technical approach of the treatment of chemistry in SCICHEM can be found in EPRI report 300202285, *SCICHEM 3.3 Technical Documentation*.

The core SCICHEM model executable is called *runSCI*. In addition, the distribution package includes several other executables that may be used for pre-processing and post-processing, depending on the user application. The METSCI executable is a meteorological pre-processor that converts standard surface and upper air sounding observations to SCICHEM-ready inputs. Note that a meteorological pre-processor, referred to as *MMIF*, is also available from the U.S. EPA SCRAM website. It is not included in this distribution. This pre-processor converts prognostic meteorological model (MM5 and Weather Research and Forecasting [WRF]) outputs to SCICHEM-ready gridded meteorological files. The TERSCI executable is a terrain pre-processor that reads digital elevation model (DEM)/national elevation dataset (NED) data in GeoTIFF format and the user's lat-lon grid information to create a terrain file in SCICHEM format.

In addition to the METSCI and TERSCI pre-processors, a post-processor (SCIDOSPOST) is provided to process the SCICHEM output files. This post-processor processes the SCICHEM surface concentration and deposition dosage output files to extract information relevant to a user's application (e.g., Class I area analysis, PSD increments, 8-hour or maximum hourly ozone values, $PM_{2.5}$ increments, etc.). SCIDOSPOST can create POSTFILES for surface concentrations at user-specified receptor locations. Using SCIDOSPOST as a post-processing step avoids the computational burden of calculating surface concentrations at sampler locations during a SCICHEM run. However, if there is a need to calculate concentrations above the surface (e.g., for comparisons with aircraft measurements or to calculate vertical profiles), then SCIDOSPOST cannot be used. In this scenario, a sampler file needs to be provided for the SCICHEM simulation that specifies sampler locations and altitudes. The sampler output for receptors above ground level is an ASCII file that can be imported into a spreadsheet and analyzed as needed.

This user's guide describes, in a step-by-step approach, how to use the various executables provided in the SCICHEM distribution package and the format of the input and output files required for running the model. In addition to these programs, a limited version of the graphical user interface (GUI), named *SCIPUFFgui*, is provided for the Windows operating system as an aid to the user to visualize model results. The GUI can plot concentration contour plots for

surface, horizontal, or vertical slices for all source types. Note that SCIPUFFgui can also be used to create and run SCICHEM 2.0 namelist-type projects, but this capability has not been extended to support keyword-type projects introduced in SCICHEM 3.0 that are required for dealing with some new source types such as area and volume. Therefore, it is recommended that the GUI should be used primarily for viewing simulation results.

1.1 Overview of the SCICHEM Model

This section provides an overview of SCICHEM, including a description of the basic options available for running the model and an explanation of the basic input data and hardware requirements needed for running the model. The model can be used for both short-range and long-range applications with or without full chemistry options.

1.1.1 Basic Input Data Requirements

Versions of SCICHEM prior to SCICHEM 3.1 used a set of input files in Fortran NAMELIST format with filename extensions ".inp", ".scn", and ".msc". SCICHEM 3.1 and later allow an alternative keyword setup file as a basic input. This keyword file must have the ".sci" extension in its name and is similar to the keyword format used in AERMOD. For multicomponent runs with the full chemistry option, or for 1-hour NO_2 applications with explicit treatment of near-source plume chemistry, another file with extension ".imc" is required for providing the details of the chemical mechanism (chemical species names, gas-phase chemical reactions, aerosol and aqueous-phase chemistry options). The keyword file or the namelist input files contain the selected modeling options as well as source location and parameter data, receptor locations, meteorological data file specifications, and output options. Another type of basic input data needed to run the SCICHEM model is the meteorological data. SCICHEM can use AERMOD surface and profile data, meteorological output data from WRF (ARW), and gridded MEDOC (Multiscale Environmental Dispersion Over Complex terrain) meteorological data files. The SCICHEM meteorological pre-processor, METSCI, can also be used to read upper air files in FSL format, surface files in TD-3505 or ISD format, and/or onsite data to create surface and profile meteorological input files for SCICHEM.

SCICHEM meteorological files in MEDOC format can be created from WRF and MM5 outputs using the Mesoscale Model Interface Program (MMIF), developed for EPA by Ramboll. The MMIF source code and user's guide are available at EPA's SCRAM website (https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#mmif). It is recommended that the latest version of MMIF be used when running SCICHEM.

1.1.2 Computer Requirements

SCICHEM can be run on 64-bit Windows 8/Windows 8.1/Windows 10 or Linux computers using the prebuilt executable files provided in the distribution package. The prebuilt files are provided for 64-bit operating systems only and will not run on 32-bit systems. However, the SCICHEM source code is provided with the distribution, and it can be compiled on any computer with a standard FORTRAN 90 compiler on operating systems such as Windows, Linux, or Mac OS X. The developers have used the Intel compiler to build the code on both Windows and Linux systems; the code has not been compiled and tested using other compilers.

Note that SCICHEM 3.3 has been compiled to run with the OpenMP library, allowing for multithreaded calculations. However, this is only valid for non-chemistry runs.

1.1.3 Modeling Options

SCICHEM includes a wide range of options for modeling air quality impacts of pollution sources. The following sections provide a brief overview of the available options.

1.1.3.1 Source Options

SCICHEM is capable of handling instantaneous and continuous sources, including point, volume, and area source types. Line sources may also be modeled as a string of volume sources or as elongated area sources.

Source emission rates can be constant or variable throughout the modeling period. These emission rates may be specified for a single source or for a group of sources. The user may also specify a separate file of hourly emission rates for some or all of the sources included in a particular model run. This may be done using either the keyword setup file ("sci" extension) or NAMELIST input (new in SCICHEM 3.2 and later).

1.1.3.2 Receptor Options

SCICHEM has considerable flexibility in the specification of receptor locations. The user must specify the locations for elevated receptors to model flagpole receptors or receptors at aircraft heights. The sampler concentration output file from the SCICHEM simulation is an ASCII file that can be imported into a spreadsheet or analyzed using Python scripts. Note that specifying a large number of samplers results in large increases in SCICHEM run times. Thus, if only surface concentrations are desired, it is not necessary to specify receptor locations for the SCICHEM simulation, because the SCIDOSPOST post-processor can be used to determine the average surface concentration and important statistics for any arbitrary network of receptors (gridded or discrete). This avoids the runtime penalty of calculating surface concentrations at user-specified sampler locations during the SCICHEM simulation. See Section 1.1.3.4 for additional details.

1.1.3.3 Meteorology Options

SCICHEM supports a wide variety of formats for meteorological inputs, including standard surface and upper air observations, on-site observations (the format of on-site data is provided by the user as in AERMET), or three-dimensional meteorological outputs from prognostic models. Planetary boundary layer turbulence is represented explicitly in terms of surface heat flux and shear stress using parameterized profile shapes.

1.1.3.4 Output Options

The basic outputs from SCICHEM are the sampler output files, the surface concentration (dosage) output files containing total and ambient concentrations, and the dry and wet deposition files. The sampler output files provide the time average total and background for the tracer and chemical species at desired receptor locations. Note that it is not recommended to specify a large number of samplers during a SCICHEM simulation because of the impacts on runtimes. Currently, the model does not allow more than 5000 samplers in a SCICHEM run. For surface concentrations, the user is advised instead to use the SCIDOSPOST post-processor.

SCIDOSPOST can also be used to conduct a Class I area analysis using the surface dosage and deposition files.

1.1.4 Starting SCICHEM

The SCICHEM model is usually run using a command-line executable named *runSCI*. In the command-line run mode, the model can be run using either of two types of input formats: the KEYWORD input format or the NAMELIST input format. As a result of recent enhancements, all source options can be run with both formats.

On a Windows operating system, the GUI, SCIPUFFgui, can also be used to create and run certain projects in the original NAMELIST format. However, as mentioned previously, the GUI has not been updated to create and run projects in the KEYWORD format that is most familiar to AERMOD users. The GUI can be launched using the executable file (SCIPUFFgui.exe) from a DOS window or by double-clicking the SCIPUFFgui icon. The project NAMELISTS files can be created and run using the GUI. SCIPUFFgui can also be used to review and plot all projects after the successful completion of the run. Note that the GUI can be used to view model results regardless of the input type (NAMELIST or KEYWORD) even though it cannot be used to create or run projects with KEYWORD input files.

Details of setting up input files for runSCI and SCIPUFFgui are provided in Section 5.

1.1.5 Namelists Approach

For the namelists input format, parameters are specified through Fortran NAMELIST groups and free formatted data located in the input ("project".inp), release scenario ("project".scn), meteorology scenario ("project".msc) files.

All NAMELIST parameters must be contained within the "**&groupname**" and "/" lines of the given input file. All lines contained outside the NAMELIST section are considered comments and are disregarded by SCICHEM, except in the multicomponent input file. Some input parameters have default values that are used if the parameter is not included in the NAMELIST. If a parameter does not have a default value, the program will abort if the parameter is not included in the NAMELIST.

The namelists format file is described in more detail in Section 4.1.

1.1.6 Keywords Parameter Approach

The basic input file for SCICHEM for the keyword format must be named "Project".sci, where "Project" is the name of the project specified by the user. The user must specify the options and input data for running the model in this file. The keywords specify the type of option or input data being entered on each line of the input file, and the parameters following the keyword define the specific options selected or the actual input data. Some of the parameters are also input as descriptive secondary keywords. The keywords are grouped by pathway and are in a logical order based on their function within the model. The syntax for each keyword is provided, and the keyword type is specified—either mandatory or optional and either repeatable or non-repeatable. Unless noted otherwise, there are no special requirements for the order of keywords within each pathway, although the order in which the keywords are presented here is recommended. Any keyword that has special requirements for its order within the pathway is so noted following the syntax and type description. The syntax descriptions in the following

sections use certain conventions. Parameters that are in all capital letters and underlined in the syntax description are secondary keywords that are to be entered as indicated for that keyword. Other parameters are given descriptive names to convey the meaning of the parameter and are listed with an initial capital letter. Parentheses around a parameter indicate that the parameter is optional for that keyword. The default that is taken, when an optional parameter is left blank, is explained in the discussion for that keyword.

The keyword format file is described in more detail in Section 4.2.

1.1.7 Multicomponent File

For both the keyword and namelists formats, a multicomponent input file (referred to as the *IMC file*) is required for simulating multiple pollutants. This file is also in a special NAMELIST format. The name of the IMC file is specified in the "project".inp file (for namelists format) and in the "project".sci file (for keyword format). There are no naming requirements for this file, but it typically has an extension of "imc" in the file name.

While the multicomponent file is primarily designed for multi-pollutant SCICHEM simulations with chemistry, we recommend that it be included even for non-chemistry single component simulations for consistency. A logical flag in the file specifies if the calculations will include chemistry or not (the default value is TRUE, i.e., chemistry calculations will be performed if this flag is not set to FALSE). The tutorials provided with the SCICHEM distribution (see Appendix A) include IMC files for two types of SCICHEM multicomponent chemistry simulations. The first IMC file contains the specifications for the full chemistry version of SCICHEM for simulating ozone and secondary $PM_{2.5}$ increments. The second file is specifically for near-source plume chemistry of NOx sources and is applicable for calculating 1-hour NO_2 increments at short distances from the source. These are the only two types of chemistry IMC files currently supported in this version of SCICHEM. An example of a non-chemistry IMC file for a chemically inert single component simulation (chemistry flag set to FALSE) is provided in the tutorial for 1-hour SO_2 concentrations. A similar non-chemistry file can be used for simulating primary $PM_{2.5}$ or PM_{10}. The chemistry flag should also be set to FALSE when simulating multiple inert pollutants in a single run.

The multicomponent file is described in more detail in Section 4.3.

2
INSTALLING AND RUNNING SCICHEM

2.1 Installation

SCICHEM can be run on Windows or Linux from the command line using the runsci.exe executable (runsci on Linux). The prebuilt binaries of the five executable files METSCI.exe, TERSCI.exe, RUNSCI.exe, SCIDOSPOST.exe and SCIPUFFgui are available for Windows and metsci, runSCI, and sciDOSpost are available for Linux. The runsci executable requires the scipuff.ini file, which is located in the bin/windows/x64 or bin/Linux directories. The landuse file named "landuse_scichem.dat" is located in the sciData directory, and the files required for Class1 analysis and the Flag2010 files are provided in the Class1Area and Flag2010 sub-directories in the sciData directory. The scipuff.ini file must be edited so that the variable LandUseDataFile under the "Land_Use" section points to the landuse_scichem.dat file with the full path name. The sciDataDir variable under the "[Paths]" must also be edited in the scipuff.ini file to point to the sciData directory.

These files (and others) are distributed together in zip files which may have extensions "tgz", "tar", "zip" or "7z" depending on the application used to generate the files. (Most file archive applications can open these, including free and open-source 7-Zip.) The following instructions will allow the user to properly install SCIPUFFgui and the executable files onto his or her PC. The steps for installing the executables for Linux are similar except for the default installation directory name:

1. Make a main directory for SCICHEM, for example, C:\EPRI\SCICHEM_3.3 (~/EPRI/SCICHEM_3.3 for Linux), which will be referred to as $SCICHEM_BASEDIR
2. Extract all files from the zip file to $SCICHEM_BASEDIR
3. If the $SCICHEM_BASEDIR is not "C:\EPRI\SCICHEM_3.3", edit the scipuff.ini file to replace "C:\EPRI\SCICHEM_3.3" with the actual directory name

A developmental version of a GUI executable, SCIPUFFgui.exe, is also available on the Windows platform. This GUI can be used for reviewing a completed project or for plotting the species total concentrations for all projects. The GUI can be launched from a DOS window, or the user can simply double-click on the icon. To use the SCIPUFFgui executable, the user must also have the following files:

- SCIPUFFgui.exe - model executable file
- SCICHEM.chm - SCICHEM help file
- SCIPUFF.INI - initialization file to set directories and array sizes
- MASSC.GRD - default vertical grid for mass-consistent runs
- SCIPUFF.PAL - defines colors for the GUI
- MAPS Directory - includes all the data files required for drawing maps

The SCIPUFF GUI files are provided with the Windows zip files. The SCIPUFFgui can be run from a DOS window in the main directory by typing SCIPUFFgui or by double-clicking the SCIPUFFgui icon.

The details for running the command-line executable runsci.exe are provided in Section 2.2.

2.2 Running the Model

2.2.1 Run scripts

An example run_scichem.bat file has been provided for Windows, and a run_scichem.sh script file has been provided for Linux. A brief description for running the runSCI executable follows.

The runSCI executable file opens the KEYWORDS input file *ProjectName*.SCI, if it is available (*ProjectName* denotes project root name); otherwise, SCICHEM looks for the NAMELISTS input files i.e., *ProjectName*.INP, *ProjectName*.SCN, and *ProjectName*.MSC and creates output files such as *ProjectName*.DOS, *ProjectName*.ADOS, *ProjectName*.DEP, *ProjectName*.PRJ, *ProjectName*.PUF, *ProjectName*.LOG, *ProjectName*.ERR, *ProjectName*.SMP, and *ProjectName*.ASMP output files on successful completion of the project. The model can be executed from the command prompt by simply typing the name runSCI, as follows:

C:\> runSCI

The runSCI executable file and the dynamic-link libraries (with extension ".dll") need to be in the directory from which the user is attempting to run the model or in a directory included on the PATH command. The KEYWORDS input file (*ProjectName*.SCI) or the NAMELISTS input files must also be located in the directory from which the model is being executed.

For multicomponent runs (with or without chemistry), an IMC file must be present, and the FILE_NAME in the MATDEF namelist section of the *ProjectName*.INP file should be set to the name of the IMC file.

The DOS version will prompt the user for the project name and the path for the scipuff.ini file. Note that some or all of the following project output files will be created or overwritten based on the run settings:

- *ProjectName*.ERR
- *ProjectName*.LOG
- *ProjectName*.PRJ
- *ProjectName*.PUF
- *ProjectName*.SMP
- *ProjectName*.ASMP
- *ProjectName*.MCW
- *ProjectName*.DEP
- *ProjectName*.DGN
- *ProjectName*.DOS
- *ProjectName*.ADOS

The tutorials accompanying this user's guide provide a step-by-step approach to running the model for several situations. The inputs and, in some cases, limited outputs from these case studies are also provided as part of the distribution. All the outputs are not provided because of file size restrictions.

Array limits that affect numerical resolution and computational time may be set in the Scipmode section of the initialization file SCIPUFF.INI. In particular, these limit the number of puffs (MAXPUFF) in the dispersion calculation and the number of grid cells used to store surface time-integrated concentration and/or deposition (MAXGRID). Several predefined limits are available by setting GUIMode according to the table below; custom values may also be defined.

GUImode	MAXPUFF	MAXGRID
Standard or Operational	20000	25000
Extended	40000	85000
Ultimate	60000	100000
Custom	*User-specified*	*User-specified*

The number of threads used for parallel calculations (non-chemistry only) can also be set in this section with the variable name NumThreads. The default value is 1. While there is strictly no upper limit, it has been found there is little speed-up beyond 8 threads, depending on the project and computer resources. An error will occur if a chemistry calculation is attempted with NumThreads greater than 1.

2.2.2 Restarting a run

A project can be restarted or continued by using the "RST:" string before the project name; for example, to continue or restart a project named "ProjectName" from the last output time, the name used for the project in the runSCI argument or prompt should be "RST:ProjectName". All the output files for the project, at the last output time, must be present in the directory for restarting the project.

2.3 Building from Source

2.3.1 Linux

The script name makeall.sh for building the code from source using the Intel compiler has been provided under the build/Linux directory. The script can be run using the following command:

> bash makeall.sh

This will build the executable files using the Intel compiler under the ifort directory.

2.3.2 Windows

The Visual Fortran project files and solutions for Visual Studio 2013 are provided under the build/Windows/workspace/EPRI directory. The batch file *runVS.bat* under the workspace directory can be used to load the solution for Visual Studio 2013. If Visual Studio is not installed in the default directory, the path will have to be edited to point to the local installed directory. The executable files can be built using the Intel compiler under the ifort directory by selecting "Build Solution" under the Build menu.

Note that SCICHEM has not been built and tested using other compilers.

3
SCICHEM METEOROLOGICAL PRE-PROCESSOR (METSCI) AND TERRAIN PRE-PROCESSOR (TERSCI)

This section describes the two pre-processors that have been developed to assist the user in creating SCICHEM input files. METSCI is a meteorological pre-processor that reads standard surface and upper air sounding observation files and creates files in the formats described in Section 3.1, suitable for running SCICHEM. The second pre-processor (TERSCI) creates terrain files in SCICHEM format using readily available digital elevation data files. These pre-processors are described in more detail in the following sections and are unchanged from the SCICHEM 3.1 versions.

3.1 METSCI

METSCI is similar to the AERMET pre-processor (EPA, 2004) for AERMOD and is functionally equivalent to running only Stage 1 of AERMET. In fact, it should be noted that the AERMET source code is used in METSCI to read the observation files and perform minimal processing and quality assurance. However, METSCI extracts only the basic observations and does not perform any boundary layer modeling as would be the case for full AERMET processing. The boundary layer calculations are conducted within SCICHEM as described in the SCICHEM Technical Document (Chowdhury et al., 2013).

The input for METSCI is similar to the Stage 1 AERMET format and employs a pathway and keyword format. These are read from a file specified on the command line with no particular file name or extension assumed. This file will contain up to four pathways: JOB, SURFACE, UPPERAIR, and ONSITE. They may appear in any order. Input that follows a pathway is associated with that pathway until another recognized pathway is given. Lines beginning with an asterisk are ignored. Note that surface observations files are currently limited to those in ISHD (DS-3505) format and the upper air observations are limited to FSL Rawinsondes. The use of on-site data closely follows that of AERMET.

Progress messages, including certain error messages, are displayed to the standard output device, typically the monitor. In particular, default settings are displayed in this way. This display can be sent to a user-specified file by redirecting the output as follows:

METSCI *inputFile* > *outputFile*

where *inputFile* is the basic METSCI input file and *outputFile* is the file name for the output.

3.1.1 Job Pathway

This pathway gives file names for reports and messages. The two keywords are:

MESSAGES file name where errors, warnings, and other messages are written by the AERMET-utilized subroutines. Mandatory.

REPORTS file name where a simple summary is written by the AERMET subroutines. Optional.

3.1.2 Surface Pathway

This pathway indicates that the keywords defining the processing of surface observations will follow. The keywords and associated input are:

DATA	surface file name and file format. The file name must include the path (if any) and is limited to 512 characters. The file type is a character string limited to 8 characters. Currently only type "ISHD" (DS-3050) is valid. Mandatory.
EXTRACT	file name of SCICHEM surface meteorological file. Mandatory.
XDATES	start and end dates of the data to be processed. The format is YY/MM/DD TO YY/MM/DD. Leading zeros in the year, month, or day integers may be omitted, but blanks after the "/" characters will result in error. The word "TO" is optional. Mandatory.
LOCATION	station identifier, latitude, longitude. The station identifier is limited to 16 characters. The latitude and longitude are given in decimal degrees appended with conventional direction abbreviations ("E", "W", "S", or "N"). ("+" and "–" symbols are not recognized.) Optional. If this pathway is not given, the station identifier and location are taken from the observation file.
RANDOM	character string "TRUE" or "FALSE" (synonyms "YES" or "NO") that applies a pseudo-random perturbation to wind direction to mitigate the biases of quantized data reporting. An optional argument can follow "TRUE" and gives the spread of the perturbation in degrees. The default spread is 10°. Optional.
QAOUT	character string "TRUE" or "FALSE" (synonyms "YES" or "NO") that invokes a limited quality assurance check of the observations. The results are given in the report and message files specified in the JOB pathway. (Unlike AERMET, no corresponding output file is generated.) Optional.
LANDUSE	character string describing the local surface conditions. Recognized strings are "CULTIVATED", "URBAN", "FOREST", "DESERT", "WATER", and "GRASSLAND". Optional. If not specified, "CULTIVATED" is assumed.

3.1.3 Upper Air Pathway

This pathway indicates that the keywords defining the processing of upper air observations will follow. The keywords and associated input are:

DATA	upper air file name and file format. The file name must include the path (if any) and is limited to 512 characters. The file type is a character string limited to 8 characters. Currently only type "FSL" is valid. Mandatory.
EXTRACT	file name of SCICHEM profile meteorological file. Mandatory.
XDATES	start and end dates of the data to be processed. The format is YY/MM/DD TO YY/MM/DD. Leading zeros in the year, month, or day integers may be omitted, but blanks after the "/" characters will result in error. The word "TO" is optional. Mandatory.
LOCATION	station identifier, latitude, longitude. The station identifier is limited to 16 characters. The latitude and longitude are given in decimal degrees appended with conventional direction abbreviations ("E", "W", "S", or "N"). ("+" and "–"

symbols are not recognized.) Optional. If this pathway is not given, the station identifier and location are taken from the observation file.

RANDOM character string "TRUE" or "FALSE" (synonyms "YES" or "NO") that applies a pseudo-random perturbation to wind direction to mitigate the biases of quantized data reporting. An optional argument can follow "TRUE" and gives the spread of the perturbation in degrees. The default spread is 10°. Optional.

QAOUT character string "TRUE" or "FALSE" (synonyms "YES" or "NO") that invokes a limited quality assurance check of the observations. The results are given in the report and message files specified in the JOB pathway. (Unlike AERMET, no corresponding output file is generated.) Optional.

3.1.3 Onsite Upper Air Pathway

This pathway indicates that the keywords defining the processing of site-specific observations will follow. Note that the recognized keywords represent a subset of those used in AERMET, and the AERMET User's Guide should be consulted for a description of the FORMAT keyword options and ways of specifying observation heights. The keywords and associated inputs are:

DATA onsite data file name. The file name must include the path (if any) and is limited to 132 characters. Mandatory.

EXTRACT file name of SCICHEM meteorological file. Either upper air or surface files may be generated depending on the input data. Therefore, a generic file extension of "obs" may be used, but any extension is valid. Mandatory.

XDATES start and end dates of the data to be processed. The format is YY/MM/DD TO YY/MM/DD. Leading zeros in the year, month, or day integers may be omitted, but blanks after the "/" characters will result in error. The word "TO" is optional. Mandatory.

LOCATION station identifier, latitude, longitude. The station identifier is limited to 16 characters. The latitude and longitude are given in decimal degrees appended with conventional direction abbreviations ("E", "W", "S", or "N"). ("+" and "–" symbols are not recognized.) Mandatory.

RANDOM character string "TRUE" or "FALSE" (synonyms "YES" or "NO") that applies a pseudo-random perturbation to wind direction to mitigate the biases of quantized data reporting. An optional argument can follow "TRUE" and gives the spread of the perturbation in degrees. The default spread is 10°. Optional.

READ record index (integer) followed by a list of variables names present on the data file. Up to 50 READ records may be given with appropriate record numbers. A maximum of 50 variables may be given per record. However, the maximum record length is 132. Mandatory.

FORMAT record index (integer) followed either by a list of Fortran-like format specifications for reading the variables in the corresponding READ records or the string "FREE" to denote Fortran-free format. The maximum record length is 132. Mandatory.

OSHEIGHTS list of heights for multi-level profile data, given in meters above ground from lowest to highest. This will supersede any heights given in the data file. Optional.

OBS/HOUR number of observations each hour. Mandatory if observations are more frequent than once per hour. (Unlike AERMET, no time-averaging is applied.)

QAOUT character strings "TRUE" or "FALSE" (synonyms "YES" or "NO") that invoke a limited quality assurance check of the observations. The results are given in the report and message files specified in the JOB pathway. (Unlike AERMET, no corresponding output file is generated.) Optional.

In addition to this meteorological pre-processor provided with the SCICHEM distribution package, a pre-processor is available from EPA to convert prognostic model (MM5 and WRF) outputs to the SCICHEM gridded MEDOC format. This processor is referred to as the *Mesoscale Model Interface Program* (MMIF). The MMIF processor and the associated user's guide can be downloaded from the EPA SCRAM website at https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#mmif.

3.2 TERSCI

TERSCI is similar to the AERMAP pre-processor (EPA, 2011) for AERMOD. TERSCI reads the same types of DEM and NED data files as AERMAP and writes a terrain (*.TER) file in the format that SCICHEM expects.

When using meteorology supplied by a MEDOC file (for example, the output from MMIF; see Section 4.5.2, MEDOC Format), there is no need to run TERSCI. The MEDOC file contains terrain information from the upstream meteorological model (for example, WRF). It is anticipated that for long-range transport analyses, the user would supply a MEDOC file. TERSCI is intended for short-range applications of SCICHEM—situations in which AERMOD could be used.

Because SCICHEM can accept only regular "XY" gridded terrain files, TERSCI does not allow the user to specify, for example, polar grids as AERMAP allows. The grid must be regularly spaced in either longitude-latitude or in UTM X-Y.

3.2.1 Usage

TERSCI will print a help message to the screen when given the **`-h`** or **`--help`** command-line option.

```
C:\> TERSCI --help
Usage: [-h | --help] [--sample] -i ctrl.inp
 Options:
    -i file    Specify control file to use
    --sample   Print a sample control file to the screen
    --version  Print the program version to the screen and exit
    --help     Print this help message
    -h         Print this help message
```

The **-h** command-line option creates a sample control file, which can be edited by the user. The control file is a keyword-driven ASCII (text) file used to control the program.

```
C:\> TERSCI --sample > tersci.inp
C:\> more tersci.inp

; Comment characters are #, ;, and !.  Blank lines are ignored.
; Values can be space-delimited OR comma-delimited, or a mix.
; Keywords are case-insensitive, filenames are not.

# USE is followed by either LATLON (alt: LL), or UTM and the UTM zone

; USE   LATLON
USE UTM    11

# DOMAIN is followed by two lower left, and two upper right, coordinates.
#   Latitude  is positive in the Northern hemisphere
#   Longitude is positive in the Eastern  hemisphere

; DOMAIN   48.865219,-98.761383 48.910038,-98.692932 ! LATLON
DOMAIN 517500  5412500  522500  5417500              ! UTM

# SPACING gives the horizontal resolution, in degrees (LL) or meters (UTM)

; SPACING  0.001  ! ~111 meters (LATLON)
Spacing 100       !  100 meters (UTM)

; NADA specifies the North American DATUM, use NADA 0 elsewhere
NADA 4

# INPUT gives the type (NED or DEM), followed by the (path+)filename.
# Can contain spaces, if enclosed in quotes. Reads the same types of
# DEM/NED files as AERMAP.  Download NED data from:
#   http://www.mrlc.gov/viewerjs/  (seamless GeoTiff)
#   ftp://rockyftp.cr.usgs.gov/vdelivery/Datasets/Staged/NED (ArcGrid)
# The ftp server has 1x1 degree ArcGrid files, which need to be converted
# to GeoTiff files (e.g. ArgGIS or gdalwarp).

INPUT  NED  n49w099.tif

# OUTPUT gives the path and filename of the output terrain file.
# Can contain spaces, if enclosed in quotes.

OUTPUT  terrain.ter
```

The file can be either space-delimited (a space between elements in a line, also called *words*) or comma-delimited, or a mixture. Blank lines, and any portion of a line after a comment character, are ignored by the program.

The order of the keywords does not matter. Keywords can be uppercase or lowercase (or a mixture) and are converted to uppercase internally. Filenames are not converted to uppercase or lowercase but are used verbatim. Case does not matter on MS Windows platforms, but for other operating systems case matters. Filenames may contain spaces if enclosed in single or double quotes: `terrain.ter`, `'terrain.ter'`, and `"terrain.ter"` are all equivalent.

Keyword	Meaning
USE	Either **UTM** or **LATLON** (or the synonym **LL**) to specify the coordinate system type. **UTM** must be followed by the UTM zone. Use negative number for the southern hemisphere.
DOMAIN	Specifies the domain using two coordinate pairs in the same units as **USE**: the lower left and upper right corners of the requested domain (X_{LL},Y_{LL}, X_{UR},Y_{UR}). This differs from the SCICHEM control file, which specifies the domain using X_{LL}, X_{UR},Y_{LL},Y_{UR}.
SPACING	Specifies the grid spacing, the distance between adjacent grid cell centers, in the same units as **USE**.
NADA	Specifies the North American DATUM for the output: 0 = No correction, useful outside of North America 1 = NAS-C, North American 1927 Clarke 1866 Spheroid (NAD-27) 4 = NAR-C, North American 1983 GRS 80 Spheroid (NAD-83)
INPUT	Gives the (path and) filename to an input NED or DEM file. This keyword is repeatable, allowing the user to feed multiple NED/DEM files to TERSCI. The path/file name may contain spaces, if enclosed in quotes.
OUTPUT	Gives the (path and) filename for the output SCICHEM-format terrain file. The path/file name may contain spaces, if enclosed in quotes.

Input NED data may be obtained from the Internet, at the servers listed above (among others). Some servers, for example, ftp://rockyftp.cr.usgs.gov/vdelivery/Datasets/Staged/NED and http://viewer.nationalmap.gov/viewer/ (the National Map Viewer), supply data only in "ArcGrid" format, which must be converted to a GeoTIFF format before TERSCI can read it (similar to AERMAP).

The SCICHEM terrain file format is as follows:

```
UTM     14
  0.51750E+03   0.54125E+04   0.10000E+00   0.10000E+00     50     50
   479   479   479   479   479   479   479   479   479   479   479   478
   478   478   478   478   478   478   477   477   477   476   477   477
…snip…
   476   476   476   476   475   475   475   475   475   475   475   476
   475   475   475   475   475   475   474   474   474   474   473   473
   473   474   473   473
```

The first line contains either "UTM" and the UTM zone, or "LATLON". The second line contains the coordinates of the lower left grid cell center (two values) followed by the grid spacing in the X- and Y-directions (currently required to be the same), followed by the number of points in the X- and Y-directions, then follows the values at the points, 12 per line.

An example using LATLON is as follows:

```
LATLON
 -0.98761E+02   0.48865E+02   0.10000E-02   0.10000E-02     68     44
   479   479   479   479   479   479   478   479   479   479   479   479
   479   479   479   478   478   479   478   479   478   478   478   478
```

Note that the lower left grid cell center is given using longitude then latitude, because longitude is the coordinate that measures eastward (that is, the X-axis).

4
INPUT FILE FORMATS

4.1 NAMELISTS Input Format

The NAMELISTS format is one of the two input formats for running SCICHEM. The second input format—that is, the KEYWORDS format—is a recent feature of the model and is described in Section 4.2.

The NAMELISTS input format consists of four input files with Fortran NAMELIST statements. Three of the input files have specific name and extension requirements. The input files are checked and re-created before starting the run (setup phase). The three input files are as follows:

ProjectName.INP	-	the main input parameter file
ProjectName.SCN	-	the release scenario file
ProjectName.MSC	-	the meteorological scenario file

where *ProjectName* is the project identifying name for the runSCI or SCIPUFFgui calculation. The fourth file is the multicomponent file, which specifies the chemistry options for the run. Although it is possible to run SCICHEM for a single-pollutant non-chemistry case without this file, the recommended approach is to include this file and to specify within this file if the run is a chemistry run or not. This is new in SCICHEM 3.3 to address confusion expressed by model users. The name of the multicomponent file is specified within the *ProjectName*.INP file above. This file is referred to as the "IMC" (for multicomponent inputs) file and conventionally has a file name extension of IMC. Examples of the multicomponent files for different applications (simple chemistry; full gas-phase chemistry; gas-phase, aerosol, and aqueous chemistry; and no chemistry with a single inert pollutant) are provided with the SCICHEM tutorial files that are part of the SCICHEM distribution (additional details below).

On Windows platforms, the GUI (SCIPUFFgui) can be used to construct the first three NAMELIST input files for SCICHEM using the "Create new project" option (See Section 5.1). The INP, SCN, and MSC files are maintained separately so that an arbitrary number of releases can be made, and multiple release material types can be defined. The fourth file (multicomponent file or IMC file) cannot be created by the GUI and must be adapted from the sample files provided with the SCICHEM distribution. As mentioned above, these examples include an IMC file suitable for long-range transport applications and calculation of ozone and primary and secondary $PM_{2.5}$ increments, an IMC file for near-source NO-NO_2-O_3 chemistry, and an IMC file for an inert case (no chemistry). The full chemistry IMC file contains the specifications for the full chemistry version of SCICHEM (the gas-phase chemistry module is based on the CB6r2 chemistry mechanism, while the aerosol and aqueous chemistry modules are based on those in the EPA model CMAQ, version 4.7.1). The inorganic aerosol module has been updated from ISORROPIA 1.7 based on the module in CMAQ 4.7.1 to the latest version ISORROPIA II. The second IMC file is provided for short-range applications to calculate near-source 1-hour NO_2 increments due to NOx sources. Only gas-phase chemistry is performed when this IMC file is used, and the gas-phase chemistry mechanism is optimized to simulate near-source NO-NO_2-O_3

chemistry. The third IMC file, for near-source SO_2 concentrations, has the chemistry flag turned off. It is not recommended to edit or change the full-chemistry IMC file provided in the distribution with the exception of changing the name for the ambient file containing background concentrations of the chemical species and deselecting aerosol and aqueous chemistry options for long-range transport applications with gas-phase chemistry only—for example, to calculate ozone impacts (described in more detail in Section 4.3).

The IMC file name must be attached to the material using the material editor in SCIPUFFgui or by changing the value of FILE_NAME in the "matdef" NAMELIST section of the INP file.

SCIPUFFgui and runSCI input parameters are specified through NAMELIST groups and free formatted data located in the input, release scenario, meteorology scenario, and multicomponent input files. All NAMELIST parameters must be contained within the "**&groupname**" and "/" lines of the given input file. All lines contained outside of the NAMELIST section are considered comments and are disregarded by SCIPUFFgui, except in the multicomponent input file. Some input parameters have default values; if a parameter does not have a default, the program will abort if the parameter is not included in the namelist.

4.1.1 Main Input File

A sample input file is shown in Figure 4-1. The following section describes the NAMELIST parameters and their defaults, if available. Some of the important NAMELIST parameters are shown in the example below.

```
&CTRL
 RESTART = F,
 FILE_RST       = ' ',
 PATH_RST       = ' ',
 TIME_RST       =  0.0000000E+00
/
 &TIME1
 YEAR_START     =       1999,
 MONTH_START    =          7,
 DAY_START      =          6,
 TSTART  =  0.0000000E+00,
 TZONE   =   18.00000    ,
 LOCAL   = T
/
 &TIME2
 YEAR_END       =       1999,
 MONTH_END      =          7,
 DAY_END =          7,
 TEND    =  0.0000000E+00,
 TEND_HR =   24.00000    ,
 DELT    =   900.0000    ,
 DT_SAVE =   1800.000
 &FLAGS
 TITLE   = Example
 CREATE  = T,
 AUDIT_CLASS    = '  '
 AUDIT_ANALYST   = '  Anonymous'
 DYNAMIC = T,
 DENSE_GAS      = F,
 STATIC  = T,
 RUN_MODE       =          0
/
 &DOMAIN
 CMAP    = 'CARTESIAN
 XMIN    =   782.0000    ,
 XMAX    =   922.0000    ,
 YMIN    =  -418.0000    ,
 YMAX    =  -278.0000    ,
 ZMAX    =   16562.24    ,
 VRES    =  9.9999996E+35,
 RES     =  9.9999996E+35,
 UTM_ZONE       =      65535,
 XREF    =  0.0000000E+00,
 YREF    =  0.0000000E+00,
 LON0    =  -88.27100    ,
 LAT0    =   35.88100
/
 &OPTIONS
 T_AVG   =  0.0000000E+00,
 CMIN    =  0.0000000E+00,
 LSPLITZ = F,
 DELMIN  =  9.9999996E+35,
 WWTROP  =  9.9999998E-03,
 EPSTROP =  3.9999990E-04,
 SLTROP  =   10.00000    ,
 UU_CALM =  0.2500000    ,
 SL_CALM =   1000.000    ,
 NZBL    =         11,
 MGRD    =          2,
 Z_DOSAGE       =  0.0000000E+00,
 SMPFILE = 'ae5.sam',
 DT_SMP  =   1800.000    ,
 SUBSTRATE_TYPE =          0
/
 &MATDEF
 CLASS   = 'GAS           ',
 MNAME   = 'TRAC          ',
 UNITS   = 'kg            ',
 FILE_NAME      =  'ae5.imc',
 FILE_PATH      = ' ',
 GROUP_DEPOSITION       = F,
 GROUP_DOSE     = F,
 MULTI_COMP     = F,
 CONC_MIN       =  0.0000000E+00,
 DECAY_AMP      =  0.0000000E+00,
 DECAY_MIN      =  0.0000000E+00,
 DENSITY =   1.200000    ,
 GAS_DEPOSITION  =  0.0000000E+00
```

Figure 4-1
Sample SCICHEM Input File

The input parameters for the NAMELIST groups are defined in the following section. Some of the parameters, marked by * , are used by the model during rewriting of the input files, and any changes to the settings by the user are ignored.

Namelist: **CTRL** - run control flag.

*restart** - Flag for run status (LOGICAL). If 'True', the old project file is used to continue the run from the last time break. The default is 'False'.

*file_rst** - name of project used to initialize current project. (CHARACTER*128). If not blank, the current project is run on from the state defined by the *file_rst* project and puff and surface files. The default is ' ' (blank).

*path_rst** - path for project *file_rst*. (CHARACTER*128). The default is ' '.

*time_rst** - time on the puff and surface files of project *file_rst* used to initialize the current project (REAL*4). The default is the last time.

Namelist: **TIME1** - time domain information.

year_start - Start year of the calculation (INTEGER*4). If the year is not specified, it is assumed to be that of the first year given in the meteorological input.

month_start - Start month of the calculation (INTEGER*4). If the month is not specified, it is assumed to be that of the first month given in the meteorological input.

day_start - Start day of the calculation (INTEGER*4). If the day is not specified, it is assumed to be that of the first day given in the meteorological input.

tstart - Start time (hours) of the calculation (REAL*4). If the time is not specified, it is assumed to be that of the first time given in the meteorological input.

tzone - Local time of midnight UTC (REAL*4). The default is zero.

local - Flag for calculation time convention (LOGICAL). If 'True', the time is taken as local instead of UTC. The default is 'False'.

time_status - This variable is not required for this version of the code; however, it will appear if the project is created with the GUI. It is not used.

Namelist: **TIME2** - supplementary time domain input used for restart.

year_end - Stop year of the calculation (INTEGER*4). If the year is not specified, it is assumed to be the same as the start year.

month_end - Stop month of the calculation (INTEGER*4). If the month is not specified, it is assumed to be the same as the start month.

day_end - Stop day of the calculation (INTEGER*4). If the day is not specified, it is assumed to be the same as the start day.

tend - Stop time (hours) of the calculation (REAL*4). If the time is not specified, it is assumed to be 1 hour past the start time.

tend_hr - Duration (hours) of the calculation (REAL*4).

delt - Maximum timestep (seconds) of the calculation (REAL*4). The default is 900.

dt_save - Amount of time (seconds) between output dumps (REAL*4). The output includes the instantaneous fields and the surface accumulation fields, as specified by the user. The default results in no output.

Namelist: **FLAGS** - run control and audit information.

title - Descriptive title of the project (CHARACTER*80). No default is available.

create - Flag for full SCIPUFFgui calculation (LOGICAL). If 'True', SCIPUFFgui only initializes the project, but does not start the calculation. The default is 'False'. If a project is created with the GUI, this will be set to 'True'. To run the command-line version, set create to 'False'.

audit_class - Classification of the current project (CHARACTER*32). No default is available.

audit_analyst - Name of the project analyst (CHARACTER*32). The default is 'anonymous'.

dynamic - Flag to including momentum and buoyancy dynamics (LOGICAL). If 'False', puffs are treated as passive. Only gaseous puffs can carry dynamics; however, all puffs will be influenced by the dynamics.

dense_gas - Flag to include dense gas effects (LOGICAL).

static - Flag to perform quasi-steady calculation of continuous sources (LOGICAL). The default is 'True'.

multicomp - Flag to perform multicomponent chemistry (LOGICAL). Must also have a multicomponent input file (*ProjectName*.IMC).

hazarea - Type of hazard area prediction (CHARACTER*4). Not required in the current version. Must be 'OFF'.

run_mode - Run mode (INTEGER*4) determined by setting certain bits. The standard run mode is used if the zero bit is not set (for example, *run_mode* = 0); if it is set (for example, *run_mode* = 1), a fast mode is used. In the fast mode, the vertical and horizontal resolution are coarsened and the merge criteria for puffs are relaxed, leading to fewer puffs and faster computation speed. [Note that bit 12 is always set internally with the result that 4096 may be added to run_mode after a calculation is performed.]

Namelist: **DOMAIN**- defines the spatial domain.

cmap - Type of spatial domain, 'UTM', 'CARTESIAN', or 'LATLON' (CHARACTER*40). The default is 'LATLON'.

xmin - Minimum horizontal coordinate (REAL*4). For a LATLON run, this value represents the minimum longitude of the domain in degrees. For CARTESIAN runs, this value represents the western boundary in kilometers.

xmax - Maximum longitude (deg) or eastern (km) boundary (REAL*4).

ymin - Minimum latitude (deg) or southern (km) boundary (REAL*4). Note that a negative UTM northing value indicates the Southern Hemisphere if a positive *utm_zone* is specified. In this case, the value is taken as 10,000 km subtracted from the standard (positive) northing value.

ymax - Maximum latitude (deg) or northern (km) boundary (REAL*4). For negative values, see *ymin* comment.

zmax - Vertical extent (meters) of the calculation domain (REAL*4). The default is 2500.

vres - Spacing parameter (meters) that limits the vertical growth of a puff (REAL*4). The default is 250.

hres - Spacing parameter that limits the horizontal growth of a puff in the same units as xmin (REAL*4). For observational data, the default is 1/10 of the domain. For gridded data, the resolution is taken as that of the meteorology.

xref - Cartesian x-coordinate (km) of the reference point when CARTESIAN coordinates are specified (REAL*4). The default is zero.

yref - Cartesian y-coordinate (km) of the reference point when CARTESIAN coordinates are specified (REAL*4). The default is zero.

utm_zone - UTM zone if *cmap* = 'UTM'. Otherwise not used. Negative value denotes Southern Hemisphere.

lon0 - Longitude of the reference point in degrees, when CARTESIAN coordinates are specified (REAL*4). The default is zero, and east is positive.

lat0 - Latitude of the reference point in degrees, when CARTESIAN coordinates are specified (REAL*4). The default is zero, and north is positive.

domain_status - This variable is not required for this version of the code; however, it will appear if the project is created with the GUI. It is not used.

Namelist: **OPTIONS** - optional parameters.

t_avg - Conditional averaging time (seconds) for defining the diffusive component of turbulence (REAL*4). The default is no conditional averaging.

cmin - Minimum puff mass (REAL*4) in user-defined units (see units under MATDEF). The default is zero.

lsplitz - Flag for vertical puff splitting within the planetary boundary layer (LOGICAL). If 'True', puffs are not split in the vertical direction within the boundary layer. The default is 'False'. This option has been disabled.

delmin - Minimum grid size (meters) for the adaptive surface grid (REAL*4). The default is zero.

wwtrop - Tropospheric vertical turbulent fluctuations (m^2s^{-2}) used as the minimum value (REAL*4). The default is 0.01.

sltrop - Tropospheric vertical length scale (meters) (REAL*4). The default is 10.

epstrop - Tropospheric energy dissipation rate (m^2s^{-3}) (REAL*4). The default is 4.0e-4.

uu_calm - Minimum horizontal velocity fluctuation variance (m^2s^{-2}) (REAL*4). The default is 0.25.

sl_calm - Horizontal length scale associated with uu_calm (m) (REAL*4). The default is 1000.

nzbl - Number of boundary layer vertical grid levels (INTEGER*4). The default is 11.

mgrd - Grid resolution parameter that limits the horizontal growth of a puff (INTEGER*4). The horizontal size of the puffs will be limited to $2^{mgrd} \times hres$, where *hres* is specified under the DOMAIN section. The default is 2.

grdmin - Minimum grid size (meters) for the puff grid resolution (REAL*4). The default is zero.

z_dosage - Elevation at which surface dosages are computed (REAL*4). Default is 0.0.

smpfile - Name of a file with sampler locations for sampler output (CHARACTER*80). See Section 5.6.

dt_smp - Minimum output time (s) to sampler file (REAL(4)). Default is large time step, *delt*.

Substrate_type - Not used.

Namelist: **MATDEF** - defines material properties (multiple copies of this namelist can be included in the input file to define multiple materials).

mname - Material name (CHARACTER*16). Any 16-character string used to identify the material. No default.

class - Material class (CHARACTER*16). Must be 'GAS' (gaseous) or 'PART' (particle).

nsg - Number of particle size groups (INTEGER*4). Only used for particle type materials.

density - Gaseous or particle material density (kg/m^3) (REAL*4). Default is nominal air density of 1.2

gas_deposition - Gas deposition velocity (m/s) (REAL*4). Only used for gaseous materials.

psize - Array of particle mass mean diameters (μm) (REAL*4). Only used for particle type materials.

pbounds - Bin boundaries (microns) that determine the range of particle sizes within the subgroup (REAL*4). Only used for particle type materials.

group_deposition - Flag for group deposition (LOGICAL). If 'True', the deposition of each subgroup is included on the output surface deposition file. The default is 'False'.

total_deposition - Flag for total deposition (LOGICAL). If 'True', the total deposition of all subgroups is included on the output surface deposition file. The default is 'False'.

group_dose - Flag for group dose (LOGICAL). If 'True', the dose of each subgroup is included on the output surface dose file. The default is 'False'.

total_dose - Flag for total dose (LOGICAL). If 'True', the total dose of all subgroups is included on the output surface dose file. The default is 'False'.

units - Material mass units for labeling plots (CHARACTER*4).

conc_min - Minimum concentration of interest for this material (REAL*4).

decay_amp - Daytime decay rate (s^{-1}) of the material (REAL*4). The default is zero.

decay_min - Nighttime decay rate (s^{-1}) of the material (REAL*4). The default is zero.

multi_comp - Flag to attach multiple chemical species to the material (LOGICAL). Must also have a multicomponent input file (*ProjectName*.IMC) specified.

nwpn_decay - Not used in this version of the code (REAL*4). If the file is created with the GUI, this variable will appear on the input file as a "not set" value of -1.E+36. It is not used.

file_name - IMC file name (CHARACTER*80) being used for a multicomponent run.

file_path - Path to the IMC file being used (CHARACTER*80). The default value is ' ' (blank).

4.1.2 Release Scenario File

A sample release scenario file is shown in Figure 4-2. The following section describes the NAMELIST parameters and their defaults, if available. Not all the NAMELIST parameters are shown in the example.

```
   &SCN
             TREL                  =  0.0000000E+00,
             XREL                  =   831.7692    ,
             YREL                  =  -357.5436    ,
             ZREL                  =   193.5480    ,
             CMASS                 =   1.000000    ,
             SUBGROUP              =          1,
             TDUR                  =   1.000000    ,
             SIZE                  =   11.73480    ,
             WMOM                  =   19.65960    ,
             BUOY                  =   48.18000    ,
             LOGNORM_MMD       = -9.9999996E+35,
             LOGNORM_SIGMA     = -9.9999996E+35,
             SLURRY_FRACTION = -9.9999996E+35,
             RELTYP                = 'CS  ',
             RELMAT                = 'TRAC          '
 /
#START_MC
             NO2   3.588982E+01
             NO   3.230084E+02
             FORM   1.560000E-03
             PAR   2.981190E+00
             CO   5.476050E+01
             OLE   2.731100E-01
             TOL   1.059300E+00
             XYL   1.142850E+00
             SO2   1.507805E+02
             SULF   1.052363E+01
             NH3   9.981000E-02
#END_MC
```

Figure 4-2
Sample SCICHEM Release Scenario File

The namelist parameters are defined as follows:

RELNAME - Release name corresponding to name specified in emissions file (*name_rel*), if used. Otherwise, optional label for release (CHARACTER*80).

RELDISPLAY - Name of prime building file, if being used. (CHARACTER*80). Otherwise, ignored.

trel - Release time (hours) (REAL*4). No default is available.

xrel - Absolute x-coordinate of the release, Cartesian (km) or Lat/Long (degrees) (REAL*4). No default is available.

yrel - Absolute y-coordinate of the release, Cartesian (km) or Lat/Long (degrees) (REAL*4). No default is available.

zrel - Release height (meters) above the surface (REAL*4). No default is available.

reltyp - Type of release: 'C' for continuous, 'I' for instantaneous, 'CM' for continuous moving, 'CS' for continuous stack with plume rise formula, 'CA' for continuous area source. (CHARACTER*4). No default is available. Appending 'F' to these strings (except 'I' and 'CM') indicates that the release rates are read from a file specified in *name_rel*.

cmass - Total mass of material for an instantaneous release, mass flux for a continuous release, or mass flux per unit area for an area source (REAL*4). In user-defined units (see *units* under MATDEF in the INP file), *units* for instantaneous and *units per second* for continuous, moving, or stack. No default. Should be set to 1 for multicomponent releases.

size - Source radius or initial Gaussian spread for Instantaneous or Continuous Releases (*reltyp* 'I' or 'C') or stack diameter (meters) for *reltyp* 'CS' (REAL*4). No default is available.

Tdur - Duration (hours) of a continuous release (REAL*4). (See *reltype*.) No default is available. Used only if not defined by an emissions file.

relmat - Name identifying the material being released (CHARACTER*4). Must be identical to a name given in the materials list in the input file. No default is available.

sigx - x-direction source diameter (m) (REAL*4) for Instantaneous release. No default is available.

sigy - y-direction source diameter (meters) (REAL*4) for Instantaneous or Continuous release. No default is available.

sigz - z-direction source diameter (meters) (REAL*4) for Instantaneous or Continuous release. No default is available.

xlena - Length of rectangular area source in the x-direction (meters) before any rotation is applied. (REAL*4).

ylena - Length of rectangular area source in the y-direction (meters) before any rotation is applied. (REAL*4).

anga - Orientation angle for the rectangular area in degrees from east, measured positive in the counterclockwise direction (REAL*4). Defines a rotation about the center of the area (*xrel*, *yrel*).

subgroup - Number of the individual material subgroup for a tracer particle release (INTEGER*4). No default is available. For tracer particle material releases if *subgroup* is equal to *nsg*+1 where *nsg* is the number of size bins defined in the MATDEF namelist in ***ProjectName*.INP**, the *cmass* is distributed among all material bins with a lognormal distribution.

horiz_uncertainty - The horizontal uncertainty (m) of the location of the source (REAL*4). The default is zero.

vert_uncertainty - The vertical uncertainty (m) of the location of the source (REAL*4). The default is zero.

urel - x-direction velocity (m/s) for a moving continuous source (REAL*4). No default is available.

vrel - y-direction velocity (m/s) for a moving continuous source (REAL*4). No default is available.

wrel - z-direction velocity (m/s) for a moving continuous source (REAL*4). No default is available.

umom - Integrated horizontal *x*-component of momentum for the release (m^4/s^2) for continuous releases and (m^4/s) for instantaneous releases; exit velocity *x*-component for stack release (m/s) (REAL(4)).

vmom - Integrated horizontal *y*-component of momentum for the release (m^4/s^2) for continuous releases and (m^4/s) for instantaneous releases; exit velocity *y*-component for stack release (m/s) (REAL(4)).

wmom - Integrated vertical momentum for the release (m^4 / s^2) for continuous releases (*reltyp 'C'*) and (m^4 / s^2) for instantaneous releases (*reltyp* ' I'*)* or exit velocity (m/s) (REAL*4) for stack or area source (*reltyp 'CS'*).

buoy - Integrated buoyancy for the release (C-m^3/s) for continuous releases and (C-m^3) for instantaneous releases or exit temperature (C) (REAL*4) for stack or area source.

lognorm_mmd - The mass mean diameter of the lognormal distribution for lognormal releases (REAL*4).

lognorm_sigma - The sigma of the lognormal distribution for lognormal releases (REAL*4).

active_fraction - Should not be modified. Default is 1.

slurry_fraction - This variable is not required for this version of the code; however, it will appear if the project is created with the GUI. It is not used.

number_random - The number of copies of this release to be randomly released (INTEGER*4). Default is 1.

random_spread - The diameter over which the releases are randomly released (m) (REAL*4). Default is 0.0.

random_seed - Random generator seed value (INTEGER*4).

name_rel - Emissions file name (including path) if *reltyp* = 'CF', 'CSF', or 'CAF' (CHARACTER*256). See Section 4.2.5.9 for a description of the emissions file format. All releases should refer to the emissions file (if using).

opid - This variable is not required for this version of the code; however, it will appear if the project is created with the GUI. It is not used.

opmod - This variable is not required for this version of the code; however, it will appear if the project is created with the GUI. It is not used.

Relstatus - This variable is not required for this version of the code; however, it will appear if the project is created with the GUI. It is not used.

Multicomponent emissions - This section should start immediately after the end of the SCN NAMELIST using the keywords "#STARTMC". The section end is marked using the keywords "#ENDMC". The emission rates of the multicomponent chemical species (REAL*4) in *emission_units* specified on the *ProjectName*.IMC are listed in this section with each species on a single line. Only the species with nonzero emissions can be listed. The non-listed species are assumed to have zero emissions.

4.1.3 Meteorology Scenario File

A sample meteorology scenario file is shown in Figure 4-3. The following section describes the namelist parameters and their defaults, if available. Not all the namelist parameters are shown in the example.

```
&MET
              MET_TYPE       = 'MEDOC',
              BL_TYPE = 'MEDOC',
              ENSM_TYPE      = 'OPER3.1',
              UU_ENSM =  0.0000000E+00,
              SL_ENSM =   100000.0    ,
              ZIMIN   =   50.00000    ,
              ZIMAX   =   1000.000    ,
              HCONST  =  0.0000000E+00,
              HDIUR   =   50.00000    ,
              H_CNP   =  -1.000000    ,
              ALPHA_CNP      =  0.0000000E+00,
              ZRUF    =  2.9999999E-02,
              SL_HAZ  =   100000.0    ,
              ALBEDO  =  0.1600000    ,
              BOWEN   =  0.6000000    ,
              CLOUD_COVER    =  0.0000000E+00,
              LOCAL_MET      = F,
              NEAREST_SFC    =      65535,
              NEAREST_PRF    =      65535,
              LMC_UA  = F,
              ALPHA_MAX      =   1.000000,
              ALPHA_MIN      =  1.0000000E-03,
              MAX_ITER_AC    =        200,
              AC_EPS  =  9.9999998E-03,
              MAX_ITER       =        100,
              P_EPS   =  9.9999997E-06,
              NZB     =         23,
              ZB    =   50.00000, 150.0000, 261.4300, 385.4140, 523.1650, 675.9950, 845.3170,
             1032.650, 239.620, 1467.990, 1719.600, 1996.440, 2300.620, 2634.360,
             3000.000, 3400.000, 3892.620, 4503.540, 5266.700, 6227.120, 7444.830,
             9000.000, 11000.00, 177*0.0000000E+00,
              FILE_TER       = '',
              LOUT_MC = F,
              LOUT_MET       = F,
              TOUT_MET       = -9.9999996E+35,
              LOUT_3D = F,
              LOUT_2D = F,
              PR_TYPE = 'METFILE',
              TBIN_MET       =   3600.000,
              I_WET   =          2,
              LANDUSE = 'NOT SET',
              MCTYPE  =      17408,
              LFORMAT = F
 /
@012metfile.mcw
```

Figure 4-3
Sample SCICHEM Meteorology Scenario File

Note: The last line in the figure provides the names of the meteorological input files and must appear as shown (@NNN*filename*) for MET_TYPE = 'OBS', 'GRIDDED', or 'MEDOC'. Here NNN is a 3-digit number with leading zeros equal to the length of the filename. For MET_TYPE = 'FIXED', the last line should contain the space-separated wind direction and wind speed.

The namelist parameters are defined as follows:

met_type - Type of meteorological input, 'OBS', 'GRIDDED', 'MEDOC', 'SCIPUFF_LIST', 'WRF', or 'FIXED' (CHARACTER*80). If MET_TYPE = 'FIXED', the last line of the MSC file must contain the wind speed and direction; otherwise, the last line must contain the file names of the

meteorological input files, as shown in Figure 4-3. Detailed description for SCIPUFF_LIST is available in Section 4.5.5. No default.

bl_type - Type of boundary layer input, 'SBL', 'CALC', 'OBS', 'OPER', 'PROF', 'MEDOC', or 'NONE' (CHARACTER*80). No default.

ensm_type - Type of large-scale meteorological input, 'INPUT', 'MODEL', 'OBS', 'OPER', or 'NONE' (CHARACTER*80). No default.

uu_ensm - Velocity variance (m^2s_{-2}) for calculating the large-scale component of the dispersion (REAL*4). Used only with 'INPUT' large-scale meteorology. The default is 0.25.

sl_ensm - Length scale (meters) for calculating the meandering component of the dispersion (REAL*4). Used only with 'INPUT' or 'OBS' large-scale meteorology. The default is 10^5.

sl_haz - Length scale (meters) for calculating dispersion due to wind uncertainty given as velocity variance on observational meteorology input files (REAL*4). Not required in the current version. The default is 10^5.

zimin - Minimum daily inversion height (meters) for calculating boundary layer parameters (REAL*4). Used only with 'SBL' boundary layers. No default is available.

zimax - Maximum daily inversion height (meters) for calculating boundary layer parameters (REAL*4). Used only with 'SBL' boundary layers. No default is available.

hconst - Minimum daily surface heat flux (Wm-2) for calculating boundary layer parameters (REAL*4). Used only with 'SBL' boundary layers. No default is available.

hdiur - Maximum daily surface heat flux (Wm-2) for calculating boundary layer parameters (REAL*4). Used only with 'SBL' boundary layers. No default is available.

h_cnp - Canopy height (meters) (REAL*4). A negative value indicates no vegetative canopy. No default is available.

alpha_cnp - Canopy exponential velocity profile parameter (REAL(4)). Used only if *h_cnp* is positive. No default is available. Varies from 0 to 10.8.

zruf - Surface roughness (meters) (REAL*4). No default is available.

albedo - Fraction of incident light that is reflected by the surface (REAL*4). Used only with 'CALC' boundary layers. No default is available.

bowen - Ratio of surface sensible heat flux to latent heat flux (REAL*4). Used only with 'calculated' 'CALC' layers. No default is available.

cloud_cover - Fractional cloud cover where complete overcast is 1 and clear sky is 0 (REAL*4). Used only with 'CALC' boundary layers. No default is available. If the fractional cloud cover is provided on an observational or gridded file, this value will be ignored.

local_met - Flag specifying the reference time for the Met files (LOGICAL). If 'True', it is assumed that the times in the Met files are local times. If 'False', the times are assumed to be UTC (GMT) times.

tbin_met - Observation time bin width in seconds (REAL*4). Observations within a bin are all given the same time. The default is no time binning.

pr_type - Global precipitation type, 'LGTRAIN', 'MODRAIN', 'HVYRAIN', 'LGTSNOW', 'MODSNOW', 'HVYSNOW', or 'METFILE' (CHARACTER). When not set to 'METFILE', it will override what has been specified on the meteorological input file for either 'PRATE' or 'PRCP'.

nearest_sfc - Number of nearest surface observation stations used for meteorology interpolation (INTEGER*4). The default is all.

nearest_prf - Number of nearest upper air profile observation stations used for meteorology interpolation (INTEGER*4). The default is all.

lmc_ua - Flag to calculate a mass-consistent adjustment to the wind fields (MCWIF) (LOGICAL). This is relevant only if *met_type* is 'OBS' and a terrain file is provided. The default is 'False'.

lout_mc - Not used in the current version (LOGICAL). If the project is created with the GUI, it will appear in the MSC file. The default is 'False'.

lout_met - Flag to output the met fields in a MEDOC-type file (LOGICAL). The default is 'False'.

tout_met - Time in seconds to output met fields (REAL*4). The default is the "not set" value of -1.E+36.

lout_2D - Flag to output the 2-D fields in a MEDOC-type file (LOGICAL). The default is 'False'.

lout_3D - Flag to output the 3-D fields in a MEDOC-type file (LOGICAL). The default is 'False'.

lformat - Flag to output the adjusted wind fields in ASCII format (LOGICAL). If 'False', a binary file is created. This is relevant only if *lout_2D* and/or *lout_3D* are 'True'. The default is 'False'.

file_ter - Name of file with path containing terrain information (CHARACTER*256) used for the mass-consistent wind field adjustment if *lmc_ua* is'True'. No default is available.

*i_wet** - Surface wetness state to associate with landuse category data from file_ter (INTEGER(4)). A value of 1 implies dry, 2 implies normal, 3 implies wet. The default value is 2.

alpha_max - Maximum value of vertical adjustment parameter for MCWIF (REAL*4). This is relevant only if *lmc_ua* is 'True', a terrain file is provided, and MCWIF is invoked. The default is 1.

alpha_min - Minimum value of vertical adjustment parameter for mass-consistent wind field calculation (REAL*4). This is relevant only if *lmc_ua* is 'True', a terrain file is provided, and MCWIF is invoked. The default is 0.

max_iter_ac - Maximum number of iterations allowed for MCWIF calculation using the point relaxation method (INTEGER*4). The default is 10000.

max_iter - Maximum number of iterations allowed for MCWIF calculation using the FFT method (INTEGER*4). The default is 30.

ac_eps - Convergence criterion for MCWIF calculation using the point relaxation method (REAL*4). The default is 1.0×10^{-2}.

p_eps - Convergence criterion for MCWIF calculation using the FFT method (REAL*4). The default is 1.0×10^{-5}.

nzb - Number of vertical grid levels used for MCWIF calculation (INTEGER*4). No default is available.

zb - Vertical grid levels used for MCWIF calculation (REAL*4). There must be *nzb* levels specified. No default is available.

dt_swift - Not used (REAL*4).

lswift - Not used (LOGICAL). Must be set to 'False'.

*mctype** - Flag used by model to set landuse type. No user settings or default is available.

4.2 KEYWORDS Input Format

This section of the SCICHEM User's Guide provides a detailed reference for the KEYWORDS input options for running SCICHEM.

4.2.1 Overview

The information in this section is organized by function; that is, the keywords are grouped by pathway and are in a logical order based on their function within the model. The format is similar to that used in EPA's AERMOD model. The syntax for each keyword is provided, and the keyword type is specified—either mandatory or optional and either repeatable or non-repeatable. Unless noted otherwise, there are no special requirements for the order of keywords within each pathway, although the order in which the keywords are presented here is recommended. Any

keyword that has special requirements for its order within the pathway is so noted following the syntax and type description.

The syntax descriptions in the following sections use certain conventions. Parameters in all capital letters and underlined in the syntax description are secondary keywords that are to be entered as indicated for that keyword. Other parameters are given descriptive names to convey the meaning of the parameter and are listed with an initial capital letter. Parentheses around a parameter indicate that the parameter is optional for that keyword. The default taken when an optional parameter is left blank is explained in the discussion for that keyword.

4.2.2 Description

The keywords specify the type of option or input data being entered on each line of the input file, and the parameters following the keyword define the specific options selected or the actual input data. Some of the parameters are also input as descriptive secondary keywords. Progress messages, including certain error messages, are displayed to the standard output device, typically the screen. In particular, SCICHEM uses default settings for some parameters that are not specified. These are displayed to the screen and can be sent to a user-specified file by redirecting the output as follows:

runSCI *inputFile* > *outputFile*

where *inputFile* is the basic runSCI input file and *outputFile* is the file name for the output.

The KEYWORDS file is divided into five functional "pathways," which are identified by a two-character ID placed at the beginning of each pathway.

The pathways and the order in which they are input to the model are as follows:

1. CO - for specifying overall job COntrol options
2. MA - for specifying MAterial information
3. SO - for specifying SOurce information
4. RE - for specifying REceptor information
5. ME - for specifying MEteorology information

Each line of the input KEYWORDS file consists of a pathway ID, an 8-character keyword, and a parameter list.

4.2.2.1 Basic Rules for Structuring Input KEYWORDS Files

Although the input KEYWORDS file has been designed to provide the user with considerable flexibility in structuring the input file, some basic syntax rules need to be followed. These rules maintain some consistency between input files generated by different users, simplify the job of error handling performed by the model on the input data, and provide information to the model in the appropriate order wherever order is critical to the interpretation of the inputs. These basic rules and the various elements of the input KEYWORDS file are as follows:

- All inputs for a particular pathway must be contiguous; that is, all inputs for the CO pathway must come first, followed by the inputs for the MA pathway, if present, and so on. The beginning of each pathway is identified with a "STARTING" keyword and the ending of the

pathway with the "FINISHED" keyword. Therefore, the first functional record of each input file must be "CO STARTING".

- Each record in the input KEYWORDS file is referred to as a pathway "image." These records are initially read into the model as 1000-character images. The information on each input image consists of a "pathway," a "keyword," and one or more "parameters." Each of these "fields" on the pathway image must be separated from other fields by at least one blank space. For most keywords, the order of parameters following the keyword is important—the exact spacing of the parameters is not important, as long as they are separated from one another by at least one blank space and do not extend beyond the 1000-character limit.
- Alphabetical characters can be input as either lower case or upper case letters. The model converts all character input to upper case letters internally, except for the title fields and file names.
- For numeric input data, it should be noted that all data are assumed to be in metric units, that is, length units of kilometers (default) or meters, speed units of meters per second, temperature units of degrees Kelvin, and emission units of grams per second.
- Certain keywords are mandatory and must be present in every KEYWORDS Input file, such as the PROJECTN keyword, which identifies the geographic projection (e.g., UTM or latitude-longitude) for the SCICHEM run. Other keywords are optional and are needed only to exercise particular options, such as the option to allow for the input of flagpole receptor heights. The keyword type (mandatory or optional) for a given keyword is provided in Section 4.2.3 below. Some of the keywords are repeatable, such as the keywords to specify source parameters, while other keywords may appear only once. With a few exceptions (described next), the order of keywords within each pathway is not critical. For the SO pathway, the LOCATION keyword must be specified before other keywords for a particular source. The MULTCOMP (for multicomponents) keyword must come before the SRCPARAM keyword and is used for runs in which chemistry calculations are required (for example, for 1-hour NO_2 concentrations, secondary pollutant impacts or Class I area analysis) or for non-chemistry runs with multiple pollutants (components). It is not strictly required for single pollutant runs without chemistry, but we recommend including it in all SCICHEM projects for consistency and to avoid confusion. The MULTCOMP chemical species list applies to all sources. For non-chemistry runs, the "step_chemistry" flag can be set to false in the multicomponent file.
- Some special provisions have been made to increase the flexibility in structuring the input files. One provision is to allow for blank records in the input file. This allows the user to separate the pathways from one another or to separate a group of images, such as source locations, from the other images. Another provision is for the use of "comment lines," identified by a "**" in the pathway field. Any input image that has "**" for the pathway ID will be ignored by the model. Because of the descriptive nature of the keyword options and the flexibility of the inputs, it is generally much easier to make modifications to an existing input KEYWORDS file to obtain the desired result than to create a new KEYWORDS file and populate it. Sample KEYWORDS files provided with the tutorials can be used for this purpose.

4.2.3 Control Pathway Inputs and Options

The Control pathway contains the keywords that provide the overall control of the model run. These include the dispersion options, averaging time options, terrain height options, and others that are described next. The CO pathway must be the first pathway in the KEYWORDS input file.

4.2.3.1 Title Information

There are two keywords that allow the user to specify up to two lines of title information that will appear on each page of the main output file from the model. The first keyword, TITLEONE, is mandatory; the second keyword, TITLETWO, is optional. The syntax and type for the keywords are summarized as follows:

```
SYNTAX:  CO TITLEONE Title1
         CO TITLETWO Title2
TYPE:    TITLEONE - Mandatory, Non-repeatable
         TITLETWO - Optional, Non-repeatable
```

The parameters Title1 and Title2 are character parameters of length 80. The title information is taken as it appears in the KEYWORDS file without any conversion of lower case to upper case letters. If the TITLETWO keyword is not included in the KEYWORDS file, the second line of the title in the output file will appear blank.

4.2.3.2 Dispersion Options

The dispersion options are controlled by the MODELOPT keyword on the CO pathway. The keyword is optional and only needs to be provided to override the default dispersion options. An example of the use of this option to specify non-default dispersion options is provided below.:

```
SYNTAX:  CO MODELOPT PASSIVE DENSEGAS NOSTATIC FASTMODE
TYPE:    Optional, Non-repeatable
```

where the secondary keyword parameters are described next (the order and spacing of these parameters is not critical):

PASSIVE - Specifies that the non-default option of no momentum or buoyancy dynamics will be used.

DENSGAS - Specifies that the non-default option of dense gas effects will be used.

NOSTATIC - Specifies that the default option of quasi-steady-state calculation of continuous sources will NOT be used.

FASTMODE - Specifies that the non-default option of a coarser resolution calculation is performed with the surface grid and vertical resolution restricted.

The default option in SCICHEM includes the use of momentum and buoyancy dynamics to calculate plume rise, no dense gas effect, quasi-steady-state calculation of continuous sources, and standard (not fast) run mode. However, if the release type is ‘CSP’, that is, continuous stack

with a plume rise formula (see Section 4.1.2 and Figure 4-2), the momentum and buoyancy dynamics calculations are not performed.

4.2.3.3 Specifying the Pollutant Type

The POLLUTID keyword is not supported in SCICHEM 3.3. The Material pathway must be used instead.

4.2.3.4 Flagpole Receptor Height Option

The FLAGPOLE keyword specifies that receptor heights above local ground level (that is, flagpole receptors) are allowed on the Receptor DISCCART pathway. The FLAGPOLE keyword may also be used to specify a default flagpole receptor height other than 0.0 meters. The syntax and type of the FLAGPOLE keyword are summarized as follows:

```
Syntax:  CO FLAGPOLE (Flagdf)
Type:    Optional, Non-repeatable
```

where Flagdf is an optional parameter to specify a default flagpole receptor height. If no parameter is provided, a default flagpole receptor height of 0.0 meters is used. Any flagpole receptor heights that are entered on the Receptor pathway will override the default value but are ignored if the FLAGPOLE keyword is not present on the Control pathway, and a non-fatal warning message is generated.

4.2.3.5 Specifying Projection

The PROJECTN keyword specifies the geographic projection for the run. The syntax and type of the PROJECTN keyword are summarized as follows:

```
Syntax:  CO PROJECTN Prjctn Datum ...
TYPE:    Mandatory, Non-repeatable
```

where the Prjctn parameter is the projection code identified by one of the secondary keywords—UTM, CARTESIAN, or LONLAT—and Datum is the 3–5 letter NIMA (National Imagery and Mapping Agency) datum.

The syntax for a UTM projection is summarized as follows:

```
Syntax:  CO PROJECTN UTM WGS84 ZONE HEM KM
```

where only WGS84 and NAD83 datums are supported, the Zone parameter is the UTM zone from 1 to 60, Hem is the Hemisphere (N or S), and Units is the horizontal distance units are in METERS and KILOMETERS.

The syntax for a CARTESIAN projection is summarized as follows:

```
Syntax:  CO PROJECTN CARTESIAN Datum Lonref Latref Xref Yref Units
```

where the Lonref and Latref parameters are the reference (origin) longitude and latitude, Xref and Yref are the reference X and Y coordinates (false easting and northing), and Units is the horizontal distance units in KILOMETERS or METERS.

The syntax for a LONLAT projection is summarized as follows:

```
Syntax:  CO PROJECTN LONLAT Datum (Units)
```

where the optional Units parameter is the horizontal distance units in DEGREES.

Following are examples of valid projections:

```
CO PROJECTN UTM WGS84 15 N KILOMETERS
CO PROJECTN CARTESIAN WGE -88.5426 44.0247 0 0 KILOMETERS
CO PROJECTN LONLAT WGC DEGREES
```

4.2.3.6 Specifying the Computational Domain

The DOMAIN keyword specifies the computational domain for the run. The syntax and type of the DOMAIN keyword are summarized as follows:

```
Syntax:  CO DOMAIN  Xmin Xmax Ymin Ymax Zmax
Type:    Optional/Mandatory, Non-repeatable
```

Following are examples of valid domain specifications:

```
** UTM domain
CO DOMAIN  559.08 562.08 4823.351 4826.351 2000.


** CARTESIAN domain
CO DOMAIN 0 292 0 292 4000


** LATLON domain
CO DOMAIN -101.00    -99.50     37.00     38.50 5000
```

The DOMAIN must be set if the terrain or meteorology domain is not available from the terrain or meteorology gridded file. If both the terrain or meteorology gridded domain and the project domain are specified and they do not match, the project domain is adjusted to the overlap region.

4.2.3.7 Specifying a Data Period to Process

The STARTEND keyword controls which period within the meteorological data file is read by the model. The keyword is optional and the default for the model if the keyword is not specified is to read the entire meteorological data file (up to a full year) and process all days within that period.

The syntax and type for the STARTEND keyword are summarized as follows:

```
Syntax:  CO STARTEND Strtyr Strtmn Strtdy (Strthr) (Strtmn) (Strtsc) Endyr
Endmn Enddy (Endhr) (Endmn) (Endsc)
Type:    Optional, Non-repeatable
```

where the Strtyr Strtmn Strtdy parameters specify the year, month, and day of the first record to be read (for example, 87 01 31 for January 31, 1987) and the parameters Endyr Endmn Enddy specify the year, month, and day of the last record to be read. The Strthr Strtmn Strtsc and Endhr Endmn Endsc are optional parameters that may be used to specify the start and end times for the

data period to be read. If either Strthr or Endhr is to be specified, both must be specified. Any records in the data file that occur before the start date are ignored, as are any records in the data file that occur after the end date. If Strthr and Endhr are not specified, processing begins with hour 0 of the start date and ends with hour 23 of the end date. If Strtmn and Endmn are not specified, processing begins with minute 0 of the start date and ends with minute 59 of the end date. If Strtsc and Endsc are not specified, processing begins with second 0 of the start date and ends with second 59 of the end date. Note that the minute and second parameters may not be necessary when using AERMET-derived meteorological data.

4.2.3.8 Specifying a Time Zone

The TIMEZONE keyword specifies the time zone of the SCICHEM scenario location. The syntax and type for the TIMEZONE keyword are summarized as follows:

```
Syntax:  CO TIMEZONE Offset
Type:    OPTIONAL, Non-repeatable
```

where the Offset parameter is the offset in hours from Coordinated Universal Time (UTC).

The following example sets the input scenario location time zone to Eastern Time (United States and Canada):

```
CO TIMEZONE -5
```

Alternatively, the LT_00UTC keyword can be used to specify the local time of midnight UTC; SCICHEM then computes the time zone offset internally. The syntax and type for the LT_00UTC keyword are summarized as follows:

```
Syntax:  CO LT_00UTC time
Type:    OPTIONAL, Non-repeatable
```

where the time parameter is the local time in hours corresponding to midnight in UTC or the offset in hours from UTC.

The following example sets the input scenario location time zone to Eastern Time (United States and Canada):

```
CO LT_00UTC 19
or
CO LT_00UTC -5
```

Both the TIMEZONE and LT_00UTC keywords are optional. The default if these options are not specified is to use UTC.

4.2.3.9 Specifying Maximum Time Step

The optional MAXTSTEP keyword specifies the maximum time step for the puff calculations. The syntax and type of the MAXTSTEP keyword are summarized as follows:

```
Syntax:  CO MAXTSTEP Maxstp
Type:    Optional, Non-repeatable
```

where Maxstp is the maximum time step in seconds. The default value if the keyword is not specified is 900 (15 minutes).

4.2.3.10 Specifying Output Interval

The optional OUTPTINT keyword specifies the output interval for the binary puff output and surface dosage and deposition files. The syntax and type of the OUTPTINT keyword are summarized as follows:

```
Syntax:  CO OUTPTINT Outint
Type:    Optional, Non-repeatable
```

where Outint is the output interval in seconds. The default value if the keyword is not specified is 3600 (1 hour).

4.2.3.11 Specifying Maximum Puffs

The optional MAXPUFFS keyword specifies the maximum puffs for the run—the default is 20,000 or as set in the SCIPUFF.ini file (see Section 2.2.1) . Input here supersedes the value set in SCIPUFF.ini. The syntax and type of the MAXPUFFS keyword are summarized as follows:

```
Syntax:  CO MAXPUFFS Maxpuf
Type:    Optional, Non-repeatable
```

where Maxpuf is the maximum number of puffs.

4.2.3.12 Specifying Horizontal Resolution

The optional HORIZRES keyword specifies the horizontal resolution of the domain used in the puff calculations. There is no default value, but it is only required in the absence of gridded meteorological or terrain input. The syntax and type of the HORIZRES keyword are summarized as follows:

```
Syntax:  CO HORIZRES Hrzres
Type:    Optional, Non-repeatable
```

where Hrzres is the horizontal resolution in the units of the domain (that is, kilometers, meters, degrees).

4.2.3.13 Specifying Vertical Resolution

The optional VERTIRES keyword specifies the vertical resolution of the domain used in the puff calculations. The default is 250 meters. The syntax and type of the VERTIRES keyword are summarized as follows:

```
Syntax:  CO VERTIRES Vrtres
Type:    Optional, Non-repeatable
```

where Vrtres is the vertical resolution in meters.

4.2.3.14 Building Downwash Option

Building downwash in SCICHEM is based on PRIME (Schulman et al., 2000). PRIME has not been updated in over 15 years and has been shown to overpredict concentrations by factors of 2 to 8 for certain building types (Petersen et al., 2017). New treatments for building downwash are

being developed (Petersen et al., 2017), and it is anticipated that future releases of SCICHEM will include these improvements. Therefore, **the current default in SCICHEM is to ignore building downwash effects (RUNPRIME = N).** However, if the user wishes to activate the building downwash option for point sources, he or she can do so by setting RUNPRIME to Y and providing the building dimensions from the Building Profile Input Program (BPIP) output in the SO section. See Section 4.2.5.4, Source Pathway, for details.

```
Syntax:  CO RUNPRIME Y
Type:    Optional, Non-repeatable
```

The implementation of building downwash in SCICHEM 3.3 has been updated to address large over-predictions noted by model users working with SCICHEM 3.2.2. These updates include bug fixes as well as changes to the downwash treatment in previous versions (SCICHEM 3.2 and earlier).

4.2.4 Material Pathway Inputs and Options

The mandatory MAterial pathway contains the keywords that define the material (pollutant) information for a particular model run and must precede the SOurce pathway. Multiple materials can be defined for a single run and applied to different sources. SCICHEM currently handles two classes of materials: gases or particles. The input parameters vary depending on the material class.

4.2.4.1 Specifying Material Types

The MATCLASS keyword is used to identify the material class of each material to be modeled. The MATCLASS card must be the first card entered for each material because it identifies the material class and dictates which parameters are needed and/or accepted. The syntax, type, and order of the MATCLASS keyword are summarized as follows:

```
Syntax:  MA MATCLASS Matid Matcls
Type:    Optional, Repeatable
Order:   Must be first card for each material input
```

where the Matid parameter is the alphanumeric material ID defined by the user (up to 8 characters), and Matcls is the material class, which is identified by one of the secondary keywords: GAS or PART. The GAS material keyword is used to specify a gaseous material. The PART material keyword is used to specify a particle material.

The material ID entered on the MATCLASS card identifies that material for the remainder of the MA pathway inputs. Because the model accepts alphanumeric strings of up to 8 characters for the material ID, the material can be identified with descriptive names, such as SO_2, XYLENE, CHLORINE, and so on. For particle materials, the material ID should be either PM2.5 or PM10, depending on the primary particle species of interest. No other particle species names are allowed in this version of SCICHEM. Note that this applies only to the tracer material—multiple species, including PM components, can be specified in multicomponent simulations as discussed in Section 4.3.

The DESCRPTN keyword provides for a detailed description of the material. The syntax, type, and order of the DESCRPTN keyword are summarized as follows:

```
Syntax:  MA MATCLASS Matid Matdes
Type:    Optional, Repeatable
Order:   Must follow the MATCLASS card for each material input
```

where the Matid parameter is the alphanumeric material ID and Matdes is the material description contained in quotes.

4.2.4.2 Specifying Material Parameters

The material parameters are input on various Material cards. Most apply to either gas or particle materials.

The DENSITY keyword is used to define the material density. It is optional but should be included for dense gases and particle materials (which otherwise have an assumed density of 500 kg/m^3). The syntax, type, and order of the DENSITY keyword are summarized below:

```
Syntax:  MA DENSITY Matid Matden
Type:    Optional, Repeatable
Order:   Must follow the MATCLASS card for each material input
```

where the Matid parameter is the alphanumeric material ID and Matden is the material density in kg/m^3.

The GASDEPOS keyword is used to define the material gas deposition velocity (and is ignored for particle materials). The GASDEPOS keyword is mandatory for gas deposition. Note that the specification of dry deposition velocity is applicable to the tracer material. For multicomponent species, dry deposition velocities are specified in the multicomponent input file. While the multicomponent file is typically used for chemistry simulations, we recommend using this option even for non-chemistry simulations. For a non-chemistry simulation, the chemistry flag can be set to false in the multicomponent file. The syntax, type, and order of the GASDEPOS keyword are summarized as follows:

```
Syntax:  MA GASDEPOS Matid Matgdv
Type:    Mandatory for gas deposition, Repeatable
Order:   Must follow the MATCLASS card for each material input
```

where the Matid parameter is the alphanumeric material ID and Matgdv is the material gas deposition velocity in m/s.

The DECAYAMP and DECAYMIN keywords are used to define the material daytime and nighttime decay rate, respectively. The DECAYAMP and DECAYMIN keywords are optional. The syntax, type, and order of the DECAYAMP and DECAYMIN keywords are summarized as follows:

```
Syntax:  MA DECAYAMP Matid Matdcy
Syntax:  MA DECAYMIN Matid Matdcy
Type:    Optional, Repeatable
Order:   Must follow the MATCLASS card for each material input
```

where the Matid parameter is the alphanumeric material ID and Matdcy is the material decay rate in s^{-1}.

Following is an example of a valid gaseous material:

```
MA MATCLASS  MAT1 GAS
MA DESCRPTN  MAT1 "1,3,5-Trimethylbenzene"
MA DENSITY   MAT1 1.2
```

where the material ID is MAT1, the description is 1,3,5-Trimethylbenzene, and the density is 1.2 kg/m^3.

As discussed previously, for multicomponent simulations (calculations with chemistry), the IMCFILE keyword is used to give the file name that contains information on the chemical species, their units, chemistry options, deposition velocities, and chemical reactions. This must be defined as part of a gaseous material. SCICHEM 3.3 allows the option of using a multicomponent file for non-chemistry simulations as well by including a flag to determine if chemistry calculations are performed or not.

4.2.5 Source Pathway Inputs and Options

The Source Pathway contains the keywords that define the source information for a particular model run. The model currently handles three source types, identified as point, volume, and area sources. The input parameters vary depending on the source type. The user can also identify groups of sources for which the model will combine the results.

The LOCATION keyword, which identifies the source type and location, must be the first card entered for each source. The optional keyword MULTCOMP must come before SRCPARAM is specified. The only other requirement for the order of the keywords is that the SRCGROUP keyword must be the last keyword before the SO FINISHED card. The user may group all the LOCATION cards together, then group the source parameter cards together—or he or she may want to group all input cards for a particular source together. All sources are given a source ID by the user, which is used to link the source parameter inputs to the correct source or sources. The source ID can be any alphanumeric string of up to 8 characters.

4.2.5.1 Identifying Source Types and Locations

The mandatory LOCATION keyword is used to identify the source type and the location of each source to be modeled. The LOCATION card must be the first card entered for each source because it identifies the source type and dictates which parameters are needed and/or accepted. The syntax, type, and order of the LOCATION keyword are summarized as follows:

```
Syntax:  SO LOCATION Srcid Srctyp Xs Ys
Type:    Mandatory, Repeatable
Order:   Must be first card for each source input
```

where the Srcid parameter is the alphanumeric source ID defined by the user (up to 8 characters), Srctyp is the source type, which is identified by one of the secondary keywords—POINT, VOLUME, AREA, or AREACIRC—and Xs and Ys are the x and y coordinates of the source location in the units defined on the CO PROJECTN keyword.

The source ID entered on the LOCATION card identifies that source for the remainder of the SO pathway inputs. Because the model accepts alphanumeric strings of up to 8 characters for the source ID, the sources can be identified with descriptive names, such as STACK1, STACK2, BOILER3, SLAGPILE, and so on.

The MATERIAL keyword identifies the material, defined in the MAterial pathway, to be modeled by each source. The LOCATION card must be the first card entered for each source because it identifies the source type and dictates which parameters are needed and/or accepted. The syntax, type, and order of the MATERIAL keyword are summarized as follows:

```
Syntax:  SO MATERIAL Srcid Matid
Type:    Mandatory when using MAterial pathway, Repeatable
Order:   Must follow the LOCATION card for each source input
```

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source and Matid is a material ID present in the MAterial pathway.

4.2.5.2 Specifying Multicomponent Releases

The MULTCOMP keyword is used to specify multicomponent species. This card must follow all LOCATION cards and precede all SRCPARAM cards. The list of species applies to all sources. Species names must match those in the SCIPUFF multicomponent/chemistry reaction file provided with the MA IMCFILE keyword.

```
Syntax:  SO MULTCOMP species1, species2, …
Type:    Optional, Non-repeatable
Order:   Must follow all LOCATION cards and precede all SRCPARAM cards
```

4.2.5.3 Specifying Source Release Parameters

The main source parameters are input on the SRCPARAM card, which is a mandatory keyword for each source being modeled. Because the input parameters vary depending on the source type, the different source types handled by the SCICHEM model are discussed separately. Note that the buoyancy and vertical momentum defined with a POINT source, and optionally for a VOLUME source, must be carried by a gaseous material. Therefore, if a particle material is to be released from a source with buoyancy and momentum, a co-located gaseous source must also be defined. (Buoyancy and momentum from a particle source are ignored.)

4.2.5.4 POINT Source Inputs

The SCICHEM POINT source algorithms are used to model releases from stacks and isolated vents, as well as other kinds of sources. The syntax, type, and order for the SRCPARAM card for POINT sources are summarized next, where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source and the other parameters are as follows:

```
Syntax:  SO SRCPARAM Srcid Ptemis Stkhgt Stktmp Stkvel Stkdia [Spemis …]
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

Ptemis - point emission rate in g/s
Stkhgt - release height above ground in meters
Stktmp - stack gas exit temperature in degrees K
Stkvel - stack gas exit velocity in m/s
Stkdia - stack inside diameter in meters
Spemis - emission rates for species listed in MULTCOMP card in g/s

The following is an example of a valid SRCPARAM input card for a point source:

```
SO SRCPARAM STACK1 16.71 35.0 444.0 22.7 2.74
```

where the source ID is STACK1, the emission rate is 16.71 g/s, the release height is 35.0 m, the exit temperature is 444.0 K, the exit velocity is 22.7 m/s, and the inside stack diameter is 2.74 m. All the parameters must be present on the input card.

Because SCICHEM uses direction-specific building dimensions for all sources subject to building downwash, there are no building parameters entered on the SRCPARAM card. Building dimensions are entered on the BUILDHGT, BUILDWID, BUILDLEN, XBADJ, and YBADJ cards described next.

Specifying Building Downwash Information

As noted, SCICHEM includes algorithms to model the effects of building downwash on emissions from nearby or adjacent point sources using the PRIME model (Schulman et al., 1997). The building downwash algorithms do not apply to volume or area sources. For a technical description of the building downwash algorithms in SCICHEM, the user is referred to Schulman et al. (2000). SCICHEM uses direction-specific information for all building downwash cases.

Note: PRIME has not been updated in over 15 years and has been shown to overpredict concentrations by factors of 2 to 8 for certain building types (Petersen et al., 2017). New treatments for building downwash are being developed (Petersen et al., 2017), and it is anticipated that future releases of SCICHEM will include these improvements. Therefore, the current default in SCICHEM is to ignore building downwash effects (RUNPRIME = N). However, if the user wishes to activate the building downwash option, he or she can do so by setting RUNPRIME to Y as described previously in Section 4.2.3.14.

Five keywords are used to specify building downwash information: BUILDHGT, BUILDWID, BUILDLEN, XBADJ, and YBADJ. This information is based on output from BPIP and is only used if RUNPRIME = Y. The syntax, type, and order for the BUILDHGT keyword, used to input direction-specific building heights, are summarized next; the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source. The user also has the option of specifying a range of sources (the Srcrng parameter) for which the building heights apply rather than identifying a single source. This is accomplished by two source ID character strings separated by a dash, for example, STACK1-STACK10. Because the model reads the source range as a single input field, there must not be any spaces between the source IDs. The model then places the building heights that follow (the Dsbh(i) parameter) into the appropriate arrays for all Srcid's that fall within that range, including STACK1 and STACK10.

```
Syntax:  SO BUILDHGT Srcid (or Srcrng) Dsbh(i),i=1,36 (16 for LT)
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

When comparing a source ID to the range limits for a Srcrng parameter, the model separates the source IDs into three parts: an initial alphabetical part, a numerical part, and the remainder of the string. Each part is then compared to the corresponding parts of the source range, and all three parts must satisfy the respective ranges for the source ID to be included. If there is no numeric part, the ID consists of only one alphabetical part. If the ID begins with a numeric character, the initial alphabetical part defaults to a single blank. If there is no trailing alphabetical part, the third part also defaults to a single blank part. If the trailing part consists of more than one alphabetical or numeric field, it is all lumped into one character field. For example, the source ID 'STACK2' consists of the parts 'STACK' plus '2' plus a single trailing blank, ' '. By comparing the separate parts of the source IDs, it can be seen that STACK2 falls between the range 'STACK1-STACK10.' For a three-part example, it can also be seen that VENT1B falls within the range of VENT1A-VENT1C. However, VENT2 does not fall within the range of VENT1A to VENT3B, because the third part of VENT2 is a single blank, which does not fall within the range of A to C. This is because a blank character will precede a normal alphabetical character.

Normally, the source ranges will work as one would intuitively expect for simple source names. Most importantly, for names made up entirely of numeric characters, the source ranges will be based simply on the relative numerical values. The user is strongly encouraged to check the summary of model inputs to ensure that the source ranges were interpreted as expected and to avoid using complex source names in ranges, such as AA1B2C-AB3A3C. Because the order of keywords within the SO pathway is flexible, it is also important to note that the building heights will be applied only to those sources that have been defined previously in the input file.

Following the Srcid or the Srcrng parameter, the user inputs 36 direction-specific building heights (Dsbh parameter) in meters, beginning with the 10-degree flow vector (wind blowing toward 10 degrees from north) and incrementing by 10 degrees in a clockwise direction. Some examples of building height inputs are as follows:

```
SO BUILDHGT STACK1 34. 34. 34. 34. 34. 34. 34. 34. 34. 34. 34. 34.
SO BUILDHGT STACK1 34. 34. 34. 34. 34. 34. 34. 34. 34. 34. 34. 34.
SO BUILDHGT STACK1 34. 34. 34. 34. 34. 34. 34. 34. 34. 34. 34. 34.
SO BUILDHGT STACK1 36*34.0
SO BUILDHGT STACK1-STACK10 33*34.0 3*0.0
SO BUILDHGT STACK1 35.43 36.45 36.37 35.18 32.92 29.66 25.50 20.56
SO BUILDHGT STACK1 15.00 20.56 25.50 29.66 32.92 35.18 36.37 36.45
SO BUILDHGT STACK1 35.43 33.33 35.43 36.45 0.00 35.18 32.92 29.66
SO BUILDHGT STACK1 25.50 20.56 15.00 20.56 25.50 29.66 32.92 35.18
SO BUILDHGT STACK1 36.37 36.45 35.43 33.33
```

The first example illustrates the use of repeat cards if more than one card is needed to input all the values. The values are processed in the order in which they appear in the input file and are identified as being repeat cards by repeating the Srcid parameter. The first and second examples produce identical results within the model. The second one illustrates the use of a repeat value that can simplify numerical input in some cases. The field "36*34.0" is interpreted by the model

as “repeat the value 34.0 a total of 36 times.” This is also used in the third example in which the building height is constant for directions of 10 degrees through 330 degrees and then is set to 0.0 (for example, the stack may be outside the region of downwash influence) for directions 340 through 360. The third example also uses a source range rather than a single source ID. The last example illustrates building heights that vary by direction and shows that the number of values on each card need not be the same as long as the total number of values equals 36. For improved readability of the input file, the user may want to put the numerical inputs into “columns,” but there are no special rules regarding the spacing of the parameters on this keyword.

The BUILDWID keyword is used to input direction-specific building widths for downwash analyses. The syntax for this keyword, which is similar to the BUILDHGT keyword, is summarized next, along with the type and order information. For a description of the Srcid and Srcrng parameters and a discussion and examples of the numeric input options, refer to the BUILDHGT keyword above. The Dsbw(i) parameter contains the 36 direction-specific building widths. The directions proceed in a clockwise direction, beginning with the 10-degree flow vector.

```
Syntax:  SO BUILDWID Srcid (or Srcrng) Dsbw(i),i=1,36 (16 for LT)
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

The BUILDLEN keyword is used to input direction-specific along-flow building lengths for downwash analyses. The syntax for this keyword, which is similar to the BUILDHGT keyword, is summarized as follows, along with the type and order information:

```
Syntax:  SO BUILDLEN Srcid (or Srcrng) Dsbl(i),i=1,36
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

For a description of the Srcid and Srcrng parameters and a discussion and examples of the numeric input options, refer to the BUILDHGT keyword above. The Dsbl(i) parameter contains the 36 direction-specific building lengths. The directions proceed in a clockwise direction, beginning with the 10-degree flow vector.

The XBADJ and YBADJ keywords are used to input direction-specific along-flow and

across-flow distances from the stack to the center of the upwind face of the projected building, respectively. The syntax for these keywords, which is similar to the BUILDHGT keyword, is summarized next, along with the type and order information. For a description of the Srcid and Srcrng parameters, refer to the BUILDHGT keyword above. The Xbadj(i) parameter contains the 36 direction-specific along-flow distances from the stack to the center of the upwind face, and the Ybadj(i) parameter contains the 36 direction-specific across-flow distances from the stack to the center of the upwind face. The directions proceed in a clockwise direction, beginning with the 10-degree flow vector.

```
Syntax:  SO XBADJ Srcid (or Srcrng) Xbadj(i),i=1,36
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
Syntax:  SO YBADJ Srcid (or Srcrng) Ybadj(i),i=1,36
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

4.2.5.5 Volume Source Inputs

The SCICHEM VOLUME source algorithms are used to model releases from a variety of industrial sources, such as building roof monitors, multiple vents, and conveyor belts. The syntax, type, and order for the SRCPARAM card for VOLUME sources are summarized as follows:

```
Syntax:  SO SRCPARAM Srcid Vlemis Relhgt Syinit Szinit
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source, and the other parameters are as follows:

Vlemis - volume emission rate in g/s
Relhgt - release height (center of volume) above ground, in meters
Syinit - initial lateral dimension of the volume in meters
Szinit - initial vertical dimension of the volume in meters

4.2.5.6 Area Source Inputs

The SCICHEM area source option is used to model low-level or ground-level releases with no plume rise, for example, storage piles, slag dumps, and lagoons. (But note that the AREA source can be defined with vertical momentum and buoyance using the namelist format.)

The SCICHEM model includes two options for specifying the shape of an area source: the AREA source type may be used to specify rectangular areas that may also have a rotation angle specified relative to a north-south orientation; the AREACIRC source keyword may be used to specify a circular-shaped area source. The source parameter inputs for each of the area source types are described next.

4.2.5.7 AREA Source Type

The rotation angle for rectangular AREA sources is specified relative to the vertex used to define the source location on the SO LOCATION card (for example, the southwest corner). The syntax, type, and order for the SRCPARAM card for AREA sources are summarized as follows:

```
Syntax:  SO SRCPARAM Srcid Aremis Relhgt Xinit Yinit Angle
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source, and the other parameters are as follows:

Aremis - area emission rate in g/(s-m^2)
Relhgt - release height above ground in meters
Xinit - length along X-axis of the rectangular area source (in the east-west direction if Angle is 0 degrees) in meters
Yinit - length along the Y-axis of the rectangular area source (in the north-south direction if Angle is 0 degrees) in meters
Angle - orientation angle for the rectangular area source in degrees from east, measured positive in the counterclockwise direction

It should be noted that the emission rate for the area source is actually an emissions flux, that is, an emission rate per unit area. This is different from the specification of point and volume source emission rates, which represent total emission rates for the source.

If the Angle parameter does not equal 0, the model will rotate the area counterclockwise around the center of the area (Xs and Ys given on the SO LOCATION card for this source). The Angle parameter may be positive (for counterclockwise rotation) or negative (for clockwise rotation), and a warning message is generated if the absolute value of Angle is greater than 180 degrees (although all configurations are described within ±90°).

The following is an example of a valid SRCPARAM input card for a rectangular area source:

```
SO SRCPARAM SLAGPILE 0.0015 5.0 50.0 100.0 30.0
```

where the source ID is SLAGPILE, the emission rate is 0.0015 g/(s-m^2), the release height is 5.0 m, the X-dimension is 50.0 m, the Y-dimension is 100.0 m, and the orientation angle is 30.0 degrees counterclockwise.

4.2.5.8 AREACIRC Source Type

The AREACIRC source type may be used to specify an area source as a circular shape. The syntax, type, and order for the SRCPARAM card for AREACIRC sources are summarized as follows:

```
Syntax: SO SRCPARAM Srcid Aremis Relhgt Radius
Type: Optional, Repeatable
Order: Must follow the LOCATION card for each source input
```

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source, and the other parameters are as follows:

Aremis - area emission rate in g/(s-m^2)
Relhgt - release height above ground in meters
Radius - radius of the circular area in meters

As with AREA sources, the emission rate for the source is an emission rate per unit area, which is different from the point and volume source emission rates, which are total emissions for the source.

4.2.5.9 Specifying an Hourly Emission Rate File

The source (SO) pathway includes an option for inputting hourly emission rates for the SCICHEM model, controlled by the HOUREMIS keyword. SCICHEM currently allows for a

single hourly emission file to be used with each model run. The syntax, type, and order for this keyword are summarized as follows:

```
Syntax:  SO HOUREMIS Emifil Srcid's (and/or Srcrng's)
Type:    Optional, Repeatable
Order:   Must follow the LOCATION card for each source input
```

where the Emifil parameter is a character field of up to 200 characters, in quotes, that identifies the hourly emission file and Srcid or Srcrng identifies the source or sources for which hourly emission rates are included. It is also possible to input a range of sources by specifying the first and last source IDs separated by a dash, for example, STACK1-STACK10. The user may include more than one HOUREMIS card in a KEYWORDS file to specify additional sources if needed, but there can be only one hourly emissions file—therefore, the filename must be the same on all HOUREMIS cards.

The format of each record of the hourly emissions file includes a pathway and keyword (SO HOUREMIS), followed by the Year, Month, Day, Hour, Source ID, and emission rate (in the appropriate units). For point sources, the stack gas exit temperature (K) and stack gas exit velocity (m/s) are also specified. The hourly emissions file is processed using the same routines used to process the KEYWORDS input file; therefore, each of the parameters must be separated by at least one space, but otherwise the format is flexible. It is also not necessary to include the SO HOUREMIS on each line as long as the parameters (Year, Month, and so on) do not begin before column 13. If MULTCOMP was specified to simulate chemically reactive species, the emission rates of emitted chemical species must be given for all sources following the gas exit velocity.

The data in the hourly emission file must include the exact same dates as are included in the meteorological input files, and the source IDs must correspond to the source IDs defined on the SO LOCATION cards and be in the same order. Multiple records are required to define the emissions for 1 hour if more than one source is referenced. The model will check for a date mismatch between the hourly emissions file and the meteorological data and for a source ID mismatch. However, it is not necessary to process the entire hourly emissions file on each model run; that is, the correct emissions data will be read if the ME STARTEND card is used, as long as all the dates (including those that are processed and those that are skipped) match the meteorological data files. An example of several lines from an hourly emissions file for two point sources is provided below:

```
SO HOUREMIS 88 8 16 1 STACK1 52.467 382.604 12.27
SO HOUREMIS 88 8 16 1 STACK2 44.327 432.326 22.17
SO HOUREMIS 88 8 16 2 STACK1 22.321 377.882 9.27
SO HOUREMIS 88 8 16 2 STACK2 42.166 437.682 19.67
SO HOUREMIS 88 8 16 3 STACK1 51.499 373.716 11.87
SO HOUREMIS 88 8 16 3 STACK2 41.349 437.276 18.77
SO HOUREMIS 88 8 16 4 STACK1 36.020 374.827 9.63
SO HOUREMIS 88 8 16 4 STACK2 43.672 437.682 18.23
```

The model will use the stack release height and stack inside diameter defined on the SO SRCPARAM card but will use the emission rate, exit temperature, and exit velocity from the hourly emission file. If the emission rate, exit temperature, and exit velocity are not included for

a particular hour—that is, any or all of those fields are blank—the model will interpret emissions data for that hour as missing and will set the parameters to zero. Because the emission rate will be zero, no calculations will be made for that hour or that source.

4.2.6 Receptor Pathway Inputs and Options

The optional REceptor pathway contains keywords that define the receptor information for a particular model run. The RE pathway contains keywords that allow the user to define Cartesian grid receptor networks as well as discrete receptor locations referenced to a Cartesian system. Alternatively, a file containing the receptor locations may be specified.

Note that, for surface receptors and time-averaged concentrations, it is recommended to minimize the number of receptors in the REceptor pathway (or eliminate the RE pathway, because no receptors are required) and instead calculate surface concentrations as a post-processing step using the supplied post-processor SciDOSPost. This will result in faster SCICHEM runtimes. This recommendation is applicable to either of the gridded or discrete receptor options discussed next.

4.2.6.1 Defining Networks of Gridded Receptors

A Cartesian grid network, defined through the GRIDCART keyword, includes an array of points identified by their x (east-west) and y (north-south) coordinates. This GRIDCART keyword has a secondary keyword XYINC that is used to define the network. The GRIDCART keyword can be thought of as a "sub-pathway," because its secondary keywords include a STA and an END card to define the start and end of inputs for a particular network.

The syntax and type of the GRIDCART keyword are summarized as follows:

```
Syntax:  RE GRIDCART Netid STA
         RE GRIDCART Netid XYINC Xinit Xnum Xdelta Yinit Ynum Ydelta

         RE GRIDCART Netid END
Type:    Optional, Repeatable
```

where the parameters are defined as follows:

Netid - Receptor network identification code (up to 8 alphanumeric characters).

STA - Indicates the STArt of GRIDCART inputs for a particular network, repeated for each new Netid.

XYINC - Keyword identifying uniform grid network generated from x and y increments.

Xinit - Starting x-axis grid location in meters
Xnum - Number of x-axis receptors
Xdelta - Spacing in meters between x-axis receptors
Yinit - Starting y-axis grid location in meters
Ynum - Number of y-axis receptors
Ydelta - Spacing in meters between y-axis receptors

END - Indicates the END of GRIDCART inputs for a particular network, repeated for each new Netid.

Note that the receptor heights are set to the flagpole height defined in the CO pathway. (Zero is used if no flagpole height is set..

Below is an example setting up a 9 x 5 Cartesian grid network:

```
RE GRIDCART CAR1 STA
RE GRIDCART CAR1 XYINC  -400  9  100  -400  5  200
RE GRIDCART CAR1 END
```

4.2.6.3 Specifying Discrete Receptor Locations

In addition to the receptor networks defined by the GRIDCART keyword described previously, the user may also specify discrete receptor points for modeling impacts at specific locations of interest. This may be used to model critical receptors, such as the locations of schools or houses, near Class I areas, or locations identified as having high concentrations by previous modeling analyses. The discrete receptors must be input as Cartesian x, y points (DISCCART keyword).

Discrete Cartesian Receptors

Discrete Cartesian receptors are defined by use of the DISCCART keyword. The syntax and type of this keyword are summarized as follows:

```
Syntax:  RE DISCCART Xcoord Ycoord (Zflag)
Type:    Optional, Repeatable
```

where the Xcoord and Ycoord parameters are the x-coordinate and y-coordinate (km, m), respectively, for the receptor location. The Zflag parameter is the optional receptor height above ground (m) for modeling flagpole receptors.

If the flagpole receptor height option (CO FLAGPOLE) is not used, the optional parameter is ignored if present. The default value for Zflag is defined by the CO FLAGPOLE card.

4.2.6.4 Receptor Output Time Interval

In this version, the instantaneous concentrations at the receptors of interest are output at intervals corresponding to the maximum puff time step. The default value of this maximum puff time step is 900 seconds, as noted in Section 4.2.3.9. Time-averaged values at the receptors can be output by specifying a sampler location file with AVERAGE header as described in Section 4.4 with the SAMPFILE keyword. The syntax of this keyword is summarized as follows:

```
Syntax:  RE SAMPFILE FILENAME.SAM
Type:    Optional
```

4.2.6.5 Multicomponent Species Output

In a multicomponent run with or without chemistry, all multicomponent species are printed by default at the interval described in Section 4.2.6.4. However, the user can override this and select specific multicomponent species by using the MULTLIST keyword to specify the list of species

to be printed. In the following example, this keyword is used to specify that only NO_2 and NO concentrations should be output:

Syntax: RE MULTLIST (NO_2, NO)

Type: Optional

4.2.6.5 Receptor File

As described in Section 4.4, a file defining receptor locations and species can specified. As noted in 4.2.6.4, this file also allows for the specification of output intervals and/or averaging time.

```
Syntax:  RE SAMPFILE FILENAME.SAM
Type:    Optional
```

4.2.7 Meteorology Pathway Inputs and Options

The mandatory MEteorology pathway contains keywords that define the input meteorological data for a particular model run. Many of the keywords are the same as those used in AERMOD; others are used to provide input similar to that given using namelist input as described in Section 4.1.3.

The SCICHEM model uses meteorological data in various formats. The input meteorological data filenames for SCICHEM are specified along with various keywords describing the file type and other relevant data. These are given in Table 4-1. The syntax and type for this keyword are summarized as follows:

```
Syntax:  ME Mettyp [Metid] Metfile [Metfile2] [lat lon]
Type:    Mandatory, Repeatable
```

where the Mettyp parameter is the met type keyword and the Metfile parameter is a character field of up to 200 characters, in quotes, that identifies the filename for the input meteorological data file. To run the model on an IBM-compatible PC, the filename parameters may include the complete DOS pathname for the file or will assume the current directory if only the filename is given. For AERMET-style files, the alphanumeric meteorology station ID must be given before the file name. These also require additional keyword input for specifying station information. If METFILE is specified, the Metid must be set to MEDOC. The optional input of a second file METFILE2 and optional input of location apply only to ASOS1MIN Mettype input.

Although SCICHEM can directly use certain types of AERMET files, it is recommended that the supplied processor, METSCI, be used to create input files in standard SCICHEM format (SCISRF and SCIPRF file types in Table 4-1). METSCI reads the same input files as AERMET to create SCISRF and SCIPRF type files.

Table 4-1
SCICHEM ME Pathway Input File Types

Mettype Keyword	File Type Description
SURFILE	AERMET surface file. Requires station ID.
PROFILE	AERMET profile file. Requires station ID.
ASOS1MIN	ASOS 1 minute surface data.
SCISRF	'SURFACE' observation file. See Section 4.5.1.
SCIPRF	'PROFILE' observation file. See Section 4.5.1.
METFILE	MEDOC gridded meteorology file or list of files (see Sections 4.5.2 and 4.5.5). Must be followed by MEDOC or .MEDOC_LIST
SCILIST	Meteorology list file. See Section 4.5.4.

4.2.7.1 Specifying Information for ASOS 1 Minute

Automated Surface Observing System (ASOS) 1 minute data files (downloaded from ftp://ftp.ncdc.noaa.gov/pub/data/asos-onemin) can be specified with the ASOS1MIN keyword, followed by the name of the DSI-6405 file containing the wind observations. Optionally, this may be followed by the name of the corresponding DSI-6406 file containing temperature, pressure, and humidity observations. In addition, the location in latitude and longitude may be given. If they are not, the location is found from a table of stations and locations in the file "isd-history.csv", which may be downloaded from ftp://ftp.ncdc.noaa.gov/pub/data/noaa and placed in the `SciDataDir` directory (as defined in SCIPUFF.INI). A copy is also delivered with SCICHEM. Given that stations and their locations change over the years, it is not guaranteed that a station will be found in the table; it is recommended that the location be specified explicitly.

The quality of the ASOS 1 minute data is quite variable. There may be extended gaps, invalid data, and duplicate times with disparate observations. SCICHEM gives information regarding these issues, if encountered, in the "caution" log file. The use of this high-frequency data will typically involve time-averaging (See TIMEBIN below). Note that these data represent 2-minute averages given every minute—therefore, SCICHEM will typically use every other time when computing averages. Periods in which missing values result in an average with substantially fewer observations than nominal are noted in the caution log file.

4.2.7.2 Specifying Station Information for AERMET-Style Files

Two keywords are used to specify information about the meteorological stations given with SURFILE and PROFILE keywords: SURFDATA for the surface meteorological station and UAIRDATA for the upper air station, respectively. The syntax and type of these keywords are summarized as follows:

```
Syntax:  ME SURFDATA Metid Stanum Year Xcoord Ycoord (Name)
Syntax:  ME UAIRDATA Metid Stanum Year Xcoord Ycoord (Name)
Type:    Mandatory (for PROFILE and SURFILE), Repeatable
```

where the Metid parameter is the alphanumeric met ID, Stanum is the station number (for example, the 5-digit WBAN number for NWS stations), Year is the year of data being processed (either 2 or 4 digits), Xcoord and Ycoord are mandatory parameters for specifying the x and y coordinates for the location of the stations, and Name is an optional character field (up to 40 characters with no blanks) specifying the name of the station. The METSCI processor compares the station numbers input using these keywords with the numbers included in the header record of the surface meteorological data file and issues non-fatal warning messages if there are any mismatches.

4.2.7.3 Specifying the Base Elevation for Potential Temperature Profile for AERMET-Style Files

The user must define the base elevation for the AERMET-style PROFILE file with the PROFBASE keyword. The syntax and type for the PROFBASE keyword are summarized as follows:

```
Syntax:  ME PROFBASE Metid BaseElev
Type:    Mandatory (for PROFILE), Non-repeatable
```

where the Metid parameter is the alphanumeric met ID and the BaseElev parameter specifies the base elevation (m) above MSL for the potential temperature profile. The base elevation should correspond with the base elevation of the primary meteorological tower.

4.2.7.4 Specifying the Surface Roughness

The user has the option of specifying a constant surface roughness in meters. If this is not given, it will be taken from AERMET surface files if appropriate or a default value of 0.1 m assumed. The syntax is as follows:

```
Syntax:  ME ROUGHNES roughness
Type:    Optional, Non-repeatable
```

4.2.7.5 Specifying the Calculated Boundary Layer

The user has the option of specifying that the boundary layer depth and surface heat flux be calculated internally by SCICHEM instead of using values on the meteorology input (if any). The syntax is as follows:

```
Syntax:  ME CALCULBL ON/OFF
Type:    Optional, Non-repeatable
```

4.2.7.6 Specifying a Terrain File

A previously generated file with the terrain elevation data defined on a regular two-dimensional grid can be specified for use with the SCICHEM model using the TELUFILE keyword in the TE pathway as shown:

```
Syntax:  TE TELUFILE   terrain_file
Type:    Optional, Non-repeatable
```

where the TELUFILE parameter is the TE type keyword and the terrain_file parameter is a character field of up to 200 characters, in quotes, that identifies the filename for the input terrain data file. The terrain file is an ASCII text file and is described in detail in Section 4.5.4. Note that the TE pathway must follow the ME pathway.

4.2.7.7 Specifying a Time Reference

The TIMEREF keyword specifies the time reference of the input meteorological data. The default for the model is to set the time reference to UTC. The syntax and type for the TIMEREF keyword are summarized as follows:

```
Syntax:  ME TIMEREF UTC or LOCAL
Type:    Optional, Non-repeatable
```

4.2.7.8 Specifying Observation Time Bin

The TIMEBIN keyword specifies the observation time bin width in seconds. Observations within a bin are all given the same time. Multiple observations for the same station are averaged. The default is zero. The syntax and type for the TIMEBIN keyword are summarized as follows:

```
Syntax:  ME TIMEBIN averaging period
Type:    Optional, Non-repeatable
```

4.3 Multicomponent Input File

Nonlinear chemistry is performed by defining a multicomponent material that will carry a set of reactive chemical species. The attached chemical species that are transported and diffused with the conserved tracer will also be transformed through chemical reaction. The gas-phase chemical mechanism and rate constants are provided by the model developers in the multicomponent input file (*ProjectName.*IMC, referred to hereafter as the *IMC file*) and are required for both KEYWORDS and NAMELISTS input formats. The CB6r2 chemistry mechanism is included in the provided IMC file for the long-range application case studies for ozone and secondary $PM_{2.5}$ calculations. For short-range 1-hour NO_2 applications, a shorter version of the mechanism—appropriate for near-source plume chemistry—is also provided (see the tutorial for the 1-hour NO_2 application). The aerosol and aqueous-phase chemistry modules in SCICHEM are based on the AERO5 option available in CMAQ. Since using the multicomponent option is also recommended for non-chemistry applications, an IMC file with the chemistry flag set to false is provided with the 1-hour SO_2 application.

The IMC file specifies the chemical species names, how they will be modeled, the chemical reactions they will undergo, and the associated reaction rate constants. It can be made up of the following five sections: Control, Aqueous-Aerosol, Species, Equations, and Table, in any order. Each section begins with "#Section name" (for example, #Control). All sections are unformatted and need only be space-delimited. The section headings are as follows: Control Section, Aqueous-Aerosol Section, Species Section, Equation Section, and Table Section. An example IMC file is shown in Appendix B. Dry deposition velocities for the various gaseous multicomponent species can be specified in the IMC file. Alternatively, gaseous species' dry deposition velocities are calculated internally using the Zhang et al. (2003) scheme. For this option, the user needs to specify properties of the species in the IMC file. The IMC file provided with the SCICHEM distribution includes these properties. Additional details are provided later in Section 4.3.3. Dry deposition velocities of particle species are calculated based on the approach used in CMAQ.

Aerosol equilibrium chemistry may be treated optionally, either by itself or in combination with aqueous-phase chemistry. Aqueous-phase chemistry may be treated if cloud liquid water content has been provided on the meteorological input files. Note that selecting the aqueous-phase chemistry option requires the selection of the aerosol chemistry option. Wet scavenging coefficients are calculated internally as part of the aqueous-phase chemistry/scavenging module, using algorithms similar to those used in CMAQ. If the aqueous-phase chemistry option is not selected, user-specified wet scavenging coefficients in the IMC file are used.

The user is encouraged to use one of the three IMC files provided with the case studies (that is, the IMC file for full chemistry calculations for long-range impacts; the IMC file for near-source

NOx chemistry calculations for short-range impacts; and the IMC file for near-source SO_2 without chemistry) and to **only change the name and/or path of the file containing the ambient or background concentrations (for the first two types of runs with chemistry)**. The **user may also opt to turn off the aerosol and aqueous chemistry options** if only gas-phase chemistry calculations are relevant for the user's application, for example, for ozone calculations (these options are already turned off in the IMC file provided for the near-source NOx chemistry calculations). **It is recommended that only the parameters listed in Sections 4.3.1 and 4.3.2 in bold font should be changed by the user. No other changes are supported in this release of SCICHEM and should be made after consultation with the model developers**.

4.3.1 Multicomponent Control Section

The Control Section (#Control) has the control namelist, which begins with "&CONTROL" and ends with "/". If parameters are not set under this section, the default values will be assumed. The following control namelist parameters are specified:

ambient_file - Name of file (CHARACTER*128), including path, that contains the 3-D time-dependent ambient species concentrations (optional). The data must be in the format as described in Section 4.3.6. The default is no ambient file. As mentioned, this is the only user-changeable parameter in the Control Section recommended for this release of SCICHEM. Note that a relative path must be based on the run directory, not the directory of the IMC file.

species_units - Concentration units (CHARACTER*80) for ambient concentrations of non-particle species. Aerosol particle species concentrations are always assumed to be in $\mu g/m^3$ or $\#/m^3$ or m^2/m^3 for types *P* (particle mass), *PN* (particle number), and *PA* (particle surface area), respectively. The options for non-particle species types are either 'ppm' or 'molecules/cm^3'. The default is 'ppm'.

emission_units - Emission rate units for the release specified in *rel_mc* in the *Projectname*.SCN file (CHARACTER*80). Options are either 'ppm-m^3/s','molecules-m^3/cm^3-s', or 'g/s'. Aerosol particle species emissions are always assumed to be in *g/s* or *#/s* or m^2/s for types *P*, *PN*, and *PA*, respectively. Note that the default emission units for gaseous species are 'ppm-m^3/s', but the imc files provided with the distribution specify the more standard g/s units.

rate_species_units - Concentration units (CHARACTER*80) for the rate constants given under the equations section. Options are either 'ppm' or 'molecules/cm^3'. The *rate_species_units* will be converted to match the *species_units*. The default is 'molecules/cm^3'.

rate_time_units - Time units (CHARACTER*80) for the rate constants given under the equations section. Options are 'seconds', 'minutes', or 'hours'. The default is 'seconds'.

particle_types - String consisting of comma-separated particles types (See Table 4-2 for a description of allowed particle types) specified in the species section. If no particle type is specified, a default type of 'P' is assumed.

particle_units - String consisting of comma-separated units for corresponding particle types specified previously (CHARACTER*80). The default is $\mu g/m^3$. The particle types and units are used only for the GUI plots. The units are not used for converting the emissions or the output concentrations.

rtol - Relative tolerance (REAL*4) used to solve chemical reaction equations. The default is 1.e-2.

step_chemistry - Flag for conducting a simulation with chemistry. The default is .TRUE.

An example of a Control Section is shown in Figure 4-4.

```
#CONTROL
  &CONTROL
      ambient_file = 'VISTAS_WEST.amb'
      emission_units = 'g/s'
      species_units = 'ppm'
      rate_time_units = 'min'
      particle_types = 'P, PA, PN',
      particle_units = 'ug/m3, m2/m3, #/m3',
      rtol = 1.e-3
      step_chemistry = .TRUE.
  /
```

Figure 4-4
Sample Control Section of the IMC File

4.3.2 Aqueous-Aerosol Section

The Aqueous-Aerosol module included in SCICHEM 3.3 is based on the CMAQ4.7.1 AERO5 module. Using parameters in the Aqueous-Aerosol Section (#Q), the modules can be turned on or off. The following namelist and namelist parameters are specified for the AERO5 aqueous-aerosol module.

Namelist: **AQAER** – Aqueous and Aerosol module control flags

aqueous - Specifies whether aqueous-phase chemistry will be performed (LOGICAL). Must have certain species defined in the Species Section, as described in the following section. If set to 'True', the species names listed will be checked with the SCICHEM species list (see Section 4.3.3) in the multicomponent file to determine if the aqueous module can be used; if so, aqueous-phase chemistry will be performed in addition to gas phase. Liquid cloud content must be provided on a meteorological input file (Observations or Gridded). The default is 'False'. Requires the aerosol control flag (see below) to be true.

aerosol - Specifies whether aerosol equilibrium chemistry will be modeled (LOGICAL). Must have certain species defined in the Species Section, as described in the following section. If set to 'True', the species names listed will be checked with the SCICHEM species list (see Section 4.3.3) in the multicomponent file to determine if the aerosol module can be used; if so,

aerosol equilibrium chemistry will be performed in addition to gas phase. The default is 'False'.

Namelist: **AERSPEC**

aerp_names - Names of species in particle phase for Aerosol module. Use as provided without any changes.

Namelist: **G2AE_SPEC**

g2ae_names - Names of gas-phase species that participate in aerosol chemistry. Use as provided without any changes.

Namelist: **NAQSSPEC**

n_g2aq_spc - Number of gas-phase species that participate in aqueous chemistry. Use as provided without any changes.

Namelist: **G2AQ_SPEC**

g2aq_names - Names of gas-phase species that participate in aqueous chemistry. Use as provided without any changes.

4.3.3 Multicomponent Species Section

Each line of the Species Section gives the species name, the species type (F, S, P, or A), the ambient concentration (ppm or molecules/cm^3), the absolute tolerance (ppm or molecules/cm^3), the gas deposition velocity (m/s), the wet scavenging coefficient (s^{-1}), the molecular weight (g/mole) to be used in solving for the concentration, and flags (T/F) for turning on or off the dosage and deposition outputs. Note that both dep and dose output flags are set to true if either the dose or dep flag is true to maintain the same order of species in both output files. There are no defaults for these parameters. The species types are shown in Table 4-2.

Table 4-2
SCICHEM Species Types

F	Fast	Species concentrations change rapidly, and species rate equations will be integrated using LSODE.
S	Slow	Species concentrations change slowly and will be integrated explicitly using a predictor-corrector scheme.
P[N|A]	Particle	Species concentrations are determined through aerosol equilibrium. Species name must match aerosol particles set by aerosol module. If N or A is present after P, the species is particle number type or particle area type.
A	Ambient	Species concentrations do not change by the reaction, such as H_2O or O_2.

The wet scavenging coefficient, s (s^{-1}), is used to define the scavenging rate, sr (s^{-1}), as:

$$sr = s\ (R/R_0)$$

where R is the precipitation rate in mm/hr and R_0 is the reference precipitation rate of 1 mm/hr. The scavenging rate is applied to the gas-phase species after the gas-phase chemistry has been advanced. Scavenging coefficients for aerosol particles specified in the IMC file are ignored. Particle scavenging rates are determined internally based on particle size and precipitation rate based on the approach of Seinfeld (1986). Similarly, dry deposition velocities for aerosol particles are also ignored, and dry deposition is computed internally following the approach of Slinn (1982). Note that if the aqueous-phase chemistry option is selected, all the wet scavenging coefficients specified in the IMC file will be ignored and the wet removal of both gases and particles will be carried out inside the aqueous-phase module.

Every species that appears in the Equation Section must also appear in the Species Section. The ambient concentration of H_2O may be set on the species line to a desired concentration or set to –1.0 to be set internally by the meteorological conditions. When set internally, the H_2O concentration is obtained from the humidity given in the meteorological input files, or a default value of 30% relative humidity is used. Note that if species other than H_2O are specified as ambient, such as O_2, the correct ambient concentration must be given on the species line. If an ambient file has been specified under the Control Section, the ambient concentrations given in the Species Section will be overridden by the 3-D ambient file.

Molecular weights are used to convert the gas-phase emissions to the desired species units and for other unit conversions. Emission rates provided in 'g/s' will be converted to 'ppm-m^3/s' using the molecular weight. Standard temperature and pressure (STP; 298 K and 1 atm) are used in the conversion, and the output concentrations are provided in µg/m^3. The molecular weights for all 'Fast' and 'Slow' species must be provided in the IMC file. Molecular weights are not required for particle species, because equilibrium concentrations are determined from the 'Fast' and 'Slow' species concentrations. For aerosol particle species, concentrations are always assumed to be in µg/m^3, #/ m^3, and m^2/m^3 for types P, PA, and PN, respectively. The corresponding emission rates for the particle types are in µg/s, #/s, and m^2/s.

One example of a Species Section from SCICHEM 3.1 (and later) is shown in Figure 4-5. In the example, only HNO_3 has a non-zero wet scavenging coefficient; therefore, there will be no wet deposition or scavenging of any species other than HNO_3. HNO_3 is modeled as a fast species with a background concentration of zero and a relative tolerance of 1.e-8. The deposition velocity is 0.02 m/s, and the wet scavenging coefficient is 6.e-5 s^{-1}. The ambient H_2O concentration will be determined from the meteorological input data.

SCICHEM 3.1 added a new dry deposition velocity scheme for gaseous species based on Zhang et al. (2003). This option is invoked if the Species section includes additional species properties (for example, Henry's Law constant) that are required to calculate the surface resistance. The provided IMC files include these additional properties. Using HNO_3 as an example again, the differences between the SCICHEM 3.0 and SCICHEM 3.1 inputs in the IMC file are highlighted as follows:

SCICHEM 3.0:

HNO3 F 2.1000E-03 1.0000E-08 0.0200 0.0 63.00 T T

SCICHEM 3.1:

HNO3 F 2.1000E-03 1.0000E-08 (2.10E+05 -8700. 0.0 0.) 0.0 63.00 T T

As shown, the dry deposition velocity is specified as 0.02 m/s in the SCICHEM 3.0 version of the IMC file. In SCICHEM 3.1 and later, the dry deposition velocity is not specified; instead, the species properties for the dry deposition velocity calculations are provided within parentheses. The four species parameters are the Henry's Law constant at 298K (2.1E+05 for HNO_3, the temperature correction factor for the Henry's Law constant (-8700 for HNO_3), and the reactivity and surface resistance scaling factors.

```
#Species,Type,Ambient,Tolerance,deposition vel,wet scav,mw,dos,dep
NO2       F           2.4000E-03        1.0000E-08   0.0025   0.0  46.00 T T
NO        F           2.8000E-05        1.0000E-08   0.0015   0.0  30.00 T T
O         F           1.0300E-26        1.0000E-12   0.0      0.0  16.00
O3        F           6.3000E-02        1.0000E-08   0.0      0.0  48.00 T T
NO3       F           2.2000E-05        1.0000E-12   0.0      0.0  62.00 T T
O1D       F           1.0000E-30        1.0000E-12   0.0      0.0  16.00
OH        F           3.2700E-09        1.0000E-12   0.0      0.0  17.00
HO2       F           6.8900E-06        1.0000E-12   0.0      0.0  33.00
N2O5      F           5.3000E-05        1.0000E-12   0.0      0.0 108.00 T T
HNO3      F           2.1000E-03        1.0000E-08   0.0200   0.0  63.00 T T
HONO      F           4.6400E-06        1.0000E-08   0.0020   0.0  47.00 T T
PNA       F           1.4243E-05        1.0000E-08   0.0020   0.0  79.00 T T
H2O2      F           3.4100E-03        1.0000E-08   0.0030   0.0  34.00
XO2       F           2.1800E-10        1.0000E-12   0.0      0.0   1.00
XO2N      F           4.4200E-10        1.0000E-12   0.0      0.0   1.00
NTR       F           6.2879E-05        1.0000E-12   0.0      0.0 130.00 T T
ROOH      F           1.0000E-04        1.0000E-12   0.002    0.0  62.00
FORM      F           3.4970E-06        1.0000E-08   0.0020   0.0  30.00 T T
ALD2      F           2.5176E-06        1.0000E-08   0.0020   0.0  44.00
ALDX      F           5.7932E-06        1.0000E-08   0.0020   0.0  44.00
PAR       F           1.7677E-02        1.0000E-08   0.0010   0.0  14.00
CO        S           2.2000E-01        1.0000E-04   0.0010   0.0  28.00 T T
MEO2      F           6.8900E-10        1.0000E-12   0.0      0.0  47.00
MEPX      F           6.8900E-06        1.0000E-12   0.002    0.0  48.00
MEOH      F           0.0000E+00        1.0000E-12   0.001    0.0  32.00
HCO3      F           0.00000+00        1.0000E-12   0.0      0.0  63.00
FACD      F           1.0000E-06        1.0000E-08   0.0020   0.0  46.00
C2O3      F           3.1300E-06        1.0000E-12   0.0      0.0  75.00
PAN       F           1.5300E-03        1.0000E-08   0.0020   0.0 121.00 T T
…….
AH2OK     P           1.0000E-01        1.0000E-08   0.0      0.0  18.00 T T
NH3       S           6.6853E-04        1.0000E-08   0.0      0.0  17.00 T T
SV_ALK    S           1.0000E-30        1.0000E-08   0.0      0.0 150.00
SV_XYL1   S           2.2881E-06        1.0000E-08   0.0      0.0 192.00
SV_XYL2   S           9.7113E-06        1.0000E-08   0.0      0.0 192.00
SV_TOL1   S           3.7395E-06        1.0000E-08   0.0      0.0 168.00
SV_TOL2   S           6.9515E-06        1.0000E-08   0.0      0.0 168.00
SV_BNZ1   S           3.7395E-06        1.0000E-08   0.0      0.0 144.00
SV_BNZ2   S           6.9515E-06        1.0000E-08   0.0      0.0 144.00
SV_TRP1   S           2.8001E-05        1.0000E-08   0.0      0.0 168.00
SV_TRP2   S           1.1231E-04        1.0000E-08   0.0      0.0 168.00
SV_ISO1   S           1.0000E-30        1.0000E-08   0.0      0.0  96.00
SV_ISO2   S           1.0000E-30        1.0000E-08   0.0      0.0  96.00
SV_SQT    S           4.7256E-06        1.0000E-08   0.0      0.0 378.00
CL2       A           1.0000E-10        1.0000E-08   0.0050   0.0  71.00
CL        A           1.0000E-10        1.0000E-08   0.0050   0.0  35.50
HOCL      A           1.0000E-10        1.0000E-08   0.0050   0.0  52.50
CLO       A           1.0000E-10        1.0000E-08   0.0050   0.0  51.50
FMCL      A           1.0000E-10        1.0000E-08   0.0050   0.0  64.50
HCL       A           1.0000E-10        1.0000E-08   0.0      0.0  36.50
CO2       A           3.8412E+02        1.0000E-08   0.0      0.0  28.00
H2O       A           -1.0              1.0000E-06   0.0      0.0  18.02
```

Figure 4-5
Sample Species Sections of the IMC File

If either the aerosol equilibrium chemistry is turned on (aerosol flag is 'True' under the AqAer Section) or the aqueous-phase chemistry is turned on (aqueous and aerosol flags are 'True' under the AqAer Section), the species shown in Table 4-3 must appear in the Species Section, even if they do not all appear in the gas-phase mechanism (for example, the aerosol species). Note that the aerosol option can be selected without selecting the aqueous-phase chemistry option, but the converse is not true.

AERO5 uses the modal aerosol treatment with three modes: Aitken, Accumulation, and Coarse. It is not necessary that all aerosol species will have all three modes. For multiple particle modes, the aerosol species names must appear in the Species Section of the IMC file with the mode character. The naming convention used for modal treatment follows that used in CMAQ and is "I" for the Aitken mode, "J" for the accumulation mode, and "K" for the coarse mode. Note that the chemical species in the provided IMC file are specifically for the AERO5 module and CB6r2 mechanism and cannot be updated to other schemes without corresponding changes in the SCICHEM code. The required names for either aqueous chemistry or aerosol equilibrium will be as they appear in Table 4-3. The total number of species needed for the aerosol module is 80 (51+29) and 67 (51+16) for the aqueous chemistry module.

Table 4-3
Required Species Names for the Aerosol Equilibrium Module and Aqueous-Phase Chemistry Module

Module	Required Species Names
Both[1] (51)	ASO4J, ASO4I, ANH4J, ANH4I, ANO3J, ANO3I, AALKJ, AXYL1J, AXYL2J, AXYL3J, ATOL1J, ATOL2J, ATOL3J, ABNZ1J, ABNZ2J, ABNZ3J, ATRP1J, ATRP2J, AISO1J, AISO2J, AISO3J, ASQTJ, AOLGAJ, AOLGBJ, AORGCJ, AORGPAJ, AORGPAI, AECJ, AECI, A25J, A25I, ACORS, ASOIL, NUMATKN, NUMACC, NUMCOR, SRFATKN, SRFACC, SRFCOR, AH2OJ, AH2OI, ANAJ, ANAI, ACLJ, ACLI, ANAK, ACLK, ASO4K, ANH4K, ANO3K, AH2OK
Aerosol (29)	NO2, N2O5, HNO3, HONO, SULF, HCL, NH3, ISOPRXN, TRPRXN, SULRXN, TOLNRXN, TOLHRXN, XYLNRXN, XYLHRXN, BNZNRXN, BNZHRXN, SESQRXN, SV_ALK, SV_XYL1, SV_XYL2, SV_TOL1, SV_TOL2, SV_BNZ1, SV_BNZ2, SV_TRP1, SV_TRP2, SV_ISO1, SV_ISO2, SV_SQT
Aqueous (16)	O3, OH, HO2, N2O5, HNO3, H2O2, MEPX, FACD, PACD, MGLY, SO2, SULF, CL2, HOCL, HCL, NH3

Note: [1]Aerosol particles must be specified as species type "P[N|A]" (particle).

4.3.4 Multicomponent Equation Section

Each line of the equations section gives the equation number followed by the chemical reaction. Species names must be placed in square brackets, such as [NO], and stochiometric coefficients are given in parentheses, as in (2.0) [NO]. The maximum number of reactants is 2, and the maximum number of products is 10. The reaction is terminated by a semicolon followed by the reaction rate coefficient type. The following rate coefficient types are available (not all types are used in the current mechanism, CB6r2):

D	Description	Number of Parameters
0	Radiation dependent	0 (Need table)
1	Constant	1 (k_0)
2	Temperature dependent	3 or 2 (*A*, *B,* and *C*)
3	Temperature and pressure dependent	4 (k_0, m_0, k_∞, and m_∞)
4	Temperature dependent and multiplied by the concentration of H_2O (for compatibility with previous version)	3 (*A*, *B,* and *C*)
5	Air concentration dependent	3 (*A*, *B,* and *C*)
6	Cloud liquid water content dependent	1 (k_0)
7	Pressure dependent (type B)	1 (k_0)
8	Equilibrium rate	3 (k_0, k_1, and N_p)
9	O_2 concentration dependent	3 (*A*, *B,* and *C*)
10	N_2 concentration dependent	3 (*A*, *B,* and *C*)
11	Falloff reaction rate (type 1)	4 (*A*, m_0, *B,* and m_∞)
12	Falloff reaction rate (type 2)	4 (*A*, m_0, *B,* and m_∞)
13	Falloff reaction rate (type 3)	6 (*A*, *B*, *C*, *D*, *E,* and *F*)
14	CH_4 concentration dependent	3 (*A*, *B,* and *C*)
15	H_2O concentration dependent	3 (*A*, *B,* and *C*)
16	O_2 and air concentration dependent	3 (*A*, *B,* and *C*)
17	H_2O concentration dependent (type 3)	3 (*A*, *B,* and *C*)
18	Falloff reaction rate (type 4)	7 (*A*, *B*, m_1, C, *D*, m_2, and *F*)
19	Falloff reaction rate (type 5)	4 (*A*, *B*, *C,* and *D*)
20	Falloff reaction rate (type 6)	4 (*A*, *B*, *C,* and *D*)
21	H_2 concentration dependent	3 (*A*, *B,* and *C*)
22	Temperature dependent (type B)	3 (*A*, *B,* and *C*)
23	Falloff reaction rate (type 7)	8 (*A*, *B*, m_1, C, *D*, m_2, *F, and G*)
24	Air concentration dependent	3 (*A*, *B,* and *C*)

For the radiation-dependent rate constants (Type 0), a table must be provided listing the rate constants as a function of zenith angle (see Section 4.3.5).

For the other reactions, the necessary constants are given after the type number. For type 1, the rate constant itself is provided; for type 2, the constants *A* and *B*, and optionally *C*, are provided, satisfying the following equation for the rate constant:

$$k = AT^{-C}e^{(B/T)}$$

Reaction type 22 is similar to type 2 with provided constants *A*, *B*, and *C* satisfying the following equation for the rate constant:

$$k = A\left(\frac{T}{T_{ref}}\right)^{C} e^{(B/T)}$$

where

$$T_{ref} = 300.$$

For reaction type 16, the form of the equation is similar to type 22. The rate constant is multiplied by the air and oxygen concentration as given by the following equation:

$$k = A\left(\frac{T}{T_{ref}}\right)^{C} e^{(B/T)}[M][O_2]$$

where $[M]$ and $[O]$ are the concentrations of air and oxygen in molecules/cm^3, respectively.

For reaction type 24, the form of the equation is similar to type 16. The rate constant is multiplied by the air concentration as given by the following equation:

$$k = A\left(\frac{T}{T_{ref}}\right)^{C} e^{(B/T)}[M]$$

where $[M]$ and $[O]$ are the concentrations of air and oxygen in molecules/cm^3, respectively.

For reaction type 3, constants k_0, m_0, k_∞, and m_∞ are provided. The rate constant for this type of reaction is calculated as follows:

$$k = \left[\frac{k_0 T^{m_0}[M]}{1+b}\right] F^{z}$$

where

$$b = \frac{k_0 T^{m_0}[M]}{k_\infty T^{m_\infty}}$$

$$z = \left[1 + \left(\log_{10} b\right)^2\right]^{-1}$$

$$F = 0.60$$

$$[M] = 7.34 \times 10^{21} \frac{P}{T}$$

and $[M]$ is the concentration of air in molecules/cm^3, P is the ratio of the pressure to standard atmospheric pressure, and T is the temperature in degree Kelvin.

Reaction type 18 (Falloff 4) is similar in form to type 3 but uses 7 constants, and the values of k_0 and k_∞ are calculated from the constants A, B, m_1, C, D, m_2, and F using the following equations:

$$k_0 = [M] A \left[\frac{T}{T_{ref}}\right]^B e^{\frac{m_1}{T}}$$

$$k_\infty = C \left[\frac{T}{T_{ref}}\right]^D e^{\frac{m_2}{T}}$$

$$b = \frac{k_0}{k_\infty}$$

$$z = \left[1 + \left(\log_{10} b\right)^2\right]^{-1}$$

$$k = \left[\frac{k_0}{1+b}\right] F^z$$

Reaction type 23 (Falloff 7) is similar in form to type 18 but uses 8 constants, and the values of k_0 and k_∞ are calculated from the constants A, B, m_1, C, D, m_2, F, and G using the following equations:

$$k_0 = [M] A \left[\frac{T}{T_{ref}}\right]^B e^{\frac{m_1}{T}}$$

$$k_\infty = C \left[\frac{T}{T_{ref}}\right]^D e^{\frac{m_2}{T}}$$

$$b = \frac{k_0}{k_\infty}$$

$$z = \left[1 + \left(\frac{\log_{10} b}{G}\right)^2\right]^{-1}$$

Reaction types 4, 5, 9, 10, 14, 15, 17, and 21 represent reactions with $[H_2O]_{ppm}$, [M], $[O_2]$, $[N_2]$, $[CH_4]$, $[H_2O]$, $[H_2O]^2$, and $[H_2]$ dependent rate constants, respectively. Here [S] is the concentration of species 'S' in molecules/cm^3 and $[S]_{ppm}$ is the corresponding concentration in ppm. The equations follow the same form as those for type 2. This type must be used for third-order reactions in which 2 SCICHEM chemical species are also reacting with air, O_2, N_2, CH_4, H_2O, or H_2, because the maximum number of reactants is 2. Even if the rate constant is independent of temperature, instead of using type 1 for two species reacting with M, O_2, N_2, CH_4, or H_2O, use type ID 4, 5, 9, 10, 14, 15, 17, or 21 with $B = 0$. The rate constant will be multiplied by $[H_2O]_{ppm}$, [M], $[O_2]$, $[N_2]$, $[CH_4]$, $[H_2O]$, $[H_2O]^2$, and $[H_2]$ for reactions of type 4, 5, 9, 10, 14, 15, 17, and 21, respectively.

Reactions of type 6 represent those that depend on the cloud liquid water content (not used in the current CB05 mechanism). The rate data provided on the equation line indicate the diffusivity of the reacting species in air. An example is the heterogeneous conversion of N_2O_5 to HNO_3. The diffusivity of N_2O_5 should be provided on the equation line for this reaction in units of cm^2/s. The reaction rate will be calculated internally as the product of a conversion constant, the diffusivity (cm^2/s) and the cloud liquid water content (g/m^3) divided by the square of the cloud droplet size (m), as follows:

$$k = 1.2e-9(LWC)(k_0)/(D_P)^2$$

For reactions of type 7, the reaction rate constant is calculated from the provided constant k_0 so that

$$k = k_0(1 + 0.6P)$$

The equilibrium rate constant for type 8 is dependent on the rate of a previous reaction using the provided constants k_0, k_1, and N_p so that

$$k = k(N_p) \Big/ \left(k_0 e^{k_1/T}\right)$$

where $k(N_p)$ is the reaction rate constant for reaction number N_p. The value of N_p must be less than the current reaction number and preferably the one immediately preceding the current reaction.

The rates for reaction types 11 and 12 (Falloff reaction types 1 and 2, respectively) are obtained from the values of constants A, m_0, B, and m_∞. For type 11, the rate is

$$k = \left[\frac{k_0}{1 + k_0/k_\infty}\right] F^z$$

where

$$k_0 = A\left(\frac{T}{T_{ref}}\right)^{m_0}[M]$$

$$k_\infty = B\left(\frac{T}{T_{ref}}\right)^{m_\infty}$$

$$z = \left[1+\left(\log_{10}\frac{k_0}{k_\infty}\right)^2\right]^{-1}$$

$$F = 0.6$$

$$T_{ref} = 300.$$

For reaction type 12, the reaction rate is multiplied by the O_2 concentration to give

$$k = \left[\frac{k_0}{1+k_0/k_\infty}\right]F^z[O_2]$$

The reaction rate for Type 13 reactions (Falloff reaction type 3) is obtained using the constants *A*, *B*, *C*, *D*, *E*, and *F*, so that

$$k = k_0 + \left[\frac{k_3}{1+k_3/k_2}\right]$$

where

$$k_0 = Ae^{\frac{B}{T}}$$

$$k_2 = Ce^{\frac{D}{T}}$$

$$k_3 = Ee^{\frac{F}{T}}[M]$$

The reaction rates for reaction types 19 and 20 (Falloff reaction types 5 and 6, respectively) are of the same form and are obtained similarly using the three constants *A*, *B*, and *C* so that

$$k = k_0 + k_2$$

for reaction type 19, and the rate is multiplied by [H_2O] for reaction type 20, as shown below:

$$k = (k_0 + k_2) * [H_2O]$$

An example Equation Section is shown in Figure 4-6. Spaces must separate different components of the equation line. A plus sign ("+") is used to separate species, a minus sign followed by a greater than sign ("->") separates the reactant species from the product species, and a semicolon (";") begins the rate constant information.

In the example,

k_1 is radiation dependent

k_2 is oxygen and air concentration dependent and is given by

$$\mathrm{k}_2 = 3.6\mathrm{e}^{-32}\left(\frac{T}{300}\right)^0 e^{-\frac{2.4}{T}}[O_2][M]$$

k_3 and k_4 are temperature dependent and are given by

$$k_3 = 1.8\mathrm{e}^{-10}T^0 e^{-\frac{-1500.}{T}},$$

$$k_4 = 3.36\mathrm{e}^{-10}T^0 e^{-\frac{-1800.}{T}},$$

k_5 is falloff type 1 reaction rate

$$k_5 = \frac{0.6^z \mathrm{k}_0}{1+\left(\frac{\mathrm{k}_0}{\mathrm{k}_\infty}\right)},$$

where $z = \dfrac{1}{1+\left[\log\left(\dfrac{\mathrm{k}_0}{\mathrm{k}_\infty}\right)\right]^2}$

and

$$k_0 = 1.5\mathrm{e}^{-29}\left(\frac{T}{T_{ref}}\right)^{-1.8}[M]$$

$$k_\infty = 1.32\mathrm{e}^{-9}\left(\frac{T}{T_{ref}}\right)^{-0.7}$$

The concentration and time units of the rate constants must be the same for all and are specified in the Control Section.

```
#Equations -- CB6R2 from CAMx

1 [NO2]  -> [NO] +  [O]      ;  0  0.000E+00  0.0000E+00
2 [O]    -> [O3]                ; 16  3.410E-32  0.0000E+00 -2.6
3 [O3]  + [NO]  ->  [NO2]   ;  2  8.400E-11 -1.3100E+03
4 [O]   + [NO]  ->  [NO2]   ; 24  6.000E-30  0.0000E+00 -1.6
5 [O]   + [NO2] ->  [NO]    ;  2  3.300E-10  1.8800E+02
```

Figure 4-6
Sample Equation Section of the IMC File

4.3.5 Multicomponent Table Section

Radiation dependent rate constants appear in the Table Section. The table is of the form:

0, zenith angles(i) , i = 1, no. zenith angles
equation number, radiation constants(i), i = 1, no. zenith angles

A zero in the equation number field indicates that the values to follow are the zenith angles. Each line must begin with a zero or an equation number.

An example of a radiation constant table is shown in Figure 4-7 for 2 reactions and 10 zenith angles. In the example, $k_1 = 3.589\text{s}^{-1}$ at a zenith angle of 60°. The zenith angle is 0° at noon and 90° at sunrise and sunset. A maximum of 20 zenith angles can be input. The radiation-dependent rate constants are set to zero before sunrise and after sunset. Every equation that has a rate constant type 0 must have a corresponding entry in the Table Section.

```
#Table
 0       0.          10.         20.          30.          40.          50.         60.          70.          78.         86.
 1  6.033E-01   5.993E-01   5.862E-01   5.630E-01   5.249E-01   4.660E-01   3.779E-01   2.492E-01   1.253E-01   3.070E-02
 8  2.556E-02   2.546E-02   2.514E-02   2.458E-02   2.366E-02   2.224E-02   2.000E-02   1.612E-02   1.073E-02   2.560E-03
```

Figure 4-7
Sample Table Section of the IMC File

4.3.6 Ambient Concentration Input

Three-dimensional time-dependent ambient concentrations may be provided in binary or ASCII MEDOC format to a multicomponent project. A detailed description of the MEDOC format is given in Section 4.5.2 for the meteorological inputs and next for the ambient concentration inputs. The ambient concentration filename is set using the *ambient_file* parameter in the Control Section of the IMC file. For species ambient concentrations that are not available in the ambient data file, the concentrations from the IMC file are used. If the modeling domain goes further than what is provided in the ambient file, SCICHEM will use the nearest point in space. Likewise, if the calculation begins before the time given on the ambient file, the first time will be used; if it begins after the last time on the file, the last time will be used. A three-dimensional ambient file must hold a minimum of one point in space at one time. Units for the concentrations must be in *species_units* as set in the Control Section of the IMC file. To use the relative humidity provided in the meteorological observation file for the concentrations of water, negative concentrations for

water must be specified on the 3-D ambient file. This will indicate that the water concentrations should be calculated internally. If relative humidity is not provided on the observation file, a default value of 30% is assumed.

As part of the SCICHEM distribution package, annual ambient concentration files are provided at the state level for the contiguous United States (CONUS), as shown in Figure 4-8. For large states (Texas and California), the concentrations are provided at the sub-state level, while a common background file is provided for the five small states in the northeastern United States (Vermont, New Hampshire, Massachusetts, Rhode Island, Connecticut). The concentrations are calculated from a 12-km CONUS simulation for 2011 with CAMx, using the 2011v6.2 modeling platform. The CAMx results are horizontally averaged over a given region, and hourly varying concentrations are provided for 18 vertical layers from the surface to about 3 km with higher resolution near the surface (the surface layer is about 20-m thick, and there are 10 layers between the surface and 1 km). The hourly values are the same for each day of the month.

The SCICHEM 3.3 distribution package also includes a processor that can create annual ambient concentration files, similar to those provided with the package, from 3-D PGM (CAMx or CMAQ) outputs. The user can select the region over which the PGM outputs are horizontally averaged. A brief user's guide is provided with the processor, and the package with documentation is available in the "CTM2SCICHEM" folder in the SCICHEM base directory.

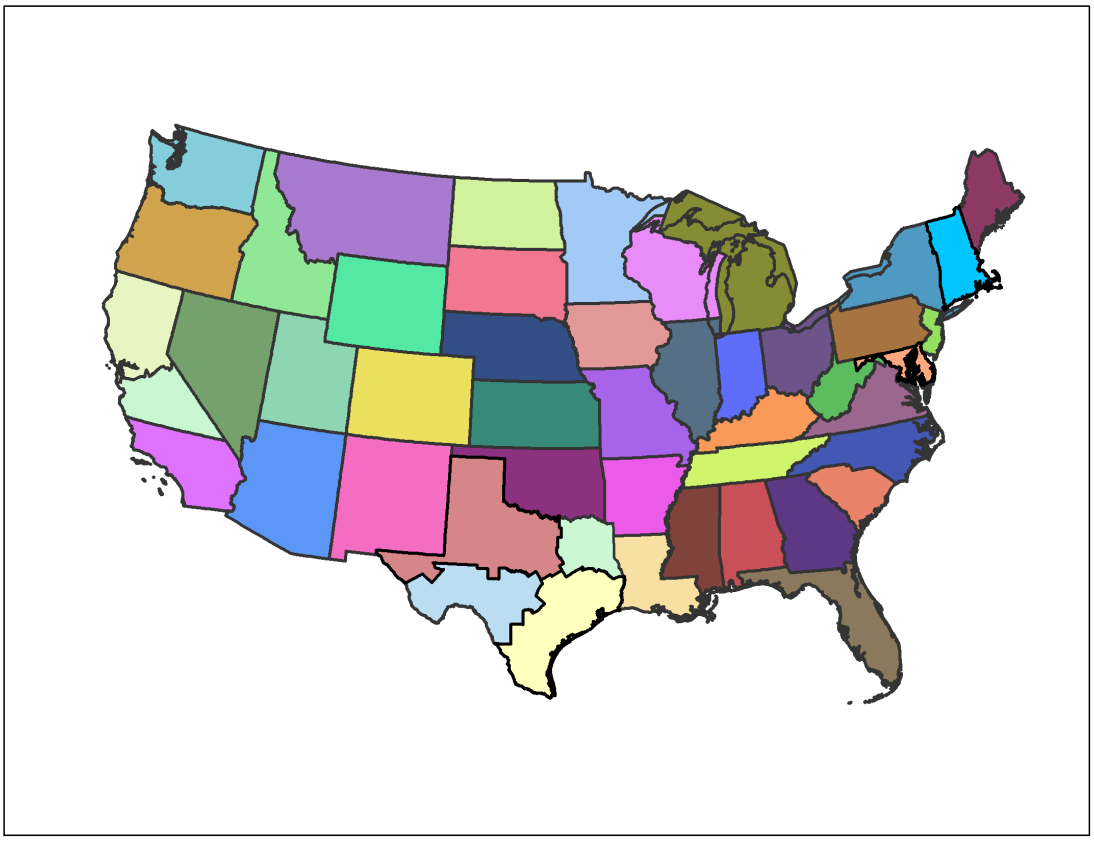

Figure 4-8
Regions for Which CMAQ-Based Background Chemistry Files Are Provided with SCICHEM

4.3.6.1 Ambient Concentration File Format

The 3-D ambient file contains a header section followed by numerical data for each time. The general format structure is illustrated in Figure 4-9, which shows the FORTRAN code used to read the file. For binary files, the read statement is unformatted.

```
!   RECORD 1 - FILE FORMAT ('FFFFFFFF' or 'BBBBBBBB')
     READ (1,'(A8)') FFLAG

!    RECORD 2 - NAME OF CODE - NOT USED IN SCICHEM
     READ (1,'(A8)') CODENAME

!    RECORD 3 - TIME
     READ (1,'(6(I12,1x))') IDAY,IMONTH,IYEAR,IHOUR,IMIN,ISEC

!    RECORD 4 - INITIAL TIME OF CALCULATION - NOT USED IN SCICHEM
     READ (1, '(6(I12,1x))') JDAY,JMONTH,JYEAR,JHOUR,JMIN,JSEC

!    RECORD 5 - NUMBER OF GRID POINTS, KEY POINTS, VARIABLES
     READ (1, '(6(I12,1x))') NXA,NYA,NZA,NDUM,NAMB3D,NVAR2D

!    RECORD 6 - NOT USED FOR SCICHEM AMB FILE
     READ (1, '(6(I12,1x))') IDUM,IDUM,IDUM,IDUM,IDUM,IDUM

!    RECORD 7 - NOT USED FOR SCICHEM AMB FILE
     READ (1, '(3(I12,1x))') IDUM,IDUM,IDUM

!    RECORD 8 – AMB CONC GRID AND TIMING INFORMATION  (KMAX+11 VALUES)
     READ (1,9003) (AMBZ(K),K=1, NZA),DXA,DYA,XOA,YOA,LAT0,LON0,
    &            DUM,DUM,DUM,DUM,ZTOPA

!    RECORD 9 – AMB SPECIES NAMES AND DUM UNITS (2*NAMB3D +2*NVAR2D VALUES)
     READ (1,9001) (NAME3D(N),N=1,NAMB3D),(NAMDUM,N=1,NAMB3D),
    &                    (NAM2D(N),N=1,NVAR2D),(NAMDUM,N=1,NVAR2D)

!    RECORD 10 - NOT USED IN SCICHEM AMB FILE
     READ (1,9003) (DUM,N=1,3*NDUM)

!    RECORD 11 - 3D VARIABLES
!                  (NAMB3D SETS OF NXA * NYA * NZA VALUES)
     DO N=1,NAMB3D
        READ (1,9003) (((CONC3D(I,J,K,N),I=1, NXA),J=1, NYA),K=1, NZA)
      END DO

!    RECORD 12 - 2D VARIABLES  (NVAR2D SETS OF NXA * NYA VALUES)
     DO  N=1,NVAR2D
       READ (1,9003) ((VAR2D(I,J,N),I=1, NXA),J=1, NYA)
     END DO

!
 9001 FORMAT(6(A8,1X))
 9002 FORMAT(6(I12,1X))
 9003 FORMAT(6(F12.4,1X))
```

Figure 4-9
Fortran Pseudo-Code for Reading a Formatted Ambient Concentration File in MEDOC Format

The definitions of the input variables for the rest of the records are as follows:

IDAY, IMONTH, IYEAR, IHOUR, IMIN, ISEC: The day, month, year, hour, minute, and second for the ambient concentrations. The time convention used must be the same as specified in the input file as described in Section 4.1.1 or 4.2.3.8. If LOCAL is set to true in the inp file, the time is assumed to be LOCAL instead of UTC. For monthly input files, where the hourly concentrations are the same over the whole month, the value of iday and iyear should be set to 99 and 9999, respectively, similar to the ambient files provided with the SCICHEM distribution. Because the monthly values are from a CMAQ simulation covering the United States, the hourly values in the included files are in UTC.

NXA, NYA, NZA: Number of grid points in the (*x, y, z*) directions, respectively.

NREPER: Number of special points. This information is not used for the SCICHEM input, and NREPER should be set to zero.

AMBZ: Array of **NZA** vertical grid coordinates in meters. SCICHEM assumes a terrain-following coordinate transformation.

DXA, DYA: Horizontal grid spacing in meters.

XOA, YOA: Horizontal grid origin (SW corner) coordinates in km.

LAT0, LON0: Horizontal grid origin (SW corner) coordinates in degrees.

ZTOPA: Vertical meteorology domain height in meters. If the parameter is not specified, the domain height is assumed to be **AMBZ(NZA)**.

NAMB3D: Number of species with three-dimensional ambient concentration fields.

NAME3D: Names of the multicomponent species with three-dimensional ambient concentration fields.

NVAR2D: Number of two-dimensional fields.

NAM2D: Names of the two-dimensional variables. SCICHEM recognizes the two-dimensional field ‘REL’ or ‘TOPO’, for reading the terrain elevation in meters.

CONC3D: The 3-D (NXA*NYA*NZA) ambient concentrations of NAMB3D species. The concentrations units for non-particle species are assumed to be *species_units*, as set under the control section of the IMC file (Section 4.3.1). Aerosol particle species concentrations are always assumed to be in $\mu g/m^3$ or $\#/m^3$ or m^2/m^3 for types *P*, *PN*, and *PA*, respectively. Note that any units specified in the *ambient_file* (DUM UNITS) are ignored.

The MEDOC file format described in Section 4.5.2 is more general than that used by the SCICHEM ambient concentration file format. Variables not used in the SCICHEM ambient concentration file format are indicated as dummy variables in the figure.

4.4 Sampler Location File

Time histories of concentration, dosage, line-of-sight integrals, and surface deposition for a set of locations can be obtained by specifying a sampler location file in the OPTIONS namelist of the main input data file (Section 4.1.1) or the RE pathway (Section 4.2.6). The location file is an ASCII text file using a format that allows the specification of moving sensors, multiple materials, and a variety of sensor outputs. The first line in the location file must begin with the case-insensitive string "SCIPUFF SENSOR" (read with Fortran 'A11' format).

The general structure of the SCIPUFF format is illustrated in Figure 4-10, where it is shown that the header record begins with the string 'SCIPUFF SENSOR' and contains optional keyword input. Depending on those keywords, the header record may be followed by a list of output times. There follows an unlimited list of sensor definition records; input varies depending on specific sensor characteristics. As also shown in the figure, "moving" sensors require a list of waypoints following the basic sensor definition record.

```
SCIPUFF SENSOR [keywords]
[outputTime [units]   !Optional list of output times
...
END]
[type] input class choice [name]  !Define individual sensors
[time location [orientation]  !Waypoint list (only for moving sensor)
...
END]                          !Terminates waypoint records
..
```

Figure 4-10
General Structure of the SCIPUFF Format Sensor Location File

User-defined inputs are shown in italics; non-italicized strings must appear exactly as shown. Brackets denote optional inputs. (Comments shown after exclamation points are not present in an actual file.)

The optional keywords on the header record can be used to specify the coordinate system of the sensor locations and control output times and format. Specific keyword descriptions are given in Table 4-4.

Table 4-4
Header Record Keywords and Input for SCIPUFF Sensor Location Format

Keyword Description	Keyword	Input	Result
Coordinate system for sensor locations, which may be different from project coordinates. The absence of any of these keywords implies that locations are in project coordinates.	LATLON LL	None	Sensor coordinates in spherical (lat/lon) system.
	UTM	Zone (INTEGER)	Universal Transverse Mercator.
	CART KM	None	Cartesian system with origin at project reference location.
Start time for sensor output. No output will be given before this time. Default is project start time. Will be superseded if list of output times defined. See below.	START	Time (REAL or [YYYYMMDD:] HH:MM:SS.SS)	Simple real number interpreted as time relative to project start time. Otherwise absolute time used with the same time convention (local or UTC) as for the dispersion calculation. If date is not given, project start date assumed.
		[*Time units*]	Optional time units for relative start time. Valid units are S, SEC, SECONDS, M, MIN, MINUTES, H, HRS, HOURS. Default is seconds.
Specifying averaging times, either for fixed interval or list of specific times.	AVERAGE TAVG AVG	Averaging time (REAL) followed by optional time units or character string 'LIST'	A real number is interpreted as the time-averaging period. 'LIST' requires a list of averaging periods immediately following the header record.
		[Time units]	Optional units for time interval. Valid units are S, SEC, SECONDS, M, MIN, MINUTES, H, HRS, HOURS. Default is seconds.
Specifying output times, either by fixed interval or list of specific times.	OUTPUT	Time interval (REAL) or character string 'LIST'	A real number is interpreted as the output time interval. 'LIST' requires a list of times to immediately follow the header record.
		[Time units]	Optional units for time interval. Valid units are S, SEC, SECONDS, M, MIN, MINUTES, H, HRS, HOURS. Default is seconds.

Note that some of the keywords require input, which then must immediately follow that keyword. No check is made for conflicting keywords, for example, specifying both 'LL' and 'UTM'. In such cases, the last keyword supersedes. Unrecognized strings are ignored. The absence of these keywords results in the default settings described in the table.

Some examples of valid header records are given in Figure 4-11. Note that most of the keywords and input in the examples could be combined; for example, 'UTM 18' and 'OUTPUT LIST' could go on the same header record.

```
SCIPUFF SENSOR UTM 18            !Sensor locations in UTM zone 18
...
SCIPUFF SENSOR OUTPUT 1 HOUR     !Sensor output in one hour intervals
...
SCIPUFF SENSOR AVERAGE 1 HOUR    !Sensor output averaged over one hour
                                 !periods
...
SCIPUFF SENSOR OUTPUT LIST       !List of output times must follow
...
SCIPUFF SENSOR START 60 MIN      !Output commences one hour after start
                                 !of dispersion calculation
...
SCIPUFF SENSOR START 20070101:12:00:00  !Output commences at
                                        !12:00 January 1, 2007
```

Figure 4-11
Examples of Header Records in a SCIPUFF Sensor Location File

As shown in Figure 4-11, the header record must be followed by a list of output times if the string 'OUTPUT LIST' is present. As with the input associated with the 'START' keyword, output times given as simple real numbers are interpreted as relative to the project start time while those given in [YYYYMMDD:]HH:MM:SS.SS format are absolute. Note that the list cannot have mixed relative and absolute times. In addition, as with the 'START' keyword, optional units can be given for relative times. The list of output times is terminated by a line containing the single string 'END'. Two examples of valid output time lists are given in Figure 4-12. The first uses time relative to the start of the calculation; the second uses the date and absolute time format.

```
SCIPUFF SENSOR OUTPUT LIST
 30 SEC      !First output 30 seconds after start of calculation
 5 MIN       !Second output at 5 minutes
 0.5 HOUR
 2 HRS       !Last output at 2 hours; no subsequent output
END
...

SCIPUFF SENSOR OUTPUT LIST
 20070101:16:00:00   !First output at 16:00 January 1, 2007
 20070101:17:30:00
 20070101:20:00
 20070102:01:00:00   !Final output at 0100 January 2, 2007
END
...
```

Figure 4-12
Two Examples of Output Time Lists in a SCIPUFF Sensor Location File

Following the header record and output time list, if present, are the records defining specific individual sensor parameters such as location, output characteristics, and material. Because there are so many combinations of sensor types and outputs, it is not possible to illustrate them all concisely in Figure 4-12. The general structure of a sensor definition record is shown consisting of optional sensor type keywords followed by input (mostly numerical) that may depend on the sensor type, a class giving the general nature of the sensor output, followed by input choices that depend on the sensor class. Finally, an optional name may be associated with the sensor. Note that all keywords and input must be space-delimited; numerical inputs are read in free format.

Table 4-5 describes the sensor type keywords; Table 4-6 gives the corresponding input requirements. Single-point (defined without a sensor type keyword), moving, and line-of-sight (LOS) sensors all require the sensor location; it is the starting location for moving sensors. LOS sensors additionally need parameters that define the orientation and range of the line integral. (Note that LOS sensors can also move.)

Table 4-5
Sensor Type Keywords

Sensor Type Keyword	Description
*None (*Default)	The absence of a sensor keyword implies a single-location, stationary, point sensor.
MOVING	Denotes a non-stationary sensor and requires a list of waypoints to follow. Must come first if used with 'LOS' keyword.
LOS	Denotes a "line-of-sight" sensor that outputs a concentration line integral. Keyword 'MOVING', if present, must come first.

Table 4-6
Required Sensor Input for Various Sensor Types

Sensor Type Keyword	Input	Input Description
None (Default) MOVING LOS	*X* (REAL) *y* (REAL) *z* (REAL) [*zRef*]	Horizontal location (*x, y*) in project coordinates, unless specified with a coordinate system keyword (Table 4-4). For lat/lon coordinates, *x* refers to East longitude, *y* to North latitude. Vertical location, *z*, is in meters. *zRef* is an optional keyword indicating the height reference: 'AGL' for height above local ground level; 'MSL' relative to mean sea level. 'AGL' is used if no reference is given.
LOS	*azimuth* (REAL) *elevation* (REAL) *range* (REAL)	Parameters defining line orientation and length. Must follow location input. *azimuth* is the clockwise rotation in a horizontal plane from North (degrees), *elevation* is the rotation above the horizon in a vertical plane (degrees), and *range* is the path length (meters). Setting *range* ≤0 implies an infinite path length (or terminated by intersection with the ground).

Table 4-7 gives the sensor classes that generally characterize sensor output. Note that for some classes, the character of the output is modified by appending certain strings to the basic class string, for example, 'CONC:INT' modifies concentration output (class 'CONC') so that it is integrated in time (':INT').

Table 4-7
Sensor Classes

Class	Description
CONC[:INT][1]	Instantaneous concentration
MC[:INT][1, 2]	Multicomponent species concentrations
MET[2]	Output of wind velocity and other meteorological quantities

Notes:
[1] Appending ':INT' to class string results in time-integrated output. Invalid with LOS sensor.
[2] Not valid with LOS sensor type.

The input choices for a given sensor class usually consist of material names, except for 'MET' class, where only a single, optional choice is available (see Table 4-8). For some sensor classes, additional optional input can be encoded into the choice string by appending appropriate numerical or character input after a colon. These are fully described in Table 4-7. The optional sensor name is limited to 64 characters without spaces. It is basically used to annotate the list of sensors because it does not appear on the output file.

Table 4-8
Choices for Various Sensor Classes

	Choice	Description
CONC	*MatName*[:*igrp*].	Material name (CHARACTER); must match one of the material names in the project input file. The subgroup identifier (INTEGER), appended after a colon, is optional and can be used to select a particular size group for a particle material, or select vapor (*igrp* = 1) liquid droplet (*igrp* = 2) for a liquid material. A value of zero (default value if *igrp* is missing) implies total concentration for the specified material, that is, sum over all subgroups.
MC	*MatName*:(s_1, s_2, ... ,s_{n+1})	Material name (CHARACTER); must match the multicomponent material name. s_1, s_2,... (CHARACTER) represent names of multicomponent species. The names are comma-delimited and must be contained within parentheses following the colon. In the absence of any name inputs, all multicomponent species values are output. All MC type samplers must have the same list of multicomponent species.
MET	[TURB]	The only valid (optional) choice for a MET class sensor is 'TURB', which results in the output of turbulence and boundary layer quantities.

Figure 4-13 shows that MOVING sensors require a list of waypoints giving location (and orientation for LOS sensors) for times relative to the project start time (unlike with output start time or time list, absolute times cannot be specified). This list must immediately follow the basic sensor definition record. There is no limit to the number of waypoints. The format of the location and orientation input is as given in Table 4-5 for the MOVING and LOS sensor input. The trajectory of a moving sensor is defined by linear interpolation in time within the sequence of waypoints.

```
SCIPUFF SENSOR UTM 18
336 4250 0 CONC TRACER                      Sensor1
MOVING 338 4250 0 CONC:INT TRACER           Sensor2
 0.3 336 4251 10
 0.5 330 4252 100
 0.9 326 4251 10
END
LOS 336 4250 0 150 15 -999 CONC SF6         Sensor3
MOVING LOS 338 4254 0 270 30 -999 CONC SF6 Sensor4
 0.25 338 4254 0 360 30 -999
 0.50 338 4254 0  90 30 -999
 0.75 338 4254 0 180 30 -999
 1.00 338 4254 0 270 30 -999
END
336 4250 100 MET                          Sensor5
336 4250 10  MET     TURB                 Sensor6
336 4250 0   MC TRACER:(NO2,SO2,O3)      Sensor7
```

Figure 4-13
SCIPUFF SENSOR Location File Showing Several Examples of Sensor Input

Figure 4-13 is an example of a sensor input file using several input options. All sensor locations are in UTM coordinates. The first sensor, labeled 'Sensor1', gives a simple concentration time history of the material 'TRACER' at ground level. Sensor2 is a moving sensor giving the time-integrated concentration of 'TRACER' along the trajectory. Waypoints for the sensor are specified at 0.3, 0.5, and 0.9 hours after the start of the calculation: the sensor begins at ground level, moves up to 100 m at 0.5 hours, and moves back down to 10 m at 0.9 hours. The sensor remains fixed at the last location after 0.9 hours.

Also shown are two LOS sensors for the material 'SF6'; the first, Sensor3, is stationary while the second has a fixed location and elevation angle but rotates through 360° over 1 hour. Both LOS sensors have unlimited range.

Sensor5 and Sensor6 are examples of meteorological sensors. The first gives mean velocity and temperature, while the latter also gives turbulence and boundary layer information.

The last sensor, Sensor7, shown in Figure 4-13 is 'MC' and samples the concentrations of three species NO_2, SO_2, and O_3 for the multicomponent material 'TRACER'.

Note that model runtimes increase when the user specifies a large number of samplers and desires time-averaged concentrations at these samplers. If the user is interested in calculating only time-averaged concentrations at surface locations, it is recommended that a minimum of samplers be specified in the sampler file and to use the new post-processor, sciDOSPost, that can calculate time-averaged surfaced concentrations at specified receptor locations after the SCICHEM simulation is completed.

4.5 Meteorology Input

4.5.1 Observation File Format

A meteorological observation input file consists of a header section that specifies the file type, the number of observation variables, their names and units, followed by the numerical data.

The header structure is shown in Figure 4-14, and individual records are described in the text that follows.

```
[# comment]
...
ftype
nvar [nvarp]
name_1  name_2  name_3 ... name_nvar
unit_1  unit_2  unit_3 ... unit_nvar
[pname_1  pname_2  pname_3 ... pname_nvarp]
[punit_1  punit_2  punit_3 ... punit_nvar]
missing [zref]
```

Figure 4-14
Header Structure for a Meteorology Observation File; Records and Variables in Brackets Are Optional or Required Only if *nvarp* Is Given

comment: Optional comments are indicated by '#' in the first column. There is no limit to the number of comment lines.

ftype: The file type, which can be 'PROFILE' or 'SURFACE'. (Only these two types are recognized by SCICHEM.) A *SURFACE* file has only one observation for each station and is typically associated with near-surface measurements of wind and/or boundary layer parameters such as surface heat flux or mixing-layer height. A *PROFILE* file generally has more than one observation height at a station and is used when vertical profiles of wind, temperature, and so on are available, for example, from upper air soundings.

nvar: The number of observation variables given in the file, read with free format. If **nvarp** is given, **nvar** is the number of fixed variables for a *PROFILE* file. Fixed variables are not functions of height, and these are indicated in Table 6-1. **nvar** must be at least 4 (station id, time, and horizontal position are the minimum requirements). **nvar** + **nvarp** cannot exceed 30 for a *PROFILE* file; **nvar** cannot exceed 22 for a surface file.

nvarp: The number of profile observation variables, read with free format. This is an option for *PROFILE* files only. Profile variables typically vary with height. Examples are height, pressure, temperature, humidity, and wind velocity. The minimum number is 3 (height and velocity).

$\mathbf{name_1}$, ... , $\mathbf{name_{nvar}}$: The observation variable names are read using **(30a8)** format.

There must be **nvar** names specified, and the order here determines the order in which variables are given in each record of the numerical data. Names recognized in SCICHEM are defined in Table 4-9; multiple specific names indicate synonyms. Other names will be ignored without causing an error so that input files with variables not needed in SCICHEM may still be used.

If **nvarp** is given, these are the names of the fixed variables. Acceptable fixed variable names are indicated in Table 4-9. Not all combinations of recognized variable names are permitted. This is discussed next.

$\mathbf{unit_1}$, ... , $\mathbf{unit_{nvar}}$: The observation variable units are read using **(30a8)** format. Only certain variables require that units be specified; otherwise, blank spaces are acceptable. Variables requiring units are indicated in Table 6-1 along with those units recognized by SCICHEM. An error message is given if a unit is unrecognized (but only for those requiring units).

$\mathbf{pname_1}$, ... , $\mathbf{pname_{nvarp}}$: The profile observation variable names are read as described for **name**, if **nvarp** is given. There must be **nvarp** names specified.

$\mathbf{punit_1}$, ... , $\mathbf{punit_{nvarp}}$: The profile observation variable units are read as described for **unit**, if **nvarp** is given.

missing: A character string of up to 8 characters used to indicate a missing or bad value in the numerical data.

zref: Optionally, the reference height in meters above the surface can be specified for *SURFACE* observations. If the reference height is omitted, a standard value of 10 m is assumed, unless the height for each observation is specified in the data record.

Table 4-9
Meteorological Variables and Their Units Recognized in SCICHEM

Variable Description	Specific Name	Units	Units as They Should Appear
Station ID[1],[2]	ID	None	None
Time[2] (intended for laboratory or other idealized situations in which date and time of day are irrelevant)	TIME	HOURS HRS MIN SEC	HOURS HRS MIN SEC
Time of Day[2]	HOUR	HOURS[3]	HOURS
Year[2]	YEAR	None	
Month[2]	MONTH	None	
Day[2]	DAY	None	
Year-Month-Day[2]	YYMMDD	None	
Julian Day[2]	JDAY	None	
X-location[2]	X	KM[3]	KM
Y-location[2]	Y	KM[3]	KM
Longitude[2]	LON	E[4] W	E W
Latitude[2]	LAT	N[4] S	N S
Wind Speed	WSPD or SPEED or SPD	KNOTS KTS M/S MPH	KNOTS KTS M/S MPH
Wind Direction	DIR or WDIR	DEG[3]	DEG
Velocity Along X- or Longitude-Axis	U	KNOTS KTS M/S MPH	KNOTS KTS M/S MPH
Velocity Along Y- or Latitude-Axis	**V**	**KNOTS KTS M/S MPH**	**KNOTS KTS M/S MPH**
Height	Z	M FEET FT	M FEET FT
Pressure	P	MB[3]	MB
Temperature	T	C K F	C K F
Humidity	H HUMID Q	GM/GM G/G GM/KG G/KG %	GM/GM G/G GM/KG G/KG %
Boundary Layer Mixing Height(2)	ZI	M FEET FT	M FEET FT

Table 4-9 (continued)
Meteorological Variables and Their Units Recognized in SCICHEM

Variable Description	Specific Name	Units	Units as They Should Appear
Pasquill-Gifford-Turner Stability Class[2]	PGT	None[5]	
Surface Heat Flux[2]	HFLUX	K-M/S C-M/S W/M/M W/M2	K-M/S C-M/S W/M/M W/M2
Monin-Obukhov Length[2]	MOL	M	M
Precipitation Index[2],[6]	PRCP	None	None
Precipitation Rate[2],[7]	PRATE	MM/HR	MM/HR
Fractional Cloud Cover[2]	FCC	None	None
Cloud Liquid Water Content[8]	CLOUD or CLOUD1 to CLOUD*ncld*	G/M^3 G/G	G/M^3 G/G
U-Velocity Std. Deviation, Large-Scale Variability	UL	KNOTS KTS M/S MPH	KNOTS KTS M/S MPH
V-Velocity Std. Deviation, Large-Scale Variability	VL	KNOTS KTS M/S MPH	KNOTS KTS M/S MPH
Large-Scale Variability Velocity Correlation Coefficient	UVL	None	None
Shear-Driven Lateral Velocity Variance	UU	M2/S2	M2/S2
Shear-Driven Lateral Velocity Variance	UU	M2/S2	M2/S2
Buoyancy-Driven Lateral Velocity Variance	VV	M2/S2	M2/S2
Vertical Velocity Variance	WW	M2/S2	M2/S2
Boundary Layer Heat Flux	WT	K-M/S C-M/S	K-M/S C-M/S
Turbulence Scale (Buoyancy-Driven)	SL	M	M
Turbulence Scale (Shear-Driven)	SZ	M	M

Notes:

[1] ID can be an 8-character alphanumeric string if it is the first variable given; otherwise, it must be an integer.

[2] Variable can be specified as fixed data on a *PROFILE* file.

[3] Unit assumed regardless of input.

[4] Default unit if none specified.

[5] Standard PGT classes converted to numerical values, that is, class A = 1, B = 2, ..., G = 7 (non-integer values are permitted).

[6] Precipitation index specified as follows: light rain 1, moderate rain 2, heavy rain 3, light snow 4, moderate snow 5, and heavy snow 6.

[7] Precipitation rate specifies only a liquid form of precipitation (that is, not frozen).

[8] If *ncld* is 1, variable may be specified as either CLOUD or CLOUD1.

The minimum requirements for meteorological observation files are that the station ID, time, location, wind speed, and height (for a *PROFILE* file only) must be specified. In addition, if certain input options are chosen—such as observational large-scale variability or observational or profile boundary layer—specific combinations of variables must be given. In particular, then, the following variables (or some combination thereof) are required as a minimum:

6. ID
7. Time (TIME, HOUR, YEAR, MONTH, DAY, YYMMDD, JDAY)
8. Wind velocity (U, V, WSPD, SPEED, SPD, DIR, WDIR)
9. Horizontal location (X, Y, LON, LAT)
10. Z if file type is PROFILE
11. UL, VL, and UVL if observational large-scale variability is specified (ENSM_TYPE='OBS')
12. Both ZI and HFLUX together or PGT or Monin-Obukhov length (MOL) if observational boundary layer is specified (BL_TYPE='OBS')
13. UU, VV, WW, WT, SL, and SZ if profile boundary layer is specified (BL_TYPE='PROF')

Cloud names are read with (A5,1.1) format to determine which cloud droplet size section the variable refers to; however, if *ncld* (specified on the MSC file) is 1, either 'CLOUD' or 'CLOUD1' may be given in the header. If *ncld* is less than the number of sections given on the observation file, a warning is displayed and the sections greater than *ncld* will be ignored.

Some combinations of variables—particularly those concerning time—are not allowed, are mutually exclusive, or result in some of the variables being ignored. In addition, the presence or absence of certain variables dictates that others be given. These situations are now enumerated:

14. Specifying TIME supersedes HOUR, DAY, MONTH, YEAR, YYMMDD, and JDAY. No error message is given, but all other time variables are ignored.
15. HOUR must be specified in the absence of TIME. HOUR must be combined with either YYMMDD, the combination of DAY, MONTH, YEAR, or JDAY. Note that YYMMDD supersedes DAY, MONTH, YEAR, which supersedes JDAY. All three variables DAY, MONTH, and YEAR must be given together. The value of the HOUR is a real number, so if the user wants to use sub-hourly meteorological data, the hour value must be specified as a fraction of an hour.
16. X and Y must be specified together. X and Y supersede LON and LAT.
17. LON and LAT must be specified together and are required if X and Y are not given.
18. U and V must be specified together. U and V supersede WSPD, and so on as well as DIR or WDIR.
19. WSPD, and so on as well as DIR or WDIR must be specified together and are required in the absence of U and V.
20. UL, VL, and UVL must be specified together. These can be used only in combination with U and V; an error occurs if they are used with WSPD and WDIR.
21. MOL supersedes PGT and HFLUX; PGT supersedes HFLUX.

The numerical data are given after the header section in the order dictated by the list of variable names. The general structure of the numerical data is shown in Figure 4-15. If **nvarp** is given, individual profiles must be separated by the fixed data record, which must begin with the string "ID:". Vertical profiles must be given with height monotonically increasing. This is also true for time, and it is further necessary that all observations at a particular time be grouped together. All **nvar** and **nvarp** variables, if applicable, for each station and/or height at a particular time must be contained on a single line of no more than 256 characters. The figure illustrates that all *nz* heights for station id_1 at $time_1$ are given before station id_2 and that those data from all *nsta* stations at $time_1$ are given before $time_2$.

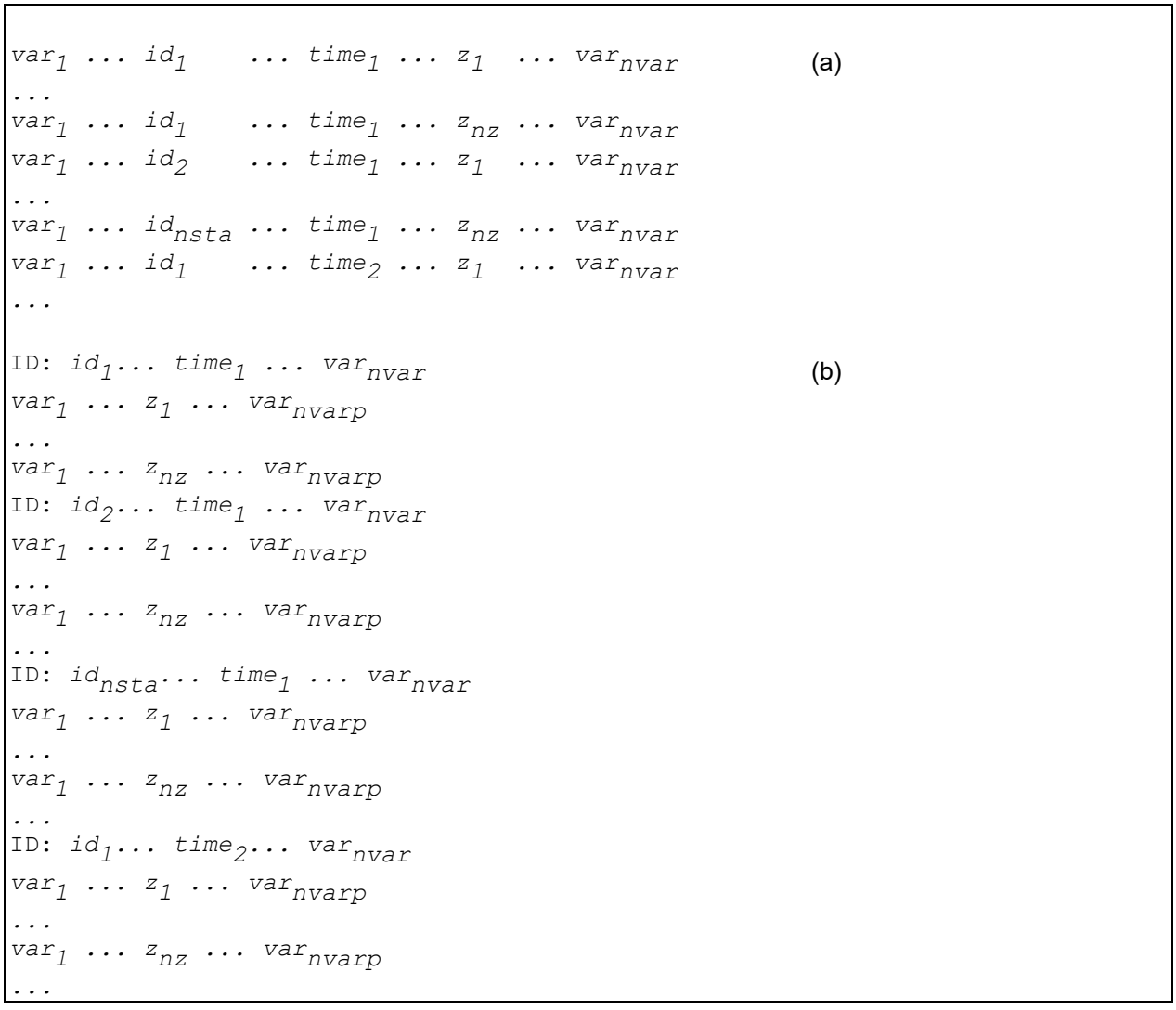

Figure 4-15
General Structure of the Numerical Data in a Meteorological Observation File: (a) Without nvarp Specified; (b) With nvar Fixed Variables and nvarp Profile Variables

4.5.2 MEDOC Format

Gridded meteorology is typically input as a MEDOC file. The original "standard" MEDOC format consists of a header section followed by numerical data for each time. An extension to this format allows SCICHEM to use meteorological fields defined in a variety of map projections, vertical coordinates, and staggered grid configurations. This information is contained in an optional header section at the beginning of the file. This will be described in the next section, after the standard format is described here. Note that since version 3.2, SCICHEM checks that valid units are specified; blank units, previously interpreted as "default" units, are no longer acceptable. Starting with version 3.4, the MMIF program (available from the EPA SCRAM website) writes MEDOC files with units included. Therefore, SCICHEM will stop execution if MEDOC files created with versions of MMIF earlier than 3.4 are used.

A sample Fortran code that reads the data for a single time break is illustrated in Figure 4-16. The first record must be either 'FFFFFFFF' for a formatted file or 'BBBBBBBB' for a binary file. The binary file is read with code identical to that shown in Figure 4-16, absent the format statements. The definitions of the input variables for the rest of the records are as follows:

IMAX, JMAX, KMAX: Number of grid points in the (*x, y, z*) directions, respectively.

NREPER: Number of special points. This information is not used for the SCICHEM input, and NREPER can be set to zero.

NVAR3D: Number of three-dimensional fields.

NAM3D: Names of the three-dimensional fields. SCICHEM requires at least the two horizontal velocity component fields, with the names 'U' and 'V'. SCICHEM will also read the vertical velocity component, 'W' (required if terrain elevation is given as a two-dimensional field), potential temperature 'T' or absolute temperature 'TA'. In addition, humidity ratio, 'H', pressure 'P', and cloud liquid water content, 'CLD' may be specified. All other names are ignored. Units are specified in **UNIT3D**.

UNIT3D: Units of the 3-D fields. The velocity fields 'U', 'V', and 'W' must be in meters per second 'M/S'; temperature ('T' or 'TA') in degrees Kelvin 'K'; pressure 'P' in millibars 'MB'; and humidity 'H' and cloud liquid water 'CLD' in grams moisture per grams dry air ('G/G'). Note that units must be specified; no defaults are assumed.

NVAR2D: Number of two-dimensional fields.

NAM2D: Names of the two-dimensional fields. SCICHEM recognizes the following two-dimensional fields if provided: terrain elevation above mean sea level (required if vertical velocity is given), 'REL' or 'TOPO'; surface roughness 'ZRUF' [or 'ZRUF(T)' if time-varying]; planetary boundary layer height (above ground level) 'ZI' or 'PBL_HITE'; surface heat flux, 'HFLX' or 'SFC_HTFX'; friction velocity, 'USTR'; precipitation rate, 'PRATE' or 'PRECIP'; accumulated precipitation, 'ACCPR' or 'PRECIPTOT'; fractional cloud cover, 'FCC' or 'CC'; albedo 'ALBEDO'; and leaf area index, 'LAI'. All other variables are ignored. Units are specified in **UNIT2D**.

UNIT2D: Units of the 2-D fields. Terrain ('REL' or 'TOPO'), roughness 'ZRUF' and boundary layer height ('ZI' or 'PBL_HITE') must be in meters 'M'; surface heat flux ('HFLX' or

'SFC_HTFX') must be in watts per square meter 'W/M2'; friction velocity 'USTR' in meters per second M/S; precipitation rate ('PRATE' or 'PRECIP') must be in millimeters per hour 'MM/HR'; accumulated precipitation ('ACCPR' or 'PRECIPTOT') in 'MM'. Because fractional cloud cover, 'FCC' or 'CC', 'ALBEDO', and 'LAI' are dimensionless, the recommended units are 'DIMLESS'; however, blanks are acceptable.

```
C     RECORD 1 - FILE FORMAT ('FFFFFFFF' or 'BBBBBBBB')
      READ (1,9001) FFLAG
C
C     RECORD 2 - NAME OF CODE - NOT USED IN SCICHEM
      READ (1,9001) CODENAME
C
C     RECORD 3 - TIME
      READ (1,9002) IDAY,IMONTH,IYEAR,IHOUR,IMIN,ISEC
C
C     RECORD 4 - INITIAL TIME OF CALCULATION - NOT USED IN SCICHEM
      READ (1,9002) JDAY,JMONTH,JYEAR,JHOUR,JMIN,JSEC
C
C     RECORD 5 - NUMBER OF GRID POINTS, KEY POINTS, VARIABLES
      READ (1,9002) IMAX,JMAX,KMAX,NREPER,NVAR3D,NVAR2D
C
C     RECORD 6 - NOT USED FOR SCICHEM
      READ (1,9002) IDUM,IDUM,IDUM,IDUM,IDUM,IDUM
C
C     RECORD 7 - NOT USED FOR SCICHEM
      READ (1,9002) IDUM,IDUM,IDUM
C
C     RECORD 8 - GRID AND TIMING INFORMATION  (KMAX+11 VALUES)
      READ (1,9003) (SZ(K),K=1,KMAX),DX,DY,XO,YO,LAT,LON,
     &              DUM,DUM,DUM,DUM,ZTOP
C
C     RECORD 9 - NAMES AND UNITS (NREPER+2*NVAR3D+2*NVAR2D VALUES)
      READ (1,9001) (NAMDUM,N=1,NREPER),
     &              (NAM3D(N),N=1,NVAR3D),(UNIT3D(N),N=1,NVAR3D),
     &              (NAM2D(N),N=1,NVAR2D),(UNIT2D(N),N=1,NVAR2D)
C
C     RECORD 10 - NOT USED IN SCICHEM
      READ (1,9003) (DUM,N=1,3*NREPER)
C
C     RECORD 11 - 3D VARIABLES
C                       (NVAR3D SETS OF IMAX*JMAX*KMAX VALUES)
      DO 21 N=1,NVAR3D
21      READ (1,9003) (((VAR3D(I,J,K,N),I=1,IMAX),J=1,JMAX),K=1,KMAX)
C
C     RECORD 12 - 2D VARIABLES  (NVAR2D SETS OF IMAX*JMAX VALUES)
      DO 41 N=1,NVAR2D
41      READ (1,9003) ((VAR2D(I,J,N),I=1,IMAX),J=1,JMAX)
C
 9001 FORMAT(6(A8,1X))
 9002 FORMAT(6(I12,1X))
 9003 FORMAT(6(F12.4,1X))
```

Figure 4-16
Fortran Pseudo-Code for Reading a Formatted MEDOC Input File

SZ: Array of **KMAX** vertical grid coordinates in meters. SCICHEM assumes a terrain-following coordinate transformation.

DX, DY: Horizontal grid spacing in meters.

XO, YO: Horizontal grid origin (SW corner) coordinates in km.

LAT, LON: Horizontal grid origin (SW corner) coordinates in degrees.

ZTOP: Vertical meteorology domain height in meters. If the parameter is not specified, the domain height is assumed to be **SZ(KMAX)**.

The MEDOC file format described in Figure 4-16 is more general than that used by SCICHEM. Variables not used in the SCICHEM application are indicated as dummy variables in the figure.

4.5.3 Extended MEDOC Header Format

As mentioned in the previous section, the MEDOC format has been extended to use a variety of map projections, vertical coordinates, and staggered grids by means of a header section appearing at the beginning of the file. This section is not required for models using spherical or Cartesian (UTM) horizontal coordinates if they also use the standard terrain-following height vertical coordinate (though these too can be defined in the header).

The first line in this section (and, therefore, of the file) consists of a keyword denoting the horizontal map projection. The number of lines in the section varies depending on the specifics of the vertical coordinates and grid. The standard MEDOC header lines will then follow, beginning with the format definition string 'FFFFFFFF' or 'BBBBBBBB'; see previous section. Because the first record of the MEDOC file is used to determine the format of the file (ASCII or binary), the map projection keyword must begin with the letters 'F' or 'B', as appropriate. The remainder of the string consists of the keywords given in Table 4-10. Therefore, the first record of a file using the Lambert Conformal projection is 'FLAMBERT' for an ASCII file and 'BLAMBERT' for binary.

The records that follow contain information required to define the map projections as well as the vertical coordinates and grid staggering. The general format of these records for an ASCII file is a description of the variable beginning with the character "#" and ending with the character "="; variables are read from the characters to the right of the equal sign in free format. The maximum line length is 80, and data are space-delimited; commas are invalid. The general layout of the header section is given in Figure 4-17. *MapKeyword* gives the model map projection; recognized strings are given in Table 4-10. *lat1*, *lat2*, *UTMzone* denote optional inputs for particular map projections, also shown in Table 4-10. *VertCoordKeyword* represents the vertical coordinate types given in Table 4-11; additional input is required only for SIGMAF. The number of staggered three- and two-dimensional fields is given by *nstg3d* and *nstg2d*, respectively; they are followed by the corresponding number of grid location records. The name of the staggered variable, *FieldName*, must be the same as one of the field names defined in the standard MEDOC header. The integers *ix*, *iy*, and *iz* define the grid location of *FieldName* relative to a grid cell center for the *x*–, *y*–, and *z*–coordinate directions, respectively. For a binary file, the records will contain only the input data without the descriptions. Note that the description to the left of the equal sign (for ASCII) is ignored and the order of the lines must be as described next.

Table 4-10
Recognized Map Projections and Associated Input

Projection (Keyword)	Description/Input
Lambert Conformal (LAMBERT)	Lat1, Lat2 (REAL) – standard latitudes where map projection is true (degrees North)
Polar Stereographic (POLAR)	Lat1 (REAL) – standard latitude where map projection is true (degrees North)
Rotated Polar Stereographic (ROTPOLE, RPOLE, ROTPOLR)	None
Mercator (MERCATR, MERCATO, or MERCTR)	Lat1 (REAL) – standard latitude where map projection is true (degrees North)
Universal Transverse Mercator (UTM)	Zone (INTEGER)
Spherical latitude/longitude (LATLON or LL)	None
Rotated spherical latitude/longitude (RLATLON, ROTLL, or LLROT)	None
Cartesian (CART or CARTESI)	None

The data required to define the horizontal map projections are given on a single record following the projection keyword. These are defined in Table 4-10. Because no input is required for spherical, rotated polar, rotated spherical, and Cartesian coordinates, this record must be omitted for those cases.

```
[MapKeyword
[# Map Parameters       =  [lat1  [lat2]] [UTMzone] ]
 # Vertical Coordinate  =  VertCoordKeyword
[# Top & Nominal Press  =  Pt  P00
 # Tsrf, Lapse, Tiso    =  Ts  Tlapse Tiso]
 # No. Staggered Fields =  nstg3d  nstg2d
[# Staggered Field      =  FieldName    ix  iy  iz
...]
FFFFFFFF
...
```

Figure 4-17
General Structure of the Special Native Coordinate Header Section

Table 4-11
Recognized Vertical Coordinates and Associated Input

Vertical Coordinate (Keyword)	Description/Input
Sigma pressure, non-hydrostatic (SIGMAF) ["F" denotes that grid point heights are fixed in time]	P_t, P_{00} (REAL): top level and nominal surface pressure level (Pa) T_{s0}, A [,T_{iso}] (REAL): reference surface temperature (K), reference temperature difference (K), and optional isothermal layer temperature (K) [Input given on two records: P_t and P_{00} first followed by T_{s0}, A, T_{iso}]
Sigma height, referenced to mean sea level (SIGMAZ)	None
Sigma height, referenced to minimum terrain elevation (SIGMAZM)	None
Sigma height, referenced to minimum terrain elevation (SIGMAZM)	None
3-D, time-varying height above ground level (HEIGHT, Z3DAGL, or HGHT-AGL)	None
3-D, time-varying height above mean sea level (Z3D, Z3DMSL, or HGHT-MSL)	None

The vertical coordinate definition follows the map projection data record. Currently only two one-dimensional coordinates are recognized: terrain-following pressure (as defined for the non-hydrostatic MM5 model) and terrain-following height coordinate. Only the sigma pressure coordinate requires additional input, which follow on the next two records. To handle all other types of vertical coordinates, a three-dimensional, time-varying height field can be used. This requires the heights for all grid cell centers to be defined at each time on the file but allows the use of any of the many commonly used one-dimensional vertical coordinates not explicitly supported here—such as pressure sigma and hybrid coordinates—as long as the grid heights can be defined.

The last input of this header section defines the grid locations of the model fields (three-dimensional and two-dimensional). The default location for any variable is assumed to be a grid cell center. The shift in location of any variable from this location (grid staggering) is defined here using three integers for the coordinate directions x, y, and z: 0 for no shift; 1 for a shift in the positive directions; –1 for a shift in the negative direction. (All shifts are assumed to be a half grid length in the appropriate direction; that is, fields are defined on cell faces or corners.) Typically, only the velocity components are shifted while the scalar fields (for example, temperature) and 2-D fields (for example, terrain height) are located at cell centers. However, to be completely general, the input allows for an arbitrary number of variables to be shifted in any (or all) directions. Therefore, the first record (following the vertical coordinate definitions) gives the number of 3-D and 2-D fields that are shifted from the default cell center location. There follows a corresponding number of records giving the field name (which must match a variable

name given later in the standard MEDOC header) and appropriate integers defining its staggered location. If no fields are staggered, only the record giving that information is required. Note that SCICHEM does not currently support staggered locations for any 2-D fields. In addition, the vertical velocity field may not be staggered unless the horizontal components are also (horizontally) staggered. Some variables defined in the standard MEDOC header have modified interpretations for the map projections described in the previous section. The projections all need a reference point (latitude and longitude) that defines the origin of the horizontal model coordinates, that is, where $(x, y) = (0, 0)$. For these projections, this location is defined using the latitude/longitude variables normally giving the South-West corner of the domain. In addition, the variables normally used to give the UTM or Cartesian coordinates of the SW corner will instead define the model (x, y) coordinates (in km) of the lower left corner (cell center) relative to the origin at the reference latitude/longitude. Note that in the case of rotated spherical coordinates, this will be in terms of *model* longitude and latitude.

Another modification to a standard MEDOC variable involves the vertical coordinate. The standard MEDOC vertical coordinate is terrain-following height (corresponding to the vertical coordinate keyword "SIGMAZ") but now will be interpreted as the vertical coordinate specified in the special header section. Furthermore, the levels will be given in the order corresponding to the model vertical indexing. For example, the first computational level in some sigma pressure models corresponds to the model top, so the first level given in the MEDOC file would be 0, with subsequent levels increasing monotonically to 1 (at the ground). This implies that the first level of the 3-D fields read later from the file is the top level. (SCICHEM will re-order because it works with height increasing from the ground.) Note that some models such as COAMPS that work in sigma height coordinates still use a vertical indexing system that starts at the model top. This requires the vertical coordinate to be specified as monotonically decreasing. In all cases, the sigma levels will correspond to cell centers.

4.5.4 WRF Input

A recent enhancement allows gridded meteorology output from the WRF model to be read directly by SCICHEM without the need for pre-processing with the MMIF program. WRF input is through a list file, as described in Section 4.5.5. The particular features required of a WRF file by SCICHEM are described here. Foremost is that the files are in NetCDF binary format.

Only the velocity components U, V, and W and fields needed to compute grid cell heights (PH, PH(B), and HGT) are required. However, it is strongly recommended that temperature (T), pressure (P and PB), and humidity mixing ratio (QVAPOR) also be included.

All of the 2-D fields, aside from HGT, are strictly optional. However, because using the boundary layer as modeled by WRF results in the most accurate dispersion calculation, it is strongly recommended that all of the fields pertaining to the atmospheric boundary layer be included. These are PBLH, HFX, UST, ZNT, QFX, TH2, and Q2. Note that if ZNT is absent, surface roughness will be set based on LU_INDEX (if available). The use of LU_INDEX requires SCICHEM to associate a roughness with each category based on season, and there is some ambiguity in exactly how this should be done. Therefore, the use of ZNT directly is strongly recommended. See Table 4-12.

Table 4-12
WRF Fields Used in SCICHEM

WRF Field Name	Description
U, V	Horizontal velocity vector components (m s^{-1})
W	Vertical velocity component (m s^{-1})
T	Perturbation potential temperature (K)
P, PB	Pressure, base state, and perturbation (Pa)
QVAPOR	Humidity mixing ratio (kg kg^{-1})
PH, PHB	Geopotential, base state, and perturbation (m^{-2} s^{-2})
HGT	Terrain height (m)
HFX	Surface sensible heat flux (W m^{-2})
QFX	Surface moisture flux (kg m^{-2} s^{-1})
ZNT	Surface roughness (m)
LU_INDEX	Landuse category
ALBEDO	Surface albedo
UST	Surface friction velocity (m s^{-1})
PBLH	Boundary layer height (m above ground level)
TH2	Potential temperature at 2 m (K)
Q2	Humidity mixing ratio at 2 m (kg kg^{-1})
RAINC, RAINNC, RAINSH	Accumulated rain in mm
MAP_PROJ	1=Lambert Conformal; 2=Polar Stereographic; 3=Mercator
TRUELAT1	Latitude where the projection is true
TRUELAT2	Latitude where the projection is (also) true
MOAD_CEN_LAT	Latitude of model grid origin
STAND_LON	Longitude of model grid origin
DX	Model grid spacing (west-to-east) in meters
DY	Model grid spacing (south-to-north) in meters

Files with single or multiple times can be used. In fact, WRF files with overlapping time periods may be used. It should be noted that SCICHEM reads the time from the WRF file and ignores any time information encoded in the file name. SCICHEM looks specifically for the global attribute 'SIMULATION_START_DATE' (string with date and time encoded as YYYY-MM-DD_HH:MM:SS) and the variable 'XTIME' (minutes since the simulation start) to define time. Furthermore, it uses the length of the CHAR variable 'Times' to determine the number of times on a particular WRF file. Note that an error will occur if any of these is absent on the file.

SCICHEM uses several global attributes to define the horizontal grid, including map factors for converting model coordinates and distances to "true" values on the spherical earth. These are given in Table 4-13. (SCICHEM also reads the first (southwest) values of the fields 'XLAT' and

'XLON'.) It also checks the name of the land use scheme defined by global attribute MMINLU, along with the corresponding number of categories in NUM_LAND_CAT.

Table 4-13
WRF File Global Attributes Used in SCICHEM

WRF Global Attribute	Description
MAP_PROJ	1=Lambert Conformal; 2=Polar Stereographic; 3=Mercator
TRUELAT1 TRUELAT2	Latitudes where the projection is true
MOAD_CEN_LAT	Latitude of model grid origin
STAND_LON	Longitude of model grid origin
DX	Model grid spacing (west-to-east) in meters
DY	Model grid spacing (south-to-north) in meters
MMINLU	Name of landuse scheme
NUM_LAND_CAT	Number of landuse categories

Table 4-14
Valid File Types for "SCIPUFF_LIST" Input File

File Type	Description
MEDOC	Gridded input type. See Section 4.5.2. Specified file is a single MEDOC file.
MEDOC_LIST	Specified file contains a list of MEDOC files (Section 4.5.2) in chronological sequence, as described in this section.
WRF	Gridded input type. See Section 4.5.4. Specified file contains a list of WRF files as described in this section.
PRF, SFC, OBS	Observational input types. See Section 3.5.1. OBS is used generically for either PRF or SFC types.
AERSFC	AERMET-style surface file.
AERPFL	AERMET-style profile file.
ASOS1MIN	ASOS 1-minute surface data. See Section 4.2.7.1.
TER	Terrain file. See Section 4.5.6.

4.5.5 List Input

Meteorological files can also be specified in a "list" input file. The first record specifies one of three list types: "SCIPUFF_LIST", "WRF", or "MEDOC". The general form of a "SCIPUFF_LIST" is given in Figure 4-18, which consists mainly of a list of file type keywords and file names. Valid file types are given in Table 4-14 and generally describe the nature of the input file. Note that the file names must include full path information if appropriate. The "optional input" is relevant only for the "ASOS1MIN:" file type, as described in Section 4.2.7.1.

```
SCIPUFF_LIST
FileType1 FileName1 [optional input]
[FileType2 FileName2 [optional input]
... ]
97
```

Figure 4-18
General Structure of a SCIPUFF_LIST Input File: Square Brackets Indicate Optional Input—That Is, Multiple Files May Be Specified, but Only One Is Required

Multiple files of the same type may be given. This is most often the case for observational types but can also be done with gridded types. In all cases, the listed files are "independent," that is, they are not assumed to be sequential in time or otherwise related.

The two other list types are designed specifically for MEDOC or WRF file input. The general form is shown in Figure 4-19. Note that WRF file requirements are given in Section 4.5.4, while the MEDOC format is described in Section 4.5.2. The keyword "PATH" is used to define the path to the directory containing the files. The absence of the path record implies that the files are located in the current user directory. There follows a simple list of files in chronological order. It is also assumed that multiple files have the same domain, grid, and variables—that is, are from the same numerical model calculation.

```
ListType
[PATH=path]
FileName1
[FileName2
... ]
```

Figure 4-19
General Structure of a MEDOC or WRF List File: ListType Must Be Either "MEDOC" or "WRF"; Square Brackets Indicate Optional Input

4.5.6 Terrain File Format

The terrain input file is an ASCII text file containing a grid description header followed by terrain elevation data defined on a regular two-dimensional grid. The header consists of an optional record followed by two mandatory records. The general structure of the terrain file is illustrated in Figure 4-20. As discussed next, the first optional record is required only if the terrain file also contains landcover data. The supplied pre-processor, TERSCI, currently supports the preparation of terrain files in SCICHEM format only without landcover data (that is, it includes only elevation data).

The first record is required only if a landcover description is given on the file. In that case, the keyword "LAND_USE" followed by an equal sign must begin the record. (Any other keyword will result in an error.) The names to the right of the equal sign denote the landcover fields on the file. The permissible names and their meanings are ZRUF, surface roughness; ALBED, surface albedo; BOWEN, Bowen ratio; HCANP, canopy height; ALPHC, canopy flow index; and CATEGORY, landcover category index. Any combination of the first three fields is allowed, but the canopy height and flow index must be given together. The landcover category is given in lieu of the first five fields. Valid category indices and the corresponding landcover descriptions are

given in Section 4.5.6. Interpretation of the landcover category input is determined by the landuse data file, which is described in the following section.

```
LAND_USE = land_key1  land_key2  land_keyN
grid_type, param1, param2
x0, y0, dx, dy, nx, ny
H1,1, H2,1,...,Hnx,1, H1,2,..., Hnx,ny
land_key1
L11,1, L12,1,...,L1nx,1, L11,2,..., L1nx,ny
 ...
land_keyN
LN1,1, LN2,1,...,LNnx,1, LN1,2,..., LNnx,ny
```

Figure 4-20
General Structure of a Terrain File

The rest of the header records are defined as follows:

grid_type, **param1**, **param2**: the grid type (CHARACTER*8) can be 'LATLON', 'UTM', 'KM', 'METERS', or 'M'. If **grid_type** is LATLON, the two numerical parameters are not required. For UTM grids, **param1** (INTEGER) contains the UTM zone number; the other parameter is not required. For all other types, if **param1** (REAL) and **param2** (REAL) are specified, they contain the longitude and latitude of the grid origin, respectively. The numerical parameters are in free format.

x0, **y0**, **dx**, **dy**, **nx**, **ny**: the grid origin (REAL) for the east-west coordinate (**x0**), the grid origin (REAL) for the north-south coordinate (**y0**), grid spacings (REAL) (**dx** and **dy**), and number of grid points in the coordinate directions (INTEGER) (**nx** and **ny**). **x0** and **y0** are in degrees if **grid_type** is LATLON; otherwise, they are in kilometers. **dx** and **dy** are in the same units as the origin coordinates unless **grid_type** is METERS or M, in which case they are in meters.

Hi,j: the terrain height in meters read with (12I6) format.

The following records are given only if the first record contains the keyword "LAND_USE", as described above.

Land_KeyN: the name of the landcover field to follow, which must match one of the names given on the first record.

L1i, j, …, LNi, j: the landcover fields corresponding to land_key1, …, land_keyN, read with (12F10.0) format for all fields except "CATEGORY", which is read with (12I6) format.

The location (*i, j*) is taken to be at **x0**+(*i*-1)***dx** and **y0**+(*j*-1)***dy**.

Note that fields in both UTM and spherical coordinate systems can be included in a single terrain file essentially by combining two separate files. The UTM fields must come first and conform to the record description just given, including the header information. The spherical coordinate system records then follow, starting with the header records. The coordinate system chosen for the puff calculation will determine which fields are read.

The use of a terrain file results in a velocity field generated by interpolating either observed velocities or gridded velocity fields onto a three-dimensional grid with its horizontal extent and resolution defined by the terrain file. A calculation is then performed to ensure near-zero divergence. This calculation can be computationally time-consuming, and it is recommended that the terrain grid size generally not exceed 100 points in either direction except for special situations. Note that when used in conjunction with gridded meteorology, the terrain grid should result in significantly finer resolution, perhaps a factor of 2 or better. Otherwise, the additional calculation will not improve the dispersion calculation significantly.

4.5.7 Landuse File Format

The landuse data input file is a fixed ASCII text file containing a list of surface parameters that are to be associated with each land cover category appearing in Table 4-15. To use the category data in SCICHEM, appropriate physical parameters—surface roughness, canopy height, canopy flow parameter, albedo, and Bowen ratio—must be assigned. The values of these parameters are generally a function of season and surface moisture condition, for example, a “wet”, “normal”, or “dry”. Figure 4-21 shows the header format and a sample of the parameter values currently specified in the landuse data file; the four columns of data represent the four seasons: winter, spring, summer, and fall. The figure shows surface roughness values for the four seasons and various landuse categories. Other fields in the landuse input file include canopy height, canopy parameter, surface albedo, and Bowen ratio for dry, normal, and wet conditions. A simple algorithm determines the “season” based on Julian day and latitude; spring and fall are basically assumed to occur for 12% of the year, and their time of occurrence changes linearly from an “all summer” condition between 20°S and 20°N to an “all winter” condition at latitudes beyond 70°N or 70°S. The moisture condition is specified by the user and is applied to the entire calculation domain.

Table 4-14
Valid Indices and Associated Landuse Types for Terrain Files with First Header Record 'LAND_USE = CATEGORY'

Index	Landuse Type
1	Developed
2	Dry Cropland and Pasture
3	Irrigated Cropland
4	Missing
5	Cropland/Grassland
6	Cropland/Woodland
7	Grassland
8	Shrubland
9	Shrubland/Grassland
10	Savanna
11	Deciduous Broadleaf Forest
12	Deciduous Needleleaf Forest
13	Evergreen Broadleaf Forest
14	Evergreen Needleleaf Forest

Index	Landuse Type
15	Mixed Forest
16	Water
17	Herbaceous Wetland
18	Wooded Wetland
19	Barren
20	Herbaceous Tundra
21	Wooded Tundra
22	Mixed Tundra
23	Bare Tundra
24	Snow or Ice
25	Partly Developed
26	Not Used
27	Not Used
28	Unclassified

```
!Land Use Parameters by Season (spring,summer,autumn,winter)
!SCICHEM VERSION  3.1
num_cat=    28
num_sup=    5
super_class= 1 2 2 2 2 2 2 2 2 3 3 3 3 3 5 2 3 4 2 3 2 4 4 1 2 2 2
Roughness   (m)
1     1     1     1     !     1=Developed
0.03  0.15  0.15  0.02  !     2=Dry Cropland & Pasture
0.03  0.2   0.2   0.2   !     3=Irrigated Cropland
5.00E-02    1.00E-01    5.00E-02    1.00E-02    !     4=Missing
0.03  0.15  0.15  0.02  !     5=Cropland/Grassland
0.2   0.3   0.3   0.1   !     6=Cropland/Woodland
0.05  0.1   0.1   0.01  !     7=Grassland
0.3   0.3   0.3   0.3   !     8=Shrubland
0.15  0.15  0.15  0.15  !     9=Shrubland/Grassland
0.05  0.1   0.1   0.01  !     10=Savanna
1     1.3   1.3   0.6   !     11=Deciduous      Broadleaf   Forest
1     1.3   1.3   0.6   !     12=Deciduous      Needleleaf  Forest
1.3   1.3   1.3   1.3   !     13=Evergreen      Broadleaf   Forest
1.3   1.3   1.3   1.3   !     14=Evergreen      Needleleaf  Forest
1.1   1.3   1.3   0.9   !     15=Mixed    Forest
0.001 0.001 0.001 0.001 !     16=Water
0.2   0.2   0.2   0.2   !     17=Herbaceous     Wetland
0.5   0.5   0.5   0.4   !     18=Wooded   Wetland
0.05  0.05  0.05  0.05  !     19=Barren
0.05  0.1   0.1   0.01  !     20=Herbaceous     Tundra
0.3   0.3   0.3   0.3   !     21=Wooded Tundra
0.15  0.15  0.15  0.1   !     22=Mixed Tundra
0.05  0.05  0.05  0.05  !     23=Bare Tundra
0.002 0.002 0.002 0.002 !     24=Snow or Ice
0.4   0.4   0.4   0.3   !     25=Partly Developed
5.00E-02    1.00E-01    5.00E-02    1.00E-02    ! 26=Not Used
5.00E-02    1.00E-01    5.00E-02    1.00E-02    ! 27=Not Used
5.00E-02    1.00E-01    5.00E-02    1.00E-02    ! 28=Unclassified
1     1     1     1     !     29=Urban    Superclass
5.00E-02    1.00E-01    1.00E-01    5.00E-02    ! 30=Grassland Superclass
1.1   1.3   1.3   0.9   !     31=Forest   Superclass
0.05  0.05  0.05  0.05  !     32=Desert   Superclass
0.001 0.001 0.001 0.001 !     33=Water    Superclass


etc.
```

Figure 4-21
Format and Content of the Landuse Data File

To handle situations in which the input landcover data must be averaged over larger cells, when the model resolution is limited, a set of superclasses is defined. Each individual type appearing in Figure 4-21 is associated with one of five superclasses defined at the bottom of the figure. When combining categories from a collection of grid cells, if any category accounts for more than 50% of the total area, the entire grid cell will be assigned that category; otherwise, the grid cell is assigned the most prevalent “superclass”. The line beginning super_class provides the mapping from the basic categories into the five superclasses, which are appended to the list of 28 basic

categories and assigned indices of 1001 through 1005. Therefore, basic category 1 (Developed) maps into superclass 1001 (Urban Superclass), category 2 (Dry Cropland and Pasture) maps into superclass 1002 (Grassland Superclass), and so on.

Note that the landuse data file also contains substrate parameters for secondary evaporation modeling. This separate section of the file is added after the landuse category data and simply provides the number of predefined substrate types together with a name (for display in the User Interface) and values for porosity, tortuosity, and grain size (in meters) as required by the absorption/desorption model.

5
RUNNING SCIPUFFGUI

A GUI, SCIPUFFgui.exe, which can be used on the Windows platform, is provided as a convenience to the user for reviewing and plotting all completed projects as described in Section 7.3. This GUI can also be used to create and run namelist projects (see Section 4.1) but not keyword projects (Section 4.2). The steps for creating a new namelist project within the GUI are detailed in Appendix B. However, it should be noted that the GUI has been carried over unchanged from SCICHEM 2.0 and has not been updated to take advantage of some of the enhancements to SCICHEM 3.0 and later. The GUI may be updated in the future to be completely compatible with the latest version of SCICHEM. For the current version of the GUI, we recommend that it be primarily used to visualize model simulation results.

6
OUTPUT FILES

6.1 Surface Output Files

If deposition or dose parameters are set to true in the material definition (*group_deposition*, *total_deposition*, *group_dose*, and *total_dose* under the MATDEF namelist of the INP file; see Section 5.2), the surface integrals of dose and deposition are stored as adaptive grid files with multiple timebreaks. The dose integral, χ_T, is stored in the surface file, ***ProjectName.*DOS**, and the deposition, χ_D, in ***ProjectName.*DEP**. These files are direct-access binary files with a record length of 512 bytes (128 words) and consist of several timebreaks. Each timebreak contains a header record followed by the field data.

For multicomponent projects, SCICHEM will output additional total time-averaged concentration fields for multicomponent species in the dose file and ambient time-averaged concentration fields for multicomponent species in the ambient dose file. SCICHEM will also output incremental dry and wet multicomponent species deposition fields, if the species dosage or deposition flags have been set to *T* in the IMC file. Note that a post-processor is provided in the SCICHEM distribution to read these files, so the following descriptions are provided only for informational purposes.

The Fortran statements to write a timebreak are illustrated in Figure 6-1.

```
c----- HEADER RECORD
       write(nwrt,rec=ir) time, ngrid, nx, ny, xorg, yorg, dx, dy,
     $                    nvar, (names(i),i=1,nvar), iversion

C----- GRID INDEX ARRAY
       do ii = 1,ngrid,128
         j1 = min0(ii+127,ngrid)
         ir = ir + 1
         write(nwrt,rec=ir) (iref(j), j=ii,j1)
       end do

C----- FIELD DATA ARRAYS
       do ivar = 1,nvar
         do ii = 1,ngrid,128
           j1 = min0(ii+127,ngrid)
           ir = ir + 1
           write(nwrt,rec=ir) (fields(j,ivar), j=ii,j1)
         end do
       end do
```

Figure 6-1
Fortran Statements to Write a Surface Output File Timebreak

The header record consists of the variables:

time	(real*4)	time of the field in hours from the beginning of the calculation
ngrid	(integer*4)	total number of grid cells in the adaptive grid; a value of zero indicates the end of the file
(nx, ny)	(integer*4)	number of base grid points in the (x, y) direction
(xorg, yorg)	(real*4)	origin coordinates of the base grid
(dx, dy)	(real*4)	grid spacings of the base grid
nvar	(integer*4)	number of field variables
names	(char*4)	array of field variable identifying names
iversion	(integer*4)	SCICHEM version number

The variable names are constructed from the input material list but do not contain direct reference to the material identifier names. The field names are four-character identifiers, and the first character denotes the type of field. **M** denotes the mean field, **V** denotes the fluctuation variance, and **S** denotes the correlation length scale. Note that the scale variable is multiplied by the fluctuation variance on the output file, because the integral value is weighted by the variance. Units for the various fields are dependent on the type of surface field but are based on the material mass units (as specified as part of the material properties definitions) and SI units. For gaseous materials or individual particle size bins, the remaining three characters of the name contain the unique type descriptor number. For particle materials with multiple size bins, the total particulate mass variables are represented by a two-character integer, containing the material identifier number; the last character of the name is **T**. The material identifier is simply the position in the list of *MATDEF* namelists in the *ProjectName*.INP file. Therefore, the total mean deposition for the first material in the input file would be named **M01T**, while the variance of the fifth particle size bin for the first material would be **V005**.

The adaptive grid structure is described by the integer*4 index array, **iref,** and the field data are stored in the real*4 array **fields**. For each grid cell, **iref** points to the first refinement sub-cell, if it exists. If the grid cell, **i**, is not refined, then **iref(i) = 0**. The first **nx*ny** cells are the base grid, so **ngrid** is necessarily greater than or equal to **nx*ny**. The centers of these cells are located at

$$x_i = \mathbf{xorg} + (i - 0.5)*\mathbf{dx}, \qquad i = 1, \mathbf{nx}$$

$$y_j = \mathbf{yorg} + (j - 0.5)*\mathbf{dy}, \qquad j = 1, \mathbf{ny}$$

and the location (x_i, y_j) corresponds to cell number $(j - 1)*\mathbf{nx} + i$ in the adaptive grid.

If a cell is refined, the **iref** array contains the grid cell number of the first of four sub-cells with half the grid size of the parent cell. Suppose i_0 is the parent cell number, with grid sizes Δx_0 and Δy_0 and center location (x_0, y_0). The parent cell may be a base grid cell but is not necessarily so because the refinement process can be continued without limit. The four sub-cells are numbered

consecutively as $\{i_1 + k : k = 0, 3\}$ where **iref**(i_0) = i_1. The sub-cells are numbered counterclockwise (that is, lower left is zero, then lower right, upper left, upper right) and have center locations

$$(x_0 \pm \Delta x_0/4, y_0 \pm \Delta y_0/4)$$

and grid size ($\Delta x_0/2$, $\Delta y_0/2$).

Each cell has a complete set of field variables associated with it, so the local field value has contributions from all levels of refinement. A simple estimate of the field value at a given location (**xp**, **yp**) can be obtained using the pseudo-code illustrated in Figure 6-2. Note that this example uses a recursive subroutine call to scan the list of refinements. The **field** array in the example represents any one of the **nvar** variables in the **fields** array on the file. This estimate simply adds contributions from successive refinement levels without any interpolation across grid cells.

```
        xx = (xp-xorg)/dx
        yy = (yp-yorg)/dy

        i0 = int(yy)*nx + int(xx) + 1

        cval = 0.0

        call sum_point_val(i0,xx,yy,cval)

c ---- cval contains the local field value

c-------------------------------------------------------------------------

        subroutine sum_point_val(i0,xc,yc,cval)

        cval = cval + field(i0)

c ***  Check for refinement

        if (iref(i0) .ne. 0) then
          xc = 2.*(xc - int(xc))
          yc = 2.*(yc - int(yc))
          i1 = iref(i0) + 2*int(yc) + int(xc)
          call sum_point_val(i1,xc,yc,cval)
        end if

        return
        end
```

Figure 6-2
Fortran Statements to Calculate Field Values from the Surface Output File

6.2 Puff File

The puff file, ***ProjectName.*PUF**, is a binary file containing the complete puff data at several timebreaks together with boundary layer and continuous source information for restart purposes. The file is written using the unformatted Fortran write statement:

```
      write(lun_puf) t,
     $       npuf,((puff(i).r(j),j=1,43),i=1,npuf),
     $       npaux,(paux(i),i=1,npaux-1),
     $       nspecies,
     $       nxbl,nybl,dxbl,dybl,
     $       xbl(i=1,nxbl),ybl(i=1,nybl),
     $       zibl(i=1,nxbl*nybl),
     $       ncrel,(c_plen(i),i=1,ncrel),
     $       nsrcaux,(src_aux(i),i=1,nsrcaux)
```

where

t	(real*4)	time of the data in seconds from the beginning of the calculation
npuf	(integer*4)	total number of puffs
puff(i).r(*)	(real*4)	floating point data for puff i
npaux	(integer*4)	total number of puff auxiliary data values + 1
paux(*)	(integer*4)	floating point data auxiliary puff data
nspecies	(integer*4)	number of multicomponent chemistry species
nxbl,nybl	(integer*4)	horizontal dimensions of meteorology grid
dxbl,dybl	(real*4)	horizontal grid intervals of meteorology grid
xbl(*),ybl(*)	(real*4)	horizontal grid locations of meteorology grid
zibl(*)	(real*4)	boundary layer depth on meteorology grid
ncrel	(integer*4)	total number of active continuous releases
c_plen(*)	(real*4)	length scale associated with each release
nsrcaux	(integer*4)	total number of source auxiliary data values
src_aux(*)	(real*4)	auxiliary source data

The floating point puff data are stored as follows:

j=1-3	$\bar{x},\bar{y},\bar{z}$	puff centroid coordinates
j=4-9	σ_{ij}	puff spread moments, in the order σ_{xx}, σ_{xy}, σ_{xz}, σ_{yy}, σ_{yz}, σ_{zz}

j=10-15	α_{ij}	puff inverse moments, in the order α_{xx}, α_{xy}, α_{xz}, α_{yy}, α_{yz}, α_{zz}
j=16	$\|\sigma\|$	determinant of the puff spread moments
j=17	Q	puff mass
j=18	$\left\langle \overline{c^2} \right\rangle$	integrated mean square concentration
j=19	$\left\langle x' \overline{u'c'} \right\rangle_L$	Large-scale diagonal-*xx* turbulent flux moment
j=20	$X12$	cross-*xy* turbulent flux moment
j=21	$\left\langle y' \overline{v'c'} \right\rangle_L$	Large-scale diagonal-*yy* turbulent flux moment
j=22	$\left\langle y' \overline{v'c'} \right\rangle_B$	Buoyancy-driven diagonal-*yy* turbulent flux moment
j=23	$\left\langle y' \overline{v'c'} \right\rangle_S$	Shear-driven diagonal-*yy* turbulent flux moment
j=24	$\left\langle z' \overline{w'c'} \right\rangle$	diagonal-*zz* turbulent flux moment
j=25	$\left\langle \overline{w'c'} \right\rangle$	vertical turbulent drift moment
j=26	$\left\langle \overline{c}^2 \right\rangle$	squared mean concentration from overlap calculation
j=27-28	Λ_c, Λ_{cH}	horizontal concentration fluctuation length scales
j=29	Λ_{cV}	vertical concentration fluctuation length scale
j=30	$2T_c$	correlation time scale for the puff concentration fluctuations
j=31	f_A	linear decay factor
j=32	z_i	local mixed layer depth
j=33	z_c	puff vertical cap height; used to control puff splitting within the planetary boundary layer
j=34-36	$\overline{u}, \overline{v}, \overline{w}$	ambient wind velocity for use with Adams-Bashforth scheme

The following seven data values are integers stored as floating point values:

j=37	*type*	an identifier for the puff material and size bin type
j=38-39	*next, prev*	pointers for the linked list on the spatial grid
j=40	*grid*	grid refinement level for the spatial grid
j=41	*tlev*	refinement level for the puff time step
j=42	*tnxt*	pointers for the linked list for time stepping
j=43	*iaux*	pointer into the auxiliary array for additional puff data; the number of data values in the array for any given puff is dependent on the material type and the overall *dynamics* flags

There may be additional puff data values for each puff, depending on the user's options. These variables would appear in the following order:

j=1	$\left\langle \overline{c_T^2} \right\rangle$	mean square total concentration (for multiple size bin particle materials)
j=2	$\left\langle \overline{c}_T^2 \right\rangle$	squared mean total concentration (for multiple size bin particle materials)
j=3-10		buoyancy parameters
Next nspectot values		multicomponent species masses
Next nspectot values		multicomponent species puff overlap concentrations
Next ncorrt values		multicomponent species correlations
Next nspectot values		multicomponent species end of chemistry concentrations
j=11+3*nspectot+ncorrt		inverse puff volume
j=12+3*nspectot+ncorrt		puff chemical stage

The puff *type* identifier is simply allocated sequentially in the order that materials are specified in the *ProjectName*.INP file. Therefore, the first material is *type* = 1 if it is a gas, or the N_{bin} size bins are *type* = 1 up to *type* = N_{bin} for a particle material. Identifiers for the second material are then allocated beginning with the next available value for *type*.

6.3 Sampler Time History File

The sampler time history file is an ASCII text file containing output from the sensors specified in the sensor definition file described in Section 6.3. The output frequency is controlled by the sampler time step *dt_smp* specified in the input file. The exact output interval may vary with the adaptive puff time step described in Section 4.5 but will be between *dt_smp* and the large time

step *delt*, also given in the input file. However, if the 'OUTPUT' keyword is given in the sensor definition file header record, the output interval specified is used as described in Section 4.4.

The output format consists of a header section followed by records for each output time. All records are on a single line (no wrapping). The first line of the header section consists of a version number (for this sampler file format) followed by a record that gives the number of sensors, start time, averaging and output intervals and coordinate information. There follows a list of the sensor locations and types. Note that these lines all start with the character "#" and can be ignored when importing as a spreadsheet. Then a single header record consists of a list of variable names followed by the data, which are aligned in columns under the corresponding variable names

(CHARACTER*8). The data records consist of time (in seconds from the start of the calculation) followed by the output for sensor-1, sensor-2, and so on. Note that the output (and variable names) depends on the sensor specification, as given in Table 6-1.

Table 6-1
Sensor Output Variables

Sensor Class	Variable Names[1]	Description
CONC	C*xxx* V*xxx* T*xxx*	Mean concentration, $\overline{c}$ Concentration variance, $\overline{c'^2}$ Fluctuation correlation time scale T_c
CONC:INT	D*xxx* V*xxx*	Mean dosage, $\overline{\chi}_T = \int_0^t \overline{c}\left(t'\right) dt'$ Dosage variance, $\overline{\chi'^2}$
MC	C*sss_xxx*	Mean concentration for species *s*, $\overline{c}_s$
MC:INT	D*sss_xxx*	Mean dosage for species *s*, $\overline{\chi}_{sT} = \int_0^t \overline{c}_s\left(t'\right) dt'$
MET [*choice*=TURB] [3]	U*xxx* V*xxx* W*xxx* T*xxx* ZI*xxx* HFLX*xxx* L*xxx* UU*xxx* VV*xxx* WW*xxx* USTR*xxx*	*x*-component velocity, $\overline{u}$ *y*-component velocity, $\overline{v}$ *z*-component velocity, $\overline{w}$ Absolute temperature, T Boundary layer depth, z_i Sensible heat flux, H Monin-Obukhov length, L Shear-driven turbulence, $\overline{u_2' u_{2\,S}'}$ Buoyancy-driven turbulence, $\overline{u_2' u_{2\,B}'}$ Vertical velocity correlation, $\overline{u_3' u_{3\,S}'} + \overline{u_3' u_{3\,B}'}$ Surface friction velocity, u_*

[1] The string '*xxx*' represents a three-digit number based on the order in which the sensor was defined in the location file.
[2] Additional output for DEP class sensors for *choice* as shown. Applies only to liquid materials in projects specifying a surface substrate.
[3] Additional outputs for MET class sensors if *choice* is set to 'TURB'.

Units for mean concentration output (CONC sensors) are in mass units per cubic meter, that is, typically kg/m^3; variances units are the square of concentration units, for example, kg^2/m^6. Dosage (time-integral of concentration) is in concentration units multiplied by time, for example, kg-s/m^3, while the corresponding dosage variance is concentration units squared multiplied by time, for example, kg^2-s/m^6. For multicomponent species (MC sensors), the concentrations units depend on whether the species are particles or non-particles. For non-particle species, the units are *species_units*, as set under the control section of the IMC file (see Section 4.3.1). Aerosol particle species concentrations are always assumed to be in $\mu g/m^3$ or $\#/m^3$ or m^2/m^3 for types *P*, *PN*, and *PA* respectively.

The fluctuation correlation time is in seconds. Mean deposition output is in mass units per area, typically kg/m^2; the deposition variance unit is the square of this. The remaining surface liquid variable (R*xxx*) is in the same units as the mean deposition. The number density of BY_SIZE output units is simply per cubic meter or s/m^3 for a time-integrated sensor.

Velocities from MET sensors are in m/s regardless of the units on the meteorological input file. Temperature is absolute in degrees K. The boundary layer depth is in meters, heat flux in W/m^2, Monin-Obukhov length in meters, turbulence velocity variances in m^2/s^2, and surface friction velocity in m/s.

Examples of SCIPUFF output format are shown in Figure 6-3. Figure 6-3 (a) shows output from two sensors. The first is a concentration sensor; the second provides integrated output of some kind, that is, surface deposition or time-integrated. Figure 6-3 (b) shows output from a BY_SPECIES sensor for a single species. These examples show small numbers of sensors and species to limit the length of the output lines. Many more sensors and species can be defined, in which case the lines for each output time are simply appended (without wrapping) with appropriate sensor output.

(a)

```
   T            C001         V001         T001         D002         V002
 9.0000E+02  9.1047E-08  5.9028E-14  9.6551E+01  7.5150E-12  7.1547E-19
 1.8000E+03  1.0229E-07  9.5524E-14  9.9917E+01  1.2910E-11  9.7301E-19
 2.7000E+03  1.6559E-08  7.8615E-15  1.1125E+02  1.2908E-11  9.7268E-19
 3.6000E+03  2.1661E-11  3.0766E-18  1.5855E+02  1.2908E-11  9.7268E-19
```

(b)

```
 T              C001       V001       T001       C001_001   C052_001   C004_001   C002       V002       T002
 9.0000000E+02 0.0000E+00 0.0000E+00 0.0000E+00 2.4000E-03 3.0000E-03 6.3000E-02 0.0000E+00 0.0000E+00 0.0000E+00
 1.8000000E+03 0.0000E+00 0.0000E+00 0.0000E+00 2.4000E-03 3.0000E-03 6.3000E-02 0.0000E+00 0.0000E+00 0.0000E+00
 2.7000000E+03 0.0000E+00 0.0000E+00 0.0000E+00 2.4000E-03 3.0000E-03 6.3000E-02 0.0000E+00 0.0000E+00 0.0000E+00
 3.6000000E+03 0.0000E+00 0.0000E+00 0.0000E+00 2.4000E-03 3.0000E-03 6.3000E-02 0.0000E+00 0.0000E+00 0.0000E+00
```

Figure 6-3
Examples of Multicomponent Sensor Output

6.4 Project Log Files

The log messages from SCICHEM are output to the ProjectName.log. Information available from the log file includes SCICHEM version number, the information about meteorology used, and domain. For multicomponent projects, additional information is output to the log file—the multicomponent species list, background species read from the ambient file, and the list of species output to the DOS and DEP file. If the Aqueous-Aerosol module is used, any messages from the module are output to the ProjectName.qlog file. Lastly, any errors or warnings are written to the log file.

6.5 Project Err File

Errors, if any, encountered during the project run are also logged to the ProjectName.err file.

7
POST-PROCESSING PROGRAMS

7.1 SCIDOSPOST for Surface Values

To facilitate post-processing the SCICHEM outputs for surface concentrations and depositions, the SCICHEM distribution includes referred to as "SciDOSpost". The name is meant to indicate that it reads the DOSage file written by SCICHEM. SCIDOSPOST can generate AERMOD-style POSTFILEs that is typically required for near-source impact calculations, for example, fence line concentrations. Examples of the use of SCIDOSPOST for this purpose are provided with the 1-hour SO_2 tutorial in the SCICHEM distribution. SCIDOSPOST can also be used to calculate secondary pollutant impacts, e.g., impacts on 8-hour ozone design values, or impacts on 24-hour and annual secondary $PM_{2.5}$ concentrations. The tutorials provided with the SCICHEM distribution provide examples of these uses as well as the use of SCIDOSPOST for Class I and Class II analyses described below.

SCIDOSPOST was initially developed to perform Class I analyses for Prevention of Significant Deterioration (PSD) permit applications and Class II analyses for PSD or Minor New Source Review. Details of this type of analyses are provided below.

There are three types of "answers" required in a typical Class I analysis (as outlined in FLAG [2010][1]):

- Maximum *N*-hour average concentrations are calculated and compared to the SILs/NAAQS/increments (where *N* varies).
- Maximum design value (DV) concentrations are calculated and compared to the short-term NO_2, SO_2, and $PM_{2.5}$ SILs/NAAQS.
- Maximum annual total nitrogen and total sulfur deposition are calculated and compared to the Deposition Analysis Thresholds (DATs, Class I analyses) or other deposition criteria (Class II analyses).
- The 98th percentile change to natural background visibility extinction is calculated for each model year, with a target of no more than 5% change (Class I analyses).

It is often quite useful to know at which Class I area within one's modeling domain the maxima occurred—and even at which receptor within a Class I area the maxima occurred. SciDOSpost was designed to be flexible enough to provide these details in addition to the final "answers" required for a Class I analysis.

[1] The FLAG (2010) document is available at http://www.nature.nps.gov/air/pubs/pdf/flag/FLAG_2010.pdf.

The program requires several inputs:

1. A control file where the user requests specific answers be calculated
2. Zero or more files containing receptor sets, which can be either the Federal Land Managers (FLM)-supplied files containing receptor locations within a Class I area or user-supplied "discrete receptors", or gridded receptors specified by domain extent and grid spacing.
3. Comma-separated value files containing Tables 6–9 from FLAG (2010), which are distributed with SCICHEM (for Class I analyses)
4. A completed SCICHEM run

The SCICHEM surface dosage and deposition files, *.ADOS (ambient or background dosage), *.DOS (plume dosage), and *.DEP (deposition), are required.

A sample control file is included with the distribution and can be created at any time by the program itself using the **--sample** command-line option. See the next section for details on the control file structure.

Discrete Class II receptor location files must be prepared by the user. They should consist of ASCII (text) files containing the receptor locations, one location (point) per line, using either the longitude and latitude (in that order) or X- and Y-coordinate system. The units of X and Y can be either lon-lat or whatever other cartesian coordinate system in which SCICHEM was run, for example, UTM). The post-processor also can also read *.SAM sampler location files, ignoring all but the first two entries in each line.

Sets of gridded Class II receptors can be specified in the sciDOSpost control file by specifying the lower left and upper right (from a projected grid point of view) corners of a desired grid and the desired receptor spacing. Note that the lower left "corner" of the grid will be the location of the receptor, as opposed to the corner of a grid cell at whose center a receptor would be placed (for example, CALPUFF terminology for a grid). The upper right receptor will be some multiple of the grid spacing and may or may not match the requested upper right coordinates—but it will not exceed it. The units of the corners and spacing can be either longitude and latitude, or the X- and Y-coordinate system in which SCICHEM was run (for example, UTM).

For both discrete and gridded Class II receptor sets, the user can mix LON,LAT and X,Y (for example, UTM) coordinates—sciDOSpost will transform either set to the units used in the SCICHEM run. However, each line (starting with the keywords REC or GRID) must use self-consistent units—specifying the corners of a grid in lon-lat and the grid spacing in meters or kilometers is not supported.

The FLM-supplied modeling receptor files are included with the SCICHEM distribution but can also be downloaded from the National Park Service website.[2] The files should be used verbatim (no pre-processing or GIS re-projecting is necessary), because they contain longitude, latitude, and elevation for each point—the same file format for user-specified Class II discrete receptors. The elevation is not used by sciDOSpost. Follow the link[3] in the upper right corner with the text "Download Class I Area Receptor Data", and save and extract the contents of the ZIP file to the **Class1Area** sub-directory under the sciData directory or any other convenient location. The

[2] See https://www.nature.nps.gov/air/maps/receptors/.

[3] Direct link: https://www.nature.nps.gov/air/maps/receptors/download/ClassIData.zip.

sciData directory is set in the 'scipuff.ini' file using the SciDataDir variable under the "[Paths]" section. If SciDataDir is not defined in the 'scipuff.ini' file, sciDOSpost uses a path relative to the current run directory.

A ZIP file containing both an MS Excel Spreadsheet and CSV files with the data from Tables 5 to 10 from FLAG (2010) is included with the SCICHEM distribution. The contents of the ZIP file have been extracted to the 'Flag2010' sub-directory under the sciData directory, but the ZIP file is included for portability. If SciDataDir is not defined in the 'scipuff.ini' file, the post-processor searches the current run directory for the files by default. Note that typically Table 6 (Annual Average Natural Conditions) is preferred over Table 5 (20% Best Natural Conditions) unless otherwise recommended by the FLM or permitting authority. Table 10 is not used by SciDOSpost but is included in case it is helpful.

The user must specify a NAME for each receptor set. If the receptor set corresponds to a Class I area, the first four characters of NAME must match the Class I area receptor filename (for example, the `meve` in `meve-recep.dat` in the example that follows, representing Mesa Verde National Park) for the program to find the proper lines in the FLAG (2010) tables. Misspelling the name will likely cause the program to fail. Receptor sets containing Class II receptors have no requirements on the name.

The user may add new lines to the FLAG (2010) CSV tables, for example, to account for other areas to be treated like a Class I area or for Native American Indian lands. Care should be taken to choose a unique 4-letter code for the new area to avoid conflicting with the existing 4-letter codes.

All receptors sets (discrete or gridded) must be assigned a NAME, which must match that used in the output section (CON, DEP, VIS, and so on lines). This is different from SCICHEM 3.1 or earlier, where sciDOSpost would write the desired output for each of the receptor sets. That made sense when sciDOSpost was only a Class I post-processor but does not make sense now that it has wider applications.

7.1.1 Control File Structure

The control file for SciDOSpost is keyword-driven. Some important features of the control file are:

- Blank lines and any portion of a line after a comment character (# ; !) are ignored.
- Keywords and values can be either space-delimited or comma-delimited or a mixture.
- Any number of spaces or commas can be used between words (elements) in a line.
- All words in the control file are case insensitive, except for filenames that are used verbatim (important on Linux platforms).
- Filenames may contain spaces and commas, if enclosed by either single or double quotes.
- Keywords may be repeated. The keywords REC, CON, DEP, and VIS may be repeated as many times as desired. For other keywords, the value of the last one encountered will be used.
- The order of the lines containing keywords does not matter, except that REC and GRID lines must precede the output lines (CON, DEP, DRY, WET, or VIS) because the letter references the receptor set names defined in the former.

- Primary keywords must be the first word on a line in the control file, but leading spaces are allowed.

A typical control file is given in the following example. Note that the order of the elements of certain keywords has changed between the SCICHEM 3.1 and 3.2 releases.

```
; This file can be space-delimited or comma-delimited, or a mixture.
; Comment characters are #, ;, and !.  Blank lines are ignored.
; Keywords are not case-sensitive.  Filenames are used verbatim, and can
; include spaces if enclosed in quotes.

# The keyword PROJECT gives a space-delimited list of one or more SCICHEM
# project basenames. A list of basenames is useful if SCICHEM was run in
# sections (e.g. months of a year).

Project fc_egu1_07s3ab

# The keyword CALCulate specifies whether to include background concentrations.

calculate plume  ! plume (default) or total = ambient + plume

# Time to process. If PROJECT is a list of only 1 element (not run in sections),
# you can omit Start and Stop to process ALL data found.

Start 2010-01-01:00   ! any of these forms work, also 2010/01/01 00
stop  2010123123

# The keyword TIMEZONE specifies the timezone you want to use for the output
# concentrations, independent of the timezone used in the SCICHEM run being
# processed. If SCICHEM used LST of GMT-0500, give 0 to shift back to UTC.
# This affects N-hour concentrations (N > 1) and max daily rolling N-hour
# concentrations (because the 'day' is affected by the output timezone).
# TimeZone is relative to GMT, i.e. -5 (GMT-05) is the US East Coast.

TimeZone   -8    ! default is zero, i.e. GMT-00

# Receptor section:
# Receptor Sets can be specified by either:
#   Using the REC  keyword to specify a file containing arbitrarily-spaced points.
#   Using the GRID keyword to specify a set of regularly spaced receptors.
# NetCDF output only works with GRIDded (regularly spaced) receptor sets.
# You can give zero REC lines or zero GRID lines, but you must specify at least
# one REC or GRID to get any output.
# The Name of each receptor set is used in the Output section, below.

# RECeptors (repeatable) keyword specifies the receptor files to use.
# 2nd word is a user-specified NAME.  If the NAME matches the first 4 characters
#    in the FLAG (2010) look-up tables, it is to be treated as a Class I area
#    and VISibility obscuration can be calculated.
# 3rd word is either LONLAT (synonym: LL) or anything else for Cartesian
#    (including UTM). MUST MATCH COORDINATE SYSTEM and UNITS of the SCICHEM run!
#    NOTE: The Class I area files are lon,lat,elev so custom files must also
#    be lon,lat (elev is ignored).
# 4th word is one of:
#    1  if the receptor set is to be treated as a Class I area
#    2  if the receptor set is a Class II area (i.e. not Class I)
# 5th word is the filename. Files can be the Class I receptor files downloaded
#    from http://www2.nature.nps.gov/air/maps/Receptors/index.cfm; or can
#    contain user-specified receptors: one UTMx,UTMy, or LON,LAT pair per line.

#   Name   LL/UTM Class Filename
REC meve   LonLat 1     sciData/Class1Area/meve-recep.dat   ! Mesa Verde NP
```

```
REC wemi   LL     1     sciData/Class1Area/wemi2-recep.dat  ! Weminuche Wilderness
REC fence  UTM    2     prop_boundary.rec
rec 50m    utm    2     50m.rec

# GRID (repeatable) keyword specifies a regularly spaced receptor grid to use.
# 2nd word is a user-specified NAME.
# 3rd word is either LONLAT (synonym: LL) or anything else for Cartesian.
# 4th word is the grid spacing, DX, in cartesian units or lat-lon.
# 5th and 6th words are the coordinates of the southwest (lower left) gridpoint
# 7th and 8th words are the coordinates of the northeast (upper right) gridpoint
#   Use the same X,Y cartesian units used in SCICHEM - mostly likely km (not m).
#   If specifying a lat-lon grid, then the X's are longitude, Y's are latitude.
#   GRIDs cannot be treated as Class I areas - those REC sets are ungridded.

#     Name    LL/UTM  DX     xWest       ySouth    xEast       yNorth
GRID  2x2km   UTM     0.050  495.550     5333.400  497.550     5335.400
grid  hotspot UTM     0.005  496.123     5345.678  496.223     5345.778
grid  Example LL      0.0005 -111.059830 48.153835 -111.032951 48.171841

# Output section:
# 1st word is one of:
#    CON for concentration          (default: ug/m3)
#    DEP for total deposition       (default: kg/ha)
#    WET for wet   deposition       (default: kg/ha)
#    DRY for dry   deposition       (default: kg/ha)
#    VIS for visibility degradation (only:    percent change)
# 2nd word is one of:
#    The chemical SPECIES to process, e.g. no2 or o3 or pm25, etc.
#    dBext for the change to the background extinction coefficient for visibility
#    cont  for the contributions of each term in the equation for dBext
# 3rd word is the requested output units:
#    Gas species can be written in ug/m3, ppm, or ppb
#    Particulate species can only be written in ug/m3
#    Deposition can be written in kg/ha, g/m2, kg/m2, g/cm2, etc.
#    Visibility can only be written in Percent
# 4th word is the Receptor Set for this output, must match either a REC or GRID
# 5th word is a SPACE selection criteria, one of:
#    AllRec: Output for every receptor. If TIME=ALL, it will be like a POSTFILE.
#       This is the only choice that makes sense for GRIDs.
#    MaxRec: Output a single receptor within each receptor set, where the
#       maximum HIGH-highest (HIGH==RANK) occurred, e.g. the H8H.
#    >=N: Output all values (of HIGH==RANK) that exceed the given concentration.
#       Remember that if using 'calculate plume' you can have valid negative
#       concentrations (e.g. NOx titration of O3), so >0 might discard data.
# 6th word is a TIME or RANK selection criteria, one of:
#    All: Output values for all time Periods
#       To get a time series, use a RECeptor set with only 1 point and 'TIME=ALL'.
#    1st, 2nd,... 8th (etc) highest HIGH or RANK (which are 'synonyms').
# 7th and 8th words specify the PERIOD over which to take some STATISTIC.
# 9th word is the STATISTIC, one of:
#    Average  to take the *windowed* average (e.g. 1-8, 9-16, 17-24).
#       See the examples for 8-hr CO below.
#    MaxDaily to take the maximum PERIOD *rolling* average from each 24 hours.
#       See the examples for 8-hr O3 below. Note a rolling 1-hr MaxDaily is the
#       same as a windowed 1-hr MaxDaily value, so 1-hr NO2/SO2 use MaxDaily.
#    Sum or Total to take the sum over the PERIOD.
#        See the examples for annual N and S deposition below.
# 10th word is the output FILE TYPE:
#    CSV  Comma-separated values
#    XZY  Actually XYLLZUT: the X,Y,lat,lon, value, units, timestamp
#    POST AERMOD-style POSTFILE (values for all times and all receptors)
#    PLOT AERMOD-style PLOTFILE (a single high/rank value at all receptor)
#    NC   NetCDF gridded file in I/O API-compliant format (only for GRIDs)
```

```
#    GRD  Surfer 6 ascii grid file (only for GRIDs)
# 11th word is the FILENAME, can contain spaces if enclosed in quotes.

# Output Examples (these are just examples, you probably don't want all of them):
#
# An AERMOD-formatted POSTFILE writing every time period for every receptor.
# An AERMOD-formatted PLOTFILE writing the Design Value at every receptor.
# A data file giving all the receptors that exceed the 1-hr NO2 SIL (7.5ug/m3).
# A single line giving the NO2 Design Value at the highest 8th high receptor.
# An AERMOD-formatted PLOTFILE writing the annual average at every receptor.
#
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  no2   ug/m3  2x2km   AllRec  All    1 hr   Average    POST  no2.pst
con  no2   ug/m3  2x2km   AllRec  8th    1 hr   MaxDaily   PLOT  no2.DV.plt
con  no2   ug/m3  50m     >=7.5   1st    1 hr   MaxDaily   XYZ   no2.over.SIL.dat
con  no2   ug/m3  hotspot MaxRec  8th    1 hr   MaxDaily   CSV   no2.DV.max.csv
con  no2   ug/m3  fence   AllRec  1st    1 yr   Average    PLOT  no2.annual.plt

# An AERMOD-formatted PLOTFILE writing the Design Value at every receptor.
# A single line giving the SO2 Design Value at the highest 4th high receptor.
# A single line giving the SO2 highest 2nd-high 3hr average value.
#
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  so2   ug/m3  2x2km   MaxRec  4th    1 hr   MaxDaily   PLOT  so2.DV.plt
con  so2   ug/m3  fence   MaxRec  4th    1 hr   MaxDaily   CSV   so2.DV.max.csv
con  so2   ug/m3  hotspot MaxRec  2nd    3 hr   Average    CSV   so2.DV.max.csv

# An AERMOD-formatted POSTFILE writing every 24-hr average at every receptor.
# An AERMOD-formatted PLOTFILE writing the PM2.5 DV at every receptor.
# The highest (over space) 24-hour PM2.5 NAAQS DV (for one year).
# The highest (over space) annual  PM2.5 NAAQS    (for one year).
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  pm25  ug/m3  2x2km   AllRec  All   24 hr   Average    POST  pm25.pst
con  pm25  ug/m3  2x2km   AllRec  8th   24 hr   Average    PLOT  pm25.plt
con  pm25  ug/m3  2x2km   MaxRec  8th   24 hr   Average    CSV   pm25.DV.max.csv
con  pm25  ug/m3  2x2km   MaxRec  1st    1 yr   Average    CSV   pm25.DV.max.csv

# An AERMOD-formatted POSTFILE of the 24-hour PM10 values.
# User must manually average the output over multiple years.
#
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  pm10  ug/m3  2x2km   All     1st   24 hr   Average    POST  pm10.pst

# The highest (over space) 1-hour average CO NAAQS.
# The highest (over space) 8-hour (windowed: 1-8, 9-16, 17-24) average CO NAAQS.
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  co    ug/m3  50m     MaxRec  2nd    1 hr   Average    CSV   co.DV.max.csv
con  co    ug/m3  50m     MaxRec  2nd    8 hr   Average    CSV   co.DV.max.csv

# The 8-hour (rolling: 1-8, 2-9, ... 17-24) max daily average (MDA8).
# A gridded netCDF file of the DV
#
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  o3    ppb    hotspot MaxRec  4th    8 hr   MaxDaily   CSV   o3.DV.max.csv
con  o3    ppb    2x2km   MaxRec  4th    8 hr   MaxDaily   NC    o3.dv.nc

# Deposition (total dep) and its components dry and wet deposition,
# useful for PSD Class I analyses.
#
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
dep  N     kg/ha  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
wet  N     ug/cm2 meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
dry  N     mg/m2  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
```

```
dep  S     kg/ha  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
wet  S     kg/ha  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
dry  S     kg/ha  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
dep  N     kg/ha  wemi    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
dep  S     kg/ha  wemi    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv

# Visibility extinction coefficient (dBext) from FLAG (2010), useful
# for PSD Class I analyses. The '>5' means write each 24-hour average that
# has a dBext > 5%, useful counting the days with greater than 5% change.
#
#    Spec  Units  RecSet  Space   Time  Period  Statistic FType Filename
vis  dBext %      meve    AllRec  1st   24 hr   Average   CSV   vis_daily.csv
vis  dBext %      meve    MaxRec  8th   24 hr   Average   CSV   vis_results.csv
vis  Cont  %      meve    MaxRec  8th   24 hr   Average   CSV   vis_contrib.csv
vis  dBext %      wemi    MaxRec  8th   24 hr   Average   PLOT  vis_daily.plt
vis  dBext %      wemi    >5      1st   24 hr   Average   CSV   vis_exceedence.csv
vis  dBext %      wemi    >10     1st   24 hr   Average   CSV   vis_exceedence.csv
```

The following describes each keyword of the control file. Italics are used to indicate number values.

```
Project project_name
```

This specifies the base filename for the project. The SciDOSpost program opens and reads *project_name*.dos, *project_name*.ados, and *project_name*.dep.

```
CALC    PLUME     default, or
CALC    TOTAL
```

The CALCulate keyword specifies whether the user want to calculate plume-specific concentrations or total (plume plus background) concentrations. Plume-specific concentrations might be useful for comparison against SILs, DATs, and Class I visibility obscuration. Total (plume plus background) concentrations might be useful for comparison with the NAAQS.

```
Start 2010-01-01:00
Stop  2010-12-31:23
```

The option keywords START and STOP can be used to select the output period to process. The internal format is either **YYYYMMDDHH** or **YYYY MM DD HH**, but the program converts typical separators like **-**, /, **_**, and **:** to spaces before parsing, allowing for, for example, WRF-style time-stamps YYYY-MM-DD_HH as well as the examples above. Use the lines **START 0000 00 00 00** and **STOP 9999 99 99 99**, or omit these keywords, to process all time-stamps found in the SCICHEM output.

```
TimeZone   -8    ! default is zero, i.e. GMT-00
```

This option specifies the desired output time zone. Because the MaxDaily (see below) keyword implies a “day”, and SCICHEM can be run in either GMT or LST, the program needs to start each day in the correct time zone.

```
REC NAME   COORD  CLASS C:\path\to\NAME-recep.dat
REC meve   LonLat 1     /data/ClassI/meve-recep.dat
REC fence  UTM    2     prop_boundary.rec
```

The RECeptor keyword is repeatable. Zero or more lines starting with REC can be given. This keyword is used for specifying discrete receptors, as opposed to the GRID keyword for grids of receptors (see below).

The 2nd word gives a user-specified NAME (`NAME` in the first line above) of the receptor set. This name might be useful for distinguishing between receptors placed along a property boundary vs. grids with onsite receptors removed for a Class II analysis. For a Class I analysis, the first four characters of the name of a Class I area should match the given filename and must match the first characters found in the CSV files for the Flag (2010) look-up tables.

The 3rd word (COORD in the first line above) can be LONLAT (or LL) if the coordinates in the file are given as LON,LAT or anything else for X,Y (cartesian, most likely UTM).

Note: LON is the coordinate in the X (east) direction and so comes first. SciDOSpost will convert either to the Project Coordinate (of the SCICHEM run), so either may be specified.

The 4th word (CLASS in the first line above) specifies whether the receptors in this file are Class I (1) or Class II (2) receptors. SciDOSpost can calculate visibility obscuration for Class I receptors only.

The 5th word is the (full or relative) path and filename to the file containing the receptors. This file can contain any number of receptors, one pair of coordinates per line. It can be user-generated (Class II) or one of the FLM-specified receptor files. Note that for some Class I areas, the *xxxx* codes are only 4 characters (followed by `-recep.dat`). Other Class I areas use 4-letter codes followed by a "2" or "3", while still others are 4 letters followed by `wild-recep.dat`, regardless of whether the Class I area is a National Park or a Wilderness area. To maintain consistency, the SciDOSpost program uses only the first 4 characters of the RECeptor set filename to look up the appropriate values within the FLAG (2010) CSV files.

If the program cannot read two numerical values from the first line of the RECeptor file, it assumes that line is a comment line and skips it. This allows the SciDOSpost program to read a SCICHEM sampler (sensor) location file, *.SAM.

```
GRID  NAME    COORD   DX     xWest    ySouth    xEast    yNorth
GRID  2x2km   UTM     0.050  495.550  5333.400  497.550  5335.400
```

The GRID keyword is repeatable. Zero or more lines starting with GRID can be given. This keyword is used for specifying grids of receptors.

The 2nd word gives a user-specified NAME (NAME in the first line above) of the receptor set, similar to the NAME in the REC keyword.

The 3rd word (COORD in the first line above) can be LONLAT (or LL) if the coordinates in the file are given as LON,LAT or anything else for X,Y (for example, UTM).

Note: LON is the coordinate in the X (east) direction and so comes first. SciDOSpost will convert either to the Project Coordinate (of the SCICHEM run), so either may be specified.

The 4th word (DX in the first line above) is the spacing between receptors, in the same units as the 5th through 8th words, as specified by the 3rd word (COORD).

The 5th and 6th words give the LON,LAT or X,Y (for example, UTM) coordinates of the lower left receptor.

The 7th and 8th words give the LON,LAT or X,Y (for example, UTM) coordinates of the upper right receptor. SciDOSpost starts with the lower left receptor and adds an integer number times DX to construct the receptor grid. The resulting upper right receptor will have coordinates less than or equal to those requested (that is, rounds down, will not exceed).

```
#    Spec  Units  RecSet  Space   Time  Period  Statistic  FType Filename
con  no2   ug/m3  2x2km   AllRec  All    1 hr   Average    POST  no2.pst
con  no2   ug/m3  2x2km   AllRec  8th    1 hr   MaxDaily   PLOT  no2.DV.plt
con  no2   ug/m3  50m     >=7.5   1st    1 hr   MaxDaily   XYZ   no2.SIL.dat
con  no2   ug/m3  hotspot MaxRec  8th    1 hr   MaxDaily   CSV   no2.DV.csv
con  no2   ug/m3  fence   AllRec  1st    1 yr   Average    PLOT  no2.ann.plt
```

The `con` keyword requests the program to write a concentration to the given file. If the file exists at the time the program is run, it is overwritten.

The 2nd word is the `species` name and must be one of the species included in the SCICHEM run—and is of course converted to upper case before searching the *.DOS file.

The 3rd word is the desired `units` of the output. CON can be written in μg/m³, ppb, or ppm.

The 4th word is the `NAME` of the receptor set for this output. It must match a `NAME` given in one of the REC or GRID lines above.

The 5th word is a `SPACE` filter and can be ALLREC for all receptors, MAXREC for only the maximum receptor, or >=*N* where *N* is a numerical value. Because SCICHEM species in the plume interact with the background concentrations, concentration can be negative (for example, NOx titration of ozone), using >=0 will not necessarily "pass through" all values.

The 6th word is a `TIME` filter and can be ALL to pass through all averaging time periods, or the rank (from highest to lowest) of the output value. Non-numeric characters are optional and ignored (writing "1st" is the same as writing "1").

The 7th and 8th words define the averaging `PERIOD`. The 8th word must be "HR" or "YR".

The 9th word defines the `STATISTIC` to be taken over the `PERIOD`. Valid values are AVERAGE to take the windowed average over the `PERIOD`, MAXDAILY to take the maximum daily rolling average over the `PERIOD`, or `SUM` (or `TOTAL`) to calculate the sum over the period. A windowed 8-hour average is from hours 1-8, 9-16, and 17-24. A rolling 8-hr average is the average from 1-8, 2-9, 3-10,… 17-24, of which sciDOSpost saves only the maximum. The MaxDaily keyword is useful for calculating NO_2 and SO_2 maximum daily 1-hour concentrations or for calculating O_3 maximum daily 8-hour concentrations. Following EPA conventions, if more than 25% of the values are missing (for example, for a 24-hour average, a partial last day of a run is discarded if the SCICHEM runs ends before 18 hours have been encountered), no average is

calculated. An annual average output with only a month of inputs will write -999. as a missing value flag.

The 10th word specifies the output file format for the filename given by the 11th word and must be one of the following:

- CSV: Comma-separated values
- XZYL (actually XYLLZUT): the X,Y,lat,lon, value, units, timestamp
- POST: AERMOD-style POSTFILE (values for all times and all receptors)
- PLOT: AERMOD-style PLOTFILE (a single high/rank value at all receptors)
- NC: NetCDF gridded file in I/O API-compliant format (only for GRIDs)
- GRD: Surfer 6 ASCII grid file (only for GRIDs)

```
dep  N     kg/ha  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
dry  N     kg/ha  meve    MaxRec  1st    1 yr   Total      CSV   max_dep.csv
wet  S     kg/ha  meve    MaxRec  1st    1 yr   Sum        CSV   max_dep.csv
```

The `dep` keyword requests the program to calculate maximum *N*-hour (or year) summed or total (over time) deposition (the sum of dry and wet deposition) of total nitrogen, total sulfur, or any one chemical species in the SCICHEM run, of the requested rank, and write the answer to the given file. `species` can be either **N** or **S** for total nitrogen or sulfur (useful for Class I analyses) or one of the species listed in SCICHEM (useful for other analyses). For N, sciDOSpost will scale the deposition each nitrogen-containing species by the ratio of the molecular weight of N to that of the species—and similarly for S.

The `dry` and `wet` keywords request the program to output the maximum *N*-hour (or year) average dry deposition or wet deposition components, respectively.

```
vis  dBext %      meve    AllRec  1st   24 hr   Average   CSV   vis.csv
vis  Cont  %      meve    MaxRec  8th   24 hr   Average   CSV   contrib.csv
```

The `vis` keyword requests the program to calculate maximum *N*-hour (or year) average visibility obscuration (light extinction) of the requested rank and write the answer to the given file. The second keyword can be **dBext** to output only the change to extinction in percent or **CONT** to write the change to extinction and the contributions of each component in the calculation. The calculations implement Figure 5 of FLAG (2010)—the IMPROVE equation for calculating light extinction.

7.1.2 Usage

SciDOSpost will print a help message to the screen when given the `-h` or `--help` command-line options.

Using the `--sample` command-line option will cause a sample control file to be printed to the screen, which the user can redirect to a file (for example, `sciDOSpost --sample > my_project.inp`).

```
Usage: SciDOSpost [-h | --help] [--sample] [-I:scpuff.ini] -i ctrl.inp
Options:"
    -i file   Specify control file to use, sciDosPost.inp by default
    -I:file   Specify the location of scipuff.ini to use
   --sample   Print a sample control file to the screen
   --version  Print the program version to the screen and exit
   --help     Print this help message
   -h         Print this help message
```

Running SciDOSpost is similar to other SCICHEM programs in that it prompts the user for the PATH for a scipuff.ini file. After that, helpful messages are printed to the screen to indicate progress. Use the **--sample** command-line parameter to create a sample control file.

7.2 Reviewing Projects Using SCIPUFF GUI (SCIPUFFgui)

Once a project has been completed successfully, it can be reviewed using SCIPUFFgui. After SCIPUFFgui has been set up and launched following the instructions in Section 2.1, the following **Review Project** window will appear (Figure 7-1).

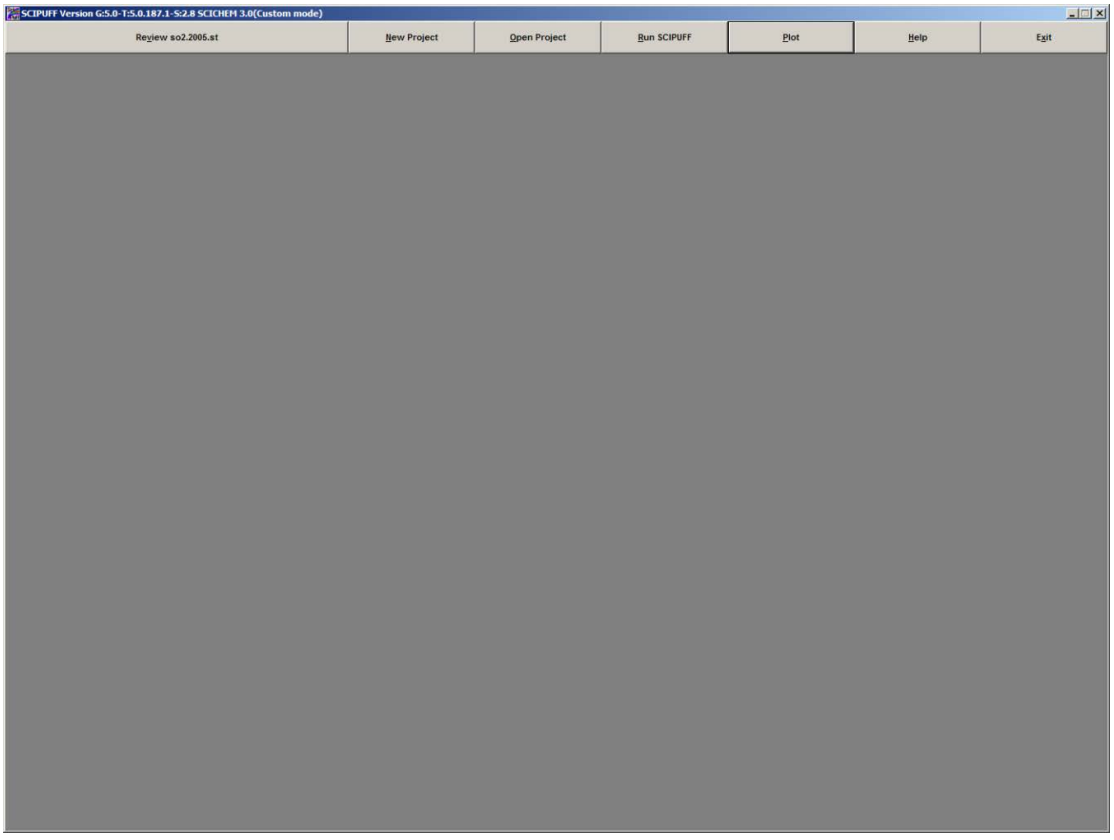

Figure 7-1
Review Project Window

Once this project is opened, the user may use the following push buttons:

- **Review** *ProjectName*
- **Plot** (See Section 7.3)

Note that the SCIPUFFgui is under development and the KEYWORDS input format type projects cannot be created or run using the present version. However, all projects—whether using KEYWORDS or NAMELISTS input—can be reviewed or plotted with SCIPUFFgui.

If the Review button is pressed, the following screen will appear (Figure 7-2).

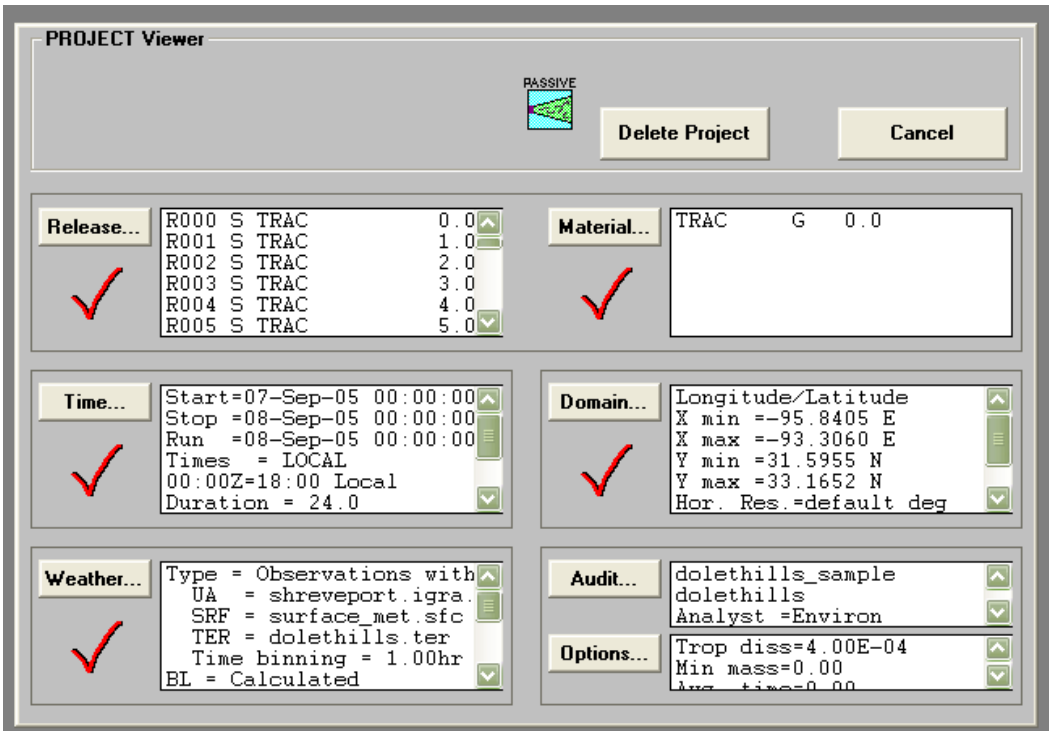

Figure 7-2
Project Viewer Window

The check marks indicate that each category has been defined. The user may then push the button for each category to simply review the project. The **Delete Project** button has been disabled and does not delete the project files.

7.2.1 Project Viewer

An icon in the upper left corner shows whether dynamic effects were included in the calculation. Dynamic effects treated are buoyant and momentum plume rise and gases that have densities different from that of air.

Passive: do not include dynamic effects

Dynamic: include dynamic effects

7.2.2 Project Coordinates

Clicking the domain button shows the project coordinate system. The possible coordinate systems are as follows:

Latitude/Longitude

This specifies the SCICHEM coordinate system as Latitude/Longitude (degrees). This is the default coordinate system.

Cartesian

This specifies the SCICHEM coordinate system as rectangular Cartesian (kilometers).

If the *reference point* box is checked for Cartesian coordinates, the following boxes will appear:

Cart. (X,Y)

This specifies the Cartesian coordinates of the reference point in kilometers.

Default: (0,0)

LLA (E,N)

This specifies the longitude and latitude coordinates of the reference point specified in the X,Y edit boxes. The coordinates can be specified in degrees or degrees/min/sec.

Default: None

7.2.3 Project Description

The Audit button shows the additional project options that were used. They include the following:

Mode

This specifies whether SCICHEM was run in *Standard* or *Fast* mode.

See Table 7-1 for a description of the two modes.

Dynamics

This specifies whether dynamics were treated. It is shown by the icon at the top.

Static Puffs

This specifies whether static puffs were used in the calculation to speed it up.

Multicomponent

This specifies whether material transformations through chemical reactions were treated.

Table 7-1
SCICHEM Run Modes

Parameter	STANDARD	FAST	Comments
VERTICAL RESOLUTION			
Default height of the vertical domain Default vertical domain resolution Default maximum vertical grid points	2500m 250m 15	5000m 1000m 7	These vertical grid parameters affect the vertical splitting of puffs, which affects the total number of puffs. These parameters can also be entered manually by the user.
HORIZONTAL RESOLUTION			
Surface resolution [DELMIN]	0.0 (As needed)	1/160 of domain	This affects the surface grid and total number of puffs if surface evaporation is occurring. This parameter can also be entered manually by the user.
MERGE CRITERIA			
SiMerge (ratio of internal scales)	1.25	1.5	This allows more merging between puffs and reduces the total number of puffs. This parameter cannot be manually entered by the user. It is changed internally when Fast Mode is selected.

The SCIPUFFgui features are described in detail in Section 4.

7.3 Plotting Using SCIPUFF GUI

This section describes how to initiate a plot after calculations are complete using the limited version of the SCIPUFFgui. The plot controls and options are defined as well as procedures for exporting plots. Once a project has finished running, or if an old project is opened, the user may click on the **PLOT** button.

If the user clicks the **DRAW** button under the Plot Control section, the default plot will appear to the right of the control area. The default plot is the vertically integrated tracer concentration. An example is shown in Figure 7-3.

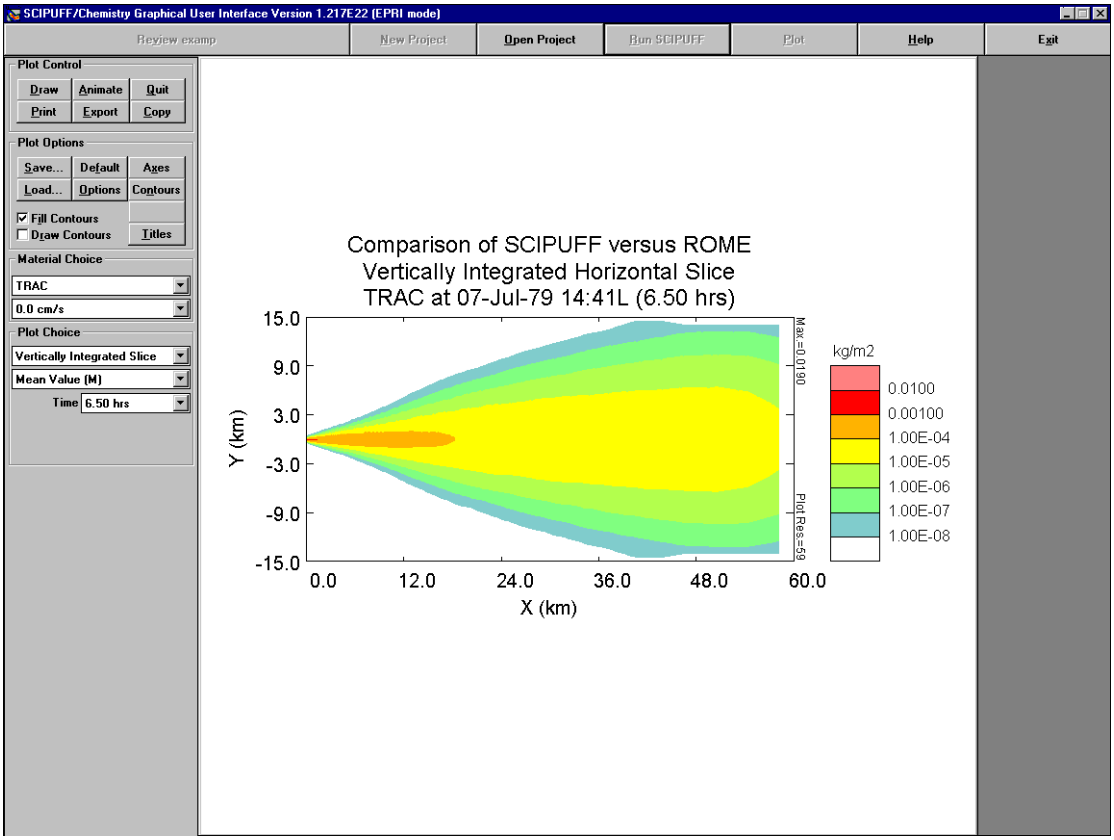

Figure 7-3
Plot Control Window

7.3.1 Plot Control

Options under the Plot Control section of the plot window are shown in Figure 7-4.

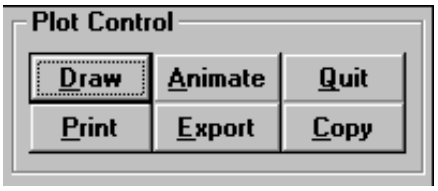

Figure 7-4
Plot Control Options

They provide the following functions:

- **DRAW** – Generates a display in the Plot Area.
- **ANIMATE** – Generates a time sequence of display bitmap files. See Section 8.2.1.
- **QUIT** – Returns to the main SCICHEM screen.
- **PRINT** – Sends the display to a specified printer.
- **EXPORT** – Saves the display to a file.
- **COPY** – Copies the current display to the clipboard.

7.3.1.1 Animate

This push button generates a sequence of bitmaps for animation display. The plot display format (type of plot, domain bounds, labels, and so on) should be defined in the normal way, but the contour levels should be fixed so that the entire sequence uses the same values. (Using default contour values can result in changing levels during the sequence.)

The bitmap file sequence uses extensions 001, 002, and so on with the file name and path selected by the user. The output files are 480x480 PCX files and are usually about 20 kB each. Existing files are not deleted but are overwritten once the procedure begins. The sequence consists of all output times between the start and stop times selected by the user.

The screen shown in Figure 7-5 will be displayed by pressing the **ANIMATE** button.

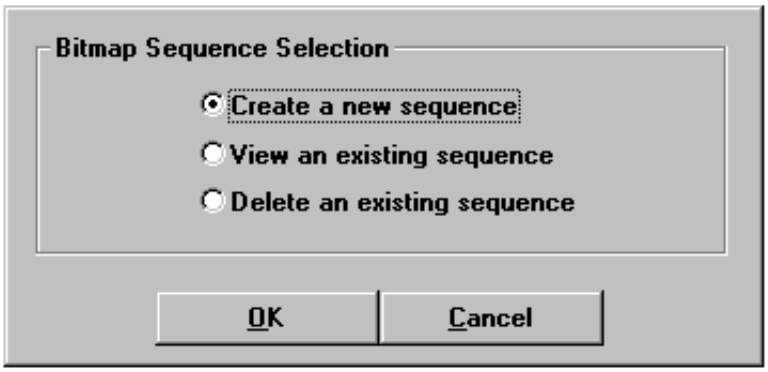

Figure 7-5
ANIMATE Window

The choices are as follows:

- ***Create a new sequence***: Generates a sequence of files that are used for animation.
- ***View an existing sequence***: Plays a sequence of files that have already been generated.
- ***Delete an existing sequence***: Deletes an animation sequence.

Once one of the radio buttons has been selected, the Open File dialog box appears. From this dialog box, you can select the name of the sequence that is to be created, viewed, or deleted. If creating a new sequence, you can also select the start and end time of the animation. When a sequence is ready for viewing (after selecting an existing sequence or generating a new one), the animation screen will appear, as shown in Figure 7-6.

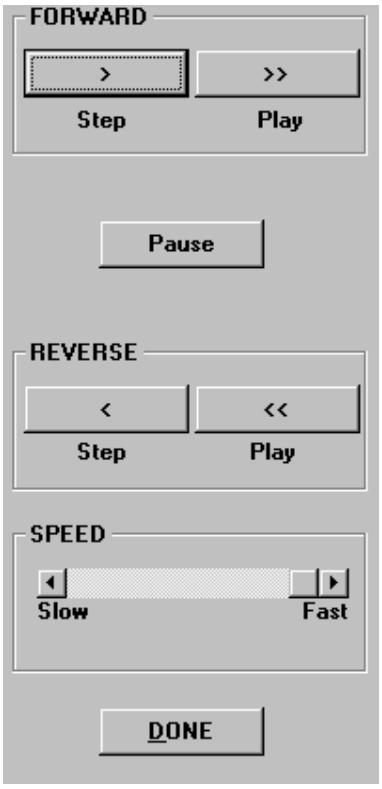

Figure 7-6
Animation Screen

This screen will consist of the plot area at the right and push buttons (shown above) that function like buttons of a tape recorder.

Pause

Temporarily stops the playing of the animation.

Done

Terminates the animation and returns to the original plot screen.

Speed

Adjusts the speed of the animation.

Forward

Step

Advances the sequence one frame.

Play

Cycles through the entire animation sequence.

Reverse

Step

Decrements the sequence one frame.

Play

Cycles through the entire animation in reverse sequence.

7.3.1.2 Export

The Open File dialog box is displayed with a section for specifying the file format. The available file types are:

- ***AVS (ASCII) file***: See Section 7.3.1.3.
- ***Bitmap file***: Standard Windows bitmap format.
- ***SCICHEM Overlay file***: File can be drawn over a plot of the same coordinate mode in SCICHEM.
- ***Table (ASCII) file***: Tabular output of the plot data in ASCII format.

7.3.1.3 AVS File

SCICHEM can export plots in the AVS (Application Visualization System)-compatible UCD (Unstructured Cell Data) file format (see Table 7-2). The format of the file is shown next.

#Comments
Nnode, Ncell, NnodeData, NcellData, NmodelData
Nid, x, y, z (*Nnode* lines)
.
Cid, Sid, Typ, N1, N2, NN (*Ncell* lines)
.
NnodV, NN1,NN2...NNNnodV
Nlabel, Nunits (*NnodV* lines)
.
Nid, Ndat1, Ndat2,...NdatNnodeData (*Nnode* lines)
.
NcelV, NC1, NC2...NCNcelV
Clabel, Cunits (*NcelV* lines)
.
Cid, Cdat1, Cdat2,...CdatNcellData (*Ncell* lines)
.
NmodV, NM1, NM2...NMNmodV
Mlabel, Munits (*Nmodv* lines)
.
Mid, Mdat1, Mdat2,...MdatNmodelData (*NMod* lines)

Table 7-2
AVS File Variables

Nnode	Total number of nodes
Ncell	Total number of cells
NnodeData	Total number of data values for each node (=1)
NcellData	Total number of data values for each cell (=0)
NmodelData	Total number of data values for each model (=0)
Nid	Node number
x,y,z	Node location
Cid	Cell number
Sid	Surface number (=1)
Typ	Cell type (=tri)
N1, N2...NN	Node numbers identifying the cell vertices (N=3)
NnodV	Number of nodal data data sets (=1)
NN1 ,NN2...NNNnodV	Number of nodal data values in each set (=1)
Nlabel	Nodal data set label
Nunits	Nodal data set units
Ndat1,Ndat2,...NdatNnodeData	Nodal data values
NcelV	Number of cell data data sets (not on file)*
NC1,NC2...NCNcelV	Number of cell data values in each set (not on file)*
Clabel	Cell data set label (not on file)*
Cunits	Cell data set units (not on file)*
Cdat1,Cdat2,...CdatNcellData	Cell data values (not on file)*
NmodV	Number of model data data sets (not on file)*
NM1, NM2...NMNmodV	Number of cell data values in each set (not on file)*
Mlabel	Model data set label (not on file)*
Munits	Model data set units (not on file)*
Mid	Model number (not on file)*
Mdat1,Mdat2,...MdatNmodelData	Model data values (not on file)*

*Although a part of the general AVS format, this does not appear on the file exported by SCICHEM because NcellData and NmodelData are 0.

SCICHEM provides comments in the header with information to identify the data (see Figure 7-7).

```
#Comments identifying data
      .
      .
      .
2257  4474  1  0  0
   1  126.200  34.2000  .000000
   2  126.600  34.2000  .000000
   3  126.600  34.6000  .000000
   4  126.200  34.6000  .000000
      .
      .
      .
2255  129.800  37.0000  .000000
2256  129.800  37.4000  .000000
2257  129.800  37.8000  .000000
   1   1 tri  1  2  3
   2   1 tri  1  3  4
   3   1 tri  4  3  5
      .
      .
      .
4472   1 tri  1900  2256  1901
4473   1 tri  1901  2256  2257
4474   1 tri  1901  2257  1902
   1   1
C, KG/M3
   1  1.000000E-30
   2  1.000000E-30
   3  1.000000E-30
      .
      .
      .
2255  1.000000E-30
2256  1.000000E-30
2257  1.000000E-30
```

Figure 7-7
Sample AVS Export File

7.3.1.4 Table (ASCII) File

Tables of point values can be exported from a plot in ASCII format. When the **EXPORT** push button is selected under the Plot Control interface area, the table (ASCII) file type (*.tab) must be selected and a file name must be entered in the Open File dialog box. After the OK push button is selected, the Tabular output Editor is displayed, as shown in Figure 7-8.

Values can be selected using the displayed *Tabular output Editor* and can also be obtained using the mouse on the plot screen with the *Get Value function*. The user can click the right mouse button anywhere on the plot to use the *Get Value function*. When values are selected, they are added to the ASCII file and not replaced. The *Get Value function* must be used prior to choosing **EXPORT**, and their values will automatically appear in the *Tabular output Viewer*.

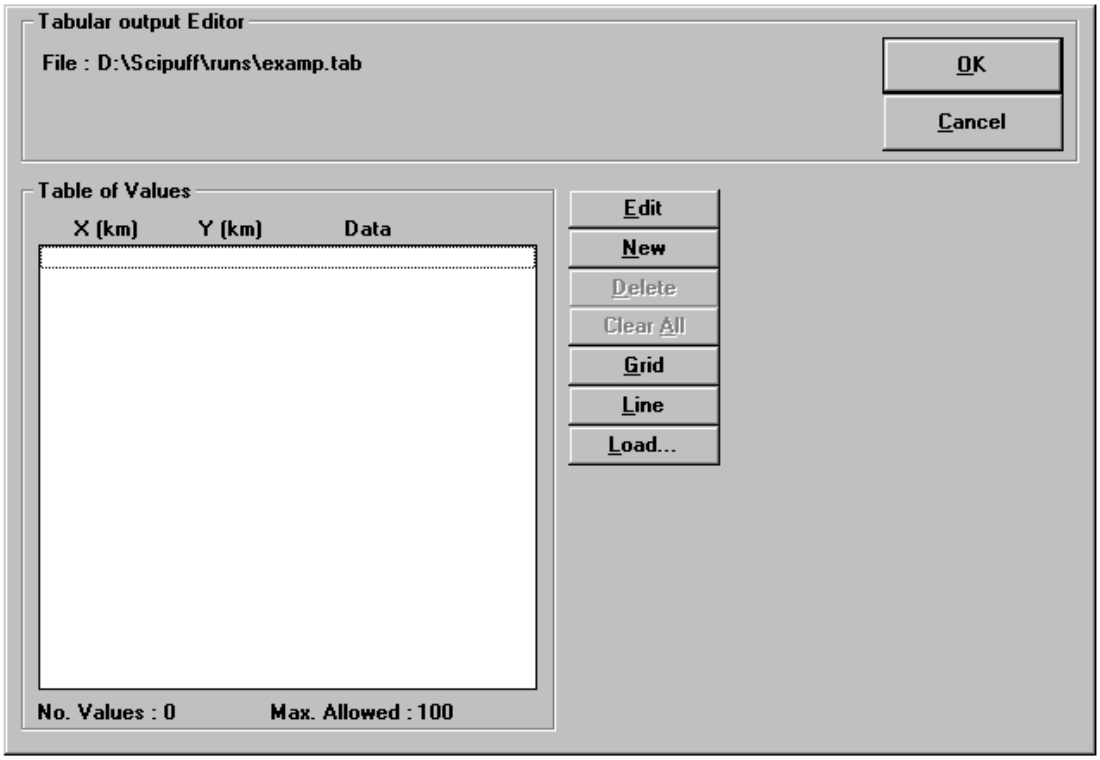

Figure 7-8
Tabular Output Editor Window

The buttons of the *Tabular output Viewer* perform the following functions:

OK

Exports the data listed in the Table of Values and returns to the main plot screen.

Cancel

Returns to the main plot screen without exporting to the Table file.

Edit

Changes the selected table value to a new value.

New

Adds a new table value to the list.

Delete

Removes a selected table value from the list.

Clear All

Removes all table values from the list.

Grid

Calculates table values based on a specified grid domain and the number of points within that domain.

Line

Calculates table values based on specified line endpoints and the number of points on that line.

Load

Copies the table values from a file into the list. This is an appending procedure, so the loaded values are added to those already in the list.

7.3.2 Plot Options

Options under the Plot Options section of the plot window are shown in Figure 7-9.

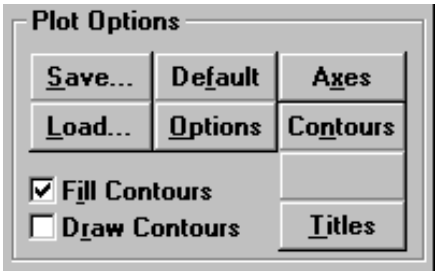

Figure 7-9
Plot Options Window

They provide the following functions:

- **SAVE** – Save selected display settings.
- **DEFAULT** – Set default display settings.
- **AXES** – Select display coordinate system, axes range, tick spacing, and labeling. See Section 7.3.3.
- **LOAD** – Load display settings (through the Open File dialog box).
- **OPTIONS** – Select additional display options. See Section 7.3.4.
- **CONTOURS** – Define display contours. See Section 7.3.5.
- **TITLES –** Modify display title text and location. See Section 7.3.6.
- **FILL CONTOURS –** Fills the area between contour levels of the displayed field using the color palette defined in SCIPAL.DAT.
- **DRAW CONTOURS –** Draws the contour levels of the displayed field using black lines.

7.3.3 Axes

The user may change the axes of the plot by pressing the AXES button. The screen shown in Figure 7-10 will be displayed.

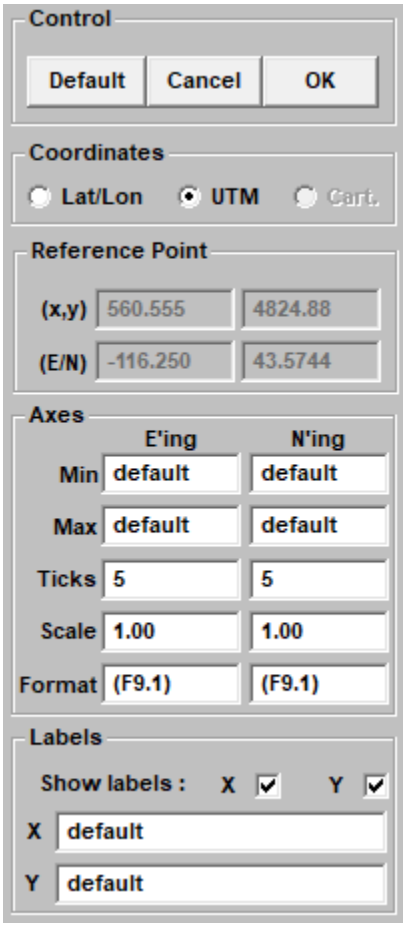

Figure 7-10
AXES Window

7.3.3.1 Control

Default

Resets all axes parameters to their defaults.

Cancel

Returns to the main plot screen without changes.

OK

Returns to the main plot screen with new settings.

7.3.3.2 Coordinates

The display coordinate system—***Lat/Lon*** (degrees), ***UTM*** (km), or ***Cartesian*** (km)—can be selected by the user. If it differs from the project coordinate system defined in the *Domain Setup*, a coordinate transformation is performed based either on the WGS84 datum or the *Reference Point* displayed (and possibly set) below.

To set the display coordinates in Lat/Lon when the project coordinates are Cartesian, the *Reference Point* must have been set in the *Domain Setup* or must be set in the *Reference Point* box (described next). This is not the case when setting Cartesian display coordinates with Lat/Lon project coordinates because a default *Reference Point* can be defined, as described in Section 8.3.1.3. The default display coordinate system is the same as that of the project. If the coordinate type is Lat/Lon, the plot boundaries are positive East and North.

7.3.3.3. Reference Points

This section is enabled only if the reference point has not been defined in the Domain Setup.

X, Y

This specifies the Cartesian coordinates of the reference point in kilometers.

Default: (0, 0)

E/N

This specifies the longitude and latitude coordinates of the reference point specified in the *X,Y* edit boxes. Default: Center of the domain if project coordinates are Lat/Lon; none if project coordinates are Cartesian.

7.3.3.4 Axes

Min X, Min Y, Max X, Max Y

This specifies the plot axes minima and maxima given in degrees for Latitude/Longitude display coordinates and km for Cartesian display coordinates. If Scale is used, the axes limits should be set accordingly; that is, the values entered here should be appropriate for the display domain after the coordinates have be multiplied by *Scale*. Default: The project domain limits used in the SCICHEM calculation (transformed if the display coordinates are different from the project coordinates).

Ticks

This specifies the number of major divisions for labeling along the X and Y axes.

Default: 5

Scale

This specifies the axes multiplication factor. For example, to convert from kilometers to meters, *Scale* is set to 1000.

Default: 1

Format

This specifies the display format of the axes values. The standard FORTRAN format convention is used and must be enclosed in parentheses.

Default: (f9.1)

7.3.3.5 Labels

Show Labels X, Show Labels Y

This specifies the character string labels displayed along the axes.

X, Y

This specifies the character string labels displayed along each axis.

Default: “Latitude” and “Longitude” for Lat/Lon display coordinates and “X (km)” and “Y (km)” for Cartesian display coordinates.

7.3.4 Options

The user may change other plotting options by pressing the OPTIONS button. The screen shown in Figure 7-11 will be displayed.

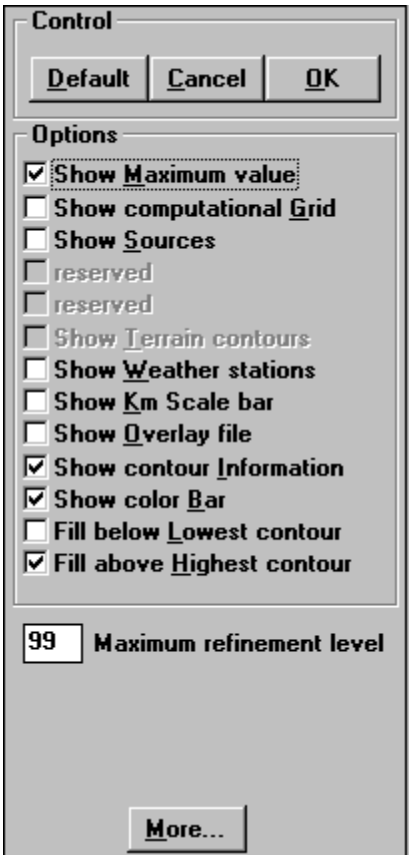

Figure 7-11
Options Window

7.3.4.1 Control

Default

Resets all parameters to their defaults.

Cancel

Returns to the main plot screen without changes.

OK

Returns to the main plot screen with new settings.

7.3.4.2 Options

Show Maximum Value

The maximum value in the selected field is displayed on the upper right-hand side of the plot.

Show Computational Grid

The SCICHEM computational grid is superimposed on the plot.

Show Sources

The sources are displayed as symbols on the plot. Continuous and instantaneous sources are represented by downward and upward pointing triangles, respectively.

Show Terrain Contours

The terrain contours are displayed on the plot. Only enabled for projects that have terrain defined.

Show Weather Stations

The locations of weather stations are displayed as boxes that are labeled with an *S* for surface observations or a *P* for profile observations. This option is available for observations type weather only.

Show Km Scale Bar

A bar that displays the distance scale in kilometers is shown at the bottom of the plot. This bar is for Cartesian coordinates only.

Show Overlay file

Overlay files are drawn on top of the current drawing. When this option is checked, the Open File dialog box will appear, and the overlay file must be specified.

Show Contour Information

The number of contours and contour level values are given below the plot. This information is displayed only when the *Show color Bar* option is off.

Show Color Bar

A color bar matching colors to contour levels is displayed on the right of the plot when filling contours.

Fill below Lowest Contour

The area having values less than the lowest contour is filled (when filling contours).

Fill above Highest Contour

The area having values greater than the highest contour is filled (when filling contours).

Maximum refinement level

This specifies the maximum level of refinement for plotting. If a large value is chosen, the plot contains finer resolution but takes more time to generate. SCICHEM automatically ignores refinement smaller than display resolution.

Default: 99

7.3.4.3 More Options

The user may change more plotting options by pressing the **MORE** button from the Plot Options edit screen. The screen shown in Figure 7-12 will be displayed.

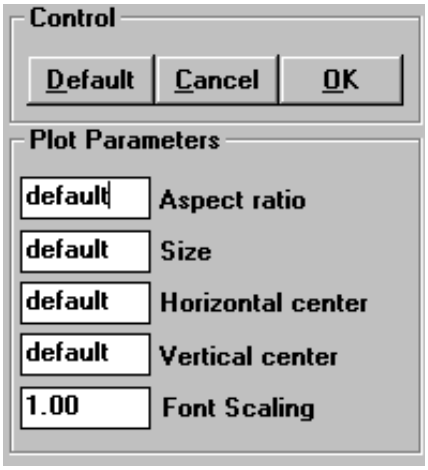

Figure 7-12
More Plot Options Window

Default

Resets all parameters to their defaults.

Cancel

Returns to the Plot Options screen without changes.

OK

Returns to the Plot Options screen with new settings.

Aspect Ratio

This specifies the ratio of the Y-axis length to X-axis length.

Default: 1

Size

This specifies the size of the plot relative to the size of the plot area (given as a fraction of the plot area). Default: To fill the plot area as much as possible.

Horizontal Center, Vertical Center

This specifies the center of the plot relative to the plot area (given in fractions of the plot area dimensions).

Default: Centered

Font Scaling

All the plot text sizes are scaled by this value.

Default: 1

7.3.5 Contours

The user may change the contours of the plot by pressing the **CONTOURS** button. The screen shown in Figure 7-13 will be displayed.

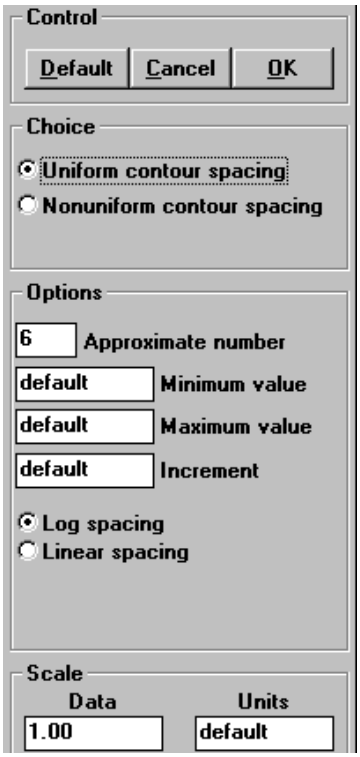

Figure 7-13
Contours Control Window

7.3.5.1 Control

Default

Resets all contour parameters to their defaults.

Cancel

Returns to the main plot screen without changes.

OK

Returns to the main plot screen with new settings.

7.3.5.2 Choice

The user may use uniform contour levels or nonuniform contour levels. The Options section of this window changes, depending on which choice is selected.

7.3.5.3 Options

Uniform Contours

Approximate Number

This specifies the approximate number of contours plotted. The actual number of contours is calculated based on the minimum, maximum, and increment, which are either specified in this group box or determined from the display field selected.

Default: 6

Minimum Value

This specifies the minimum contour level display.

Default: The minimum value of the display field.

Maximum Value

This specifies the maximum contour level display.

Default: The maximum value of the display field.

Increment

This specifies the contour spacing used for displaying the selected field.

Default: Determined from the *Minimum* and *Maximum values* and the *Approximate number* of contours.

Log Spacing

Logarithmic plot contour spacing is used. Log spacing is the default for mean value plots.

Linear Spacing

Linear plot contour spacing is used. Linear spacing is the default for probabilistic plots.

Nonuniform Contours

Contour Values

Displays contour values (Figure 7-14).

Edit

Changes the selected contour value to a new value.

New

Adds a new contour value to the list.

Delete

Removes a selected contour value from the list.

Clear

Removes all contour values from the list.

Compute

Calculates contour values based on a specified range, number of values, and an assumed distribution.

Load

Copies contour values from a file into the list. This is an appending procedure, so the loaded values are added to those already in the list.

Save

Saves the current contour value list to a file.

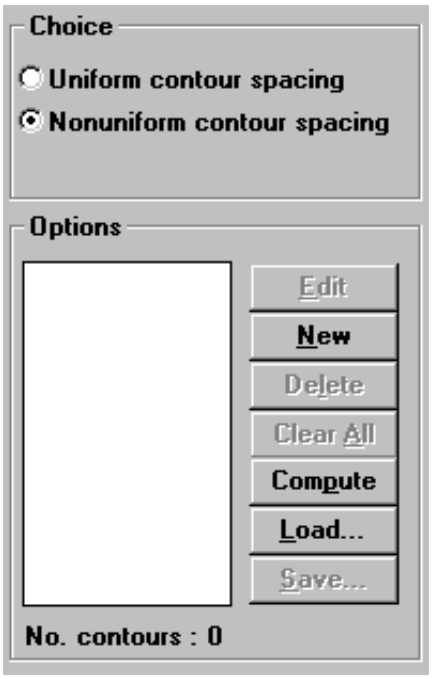

Figure 7-14
Contour Value List Window

7.3.5.4 Scale

Data

This specifies the value by which the plotted data are scaled.

Units

This specifies the units used for labeling the data contours.

7.3.6 Titles

The user may change the titles of the plot by pressing the **TITLES** button. The screen shwn in Figure 7-15 will be displayed.

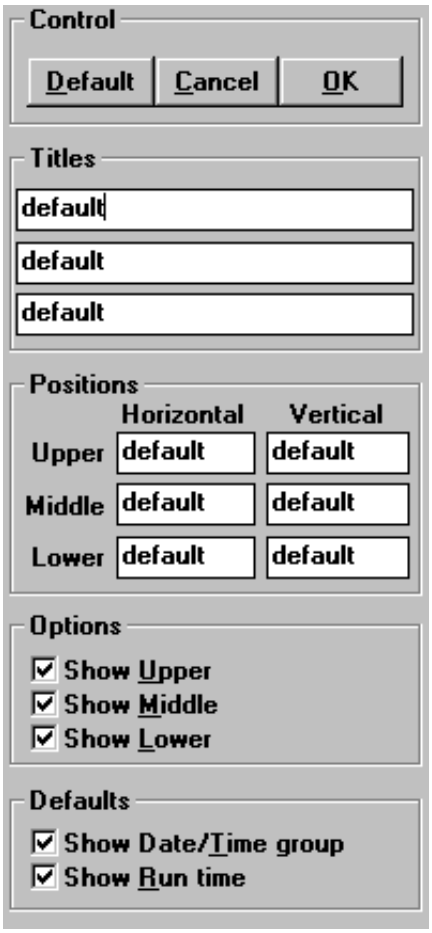

Figure 7-15
Title Window

7.3.6.1 Control

Default

Resets all parameters to their defaults.

Cancel

Returns to the main plot screen without changes.

OK

Returns to the main plot screen with new settings.

7.3.6.2 Titles

There are three edit boxes for the upper, middle, and lower titles.

Defaults:
Upper title: *Project Title*
Middle title: Plot type
Lower title: Material, size group if appropriate, and time.

7.3.6.3 Positions

Upper, Middle, Lower

There are three sets of edit boxes for the horizontal and vertical positions of the three titles. The positions are specified in fractions of the plot window and refer to the location of the center of the title string baseline. The default locations center the titles above the plot.

7.3.6.4 Options

Show Upper, Show Middle, Show Lower

There are three check boxes that control the drawing of the titles on the plot.

7.3.6.5 Defaults

Show Date/Time Group

The time in day-month-year-hour format is displayed in the lower title (default title only).

Show Run Time

The time from the start of the run is displayed in the lower title (default title only).

7.4 Material Choice

SCICHEM allows multiple materials and particle size groups as well as multicomponent materials. The user must select the material and the size group or species name, if appropriate, for display. The Material Choice section of the Plot Control window is shown next (Figure 7-16).

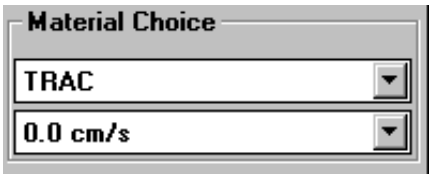

Figure 7-16
Material Choice Window

The two drop-down lists are as follows:

Material Name

This specifies that the name of the material will be displayed.

Species Name or Particle Size Group

This specifies the species name for a multicomponent material or the size group for a particle material selected for display. Total denotes the sum of all the size bin contributions when multiple size bins are specified for a particulate. This box displays the deposition velocity for a gaseous material or a single size bin particle material. For multicomponent materials, vertically integrated plots cannot be displayed because of the presence of background concentrations; therefore, species names are not available for these plots.

7.5 Plot Choice

The Plot Choice section of the Plot Control window is shown next (Figure 7-17):

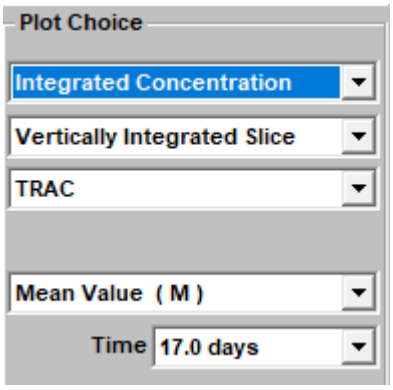

Figure 7-17
Plot Control Window

7.5.1 Plot Class/Type

Plots are defined by generic classes and more specific types, which depends on the class. The following is a complete list of plot classes and their types, along with a brief description. Some may not be available because of the selected project type and/or output flags for the selected display material.

Surface Dose (Integrated)

Surface
The time-integrated material concentration at the surface will be plotted.

Surface Deposition (Integrated)

Surface
The time-integrated mass of material deposited on the surface will be plotted.

Concentration (Instantaneous)

Horizontal Slice
A horizontal cross-section through the material concentration field will be plotted. The slice altitude in meters is specified in the associated edit box.

Vertical Slice
A vertical cross-section through the material concentration field will be plotted. The slice parameters are selected in the associated ***Select*** dialog box.

Surface
The instantaneous material concentration at the surface will be plotted (available only for runs with terrain).

Integrated Concentration

Vertically Integrated Slice
The vertically integrated material concentration will be plotted. Units are mass per area.

Horizontal Projection
The horizontally integrated material concentration will be plotted. The direction of the integration is normal to the vertical slice defined in the associated ***Select*** dialog box.

Surface
The instantaneous material concentration at the surface will be plotted (available only for runs with terrain).

Met/Terrain

Surface
Terrain elevations will be plotted (available only for runs with terrain).

3D Met

Horizontal Slice
Velocity and other meteorological fields will be plotted (available only for runs with saved meteorology fields).

7.5.2 Plot Value

Mean (M)

Displays contours of the mean field selected for display.

Prob(V>E)

Displays contours of the probability that the selected field will exceed a prescribed value. The exceedance value is entered in an associated edit box.

Exceed. Value (V[Pc>P])

Displays areas where the conditional probability of exceeding the contour value is greater than the value given in the *Probability* edit box (see below). For example, if the number in the Probability edit box is 0.5, the area inside of a contour value of 1.0 corresponds to the region where the conditional probability of values exceeding 1.0 is equal to or greater than 50%.

Exceed

This specifies the exceedance value used for probabilistic plotting. This edit box appears only when the *Prob(M>E)* plot type is selected. The units are the same as the display contours.

Default: 0

Probability

This specifies the probability value used for the *Exceed. Value (V[Pc>P])* plot type.

Default: 0.5

7.5.3 Time

The output time (in displayed units) from the start of the calculation. Only the times saved on the SCICHEM output files are available for plotting and are displayed in the list box. The default is the last time break on the output files.

7.5.4 Additional Parameters

The following additional parameters will be required, depending on the plot choice:

Height (m)

This specifies the height above the ground level (m) for an instantaneous horizontal slice. This edit box appears only when the plot type is a horizontal slice. The default is 0.

Select

This specifies the horizontal limits and vertical extent of the vertical slice, either through dialog box input or by mouse selection. This push button appears only when the plot type is a vertical slice. See Section 7.5.5.

7.5.5 Selecting Vertical Slices

Use the **SELECT** push button to define the location and extent of a vertical slice through the instantaneous concentration field or the projection plane for horizontally integrated concentration. The slice location can also be specified by dragging the mouse if the plot window is displaying a horizontal field. When the mouse is positioned in the plot area, the cursor becomes a pair of scissors (for determining the cross-sectional cut) with the "hot spot" at the intersection of the scissor blades. The vertical cross-section location is specified by clicking the mouse at the start point and dragging to the end point. The edit screen shown in Figure 7-18 appears when the **SELECT** button is pushed.

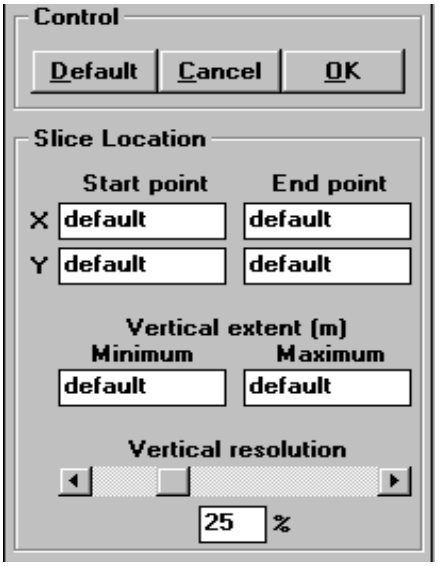

Figure 7-18
Slice Location Window

The choices are defined next.

7.5.5.1 Control

Default

Resets all parameters to their defaults.

Cancel

Returns to the main plot screen without changes.

OK

Returns to the main plot screen with new settings.

7.5.5.2 Start Location

Start Point, End Point

This specifies the start and end points of the slice in display coordinates. (The display coordinate system can be set using the *Axes* options.)

Default: The start and end points are the coordinates of the lower left and upper right corners of the horizontal calculation domain.

Vertical Extent

This specifies the *Minimum* and *Maximum* height range of the slice in meters.

Default: The defaults are the lowest and highest points in the SCICHEM domain.

Vertical Resolution

This controls the number of vertical grid points of the slice, between 0% (5 points) and 100% (105 points). A larger number improves the quality (resolution) of the display, but it also increases the plotting time. The slider bar allows the user to change the resolution.

Default: 25%

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A
TUTORIALS

A.1 Short-Range Impacts: 1-Hour SO_2

A.1.1 Introduction

This tutorial provides a step-by-step procedure for conducting an annual SCICHEM simulation to calculate 1-hour SO_2 incremental concentrations for 2005 due to SO_2 emissions from a boiler unit at a hypothetical facility. The facility is assumed to be located in an empty, grassy field slightly NW of the Boise Air Terminal landing strip (centered at 43.574152°N, 116.249741°W) near Boise, Idaho. A pseudo-property boundary is created, using a square box with 100-m sides, with the emission unit in the center. Receptors are placed every 10 m along the property boundary and every 50 m along the boundary of the modeling domain.

This tutorial uses the Linux build of SCICHEM and the associated pre-processor and post-processor. Although this tutorial focuses on running the case study on Linux, the procedure for running on Windows is similar, and a Windows batch file is also provided as part of the package. Because SO_2 is treated as an inert species in this simulation, a dummy (no reaction) IMC file is used with the chemistry flag set to false. Examples of multicomponent simulations with near-source plume chemistry are provided in Tutorial 2 for near-source 1-hour NO_2 incremental concentrations and in Tutorials 3 and 4 for full chemistry applications for long-range impacts (ozone, secondary $PM_{2.5}$, AQRV analyses).

This tutorial illustrates the use of SCICHEM inputs based on the KEYWORDS format (See Section 4.2 of this User's Guide). Tutorial 2 also illustrates the same usage, while Tutorials 3 and 4 illustrate the use of NAMELIST-type SCICHEM inputs (described in Section 4.1 of this User's Guide).

A.1.2 Case Study Setup

The sub-directories of the test cases for Tutorial 1 and all the other tutorials in this document are located in the "Linux" sub-directory of the "examples" directory. The Tutorial 1 sub-directory is named "so2_2005". The examples directory also includes a sub-directory called "Common", which contains SCICHEM data directories that are common to several of the tutorials. For this tutorial and Tutorial 2, these common directories include the following:

- The "metsci" directory, which contains the standard surface and upper air meteorological data required to run the meteorological pre-processor METSCI and the outputs of METSCI.
- The "ASOS1Min" directory, containing Automated Surface Observing System (ASOS) 1-minute meteorological data files (the DS-6405 file containing the wind observations and the corresponding DS-6406 file containing temperature, pressure, and humidity observations). These files are read directly by SCICHEM without any additional pre-processing.
- The "NED" directory, containing National Elevation Dataset (NED) data file in GeoTIFF format to create a terrain file for the modeling domain in the format expected by SCICHEM using the terrain pre-processor, TERSCI (see below).

- The “tersci” directory, which contains the output of the TERSCI pre-processor terrain data using the NED data file in the NED directory.

Figure A-1 provides a tree diagram of the directory organization in the examples directory for Tutorial 1 for the Linux demonstration.

```
examples
|-- Common
|   |-- ASOS1Min
|   |   |-- 64050KBOI2005.dat
|   |   |-- 64060KBOI2005.dat
|   |-- NED
|   |   |-- 16102713.tif
|   |-- metsci
|   |   |-- KBOI.2005.INP
|   |   |-- KBOI.2005.ISHD
|   |   |-- KBOI.FSL.2005.TXT
|   |   |-- run_metsci.sh
|   |-- tersci
|   |   |-- run_tersci.sh
|   |   |-- tersci.utm.inp
|-- Linux
|   |-- run_sciDOSpost.sh
|   |-- run_scichem.sh
|   |-- so2_2005
|   |   |-- sciDOSpost.inp
|   |   |-- so2-2005-st.emi
|   |   | --so2-2005-st.sci
|   |   | --so2-2005-st.sam
|   |   | --so2_norxn.imc
```

Figure A-1
Directory Organization for Tutorial 1

The SCICHEM run script (run_scichem.sh) for all case studies is located in the “Linux” directory. The argument to this script specifies the project name, so a single run script can be used for all the tutorials described here. **The user needs to step into the project directory (so2_2005 directory for this tutorial) and run the script from within the project directory.** In addition, this case study requires three other run scripts:

- The meteorological data pre-processing run script (“run_metsci.sh”) in the metsci directory.
- The terrain data pre-processing run script (“run_tersci.sh”) in the tersci directory.
- The post-processing run script in the Linux directory (“run_sciDOSpost.sh”). As in the case of the SCICHEM run script, the user needs to step into the project directory and run the script from within the project directory.

The meteorological pre-processing run script calls the “METSCI” pre-processor (described in Section 3.1 of this User’s Guide) to create surface and upper air meteorological files in SCICHEM format in the metsci sub-directory. (The script must be run in the examples/Common/metsci sub-directory.) This sub-directory initially contains the standard meteorological data available from NOAA (see “Meteorological Data” section below) and a configuration file (the “METSCI” input file, “KBOI.2005.INP”). After the pre-processor runs,

additional files are created as discussed later. Although no pre-processing of the ASOS 1-minute data is required in directory ASOS1Min because the 1-minute data can be read directly by SCICHEM, it should be noted that SCICHEM can read only one pair (DS-6405 and DS-6406) of ASOS files per measurement locations. Therefore, the monthly ASOS data files must be concatenated for simulations longer than a month (for example, an annual simulation as in this tutorial). The concatenation is straightforward because there are no header records. For this case study, the ASOS1Min directory contains the concatenated DS-6405 and DS-6406 files.

The terrain pre-processing run script calls the TERSCI processor described in Section 3.2 of this User's Guide to create a terrain file in SCICHEM format using as input a GeoTIFF file containing NED data. (It must be run in the examples/Common/tersci sub-directory.)

After the SCICHEM meteorological files and terrain file are created with the METSCI and TERSCI pre-processors, respectively, the SCICHEM simulation can be conducted in the "so2_2005" directory. This directory contains the SCICHEM configuration file ("so2-2005-st.sci") in KEYWORD format and the hourly emissions file ("so2-2005-st.emi") for the boiler unit referenced in the configuration file. See Section 4.2 of the Draft User's Guide for a description of these files. These are the two main user-provided input files required for this inert species application (in addition to the meteorology inputs in the METSCI directory, the ASOS 1-minute meteorology inputs in the ASOS1Min directory and the terrain file in the TERSCI directory).

The SCICHEM configuration file is required for every SCICHEM application that uses the KEYWORD format inputs. The hourly emissions file is specified in the configuration file (see Section 4.2.5.9 of the User's Guide). If not specified, the model uses the non-varying emission rates and stack parameters provided within the SO pathway in the configuration file. However, for this tutorial, even though the hourly emission rates and stack parameters are not varying, an hourly emissions file is provided for illustration.

In addition, if the user wishes to conduct a multicomponent simulation for chemically reactive pollutants, it is necessary to provide a multicomponent input file and optionally a background concentration file. However, for this tutorial—which treats SO_2 as an inert species—we use a dummy IMC file (with no reaction) named so2_norxn.imc. An example of a KEYWORD format multicomponent simulation for 1-hour NO_2 concentrations is provided in Tutorial 2.

In addition to the input files mentioned above, the model requires an initialization file ("scipuff.ini") and a land use file ("landuse_scichem.dat"), described in this User's Guide. These two files are application-independent and are required for all SCICHEM applications. The scipuff.ini file is located in the directory that contains the SCICHEM executable, as specified in the provided run_scichem.sh run script. The landuse_scichem.dat file and other auxiliary files are located in the "sciData" directory. The sciData directory is at the same level as the "examples" directory containing the tutorial test cases. **Note that the scipuff.ini file specifies the locations of the sciData directory and the landuse_scichem.dat file. These locations are specified as relative paths in the linux version but in absolute path in the windows version. Users may need to modify the scipuff.ini file for their specific configuration.**

All the SCICHEM outputs for this tutorial are created in the project ("so2_2005") sub-directory.

The final step in this tutorial is the post-processing step to read the SCICHEM surface dosage output file in the same so2_2005 sub-directory. Because of space restrictions, only the final output files from the post-processing are provided here for benchmarking.

Each of these steps in the preparation of SCICHEM input files and conducting the SCICHEM simulation is described in more detail next.

A.1.3 Meteorological Data Preparation

The first step in conducting the SCICHEM simulation is to prepare the meteorological inputs using the NCDC DS-3505[4] surface data and FSL[5] upper air data for the Boise Air Terminal (KBOI, WMO ID 726810, WBAN ID 24131) for calendar year 2005. These standard data sets are processed using the METSCI pre-processor in the metsci directory. The METSCI input file, "KBOI.2005.INP", provides the configuration for the METSCI run and is reproduced next. Sections 3.1.1 to 3.1.3 of this User's Guide describe the various components of this input file. The main outputs of the pre-processor are the surface and upper air files in SCICHEM format, called "KBOI2005.SFC" and "KBOI2005.PRF", respectively, in this case study. These files are used in the SCICHEM simulation.

```
**********************************************************
** METSCI Input
**********************************************************
JOB
   REPORT      kboi2005.rpt
   MESSAGES    kboi2005.msg

UPPERAIR

   DATA        KBOI.FSL.2005.TXT FSL
   EXTRACT     KBOI2005.PRF
   QAOUT       TRUE
   XDATES      2005/01/01 TO 2005/12/31

SURFACE

   DATA        KBOI.2005.ISHD ISHD
   EXTRACT     KBOI2005.SFC
   QAOUT       TRUE

   XDATES      2005/01/01 TO 2005/12/31

   LANDUSE     CULTIVATED
```

This version of SCICHEM can also directly read ASOS 1-minute meteorological data. **However, it is necessary to concatenate the monthly data available from the NCDC ftp site[6] when conducting simulations for periods longer than a month because SCICHEM can read only one file per measurement location.** For Tutorials 1 and 2, the concatenated ASOS 1-minute data files are located in the ASOS1Min directory.

---

[4] DS-3505 surface data are available at ftp://ftp3.ncdc.noaa.gov/pub/data/noaa.

[5] FSL upper-air data are available at http://esrl.noaa.gov/raobs.

[6] ASOS 1-minute surface data are available at ftp://ftp.ncdc.noaa.gov/pub/data/noaa.

A.1.4 Terrain Data Preparation

The TERSCI pre-processor (see Section 3.2 of this User's Guide) can read Digital Elevation Model (DEM) and/or NED data files in GeoTIFF format to create a terrain file for the modeling domain in the format expected by SCICHEM. Note that this step is optional and depends on the application requirements; that is, it can be skipped for a flat terrain application. It is presented in this tutorial for completeness. The User's Guide provides information on websites from which NED data can be downloaded. For this tutorial, the NED GeoTIFF file ("16102713.tif") was downloaded from http://www.mrlc.gov/viewerjs/ by specifying the relevant coordinates for the modeling domain. This file is located in the "NED" directory at the same level as the "tersci" directory (see tree diagram in Figure A-1). The TERSCI control file "tersci.utm.inp" specifies the location of this file and the resulting output file as well as other information required for running TERSCI (see Section 3.2.1 for additional details on the contents of this control file). The output of TERSCI for this tutorial is called "terrain.utm.ter" and is created in the "tersci" directory.

A.1.5 SCICHEM Simulation

After the SCICHEM surface and upper air meteorological data files and the terrain file are created as described previously, the SCICHEM run script ("run_scichem.sh") in the Linux directory is used to conduct the SCICHEM simulation for this case study. **Before invoking the run script, the user must first step into the project directory ("so2_2005") and invoke the run script from within the project directory.** The project name is specified as a command-line argument to the run script. For this case study, the project name is "so2-2005-st". The steps for this tutorial are as follows:

1. Change directories to the so2_2005 directory (for example, "cd so2_2005" from the Linux directory).
2. Invoke the run script with the project name as the argument (for example, "../run_scichem.sh ./so2-2005-st").

SCICHEM looks for the configuration file, which has the name *projectname*.sci, that is, "so2-2005-st.sci" for this tutorial. The various components of this file are described in detail in Section 4.2 of this User's Guide and include the following:

1. The run control section (lines starting with 'CO' or in the 'CO' block). For this tutorial, the run control section specifies UTM for the coordinate system with kilometer units (see Section 4.2.3.5) and specifies the computational domain (Section 4.2.3.6), time zone (Section 4.2.3.8), and the start and end of the simulation period (Section 4.2.3.7).
2. The material pathway (lines starting with 'MA' or in the 'MA' block). This pathway is described in Section 4.2.4.
3. The source description section (lines starting with 'SO' or in the 'SO' block). The source pathway is described in Section 4.2.5.
4. The receptor description section, specifying the receptor locations where concentration increments are to be calculated and output in the sampler file. For this example, two sets of receptors are included: the first set is placed along the boundary of the property at 10-m intervals, while the second set is placed along the computational domain boundaries at 50-m intervals. The receptor pathway is described in Section 4.2.6 of this User's Guide. In this

example, we do not use the receptor pathway but the post-processer sciDOSpost to output the post files for the receptors listed in the so2-2005-st.sam file.

5. The meteorology section, specifying the locations of the meteorological files to be used in the SCICHEM simulation. For this example, these files include both the ASOS 1-minute files as well as the files created by the METSCI pre-processor and located in the metsci directory. Section 4.2.7 of this User's Guide describes the meteorology pathway in detail.
6. The terrain section, specifying the location of the terrain file created using TERSCI. This pathway is described in Section 4.2.7.5.

The model assumes default values for the parameters that are not supplied in the provided configuration file for this test case. For example, the default maximum puff time step (MAXTSTEP) is 900 seconds— the maximum time step used in this test case—so the parameter MAXTSTEP is not specified in the configuration file. This would also be the default frequency of sampler output although in this case, the output is defined in the sampler file.

Several output files are created in the simulation with the names *projectname.*??? where "???" is the three-letter file extension identifying the file (for example, the "prj" extension specifies the project file; the "puf" extension specifies the file containing instantaneous puff incremental concentrations). These output file types are described in Section 6 of the User's Guide. The surface dosage output (specified by the "dos" extension) contains the integrated hourly species concentrations on an adaptive grid within the modeling domain. This is the file that is converted by the post-processor, described in the following section, to create various reports—including an output file in the AERMOD POSTFILE format.

For space reasons, none of the SCICHEM output files is provided in this distribution. Only the files created by the post-processor, described next, are provided for benchmarking.

A.1.6 Post-Processing of Surface Dosage Output

The last step in this tutorial is running the post-processor "sciDOSpost", which reads the SCICHEM surface dosage output in the file "so2-2005-st.dos" in the project directory. The control file for the post-processing is named "so2-2005-st.sciDOSpost.inp", and the file name is provided as a command-line argument to the post-processor run script "run_sciDOSpost.sh", located in the Linux directory. **As in the case of running SCICHEM, the user must first change directories to the project directory and invoke the post-processor run script from within the project directory.** The outputs of the post-processor depend on the reporting requirements specified in the control file. The provided sciDOSpost control file in this tutorial is self-descriptive, with comment lines preceded by the hash mark (#), semicolon (;), or exclamation point (!). The user can follow these comments to construct an application-specific control file.

For this tutorial, the post-processor creates four output files. The first file, called "so2-2005-st.sciDOSpost.samp.pst", is a file in AERMOD POSTFILE format and contains 1-hour average SO_2 concentrations for each hour at each sampler location specified in the "so2-2005-st.sam" file. The name of the sampler location file is specified in the sciDOSpost.inp control file using the "rec" keyword. The next file, "so2-2005-st.sciDOSpost.grid.pst", is also in POSTFILE format, but here the locations are arrayed on a regular grid defined with the GRID keyword in the sciDOSpost control file. The third output file, called "max_concentrations.csv", is a comma-separated values file that contains the 4^{th} highest daily 1-hour maximum SO_2 concentration, the

2nd highest 3-hour average SO_2 concentration, the maximum 24-hour average SO_2 concentration, and the maximum annual average SO_2 concentration over all receptors. Finally, "so2-2005-st.dv.plt" is an AREMOD-style PLOTFILE giving the 4th highest daily maximum concentration over all the previously mentioned grid locations.

A.2 Short-Range Impacts: 1-Hour NO_2

A.2.1 Introduction

This tutorial provides a step-by-step procedure for conducting an annual SCICHEM simulation to calculate 1-hour NO_2 incremental concentrations for 2005 due to NOx emissions from a short (less than 10-m high) fire pump at a hypothetical facility. The primary NO_2 emissions are assumed to be 15% of the NOx emissions. The location of the facility is the same as in the SO_2 case study described in Tutorial 1. The receptor locations are also the same as in the SO_2 case study. Following are the key differences between this NO_2 case study and the SO_2 case study in Tutorial 1:

1. The source characteristics (stack parameters, emission rates) are different.
2. The NO_2 case study requires the treatment of the near-source chemistry of NO, NO_2, atomic oxygen (O), and ozone (O_3). Therefore, this is an example of a multicomponent SCICHEM simulation with reactive plume chemistry for near-source calculations.

As in Tutorial 1, this tutorial uses the Linux build of SCICHEM and the associated pre-processors and post-processors. Although this tutorial focuses on running the case study on Linux, the procedure for running on Windows is similar—a Windows batch file is also provided as part of the package. In addition, like Tutorial 1, the case study described here illustrates the use of SCICHEM inputs based on the KEYWORDS format.

A.2.2 Case Study Setup

The test case for the tutorial is provided in the "examples/Linux/no2_mc_2005". The organization and file structure of the case study, including the meteorological files and terrain data, are generally similar to those for the inert SO_2 application in Tutorial 1, with some small differences that are discussed next. The reader is referred to Tutorial 1 for a description of the common features of the two case studies.

Figure A-2 provides a tree diagram of the directory organization in the examples directory for Tutorial 2 for the Linux demonstration.

```
examples
|-- Common
|   |-- ASOS1Min
|   |   |-- 64050KBOI2005.dat
|   |   |-- 64060KBOI2005.dat
|   |-- NED
|   |   |-- 16102713.tif
|   |-- metsci
|   |   |-- KBOI.2005.INP
|   |   |-- KBOI.2005.ISHD
|   |   |-- KBOI.FSL.2005.TXT
|   |   |-- run_metsci.sh
|   |-- no2_mc_2005
|   |   |-- no2.imc
|   |   |-- o3.amb
|   |-- tersci
|   |   |-- run_tersci.sh
|   |   |-- tersci.utm.inp
|-- Linux
|   |-- run_sciDOSpost.sh
|   |-- run_scichem.sh
|   |-- no2_mc_2005
|   |   |-- sciDOSpost.inp
|   |   |-- no2-2005-mc.emi
|   |   | --no2-2005-mc.sci
```

Figure A-2
Directory Organization for Tutorial 2

The same SCICHEM run script (run_scichem.sh) used for Tutorial 1 is used here. Again, the user needs to step into the project directory (no2_mc_2005 directory for this tutorial) and run the script from within the project directory. As in Tutorial 1, the case study requires three other run scripts: 1) meteorological pre-processing, 2) terrain data pre-processing, and 3) post-processing. The first two components are identical to the corresponding components in the SO_2 case study; additional details on these steps can be found in the Tutorial 1 description.

After the SCICHEM meteorological files and terrain file are created with the METSCI and TERSCI pre-processors, the SCICHEM simulation can be conducted in the "no2_mc_2005" directory. This directory contains the SCICHEM configuration file ("no2-2005-mc.sci") in KEYWORD format and the hourly emissions file ("no2-2005.mc-emi") for the fire pump referenced in the configuration file. See Section 4.2 of this User's Guide for a description of these files.

Because this is a multicomponent simulation, an additional input file ("no2.imc"), referred to as the *multicomponent input file* in Section 4.3, is required. The name of the multicomponent file is provided in the Materials (MA) section of the configuration file. The multicomponent file contains a description of the chemical species and the chemical reactions that they undergo. For the 1-hour NO_2 application, it is also necessary to specify background ozone concentrations, either as a fixed value or hourly varying values. The latter is the preferred option, and hourly ozone observations are typically available from the routine monitoring networks. Therefore, the

"no2.imc" file also specifies the name of the background ozone concentration file ("o3.amb") for this case study. For this tutorial, the "no2.imc" and "o3.amb" files are located in the "no2_mc_2005" sub-directory of the "Common" directory as shown in Figure A-2.

The configuration file, the hourly emissions file, the multicomponent input file, and the ambient ozone file are the four input files required for this multicomponent application (in addition to the meteorology inputs in the METSCI and ASOS1Min directories and the terrain data in the TERSCI directory).

In addition to these input files, the model requires an initialization file ("scipuff.ini") and a land use file ("landuse_scichem.dat"). See Tutorial 1 for more details.

All the SCICHEM outputs for this tutorial are created in the project ("no2_mc_2005") sub-directory.

The final step in this tutorial is the post-processing step to read the SCICHEM surface dosage output files in the same no2_mc_2005 sub-directory. Because of space restrictions, only the final output files from the post-processing are provided here for benchmarking.

Each of these steps in the preparation of SCICHEM input files and conducting the SCICHEM simulation is described in more detail next.

A.2.3 Meteorological Data and Terrain Data Preparation

These steps are identical to the meteorological data preparation step and terrain data preparation step for Tutorial 1 and are not described here. Details on this step can be found in Sections 2.1 and 2.2 of Tutorial 1.

A.2.4 SCICHEM Simulation

After the SCICHEM surface and upper air meteorological data files and the terrain file are created as described previously, the SCICHEM run script ("run_scichem.sh") in the Linux directory is used to conduct the SCICHEM simulation for this case study. **Before invoking the run script, the user must first step into the project directory ("no2_mc_2005") and invoke the run script from within the project directory.** The project name is specified as a command-line argument to the run script. For this case study, the project name is "no2-2005-mc". Following are the steps for this tutorial:

1. Change directories to the no2_mc_2005 directory (for example, "cd no2_mc_2005" from the Linux directory).
2. Invoke the run script with the project name as the argument (for example, "../run_scichem.sh no2-2005-mc").

SCICHEM looks for the configuration file, which has the name *projectname.*sci, that is, "no2-2005-mc.sci" for this tutorial. The various components of this file are described in detail in Section 4.2 of the User's Guide and include the following:

1. The run control section (lines starting with 'CO' or in the 'CO' block). This section is similar to the 'CO' section for Tutorial 1.
2. The material section (lines starting with 'MA' or in the 'MA' block). The path name of the multicomponent input file ("no2.imc") is provided in this section and signifies that this is a multicomponent simulation.
3. The source description section (lines starting with 'SO' or in the 'SO' block). The model calculates plume rise and initial puff dispersion dynamically. In addition, NO_2 and NO are specified as the emitted multicomponent species.
4. The receptor description section, specifying the receptor locations where concentration increments are to be calculated and output in the sampler file. As in the SO_2 case study in Tutorial 1, two sets of receptors are included: the first set is placed along the boundary of the property at 10-m intervals, while the second set is placed along the computational domain boundaries at 50-m intervals. Note that in a multicomponent simulation such as this Tutorial 2 case study, it is possible to specify the species that will be output in the sampler file using the MULTLIST keyword option. If this keyword is not provided, all multicomponent species are output.
5. The meteorology section, specifying the locations of the meteorological files to be used in the SCICHEM simulation. For Tutorial 2, this section is identical to the SO_2 case study in Tutorial 1.
6. The terrain section, specifying the location of the terrain file created using TERSCI. This is also identical to the corresponding section in Tutorial 1.

The model assumes default values for the parameters that are not supplied in the provided configuration file for this test case.

Several output files are created in the simulation with the names *projectname.*??? where "???" is the three-letter file extension identifying the file (for example, the "prj" extension specifies the project file; the "puf" extension specifies the file containing instantaneous puff incremental concentrations). These output file types are described in Section 6 of the User's Guide. The surface dosage output (specified by the "dos" extension) contains the integrated hourly species concentrations on an adaptive grid within the modeling domain. For a multicomponent run, two additional files with a four-letter file extension are also created. These files contain background (ambient) concentrations of the multicomponent species. The two files are named "*projectname.*asmp" and "*projectname.*ados". The first file contains ambient concentrations at the specified receptor locations, while the second file contains hourly surface ambient concentrations on the SCICHEM adaptive grid. The "*projectname.*dos" and "*projectname.*ados" files are read by the sciDOSpost post-processor, described in the following section, to create various reports.

For space reasons, none of the SCICHEM output files is provided in this distribution. Only the files created by the post-processor, described next, are provided for benchmarking.

A.2.5 Post-Processing of Surface Dosage Output

The last step in this tutorial is running the post-processor "sciDOSpost", which reads the SCICHEM surface dosage outputs in the files "no2-2005-mc.dos" and "no2-2005-mc.ados" in the project directory. The control file for the post-processing is named "no2-2005-mc.sciDOSpost.inp", and the file name is provided as a command-line argument to the post-processor run script "run_sciDOSpost.sh", located in the Linux directory. **As in the case of running SCICHEM, the user must first change directories to the project directory and invoke the post-processor run script from within the project directory.** The outputs of the post-processor depend on the reporting requirements specified in the control file. The provided sciDOSpost control file in this tutorial is self-descriptive, with comment lines preceded by the hash mark (#); the user can follow these comments to construct an application-specific control file.

For this tutorial, the post-processor creates four output files. The first file, "no2.over.sil.dat", contains the 8th highest daily maximum hourly NO_2 concentration at each receptor that exceeds the specified value of 7.5 μg/m^3. The receptor locations are defined in the file "no2-2005-mc.sam" as specified with the "rec" keyword. The output format is in "xyz" format, which gives locations in UTM and latitude/longitude, units, and time stamp along with the data values. The second output file, "max_concentrations.csv", is a comma-separated values file that contains the 8th highest daily maximum 1-hour NO_2 concentration and the maximum annual average NO_2 concentration over all receptors. Next, "no2.dv.samp. plot" is a file in AERMOD PLOTFILE format and contains the 8th highest daily 1-hour average NO_2 concentration at each receptor location defined in "no2-2005-mc.sam". Finally, "no2.dv.grid. plot" is similar to "no2.dv.samp. plot" but with receptor locations defined with the "grid" keyword.

A.3 Long-Range Impacts: TVA Cumberland

A.3.1 Introduction

This tutorial provides a step-by-step procedure for conducting a full chemistry simulation with SCICHEM to investigate impacts on incremental concentrations of emitted species and their secondary products downwind of a point source at distances ranging from 20 km to over 100 km. The source is the TVA Cumberland power plant located in north central Tennessee to the northwest of Nashville. This tutorial illustrates an example of a simulation of the TVA plume for a 15-hour period starting at midnight local time and illustrates the use of hourly surface and upper air meteorological observations to drive the model.

The modeling domain for this application is centered on the power plant and extends to 150 km on each side of the power plant in both the north-south and east-west directions. A Cartesian coordinate system is used for this application with the reference origin at the plant location (36.39°N, 87.6523°W). For illustration purposes, receptors are placed along the crosswind direction at 20 km, 55 km, and 110 km downwind and heights ranging from 520 m to 620 m above ground at approximately the plume centerline height.

This tutorial uses the Linux build of SCICHEM: The procedure for running on Windows is similar; a Windows batch file is also provided as part of the package. Because this is a full chemistry simulation, it uses the multicomponent option as described in the following section.

This tutorial illustrates the use of SCICHEM inputs based on the NAMELIST format (See Section 4.1 of the User's Guide). Tutorial 4 also illustrates the same usage.

A.3.2 Case Study Setup

The test case for this tutorial is provided is in the "examples/Linux/tva" directory. As with the previous tutorials, the run script ("run_scichem.sh") in the Linux sub-directory will be used. The project input files (in NAMELIST format) are located in the "tva" sub-directory. The project name for this application is " tva_080725". Figure A-3 provides the directory structure for this tutorial within the examples directory.

```
examples
|-- Common
|   |-- TVA
|   |   |-- fullchem_CB6r2_ae5_TN.imc
|   |   |-- tva_080725.sam
|-- Linux
|   |-- run_sciDOSpost.sh
|   |-- run_scichem.sh
|   |-- tva
|       |-- tva080725.prf
|       |-- tva080725.sfc
|       |-- tva_080725.inp
|       |-- tva_080725.msc
|       |-- tva_080725.scn
```

Figure A-3
Directory Organization for Tutorial 3

The following NAMELIST format input files in the project directory ("tva") are used for the SCICHEM application (see Section 4.1 of this User's Guide for a description of these files):

1. The main input parameter file ("tva_080725.inp")
2. The release scenario file ("tva_080725.scn")
3. The meteorological scenario file ("tva_080725.msc")

The main input parameter file, described in Section 4.1.1 of this User's Guide, contains information on the run duration, run time step, output time step, modeling domain, model options (default options are used if not specified in the input file), name of the sampler file containing receptor locations (optional), and name of the multicomponent input file (required for a multicomponent run) specifying the options for the chemistry calculations. This tutorial uses the "NONE" setting for the large-scale variability calculations, and the value of T_AVG in the Options section of the INP file is set to 0. This is because the project is run for a small domain and short time duration of 15 hours, and we are interested in sampling the instantaneous concentrations. For this exercise, the sampler file is called "tva_080725.sam" and contains receptor locations along three plume traverses at 20 km, 55 km, and 110 km downwind and heights ranging from 520 m to 620 m above ground. It also contains a list of the multicomponent species to be printed at the receptor locations. The sampler location file is described in Section 4.4. For this tutorial, the sampler location file is located within the "TVA" sub-directory of the "Common" directory (see Figure A-3).

The release scenario file is described in detail in Section 4.1.2 of this User's Guide and includes information on source location, stack parameters, and emission rates. For this exercise, there is only one source, located at the center of the modeling domain, which is also the origin—so the source location specified by XREL and YREL is (0,0). ZREL is the stack height in meters above the surface. The source is treated as a continuous stack (RELTYP='CS'), and plume rise is calculated within SCICHEM by solving the dynamic equations governing the evolution of freshly released puffs. For this application, the emissions and flow rates are assumed to be invariant in time, so the duration of the release is set to a sufficiently long time in hours ('TDUR=999.0') to cover the simulation period (15 hours in this exercise). For an annual simulation, this parameter would need to be increased appropriately. If hourly varying emission rates are available, the value of TDUR would be set to 1 and the information in the example release scenario file would need to be provided for each hour and each source. Other parameters in the release scenario file that would typically be changed by the user are as follows:

- Stack diameter (SIZE), 16.6 m for this exercise
- Stack exit velocity (WMOM), 19.66 m/s for this exercise
- Stack exit temperature (BUOY), 48.18^{o}C for this exercise
- Emission rates of multicomponent species, if applicable (for this exercise, emission rates of SO_2, NO, and NO_2 are provided)
- Emission rate of tracer material for a non-multicomponent run (CMASS); for a multicomponent run, this can be set to 1.0, as in the example scenario file

The meteorological scenario file is described in detail in Section 4.1.3 of the User's Guide. For this exercise, the parameter 'MET_TYPE' is set to 'OBS', indicating that the meteorology will be provided in the observation file format (see Section 4.5.1 of the User's Guide). One or more such observation files can be provided. For this exercise, two observation files are provided: a surface observation file and a profiler file containing upper air data. Both types of files are described in Section 4.5.1 of the User's Guide. The names of these files are provided in the last line of the meteorological scenario file and are called "tva080725.sfc" (containing surface observations) and "tva080725.prf" containing profiler data. These files are located in the project directory ("tva") for this tutorial. The lengths of the names of both files are 13 characters, and so the file names are prefixed with "@013" as described in the User's Guide. If the files were located in another directory, the full path name for the files would need to be provided and the prefix indicating the number of characters in the full path name would need to be changed accordingly. Because the observations do not include mixing height information, the parameter 'BL_TYPE' is set to 'CALC' in the meteorological scenario file so that the boundary layer height can be calculated internally within the model.

The multicomponent input file, referenced in the main input parameter file "tva_080725.inp", is named "fullchem_CB6r2_ae5_TN.imc" for this application. See Section 4.3 of this User's Guide for a full description of this file and its contents. For the most part, the only change that users should make to this file for their applications is the name of the ambient file containing the background chemical concentrations for the modeling domain. This file is named "TN.amb" in this application because the source is located in Tennessee. See Section 4.3.6 for a discussion of the various regions within the CONUS domain for which background chemistry profiles are provided as an aid to the user. Background chemistry files for each of these regions are provided

in the “Amb” sub-directory of the “sciData” directory (a discussion of the sciData directory follows). However, the user may optionally use application-specific background chemical concentrations if those are readily available.

In addition to specifying the ambient chemistry file for the SCICHEM simulation, the user may also opt to conduct a gas-phase-chemistry-only simulation (without aerosol and aqueous chemistry) by changing the flags for aerosol and aqueous chemistry from “True” to “False” in the multicomponent input file. Note that if the aqueous chemistry flag is set to “True”, the aerosol flag must also be set to “True” (see Section 4.3.2 of the User’s Guide). However, a run with aerosols (aerosol flag set to “True”) can be conducted without aqueous chemistry (aqueous chemistry flag set to “False”). For this tutorial, the multicomponent input file is located within the “TVA” sub-directory of the “Common” directory (see Figure A-1).

In addition to the input files discussed previously, the model requires an initialization file (“scipuff.ini”) and a land use file (“landuse_scichem.dat”), as discussed for the previous tutorials. See Section A.1.2.

Once all the input files are prepared, the run script in the “examples/Linux” directory can be used to conduct the SCICHEM simulation. **Before invoking the run script, the user must first step into the project directory (“tva”) and invoke the run script from within the project directory.** The project name is specified as a command-line argument to the run script. For this case study, the project name is “tva_080725”. The steps for this tutorial are as follows:

1. Change directories to the “tva” directory (for example, “cd tva” from the Linux directory).
2. Invoke the run script with the project name as the argument (for example, “../run_scichem.sh tva_080725”).

In the absence of a configuration file (with extension “sci”), SCICHEM looks for the three NAMELIST format files as well as for the auxiliary files (the multicomponent input file, the sampler location file, the background chemistry file, and the meteorological observation files) described previously.

Several output files are created in the project directory with the names *projectname.*??? where “???” is the three-letter file extension identifying the file (for example, the “prj” extension specifies the project file; the “puf” extension specifies the file containing instantaneous puff incremental concentrations). These output file types are described in Section 6 of this User’s Guide. For a multicomponent run, two additional files with a four-letter file extension are also created. These files contain background (ambient) concentrations of the multicomponent species. The two files are named “*projectname.*asmp” and “*projectname.*ados”. The first file contains ambient concentrations at the specified receptor locations, while the second file contains hourly surface ambient concentrations on the SCICHEM adaptive grid.

The sampler output file (“tva_080725.smp”) that is created contains plume total concentrations of tracer and multicomponent species at the sampler locations and heights specified in the “tva_080725.sam” file. For this exercise, there are 183 such sampler locations corresponding to three traverses of the Cumberland plume. The sampling interval is always the same as the maximum puff time step (DELT), which is set to 900 seconds in the main parameter input file, “tva_080725.inp” (this is also the default value if not specified). Note that the values in the “tva_080725.smp” file are total concentrations; that is, they represent the plume increment plus

the background value. A second sampler file, with the "asmp" extension ("tva_080725.asmp") contains the ambient concentrations at the sampler locations, as mentioned. Therefore, it is possible to calculate plume increments, that is, the change in concentration with respect to the ambient value as the difference between the total and ambient concentrations. Positive values represent increments, while negative values represent decrements from the background value. Therefore, plume ozone increments near the source are generally negative, because the ambient ozone is scavenged by the NOx in the plume. The sampler output files can be imported into a spreadsheet for analysis or for comparing against measurement data.

The surface total dosage and incremental deposition files ("tva_080725.dos" and "tva_080725.dep", respectively) contain hourly surface total (plume + ambient) concentrations and deposition values on the SCICHEM adaptive grid. These can be viewed with the SCICHEM GUI. An ambient surface dosage file ("tva_080725.ados") is also created as mentioned previously. The sciDOSPost processor, discussed in Tutorials 1 and 2, can be used to extract information from the surface dosage and deposition files and perform a Class I analyses for Prevention of Significant Deterioration (PSD) permit applications and Class II analyses for PSD permits or Minor New Source Review. An example of this analysis is shown in the following tutorial (Tutorial 4).

A.4 Long-Range Impacts: Four Corners

A.4.1 Introduction

This tutorial provides a step-by-step procedure for conducting a full chemistry simulation with SCICHEM to investigate impacts on incremental concentrations of emitted species and their secondary products at several Class I areas in the modeling domain. The tutorial illustrates the approach that would be used for assessing the Class I area air quality and AQRV impacts as used under the New Source Review and PSD programs or as part of an Environmental Impact Statement or Resource Management Plan under the National Environmental Policy Act.

The case study described in this tutorial is focused on the Four Corners region in the Southwest United States. SCICHEM is used to simulate the transport and chemistry of emissions from a single hypothetical source in New Mexico. A latitude-longitude coordinate system is used for this application with a domain of about 4 degrees by 4 degrees. There are several Class I areas within the modeling domain. Although an annual simulation was conducted with SCICHEM for this application, the data set provided with this tutorial and the SCICHEM distribution considers a 17-day period in July 2011 (July 15 to July 31) to keep the file sizes reasonable for the distribution. The tutorial illustrates the use of a gridded meteorological file to drive the model. The size of the gridded meteorological file for this 17-day period is about 1 GB.

This tutorial uses the Linux build of SCICHEM and the sciDOSpost processor described in Section 7.2 of the User's Guide. Although this tutorial focuses on running the case study on Linux, the procedure for running on Windows is similar; a Windows batch file is also provided as part of the package. Because this is a full chemistry simulation, it uses the multicomponent option as described in the following section.

Like Tutorial 3, this tutorial illustrates the use of SCICHEM inputs based on the NAMELIST format (see Section 4.1 of the User's Guide).

A.4.2 Case Study Setup

The test case for this tutorial is provided in the "fourCorners" sub-directory of the "Linux" directory in the "examples" directory. The Linux directory contains a run script ("run_scichem.sh"), while the NAMELIST format input files for the SCICHEM application are located in the "fourCorners" sub-directory. The project name for this application is "sw_ss" (for single source in the southwest). Figure A-4 provides the directory structure for this tutorial within the examples directory.

```
examples
|-- Common
|   |-- FourCorners
|   |   |-- SW_grid.sam
|   |   |-- fullchem_ae5_SW.imc
|   |   |-- SW.jul.scichem.bin.mcw
|-- Linux
|   |-- fourCorners
|   |   |-- sw_ss.inp
|   |   |-- sw_ss.msc
|   |   |-- sw_ss.scn
```

Figure A-4
Directory Organization for Tutorial 4

The following NAMELIST format input files in the project directory ("fourCorners") are used for the SCICHEM application (see Section 4.1 of the User's Guide for a description of these files):

1. The main input parameter file ("sw_ss.inp")
2. The release scenario file ("sw_ss.scn")
3. The meteorological scenario file ("sw_ss.msc")

The main input parameter file, described in Section 4.1.1 of the User's Guide, contains information on the run duration, run time step, output time step, modeling domain, model options (default options are used if not specified in the input file), and name of the multicomponent input file (required for a multicomponent run) specifying the options for the chemistry calculations. No sampler location file is specified in the example. The actual Class I area analysis is performed on all Class I area receptors of interest using the sciDOSpost processor and the surface dosage and deposition outputs from SCICHEM, as described later.

The release scenario file is described in detail in Section 4.1.2 of the User's Guide and includes information on source location, stack parameters, and emission rates. For this exercise, there is only one source, at the location (XREL, YREL) in latitude-longitude coordinates. ZREL is the stack height in meters above the surface. The source is treated as a continuous stack (RELTYP='CS'), and plume rise is calculated within SCICHEM by solving the dynamic equations governing the evolution of freshly released puffs. For this application, the emissions and flow rates are assumed to be invariant in time, so the duration of the release is set to a sufficiently long time in hours ('TDUR=9000.0') to cover the simulation period (408 hours in this exercise). For an annual simulation, this parameter would need to be increased appropriately. If hourly varying emission rates are available, the value of TDUR would be set to 1 and the information in the example release scenario file would need to be provided for each hour and

each source. The following other parameters in the release scenario file would typically be changed by the user:

- Stack diameter (SIZE), 6 m for this exercise
- Stack exit velocity (WMOM), 23 m/s for this exercise
- Stack exit temperature (BUOY), 156ºC for this exercise
- Emission rates of multicomponent species, if applicable (for this exercise, emission rates for 11 species are provided)
- Emission rate of tracer material for a non-multicomponent run (CMASS); for a multicomponent run, this can be set to 1.0, as in the example scenario file

The meteorological scenario file is described in detail in Section 4.1.3 of the User's Guide. For this exercise, the parameter 'MET_TYPE' is set to 'MEDOC' indicating that gridded meteorology will be provided (see Section 4.5.2 of the User's Guide for a description of the MEDOC file). When there is only one MEDOC file (for example, an annual file), its name can be specified in the meteorological scenario file. If there are multiple MEDOC files (for example, 12 monthly files), the name of a file containing the list of the monthly files is specified in the meteorological scenario file (see Section 4.5.5 of the User's Guide for the list input option). For this exercise, one MEDOC format file is provided for the 17-day period referred to earlier. MEDOC files can be prepared from WRF or MM5 outputs using the Mesoscale Model Interface Program (MMIF), developed for EPA by Ramboll. The MMIF source code and user's guide are available at EPA's SCRAM website.[7] The MEDOC file provided here was obtained by running the MMIF 3.4 processor on the 2011 EPA modeling platform 12-km CONUS WRF outputs. The name of the MEDOC file is provided in the last line of the meteorological scenario file and is called "SW.jul.scichem.bin.mcw". This file is located in the FourCorners sub-directory of the "Common" directory (see Figure A-4), so the full path to this file is "../../Common/FourCorners/". The length of the full file name (with path) is 47 characters, so the name is prefixed with "@047" (as described in the User's Guide) as follows: @047../../Common/FourCorners/SW.jul.scichem.bin.mcw. Because the MEDOC file includes mixing height information, the parameter 'BL_TYPE' is set to 'MEDOC' in the meteorological scenario file so that the model uses the provided boundary layer heights.

The multicomponent input file, referenced in the main input parameter file "sw_ss.inp", is named "fullchem_ae5_SW.imc" for this application. See Section 4.3 of the User's Guide for a full description of this file and its contents. This file is also located in the parent directory of the Linux directory. For the most part, the only change that a user should make to this file is the name of the ambient file containing the background chemical concentrations for the modeling domain. This file is named "SW.amb" in this application because the hypothetical source is located in the southwest United States. See Section 4.3.6 of the User's Guide for a discussion of the various regions within the CONUS domain for which background chemistry profiles are provided as an aid to the user. Background chemistry files for each of these regions are provided in the "Amb" sub-directory of the "sciData" directory (a discussion of the sciData directory

[7] http://www.epa.gov/ttn/scram/dispersion_related.htm#mmif.

follows). However, the user may optionally use application-specific background chemical concentrations if those are readily available.

In addition to specifying the ambient chemistry file for the SCICHEM simulation, the user may also opt to conduct a gas-phase-chemistry-only simulation (without aerosol and aqueous chemistry) by changing the flags for aerosol and aqueous chemistry from "True" to "False" in the multicomponent input file. Note that if the aqueous chemistry flag is set to "True", the aerosol flag must also be set to "True" (see Section 4.3.2 of the User's Guide). However, a run with aerosols (aerosol flag set to "True") can be conducted without aqueous chemistry (aqueous chemistry flag set to "False"). For this tutorial, the multicomponent input file is located within the "FourCorners" sub-directory of the "Common" directory (see Figure A-1).

In addition to the input files discussed previously, the model requires an initialization file ("scipuff.ini") and a land use file ("landuse_scichem.dat"), described in the User's Guide. These two files are application-independent and required for all SCICHEM applications. The scipuff.ini file is located in the directory that contains the SCICHEM executable, as specified in the provided run_scichem.sh run script. The landuse_scichem.dat file and other auxiliary files are located in the "sciData" directory. The sciData directory is at the same level as the "examples" directory containing the tutorial test cases. **Note that the scipuff.ini file specifies the locations of the sciData directory and the landuse_scichem.dat file. These locations are specified as absolute path names, so users must modify the scipuff.ini file for their configuration.**

Once all the input files are prepared, the run script in the "examples/Linux" directory can be used to conduct the SCICHEM simulation. **Before invoking the run script, the user must first step into the project directory ("fourCorners") and invoke the run script from within the project directory.** The project name is specified as a command-line argument to the run script. For this case study, the project name is "fc_egu1". The steps for this tutorial are as follows:

1. Change directories to the "fourCorners" directory (for example, "cd fourCorners" from the Linux directory).
2. Invoke the run script with the project name as the argument (for example, "../run_scichem.sh sw_ss").

SCICHEM looks for the three NAMELIST format files as well as for the auxiliary files (the multicomponent input file, the sampler location file, the background chemistry file, and the meteorological observation files) described previously.

Several output files are created in the project directory with the names *projectname.*??? where "???" is the three-letter file extension identifying the file (for example, the "prj" extension specifies the project file; the "puf" extension specifies the file containing instantaneous puff incremental concentrations). These output file types are described in Section 6 of the User's Guide. For a multicomponent run, two additional files with a four-letter file extension are also created. These files contain background (ambient) concentrations of the multicomponent species. The two files are named "*projectname.*asmp" and "*projectname.*ados". The first file contains ambient concentrations at the specified receptor locations, while the second file contains hourly surface ambient concentrations on the SCICHEM adaptive grid.

For space reasons, none of the SCICHEM output files is provided in this distribution. Only the files created by the post-processor, described next, are provided for benchmarking.

A.4.3 Post-Processing of Surface Dosage Output

The surface total dosage and deposition files ("sw_ss.dos" and "sw_ss.dep", respectively) contain hourly surface total (plume + ambient) integrated concentrations and deposition values on the SCICHEM adaptive grid. These can be viewed with the SCICHEM GUI. An ambient surface dosage file ("sw_ss.ados") is also created as mentioned. The sciDOSPost processor, discussed in Tutorials 1 and 2, is used to extract information from the surface dosage and deposition files and perform a Class I analyses. This step is described next.

For this tutorial, the "sciDOSpost" processor reads the SCICHEM total and ambient surface dosage outputs in the files "sw_ss.dos" and "sw_ss.ados", respectively, as well as the deposition file "sw_ss.dep" in the project directory. The control file for the post-processing is named "sw_ss.sciDOSpost.inp", and the file name is provided as a command-line argument to the post-processor run script "run_sciDOSpost.sh", located in the Linux directory. **As in the case of running SCICHEM, the user must first change directories to the project directory and invoke the post-processor run script from within the project directory.** The outputs of the post-processor depend on the reporting requirements specified in the control file "sw_ss.sciDOSpost.inp". The provided sciDOSpost control file in this tutorial is self-descriptive, with comment lines preceded by the hash mark (#), and the user can follow these comments to construct an application-specific control file. The "calculate plume" keyword is used to specify that plume increments are to be calculated for the concentrations (that is, the difference between the total values in the sw_ss.dos file and the ambient values in the sw_ss.ados file). The deposition is always calculated as a plume increment.

For this tutorial, the post-processor creates 16 output files based on the specification of requirements in the "sw_ss.sciDOSpost.inp" file. The "max_concentrations.csv" file is a comma-separated values file that contains several statistics for each Class I area:

- The highest 17-day (408-hour) average concentration over all receptors in the Class I area for NO_2, SO_2, $PM_{2.5}$, and PM_{10}
- The highest 3-hour average concentration of SO_2 over all receptors in each Class I area
- The highest 24-hour average concentration of SO_2, $PM_{2.5}$, and PM_{10} over all receptors in each Class I area

Note that the SCICHEM outputs for this case study contain only 408 hours of data because the simulation is for a 17-day period—therefore, annual statistics are not available. In a typical application, the model would be run for a full year and the "408 hr" period would be replaced with "1 yr".

The rest of the files are listed and described here:

- "max_dep.csv" contains the highest 17-day sulfur and nitrogen deposition over all receptors in each Class I area.
- "vis_results.csv" contains the 8^{th} highest 24-hour average change in extinction over all receptors in each Class I area.
- The "visibility_exceedances.csv" reports exceedances of >5% and >10% changes to the 24-hour extinction coefficient for all receptors in each Class I area.

- "meve.dep.xyz" gives the 17-day average total, wet, and dry deposition of nitrogen for all receptors in the Mesa Verde area, reported in "xyz" format, which additionally displays locations in UTM and latitude/longitude, units, and time stamp.
- "meve.vis_contrib.csv" is a comma-separated values file containing the contribution of each species to the 8th highest 24-hour average change in extinction over all receptors in the Mesa Verde area.
- "pso4.max.grd" contains the maximum 24-hr average concentrations of particulate SO_4 arrayed on a regular grid defined in "sw_ss.sciDOSpost.inp" with the "grid" keyword. Output is in Surfer 6 ASCII format.
- "pno3.max.grd" is the same as "pso4.max.grd" but for particulate NO_3.
- "pso4.max.smp" is similar to "pso4.max.grd" but with locations defined in the file "sw_grid.sam" (as specified with the "rec" keyword) and output in "xyz" format.
- "pno3.max.smp" is similar to "pso4.max.smp" but for particulate NO_3.
- "o3.DV.grd" gives the 4th highest rolling 8-hour average O_3 concentration arrayed on a regular grid, in Surfer 6 ASCII format.
- "o3.DV.smp"is similar to "o3.DV.grd" but with locations defined in "sw_grid.sam" and in "xyz" format.
- "no2.dv.xyz" contains the 8th highest daily 1-hour average NO_2 concentration, on a regular grid, in "xyz" format.
- "so2.dv.grd" contains the 4th highest daily 1-hour average SO_2 concentration on a regular grid, in Surfer 6 ASCII format.
- "no2.dv.smp" is the same as "no2.dv.xyz" but with locations defined in "sw_grid.sam".
- "so2.dv.smp" is similar to "so2.dv.grd" but with locations defined in "sw_grid.sam" and in "xyz" format.

B
USING SCIPUFF GUI

As mentioned in Section 5, the current version of the GUI is provided primarily as a convenience to the user to visualize model results. However, the GUI has some limited capabilities to create namelist-type projects. In this section, we describe how the GUI can be used for creating namelist projects.

B.1 Creating a New Project

To create a new project, the user will click the **New Project** button. The window shown in Figure B-1 will appear, prompting the user for a new project name.

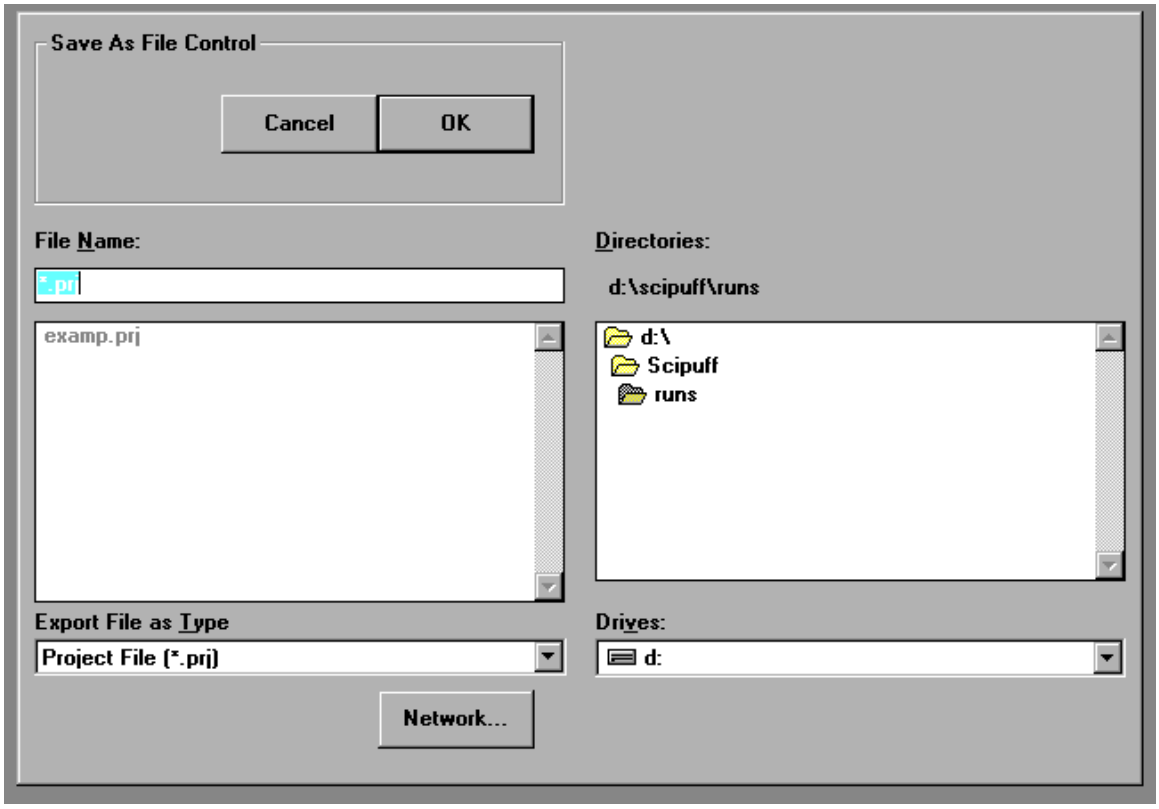

Figure B-1
New Project Window

The user can enter the project name and click **OK** to continue. Afterwards, the **New Project Setup** window will appear (Figure B-2).

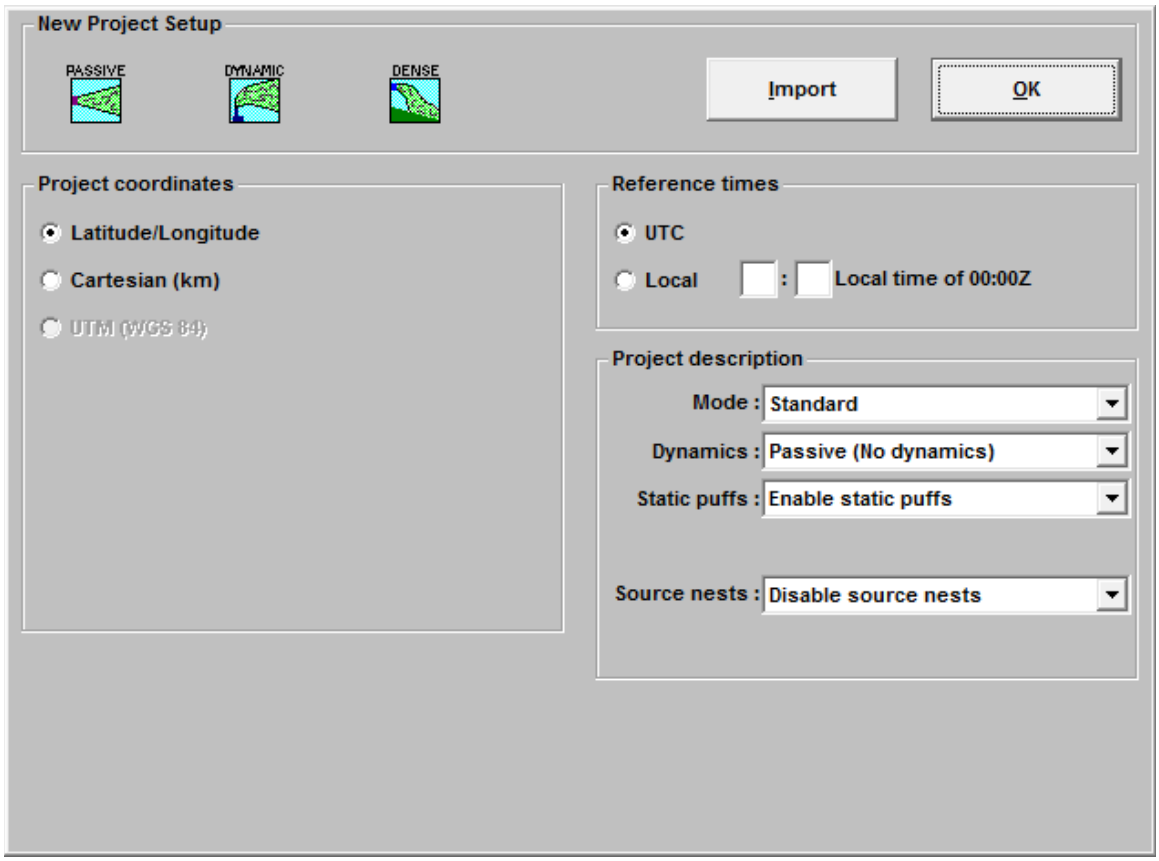

Figure B-2
New Project Setup Window

B.1.1 New Project Setup

The user must select an icon in the upper left corner that determines whether dynamic effects will be included in the calculation. Dynamic effects treated are buoyant and momentum plume rise and gases that have densities different from that of air.

Passive - do not include dynamic effects

Dynamic - include dynamic effects

Dense - include dense gas effects

The user may click **Import** to import an existing project into the current project. Otherwise, the user will enter all necessary information for the new project in this window and press **OK**. When importing files, a *Restart* check box is included with the Open File dialog box. If Restart is selected, the Restart Time Editor dialog box will appear when the ***OK*** button is pushed. The start time of the new project is then selected from the Restart time list box.

B.1.2 Project Coordinates

The user must specify the project coordinate system. The choices are as follows:

Latitude/Longitude

This specifies the SCICHEM coordinate system as Latitude/Longitude (degrees). This is the default coordinate system.

Cartesian

This specifies the SCICHEM coordinate system as rectangular Cartesian (kilometers). If this radio button is selected, you may check the "Lat./Lon. Reference Point" check box.

If the *reference* point box is checked for Cartesian coordinates, the following edit boxes will appear:

Cart. (X, Y)

This specifies the Cartesian coordinates of the reference point in kilometers.

Default: None

LLA (E, N)

This specifies the longitude and latitude coordinates of the reference point specified in the X, Y edit boxes. The coordinates can be specified in degrees or degrees/min/sec.

Default: None

B.1.3 Reference Times

The user must specify the project reference times. The choices are as follows:

UTC

This specifies the SCICHEM time to be in the Universal Time Convention, which is equivalent to Greenwich Mean Time (GMT or Z). UTC is the default time reference.

Local

This specifies the SCICHEM time to be in local time.

The following edit box appears with the *Local* time reference option:

Local Time of 00:00Z

This specifies the local time (hours:minutes) of midnight UTC. This is used to convert the meteorology time if it uses a different convention. It is also used to determine some boundary layer parameters depending on boundary layer type.

Default: None

B.1.4 Project Description

The user must specify additional project options. They include the following:

Mode

This specifies whether to run SCICHEM in *Standard* or *Fast* mode. See Table B-1 for a description of the two modes.

Dynamics

This specifies whether to treat dynamics. It is controlled by an icon at the top.

Static Puffs

This specifies whether to use static puffs in the calculation. Static puffs significantly speed up the calculation; therefore, the default is to use them.

Multicomponent

This specifies whether to treat material transformations through chemical reactions. The **Browse** button should be used to select the IMC file (see Section 4.3) if this option is activated.

Table B-1
SCICHEM Run Modes

Parameter	STANDARD	FAST	Comments
VERTICAL RESOLUTION			
Default height of the vertical domain Default vertical domain resolution Default maximum vertical grid points	2500m 250m 15	5000m 1000m 7	These vertical grid parameters affect the vertical splitting of puffs, which affects the total number of puffs. These parameters can also be entered manually by the user.
HORIZONTAL RESOLUTION			
Surface resolution [DELMIN]	0.0 (As needed)	1/160 of domain	This affects the surface grid and total number of puffs if surface evaporation is occurring. This parameter can also be entered manually by the user.
MERGE CRITERIA			
SiMerge (ratio of internal scales)	1.25	1.5	This allows more merging between puffs and reduces the total number of puffs. This parameter cannot be manually entered by the user. It is changed internally when Fast Mode is selected.

B.1.5 New Project Editor

Once a project has been set up or imported, the New Project Editor window will appear, as shown in Figure B-3.

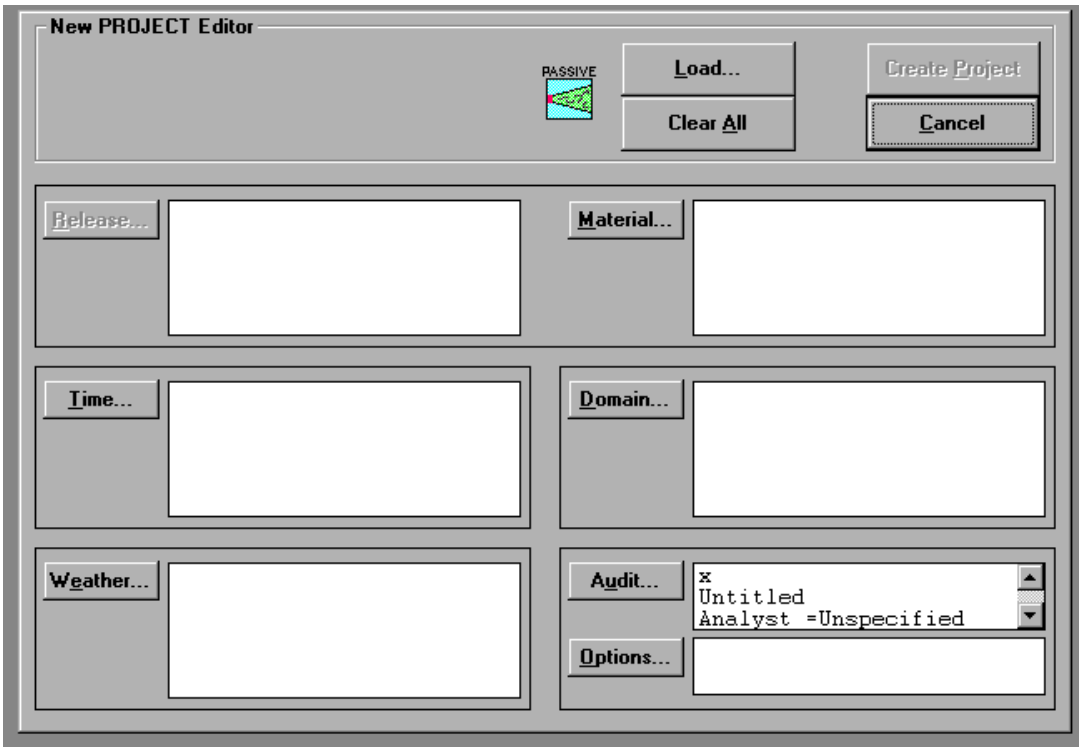

Figure B-3
New Project Editor Window

The user must define key areas of the project. A red check mark will appear next to each category once it has been edited. (A check mark will appear even if a category has not been fully filled out. Error messages may appear when the user attempts to proceed in that case.) After all categories are complete, the user may click **Create Project** to create the new project files. The key areas that must be defined include the following categories:

- Release
- Time
- Weather Material
- Domain
- Audit
- Options

B.2 Material Editor

The material editor is used to define the parameters of the material being released. The material must be defined prior to defining the release parameters; therefore, the discussion will begin with the material editor. When the user clicks Material, the Material Editor window (shown in Figure

B-4, top portion only) will appear and can be used to add, change, or delete materials and to create or change a material definition.

If the user is creating a new material by clicking New, the material dialog box will appear, as shown next, giving choices of materials as Gas or Particle. If a material has already been defined, the user may copy another material by choosing it from a drop-down list.

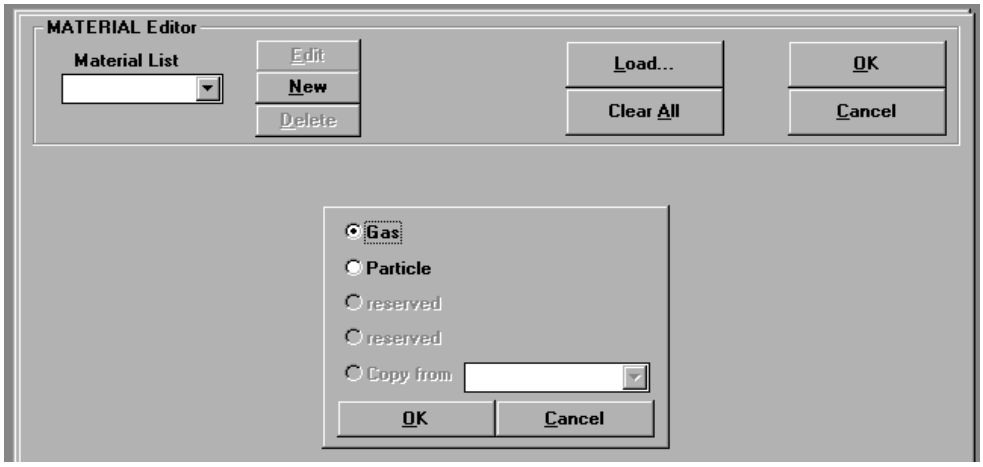

Figure B-4
Material Editor Window

B.2.1 Gas Material

This window is used to define a gas. The Material Editor window for a gas is shown in Figure B-5.

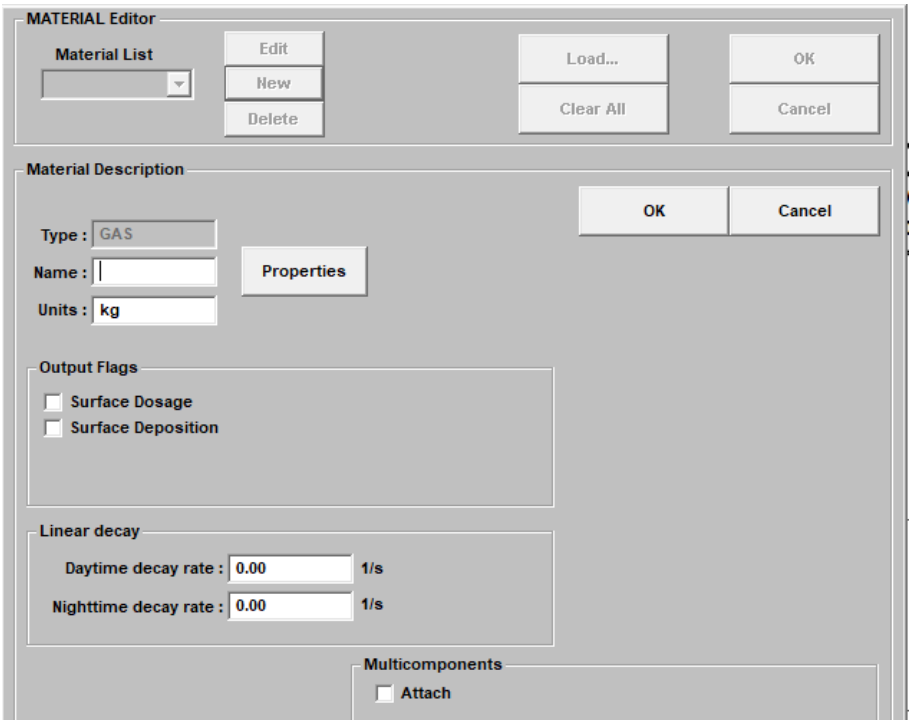

Figure B-5
Material List for a Gas Window

The input parameters are defined as follows:

Material Description

Type

This specifies the material type (GAS). This parameter cannot be edited from this box.

Name

This is the unique name identifying the material, up to 8 characters in length.

Default: NONE - Must be specified.

Units

This specifies the material mass units. The default is kg.

Output Flags

Surface Dose

This specifies that the time-integrated surface dose is written to *ProjectName*.DOS.

Surface Deposition

This specifies that the time-integrated surface deposition is written to *ProjectName*.DEP.

Linear Decay

Daytime Decay Rate

This specifies the daytime decay rate (s^{-1}) of the gas material

Default: 0.0

Nighttime Decay Rate

This specifies the nighttime decay rate (s^{-1}) of the gas material.

Default: 0.0

Multicomponents - Attach

Multicomponent species may be attached to the material using this check box. The species names are taken from the IMC file. This option is available only if the project has been defined Multicomponent.

When the user presses the Properties button, the Gas Parameter Editor window will appear, as shown in Figure B-6.

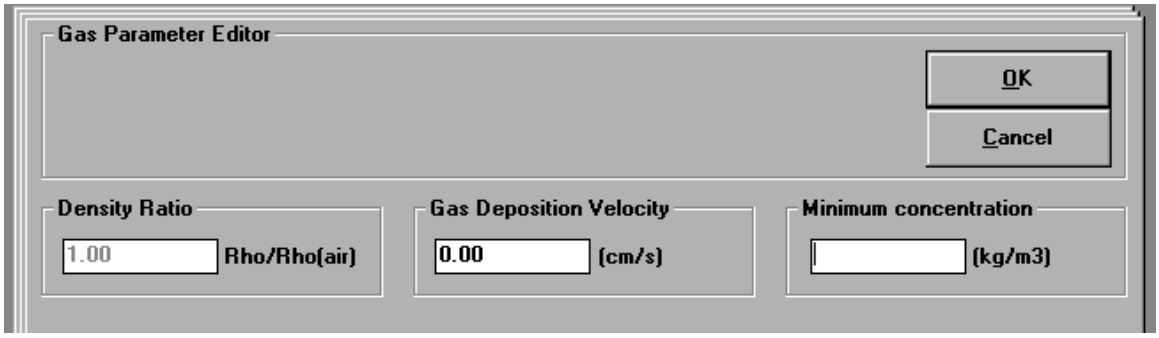

Figure B-6
Gas Parameter Editor Window

The gas properties are defined as follows:

Density Ratio

This specifies the density ratio of material-to-air that is used to determine buoyancy effects.

Default: 1.0

Gas Deposition Velocity

This specifies the velocity (cm/s) at which the gaseous material deposits to the surface. A zero deposition velocity implies no deposition.

Default: 0.0

Minimum Concentration

This specifies the minimum puff concentration (material mass units/m^3). A puff with a concentration less than this value does not split or distort because of velocity gradients, but it may merge with other puffs. Setting this minimum value may help decrease execution time.

Default: 0.0 (blank converts to zero after clicking OK)

B.2.2 Particle Material

This window is used to define a particle. The Material Editor window for a particle is shown in Figure B-7.

Figure B-7
Material Editor for a Particle Window

The input parameters are defined as follows:

Material Description

Type

This specifies the material type (PART). This parameter cannot be edited from this box.

Name

This is the unique name identifying the material, up to 8 characters in length.

Default: NONE - Must be specified.

Units

This specifies the material mass units. The default is kg.

Output Flags

Surface Dose (Size Bin)

This specifies that the time-integrated surface dose for each size bin is written to *ProjectName*.DOS

Surface Deposition (Size Bin)

This specifies that the time-integrated surface deposition for each size bin is written to *ProjectName*.DEP.

Surface Dose (Total)

This specifies that the time-integrated surface dose, summed over all the size bins, is written to *ProjectName*.DOS.

Surface Deposition (Total)

This specifies that the time-integrated surface deposition, summed over all the size bins, is written to *ProjectName*.DEP.

Linear Decay

Daytime Decay Rate

This specifies the daytime decay rate (s^{-1}) of the particle material

Default: 0.0

Nighttime Decay Rate

This specifies the nighttime decay rate (s^{-1}) of the particle material.

Default: 0.0

Size Bins

The particle size distribution for the material is defined by several discrete bins. The size bins are defined in the Bin Boundaries box by copying an existing material, computing bin boundaries based on an assumed distribution, or constructing bin boundaries explicitly. The bin boundaries may then be edited as desired.

The No. Size Bins displayed here is the number of bins used to define the size distribution. A single size bin indicates that all released particles of this material fall within the same bin. At least one bin must be defined. The maximum number of size bins is 50.

The Bin Boundaries (microns) determine the range and distribution of the particle sizes. The number of bin boundaries is always 1 greater than the number of size bins. Bin boundaries are used to calculate the increase in the vertical spread of the material due to differential gravitational settling rates; that is, large particles fall out faster than smaller particles, increasing the vertical extent of the material.

Use the buttons in the Bin Boundaries group to define the size bins:

Edit - Click to change the selected bin boundary to a new value.

New - Click to add a new bin boundary to the list.

Delete - Click to remove a selected bin boundary from the list.

Clear All - Click to remove all bin boundary values from the list.

Compute - Click to calculate bin boundaries based on a particle size range, number of bins, and an assumed size distribution.

Load - Click to copy bin boundaries from a file into the list. This is an appending procedure, so the loaded values are added to those already in the list.

Save - Click to save the current bin boundary list to a file.

When the user presses the Properties button, the Particle Parameter Editor window will appear, as shown in Figure B-8.

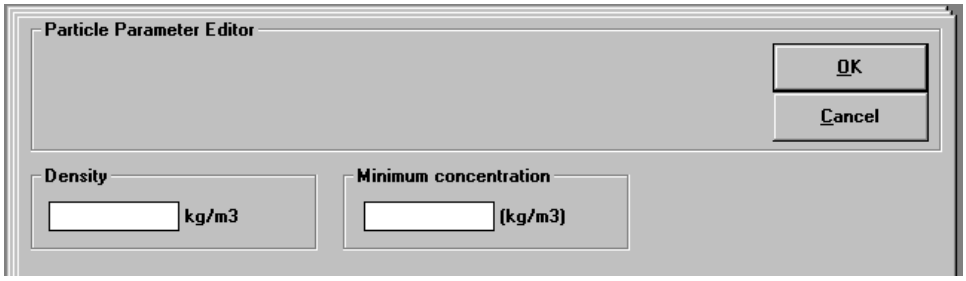

Figure B-8
Particle Parameter Editor Window

The particle parameters are defined as follows:

Density

This specifies the density of the particle material (kg/m^3).

Default: None – Must be specified.

Minimum Concentration

This specifies the minimum puff concentration (material mass units/m^3). A puff with a concentration less than this value does not split or distort due to velocity gradients, but it may merge with other puffs. Setting this minimum value may help decrease execution time.

Default: 0.0 (blank converts to zero after clicking OK)

B.2.3 Liquid Material

This window is used to define a liquid. The Material Editor window for a liquid is shown in Figure B-9.

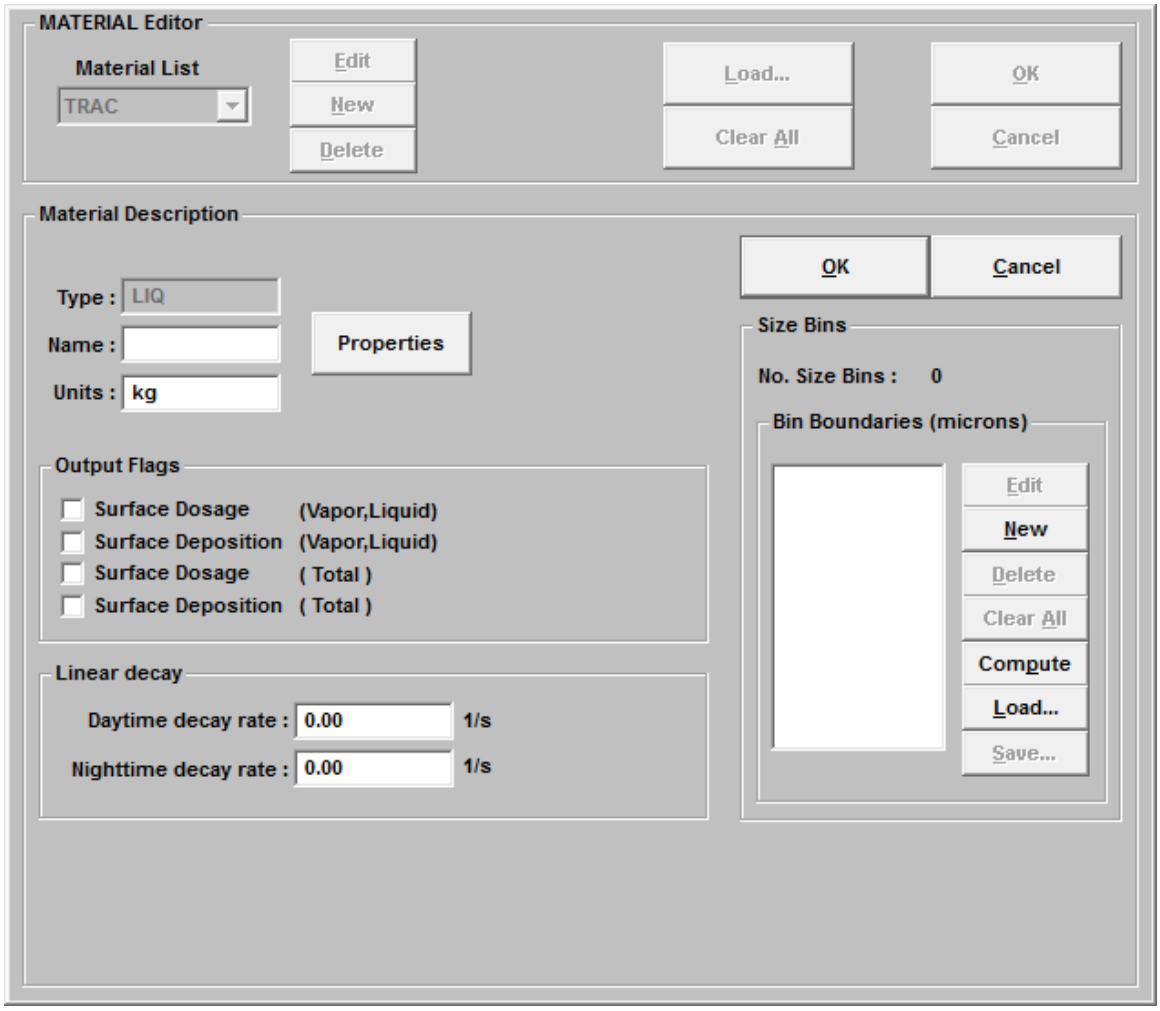

Figure B-9
Material Editor for a Liquid Window

The input parameters are defined as follows:

Material Description

Type

This specifies the material type (LIQ). This parameter cannot be edited from this box.

Name

This is the unique name identifying the material, up to 8 characters in length.

Default: NONE - Must be specified.

Units

This specifies the material mass units. The default is kg.

Output Flags

Surface Dosage (Vapor, Liquid)

This specifies that the time-integrated surface dose is written to ProjectName.DOS.

Surface Deposition (Vapor, Liquid)

This specifies that the time-integrated surface deposition is written to *ProjectName*.DEP.

Surface Dosage (Total)

This specifies that the time-integrated surface dose is written to *ProjectName*.DOS.

Surface Deposition (Total)

This specifies that the time-integrated surface deposition is written to *ProjectName*.DEP.

Linear Decay

Daytime Decay Rate

This specifies the daytime decay rate (s^{-1}) of the liquid material.

Default: 0.0

Nighttime Decay Rate

This specifies the nighttime decay rate (s^{-1}) of the liquid material.

Default: 0.0

When the user presses the Properties button, the Liquid Parameter Editor window will appear, as shown in Figure B-10.

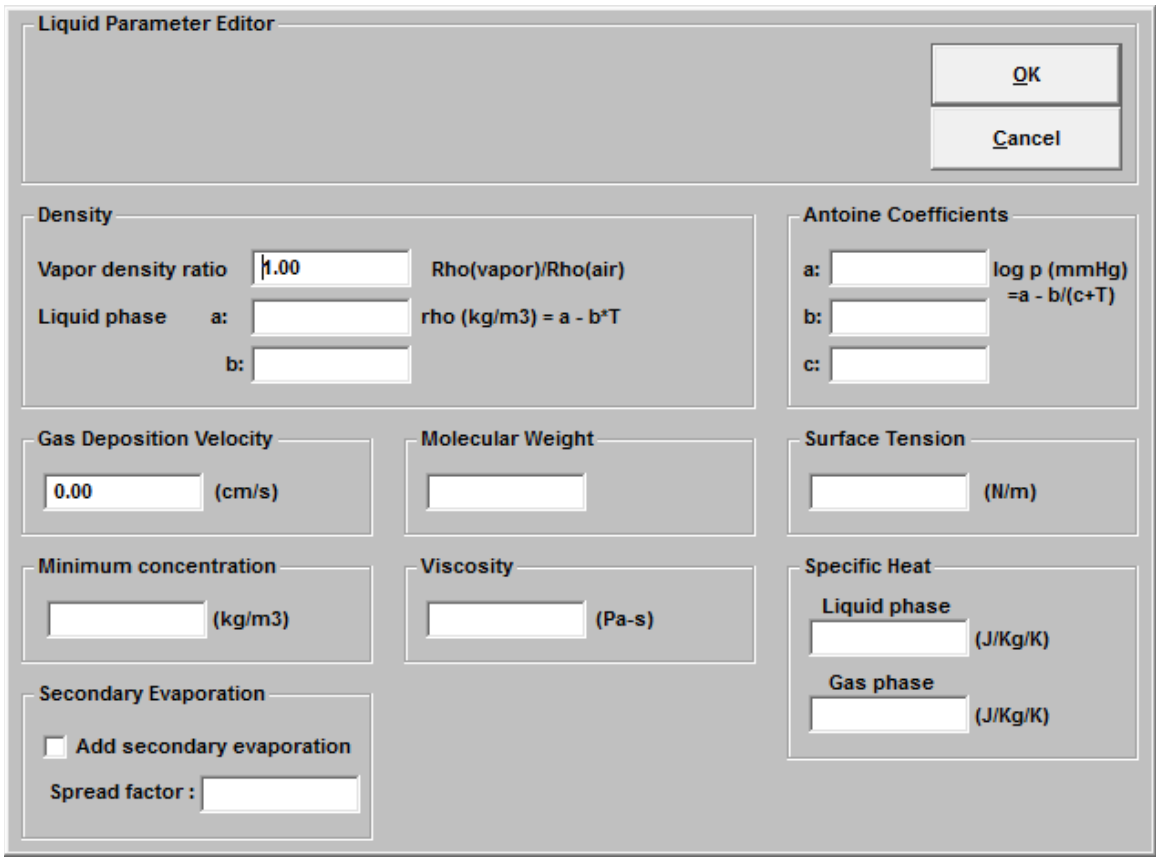

Figure B-10
Liquid Parameter Editor Window

The liquid properties are defined as follows:

Vapor Density Ratio

This specifies the density ratio of material-to-air that is used to determine buoyancy effects.

Default: 1.0

Gas Deposition Velocity

This specifies the velocity (cm/s) at which the gaseous material deposits to the surface. A zero deposition velocity implies no deposition.

Default: 0.0

Molecular Weight

This specifies the molecular weight of the gaseous material.

Surface Tension

This specifies the surface tension (N/m) of the liquid material.

Viscosity

This specifies the viscosity (Pa-s) of the liquid material.

Liquid Phase Specific Heat

The specific heat (J/Kg/K) of the material in liquid phase.

Default: 0.0

Gas-Phase Specific Heat

The specific heat (J/Kg/K) of the material in gas phase.

Secondary Evaporation

Logical to turn on evaporation of liquid from surface deposition.

Default: False

B.3 Release Editor

The Release Editor is used to define the release parameters. When the user clicks Release from the New Project, the Release Editor window (shown in Figure B-11, top portion only) will appear and can be used to add, change, or delete releases.

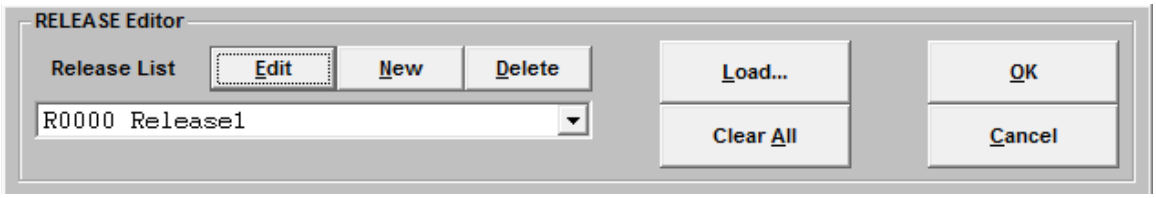

Figure B-11
Release Editor Window

If the user is creating a new release by clicking New, the release dialog box will appear, as shown in Figure B-12, giving choices of release types. If a release has already been defined, the user may copy another release by choosing it from the drop-down list. Multiple releases may be defined for a single project. Section B.2.1 shows editing windows for the release of a gas type material. Releases of particle materials are discussed in Section B.2.2.

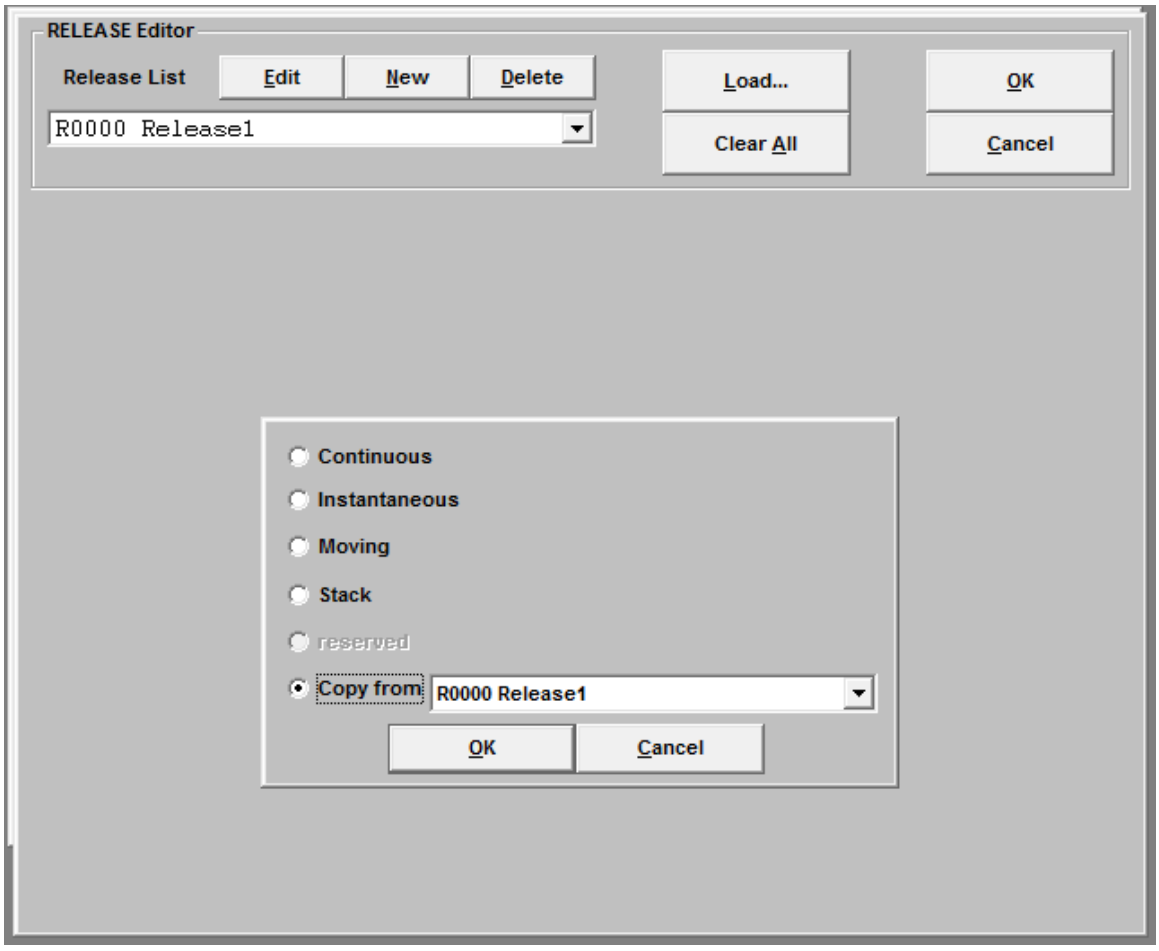

Figure B-12
Release List Window

Select the type of release from the displayed options:

- Continuous
- Instantaneous
- Moving
- Stack
- Copy from (an existing release definition)

B.3.1 Continuous Release Type

This window is used to define a continuous release of a gas. The Release Editor window for a continuous release is shown in Figure B-13.

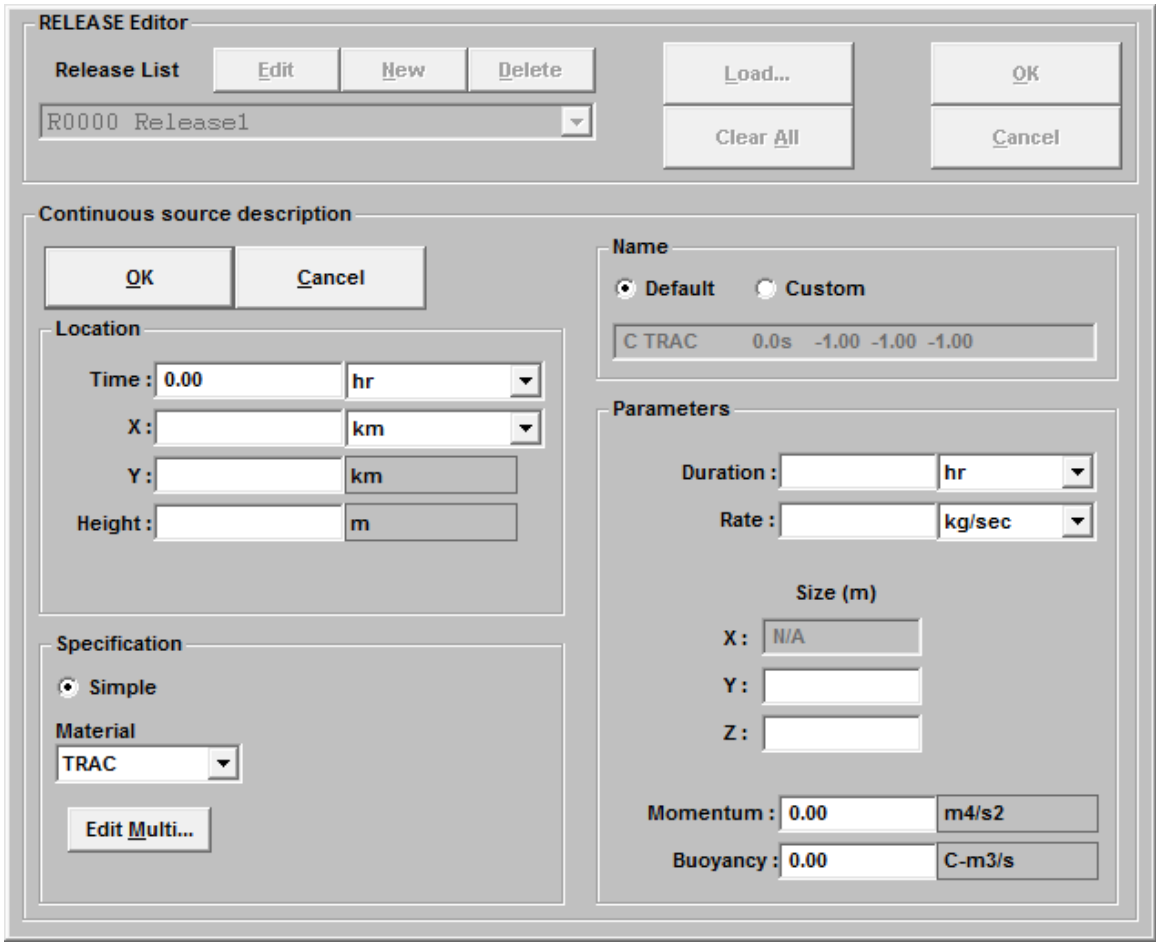

Figure B-13
Release Editor Window for Continuous Release

The release parameters are defined as follows:

Location

Time

This specifies the time (hrs) relative to the SCICHEM calculation start time at which the material is first released. For example, if a material is released at the calculation start time, the release time is 0. Releases can be input in any order because SCICHEM automatically sorts each release by its release time. The units can be changed with the combo box to the right.

Default: 0.0 hours

X

This specifies the x-coordinate, Cartesian (km), of the release. The units can be changed with the combo box to the right.

Default: Km

Y

This specifies the y-coordinate, Cartesian (km), of the release. The units are the same as the *X* units.

Default: Km

Height (m)

This specifies the height (m) of the release above the surface.

Default: None - Must be specified.

Specification

Simple

The material is released at the specified location with the mass and size defined in the **Parameters** group box. This is the only option for a continuous release.

Material

This specifies a four-character name identifying the material being released. The drop-down list contains a list of materials defined for this project.

Edit Multi

If the material multicomponent species are attached to the material, this push button will appear, allowing the user to specify multicomponent emissions.

Name

Default

Use the default release name.

Custom

This button allows the user to provide a customized name for the release.

Parameters

Duration

This specifies the length of time (hours), relative to the release time, that the material is released. The units are changed with the combo box on the right.

Default: NONE - Must be specified.

Rate

This specifies the material mass release rate (mass units/s). The mass units are taken from the Material Description.

Default: NONE - Must be specified.

X (Size)

This is not applicable for a continuous source.

Y (Size)

This specifies the lateral Gaussian spread parameter (size) of the release source (m).

Default: NONE - Must be specified.

Z (Size)

This specifies the vertical Gaussian spread parameter (size) of the release source (m).

Default: NONE - Must be specified.

Momentum

This specifies the momentum of the effluent (m^4/s^2) if the project is a Dynamic Run and the material type is Gas. To include the effect of dynamics on materials other than gases, the effluent gas must also be a defined release.

Default: NONE - Must be specified.

Buoyancy

This specifies the buoyancy of the effluent (C-m^3/s) if the project is a Dynamic Run and the material type is Gas. To include the effect of dynamics on materials other than gases, the effluent gas must also be a defined release.

Default: NONE - Must be specified.

Multicomponent Releases

If the material being released is a multicomponent material, the Edit Multi push button will appear beside the material combo box to allow editing the release rates of each species. Species emission rates should be expressed in *emission_units* (either in ppm-m^3/sec, 1.e-6 molecules/sec, or g/s). The *emission_units* are given in the IMC file under the control section. For a multicomponent species, the concentration will be displayed in *species_units* for gases (as specified in the IMC file under the control section). For aerosol particles, the emission units are always assumed to be g/s. Additional particle types are denoted by "PA" for particle area emission and have units of m^2/s, and "PN" for particle number emissions with emission units of numbers/s. See Section 4.3 for details on the IMC file.

When the Edit Multi button is clicked, the window shown in Figure B-14 will appear, allowing the user to edit the multicomponent emission rates.

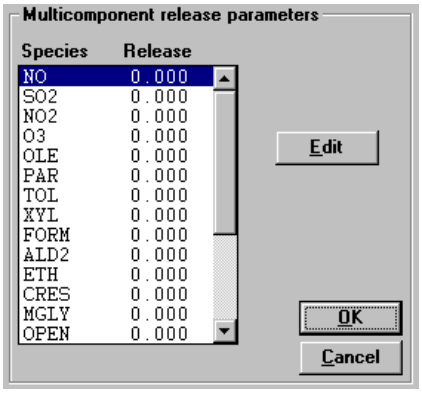

Figure B-14
Edit Multicomponent Release Parameters Window

B.3.2 Instantaneous Release Type

This window is used to define an instantaneous release of a gas. The Release Editor window for an instantaneous release is shown in Figure B-15.

Figure B-15
Release Editor Window for an Instantaneous Release

The release parameters are defined as follows:

Location

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Specification

Simple

The material is released at the specified location with the mass and size defined in the Parameters group box.

CLOUDTRANS

This is an unsupported feature in SCICHEM.

The remaining definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Name

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Parameters

Randomize Location

This allows for a randomization of the source locations within the calculation domain. If this box is checked, a Parameters push button appears.

Mass

This specifies the total mass (mass units) of the released material. The mass units are taken from the corresponding Material Description, Gas or Particle, as appropriate.

Default: NONE - Must be specified.

X (Size)

This specifies the x-coordinate Gaussian spread parameter of the release source (m).

Default: NONE - Must be specified.

Y (Size)

This specifies the y-coordinate Gaussian spread parameter of the release source (m).

Default: NONE - Must be specified.

Z (Size)

This specifies the vertical Gaussian spread parameter of the release source (m).

Default: NONE - Must be specified.

Momentum

This specifies the momentum of the effluent (m^4/s) if the project is a Dynamic Run and the material type is Gas. To include the effect of dynamics on materials other than gases, the effluent gas must also be a defined release.

Default: NONE - Must be specified.

Buoyancy

This specifies the buoyancy of the effluent ($C\text{-}m^3$) if the project is a Dynamic Run and the material type is Gas. To include the effect of dynamics on materials other than gases, the effluent gas must also be a defined release.

Default: NONE - Must be specified.

B.3.3 Moving Release Type

This window is used to define a moving release of a gas. The Release Editor window for a moving release is shown in Figure B-16.

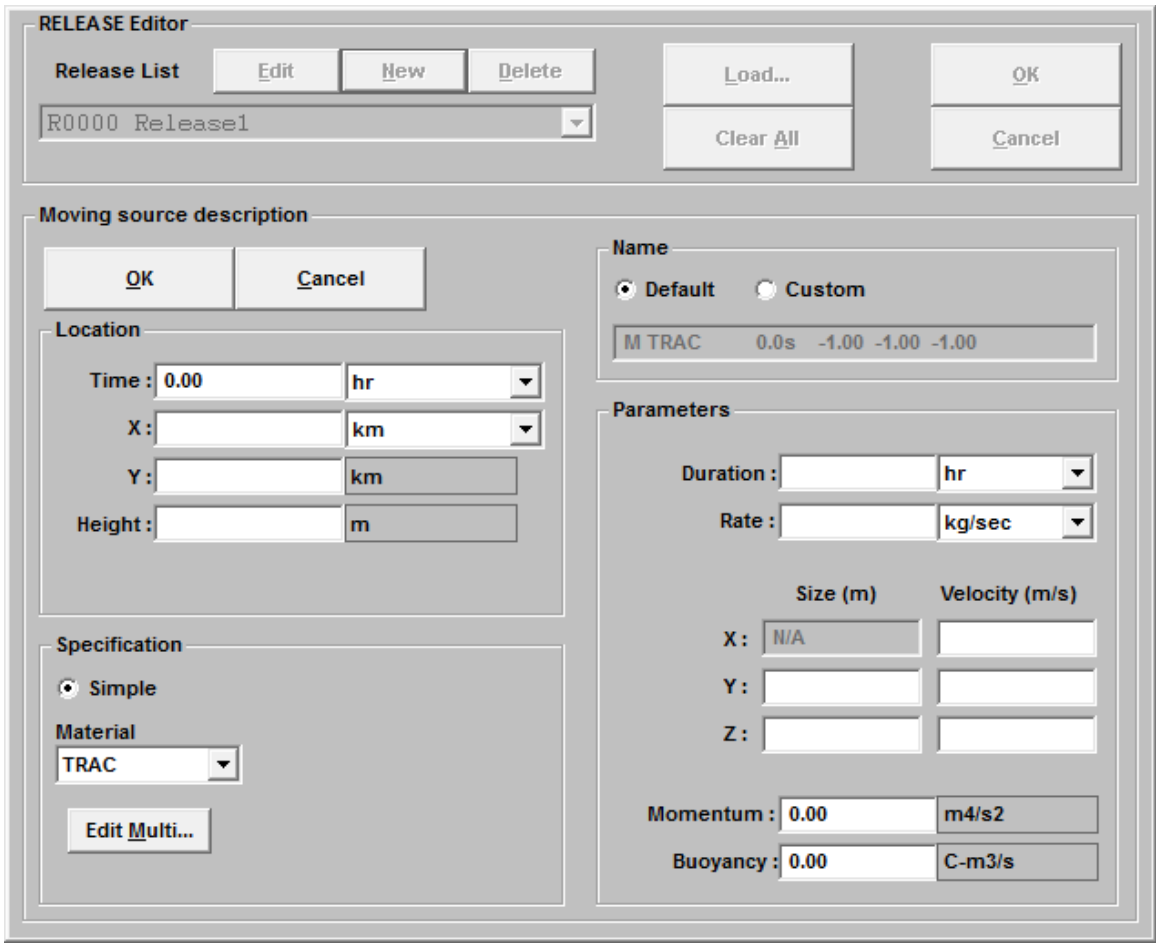

Figure B-16
Release Editor Window for a Moving Release

The release parameters are defined as follows:

Location

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Specification

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Name

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Parameters

The definitions of these parameters are the same as those for the continuous release (Section B.3.1) except that the source velocity (m/s) appears next to the source coordinates.

X (Velocity)

This specifies the source velocity component in the x-coordinate direction (m/s).

Default: NONE - Must be specified.

Y (Velocity)

This specifies the source velocity component in the y-coordinate direction (m/s).

Default: NONE - Must be specified.

Z (Velocity)

This specifies the source velocity component in the vertical direction (m/s).

Default: NONE - Must be specified.

B.3.4 Stack Release Type

This window is used to define a stack release of a gas. The Release Editor window for a stack release is shown in Figure B-17.

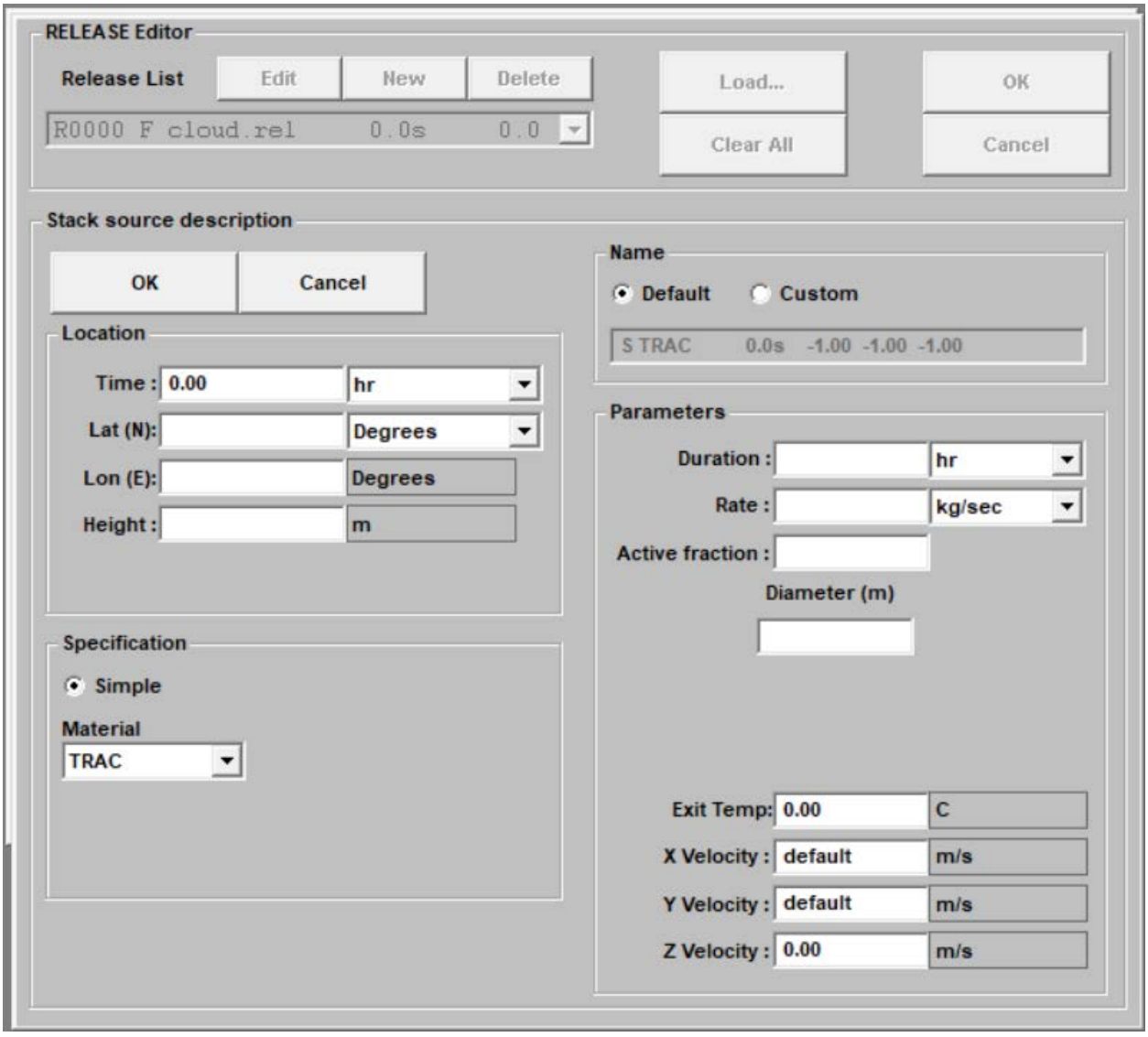

Figure B-17
Release Editor Window for a Stack Release

The release parameters are defined as follows:

Location

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Specification

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Name

The definitions of these parameters are the same as those for the continuous release (Section B.3.1).

Parameters

The definitions of the Duration and Rate are the same as those for the continuous release (Section B.3.1).

Diameter (m)

This specifies the diameter of the stack (m).

Default: NONE - Must be specified.

X-,Y-,Z- Velocity (m/s)

This specifies the exit velocity components (m/s) of the stack effluent if the project is a Dynamic Run and the material type is Gas. To include the effect of dynamics on materials other than gases, the effluent gas must also be a defined release. In a vertical stack, only the z-component is non-zero.

Default: 0.00.

Exit Temperature (C)

This specifies the exit temperature (C) of the stack effluent if the project is a Dynamic Run and the material type is Gas. To include the effect of dynamics on materials other than gases, the effluent gas must also be a defined release.

Default: 0.00

B.3.5 Release of Particle Materials

This editor shows the difference when specifying a release using particle materials. All parameters are the same as those defined in Sections 4.3.1 through 4.3.4, except under the Specification editing area if a particle material is chosen. The user may select the particle size group that is released. Figure B-18 shows an example.

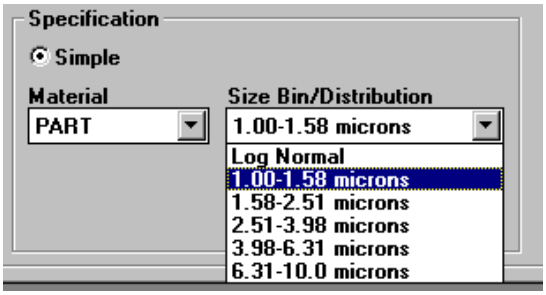

Figure B-18
Specification Box

If a Log Normal distribution is chosen, the following edit boxes will appear, as shown in Figure B-19.

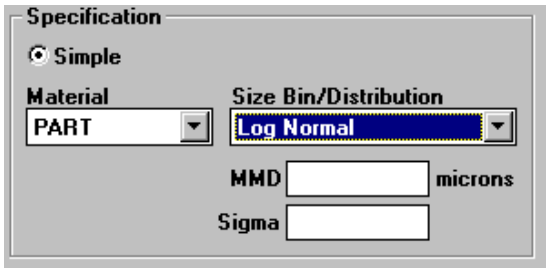

Figure B-19
Log Normal Specification Box

When this option is chosen, the user must specify the mass mean diameter, MMD, in microns and the geometric standard deviation, *Sigma*, (σ^2). The resulting lognormal size distribution is partitioned into the material size bins, as defined in the particle material description.

If more than 5% of the release mass lies outside the range of the size bins, a warning is issued. Continuing without changing the distribution or the size bins will allocate mass below the lower size bin limit into the first size bin and mass above the upper size bin into the last bin. To change the size bin boundaries, the user must return to the Material Editor.

A useful guide for determining the size bin range is that 96% of the total mass in the lognormal distribution is contained between $\frac{MMD}{\sigma^2}$ and $MMD \times \sigma^2$. A typical size bin specification would span this range using 10 bins with logarithmic spacing. The resolution of the size distribution depends on the range of the calculation; longer range calculations may need better resolution to prevent separation between bins as the material falls through the atmosphere.

B.4 Time Editor

The Time Editor is used to define the duration of the simulation and the time step and output intervals. When the user clicks Time from the New Project, the Time Editor window (shown in Figure B-20) will appear.

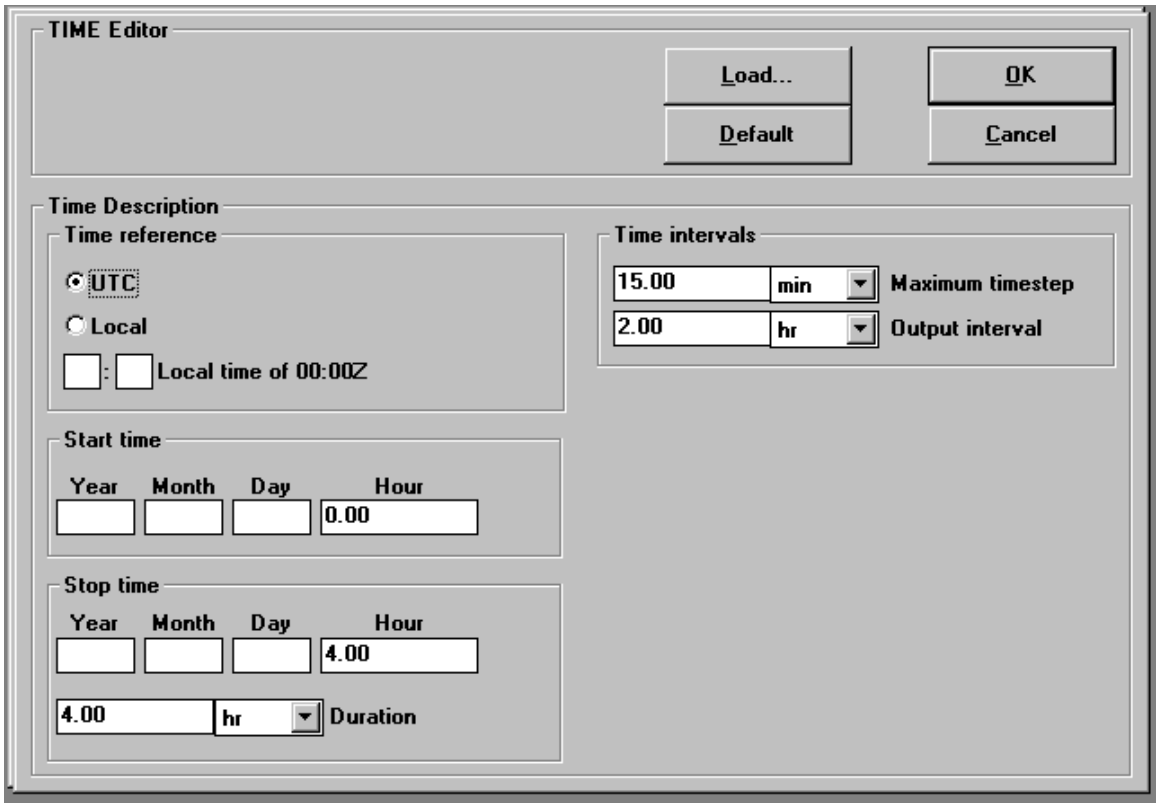

Figure B-20
Time Editor Window

The parameters are defined as follows:

B.4.1 Time Reference

UTC

This specifies the SCICHEM time to be in the Universal Time Convention, which is equivalent to Greenwich Mean Time (GMT or Z). UTC is the default time reference.

Local

This specifies the SCICHEM time to be in local time.

Local Time of 00:00Z

This specifies the local time (hours:minutes) of midnight UTC. This is used to convert the meteorology time if it uses a different convention. It is also used to determine some boundary layer parameters depending on boundary layer type.

Default: 00:00.

B.4.2 Start Time

Year, Month, Day, Hour

This specifies the start time for the SCICHEM calculation. This determines the initial release time for the dispersion calculation.

Default: If Year, Month, Day are left blank, the release is assumed to start on the first day in the meteorological file. If Year is less than 100, it is assumed to be between 1950 and 2049, for example, setting Year to 1 is equivalent to 2001 and 99 is equivalent to 1999.

B.4.3 Stop Time

Year, Month, Day, Hour

This specifies the stop time for the SCICHEM calculation. It is specified in the same way as the start time. Duration is automatically computed when this is set.

Default: 4 hours after the start time

Duration

This specifies the total calculation period for the SCICHEM calculation. The stop time is automatically computed when this is set. Time duration units are chosen with the adjacent combo box.

Default: 4 hours

B.4.4 Time Intervals

Maximum Time Step

This specifies the maximum time step for the dispersion calculation. This should be chosen to smoothly resolve any meteorological variations, including the boundary layer. SCICHEM uses an adaptive time step and reduces the step size as appropriate for each puff. The units for the time step can be changed with the adjacent combo box.

Default: 15 minutes

Output Interval

This specifies the time interval between saved outputs. The output includes the instantaneous fields and optional surface integral fields (surface dose and/or surface deposition). The units for the output interval can be changed with the adjacent combo box.

Default: 2 hours

B.4.5 Restart Time

Time

This specifies the time at which the current project is initialized when restarting from an existing project. This input area is shown for restarts only.

B.5 Domain Editor

The Domain Editor is used to specify the domain parameters. When the user clicks Domain from the New Project, the Domain Editor window (shown in Figure B-21) will appear.

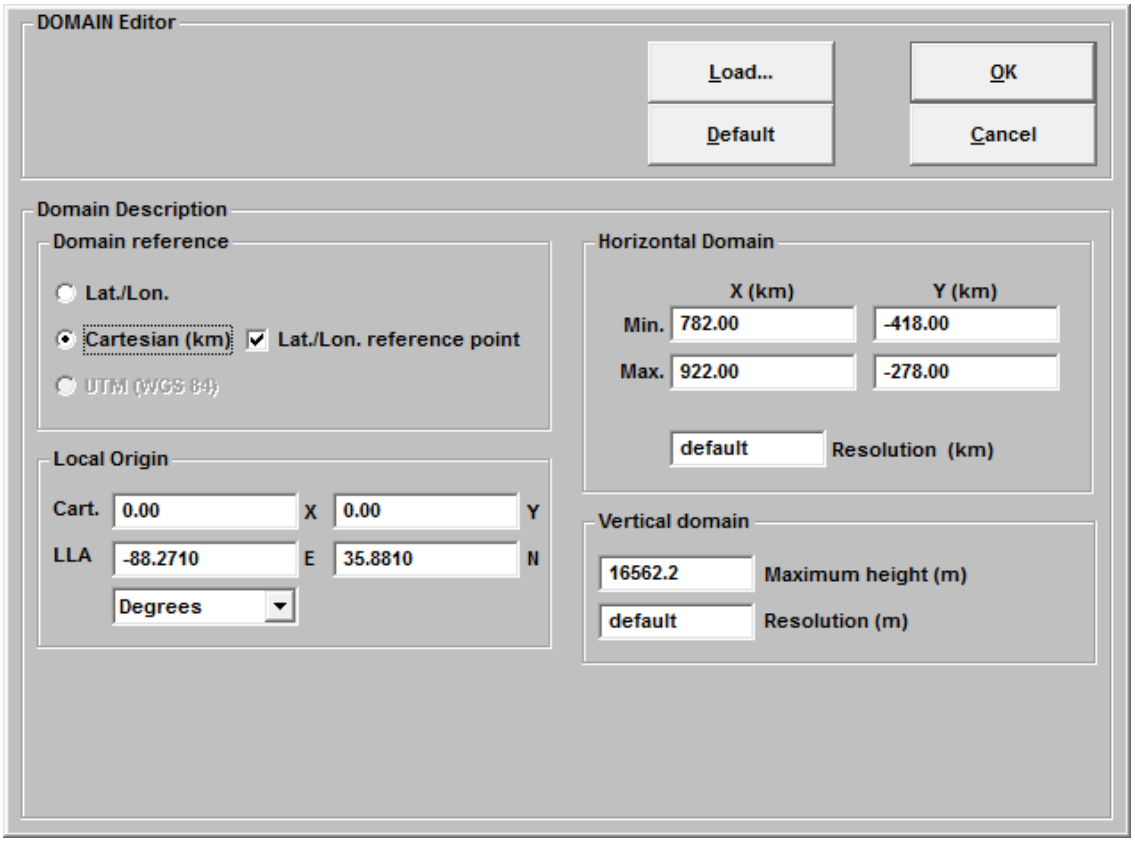

Figure B-21
Domain Editor Window

The parameters are defined as follows.

B.5.1 Domain Reference

Lat./Lon.

This specifies the SCICHEM coordinate system as Latitude/Longitude (degrees). This is the default coordinate system.

Cartesian

This specifies the SCICHEM coordinate system as rectangular Cartesian (kilometers). Optionally, the user can specify the Latitude/Longitude reference point for locating the Cartesian domain on the surface of the earth. Cartesian coordinates do not account for the curvature of the earth and should therefore be limited to domain sizes less than about 300 km.

B.5.2 Horizontal Domain

Lat. (or X), Lon.(or Y) - Minima and Maxima

This specifies the limits that determine the extent of the SCICHEM dispersion calculation domain. For Latitude/Longitude coordinates, the domain boundaries are positive values in degrees for East and North. Therefore, the minimum longitudinal coordinate is the Western edge of the domain, and the minimum latitude is the Southern edge. For Cartesian coordinates, the domain extents are specified in kilometers.

Default: Limits must be explicitly set for observational meteorology without terrain input. For gridded meteorology or observational meteorology with terrain/mass consistency, the limits will be determined from the meteorology or terrain grid.

Resolution (Deg. or km)

This box specifies the spacing (degrees or km) that defines the horizontal numerical resolution of the puff dispersion calculation. Smaller values generally result in longer computation times but allow for better resolution of the flow field. The horizontal growth of the puffs is also a measure of the horizontal resolution and is controlled by the parameter *MGRD* set in the Options editor. When using gridded meteorology or terrain/mass consistency, it is necessary that the default resolution (denoted by "default" in the edit box) be used. The horizontal resolution will be determined by the meteorological input files. (The horizontal growth of the puffs can still be controlled with *MGRD* in the Options editor.) For observational meteorology, this parameter determines the horizontal grid size used to interpolate the data.

Default: The resolution is 1/10 of the domain size for observational meteorology. For gridded data, the resolution is taken as that of the meteorology.

B.5.3 Vertical Domain

Maximum Height (m)

This specifies the vertical extent of the calculation domain (m). The lower bound of the domain is always at the surface.

Default: 2500 m

Resolution (m)

This box specifies the spacing (m) that defines the vertical numerical resolution of the puff dispersion calculation. It should be based on the meteorology grid spacing. For example, if the vertical resolution of the meteorological data is 1000 meters, this value should be approximately 1000 meters. Setting the resolution much less than the meteorology grid spacing does not significantly increase the accuracy of the SCICHEM results but does increase the execution time. If it is set larger than the meteorology spacing, the accuracy of the SCICHEM calculation may be decreased. It should be noted that the planetary boundary layer resolution is set independently in the Options section.

Default: "default" results in 250 m set internally (subject to a maximum of 200 levels up to maximum height)

B.5.4 Local Origin

Cartesian

The X and Y coordinates for local origin in km.

Default: 0.,0.

LLA

The corresponding Latitude and Longitude coordinates for the origin in degrees.

Default: None

B.6 Weather Editor

The Weather Editor is used to define the background meteorological conditions. When the user clicks Weather from the New Project Editor, the Weather Editor window (shown in Figure B-22) will appear.

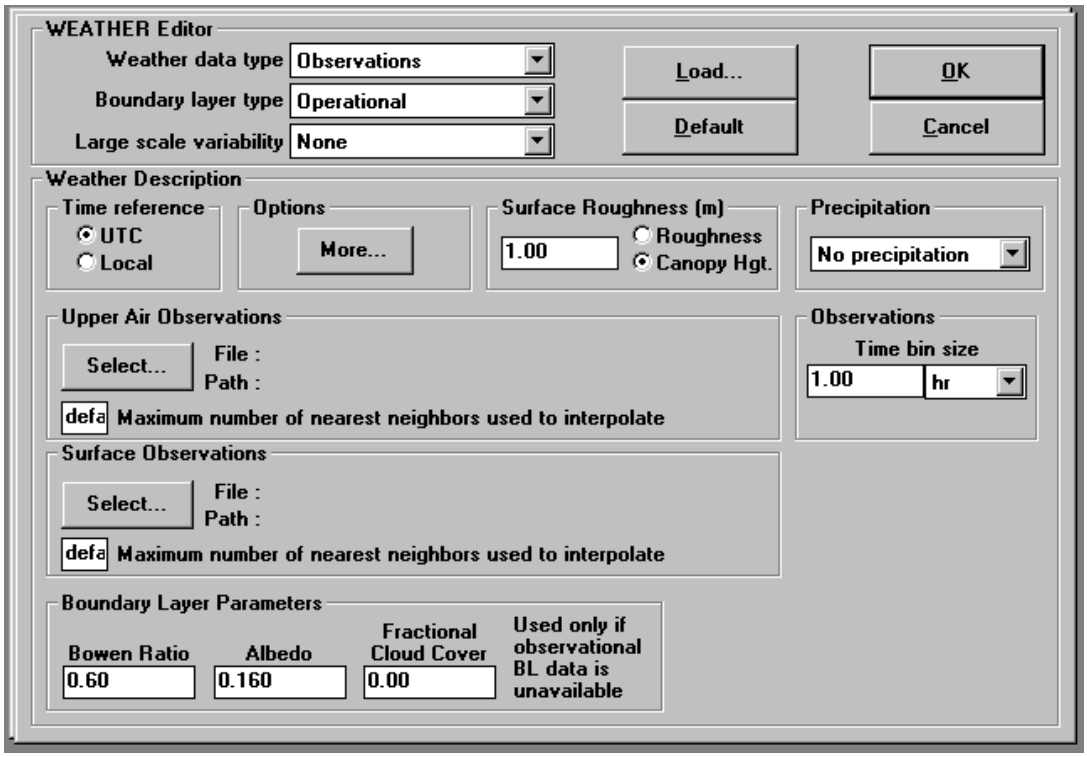

Figure B-22
Weather Editor Window

B.6.1 Weather Data Types

The choices of weather data types are as follows:

- Fixed Winds
- Observations
- Surface Observations only
- Upper Air Observations only
- List of grid/obs met files
- List of MEDOC files
- SCIP Gridded Data
- WRF Gridded Data
- MEDOC Gridded Data

Weather Data Type: Fixed Winds

When the Fixed Winds option is chosen, the user will be prompted to enter the following information (see Figure B-23).

Figure B-23
Fixed Winds Screen

Wind Speed

This specifies the wind speed (at 10 meters above the surface) used in translating the effluent. The wind speed is held constant in space and time at this value. The units are selected from the associated list box.

Default: 4.0 m/s

Direction

This specifies the wind direction (at 10 meters above the surface) used in translating the effluent. The wind speed is held constant in space and time at this value. The unit is degrees. It is the direction from which the wind is blowing.

Default: 90.0 degrees

Weather Data Type: Observations

When the Observations option is chosen, the user will be prompted to enter the following information (see Figure B-24).

Figure B-24
Upper Air Observations Window

When the user clicks the Select button, the Open File dialog box will appear, allowing the user to select the meteorological files. The user must choose both the Upper Air Observations file (PROFILE type) and the Surface Observations (SURFACE type). These files should be formatted as described in Section 4.5.1.

Maximum Number of Nearest Neighbors Used to Interpolate

This specifies the maximum number of observation locations (reporting data at a given time) that are used to interpolate the observations onto the meteorology grid. Decreasing this number will decrease the project run time.

Default: All - Standard observations
4 - Analysis or forecast

Time Bin Size

This specifies the time bins (and time units) for observational input so that all observations reported within a time bin will be assigned the same time. This feature may avoid overly frequent updating of the meteorology, most notably when SCICHEM is involved.

Weather Data Type: Surface Observations Only

The user will select only a Surface Observations file, formatted as described in Section 4.5.1.

Weather Data Type: Upper Air Observations Only

The user will select only an Upper Air Observations file, formatted as described in Section 4.5.1.

Weather Data Type: List of Grid/Obs Met Files

The user will select a meteorological list file as described in Section 4.5.5. The first line should be "SCIPUFF_LIST".

Weather Data Type: List of MEDOC Files

The user will select a meteorological list file as described in Section 4.5.5. The first line should be "MEDOC", followed by a list of sequential MEDOC files.

Weather Data Type: SCIP Gridded Data

Not used.

Weather Data Type: WRF Gridded Data

The user will select a meteorological list file as described in Section 4.5.5. The first line should be "WRF".

Weather Data Type: MEDOC Gridded Data

The user will select a MEDOC Gridded Data file, formatted as described in Section 4.5.2.

Boundary Layer Types

The choices of boundary layer types are as follows:

- None
- Simple Diurnal
- Calculated
- Observations
- Profile
- Gridded
- Operational

Boundary Layer Type: None

Specifying no boundary layer implies that no small-scale turbulence is included in the calculation. This should be used only under special circumstances, such as conducting simple advection tests. There are no input parameters.

Boundary Layer Type: Simple Diurnal

SCICHEM allows for very simple estimates of boundary layer height and surface height flux using simple functional forms with user-specified nighttime and daytime values. This option should be used only for theoretical or hypothetical studies in which either the user does not want to use the real boundary layer data or the data are not available. The input parameters are as follows (Figure B-25).

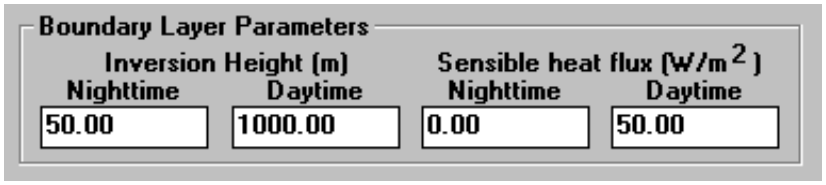

Figure B-25
Boundary Layer Parameters Window for Simple Diurnal

Inversion Height (m) - Nighttime and Daytime

This specifies the minimum and maximum diurnal inversion heights used in calculations of boundary layer parameters.

Default: Minimum = 50; Maximum = 1000

Sensible Heat Flux (W/m^2) - Nighttime and Daytime

This specifies the minimum and maximum daily surface heat fluxes used in calculations of boundary layer parameters.

Default: Minimum = 0; Maximum = 50

Boundary Layer Type: Calculated

SCICHEM calculates surface heat flux using a surface energy balance model. Boundary layer height is estimated from an evolution equation that models growth from convectively and mechanically driven entrainment into the overlying stable air. The input parameters are as follows (Figure B-26).

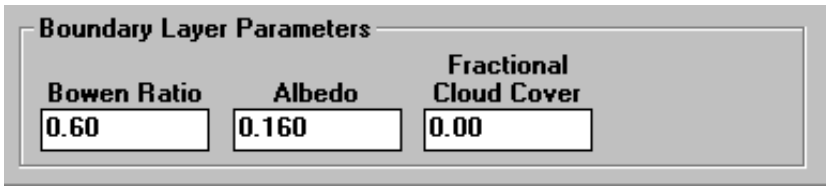

Figure B-26
Boundary Layer Parameters Window for Calculated

Bowen Ratio

This specifies the ratio of surface sensible heat flux to latent heat flux. See Table B-2 for typical values.

Default: 0.6

Albedo

This specifies the fraction of incident light that is reflected by the surface. See Table B-3 for typical values.

Default: 0.16

Cloud Cover

This specifies the fractional cloud cover where completely overcast is 1 and clear is 0.

Default: 0

Table B-2
Typical Bowen Ratios

Land Use Type	Spring	Summer	Autumn	Winter
Water	0.1	0.1	0.1	1.5
Deciduous Forest	0.7	0.3	1.0	1.5
Coniferous Forest	0.7	0.3	0.8	1.5
Swamp	0.1	0.1	0.1	1.5
Cultivated Land	0.3	0.5	0.7	1.5
Grassland	0.4	0.8	1.0	1.5
Urban	1.0	2.0	2.0	1.5
Desert Shrubland	3.0	4.0	6.0	6.0

Table B-3
Typical Albedo Values

Land Use Type	Spring	Summer	Autumn	Winter
Water	0.12	0.10	0.14	0.20
Deciduous Forest	0.12	0.12	0.12	0.50
Coniferous Forest	0.12	0.12	0.12	0.35
Swamp	0.12	0.14	0.16	0.30
Cultivated Land	0.14	0.20	0.18	0.60
Grassland	0.18	0.18	0.20	0.60
Urban	0.14	0.16	0.18	0.35
Desert Shrubland	0.30	0.28	0.28	0.45

Boundary Layer Type: Observations

SCICHEM uses observations of boundary layer mixing height (ZI) and surface heat flux (HFLUX) or Pasquill-Gifford-Turner stability class (PGT) or Monin-Obukhov length (MOL) that are contained on a SURFACE or PROFILE observations file (Table B-4). MOL supersedes PGT and HFLUX. PGT supersedes HFLUX. PGT and MOL may be used without specifying ZI, and assumed mixing heights, shown in Table B-3, will be used. ZI must be provided if HFLUX is used. See Section 4.5.1 for details regarding SURFACE or PROFILE observations files.

Table B-4
Assumed Mixing Heights for Use with PGT or MOL

Stability Index	PGT	MOL (m)	ZI (m)
1	A	-5	1000
2	B	-12.5	1000
3	C	-50	1000
4	D	-1000	1000
5	E	25	125
6	F	13	65
7	G	5	25

Boundary Layer Type: Profile

SCICHEM reads boundary layer profiles from the PROFILE observations file. In this case, the upper air file can contain only a single profile. The boundary layer variables include the shear-driven lateral velocity variance (UU), the buoyancy-driven lateral velocity variance (VV), the vertical velocity variance (WW), the boundary layer heat flux (WT), the shear-driven turbulence scale (SZ), and the buoyancy-driven turbulence scale (SL). See Section 4.5.1 for details regarding the PROFILE file.

Boundary Layer Type: Gridded

SCICHEM reads boundary layer observations (mixing heights and surface heat flux) from a MEDOC file. This option is available only if the Weather Data type is also MEDOC Gridded Data.

Boundary Layer Type: Operational

SCICHEM uses boundary layer Observations if available. If not, the boundary layer is Calculated. In addition, if one of the two required observational boundary layer variables is provided—surface heat flux (HFLUX) or boundary layer height (ZI)—SCICHEM will use the one supplied in its calculations.

Note: If Pasquill-Gifford-Turner stability class (PGT) or Monin-Obukhov Length (MOL) is provided without boundary layer mixing heights, SCICHEM uses assumed boundary layer mixing heights (Table B-4) and the boundary layer type is considered to be Observations.

B.6.2 Large-Scale Variability

The SCICHEM dispersion calculation accounts for mesoscale or synoptic scale variability in the wind field. This is important for long-range transport applications in which the range exceeds 100 km and for incorporating climatological variability or forecast uncertainties.

The large-scale velocity fluctuations are assumed to be constrained to the horizontal plane and are characterized by a variance and length scale. These parameters may be specified by the user, computed from a theoretical model, or read from a meteorology observation file. The large-scale variability is ignored by selecting None from the combo box.

The choices of large-scale variability are as follows:

- Model
- Observations
- Input
- None
- Operational

Large-Scale Variability: Model

In this mode, the length scale and variance of the large-scale variability are determined from a theoretical model based on climatological statistics. The large-scale variability model used in SCICHEM is based on research by Nastrom and Gage (1985) and a theoretical model proposed by Gifford (1988).

Nastrom and Gage analyzed GASP (Global Atmospheric Sampling Program) wind data and showed a clear spectral break at a horizontal wavelength of about 400 km, with k^{-3} spectrum at longer wavelengths and $k^{-5/3}$ for shorter scales. Gifford argues that the large-scale behavior is consistent with the predictions of two-dimensional turbulence theory, while the $k^{-5/3}$ behavior indicates three-dimensional motions in that part of the spectrum.

We assume that the upper troposphere data are representative of the entire lower atmosphere, although there is probably some vertical variation. However, no data presently exist to define these fluctuation profiles, so the simplest assumption is made.

Furthermore, the GASP data represent long-term averages and cannot provide any relationship between the local meteorological conditions and the local smaller scale velocity fluctuations. Use of the GASP data is therefore equivalent to a climatologically averaged spectrum. Using Gifford's suggestions and the GASP profiles, which show an increase in fluctuation variance toward the poles, the horizontal velocity variance is represented as

$$\overline{u_T'^2} = \overline{v_T'^2} = \begin{cases} \varepsilon_T / \left(f_o \cos\theta \right), & \theta < 75^\circ \\ \varepsilon_T / \left(f_o \cos 75^\circ \right), & \theta \geq 75^\circ \end{cases}$$

where θ is the latitude, f_O is twice the rotation rate of the earth, and ε_T is the average tropospheric energy dissipation rate. Gifford suggests a value of $4\times10^{-4} m^2 s^{-3}$ for ε_T, but the inverse cosine variation is an empirical factor to provide a match with the latitudinal variation observed in the GASP data. The turbulence length scale associated with these dissipative fluctuations is taken to be

$$\Lambda_T = \left(\overline{u_T'^2} + \overline{v_T'^2}\right)^{1/2} f^{-1}$$

where f is the Coriolis parameter defined as

$$f = f_o \times \begin{cases} \sin\theta, & \theta > 15^\circ \\ \sin 15^\circ, & \theta \le 15^\circ \end{cases}$$

The limit of 15° is necessary to avoid singularities in the equation.

The velocity variance used in the dispersion calculation depends on the resolution of the input wind fields because the turbulence input represents only the unresolved component of the wind. Using the filter scale, Λ_G ,which is related to the wind field resolution, we define

$$\Lambda_{HL} = \min\left(\Lambda_G, \Lambda_T\right)$$

and

$$\overline{u_L'^2} = \overline{u_T'^2}\left(\frac{\Lambda_{HL}}{\Lambda_T}\right)^{2/3}$$

consistent with a $k^{-5/3}$ spectral behavior. The cross-correlation, $\overline{u_L' v_L'}$, is assumed to be zero in the model.

Large-Scale Variability: Observations

The large-scale variability parameters (UL, VL, and UVL) will be read from the SURFACE and/or PROFILE observation files (see Section 4.5.1). The user must enter the length scale explicitly. The input parameter is as follows (Figure B-27).

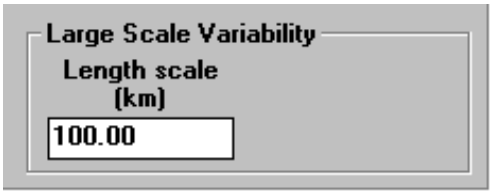

Figure B-27
Large-Scale Variability Window for Observations

Length Scale

This specifies the characteristic length scale (km) of the large-scale variability.

Default: 100

Large-Scale Variability: Input

In this mode, a single length scale and variance are used to characterize the large-scale variability. The user is prompted for the following input parameters (Figure B-28).

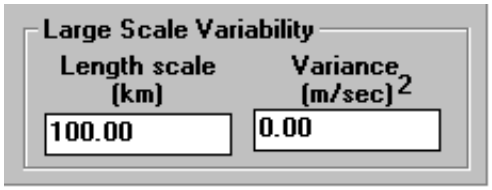

Figure B-28
Large-Scale Variability Window for Input

Length Scale

This specifies the characteristic length scale (km) of the large-scale variability.

Default: 100

Variance

This specifies the large-scale velocity variance $\left(m^2 s^{-2}\right)$.

Default: 0

Large-Scale Variability: None

In this mode, large-scale variability is ignored. This mode should be selected only for short-range transport applications, that is, ranges less than 100 km, which do not include climatological variability.

Large-Scale Variability: Operational

In this mode, the full effects of large-scale variability are applied only when the large-scale variability length scale is exceeded by the internal puff scale or by the horizontal boundary layer turbulence scale. Otherwise, a simple energy spectrum assumption is used to determine the reduced variance appropriate for diffusion on scales smaller than the cloud and boundary layer scales.

B.6.3 Additional Weather Input Parameters

The following additional input parameters may be required (Figure B-29).

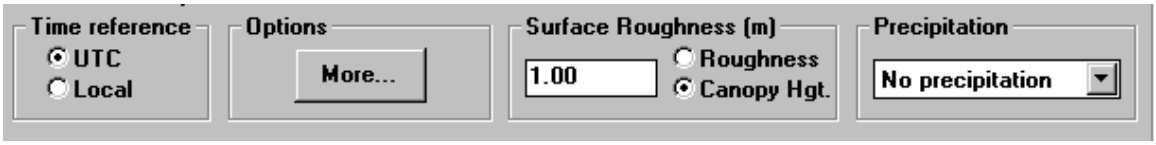

Figure B-29
Additional Weather Input Parameters Window

Time Reference

If the time reference is different from that specified in the Time setup, the local time of 00:00z must be set there.

UTC

This specifies the time on the meteorology files to be in the Universal Time Convention, which is equivalent to Greenwich Mean Time (GMT or Z). UTC is the default time reference.

Local

This specifies the time on the meteorology files to be in local time.

Surface Roughness

Roughness (m)

This specifies the surface roughness length (m). See Table B-5 for typical values. The default value for the roughness is 0.03 m.

Canopy Height (m)

This specifies the actual height (m) of the vegetative canopy. The canopy height is used only as an alternative way to specify the surface roughness length. Note that the bottom of the SCICHEM calculation domain is assumed to be at the top of the canopy. The default value for canopy height is 1 m.

Table B-5
Suggested Values for Surface Roughness (Saucier, 1987)

z_0 (m)	Surface Description
0.0005	Bare Ground, Sand Dunes, Water
0.001	Nearly Barren with Low Growing Vegetation
0.01	Grassland, Cropland, Wetlands
0.05	Grassland with Scattered Trees, Brushland, Scrub Growth
0.1	Deciduous Forest, Villages, Forest Clearings
0.5	Mixed Forest, Towns, Cities
1.0	Coniferous Forest

Precipitation

SCICHEM includes a washout calculation based on the precipitation category. For Observational meteorology, the precipitation category can be either selected from the drop-down list or specified (as an index or a rate) on an observation file. See Section 4.5 for information on providing precipitation data on an observation or MEDOC gridded meteorological file. For other weather data types, the precipitation category must be selected from the drop-down list and cannot be read from a file. The precipitation categories are shown in Table B-6.

Table B-6
Precipitation Categories

Precipitation Rate (mm/hr)	Precipitation Category
0.5 to <3.5	Light Rain
3.5 to <25.0	Moderate Rain
25.0 or greater	Heavy Rain
5.0 to <20.0	Light Snow
20.0 to <100.0	Moderate Snow
100.0 or greater	Heavy Snow

B.6.4 Meteorological Options

Options are provided for saving meteorological data used in SCICHEM and for generating mass-consistent winds. The user may click the Options button from the Weather Editor and use one or both of the check boxes provided to enable these options.

Save Meteorology Fields

If the user checks the Save Meteorology Fields check box, the following choices are shown (Figure B-30).

2-D

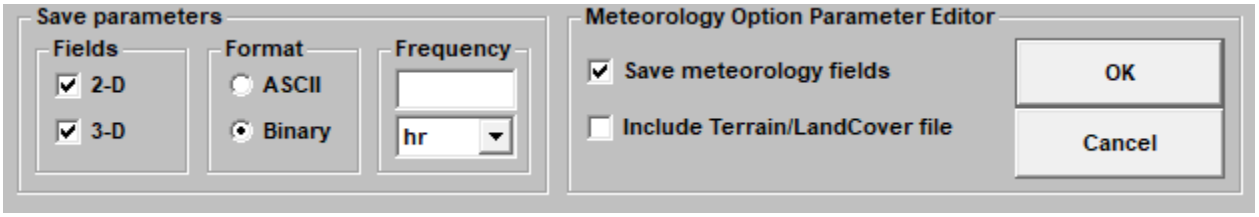

Figure B-30
Save Meteorology Fields Window

This will save the 2-D fields as a MEDOC-type named *ProjectName*.MCW. 2-D variables include ZI, USTR, HFLX, U, V, REL, PRATE, and FCC, which are the boundary layer height, surface friction velocity, heat flux, surface velocities in the x- and y-directions, relief, precipitation rate (mm/hr), and fractional cloud cover, respectively. See Section 4.5.2 for details on the MEDOC format.

3-D

This will save the 3-D fields as a MEDOC-type named *ProjectName*.MCW. 3-D variables include U, V, W, T, H, and CLD, which are the velocities in the x-, y-, and z-directions, temperature, humidity, and cloud liquid water content, respectively. See Section 4.5.2 for details on the MEDOC format.

ASCII Format

This will save meteorological fields in ASCII format.

Binary Format/ASCII Format

This will save meteorological fields in binary format. Binary format results in faster writing, smaller files, and faster reading of these files when used as meteorological input.

Frequency

This specifies the frequency for saving the meteorological data.

Include Terrain/LandCover file

When this check box is clicked, a diagnostic three-dimensional wind field is generated using meteorological observations (including upper air profiles, surface observations, and fixed input) and the specified gridded terrain file. The wind field is determined by first interpolating from the observations onto the grid and then adjusting the three-dimensional field so that it satisfies mass continuity.

SCIPUFF Mass Consistency Solver

It has been shown that the minimum adjustment (in the least-squares sense) is given by the gradient of a particular scalar potential analogous to a dynamic pressure field. Terrain effects are included using a terrain-following coordinate system. Atmospheric stability is accounted for by means of a parameter that weights adjustments to the vertical velocity.

Two methods are used in computing the adjusted wind fields. The fastest method employs a fast Fourier transform (FFT) technique but is limited by terrain slope and atmospheric stability. A point relaxation technique is used when the FFT solver is inappropriate.

The following screen will be displayed (Figure B-31).

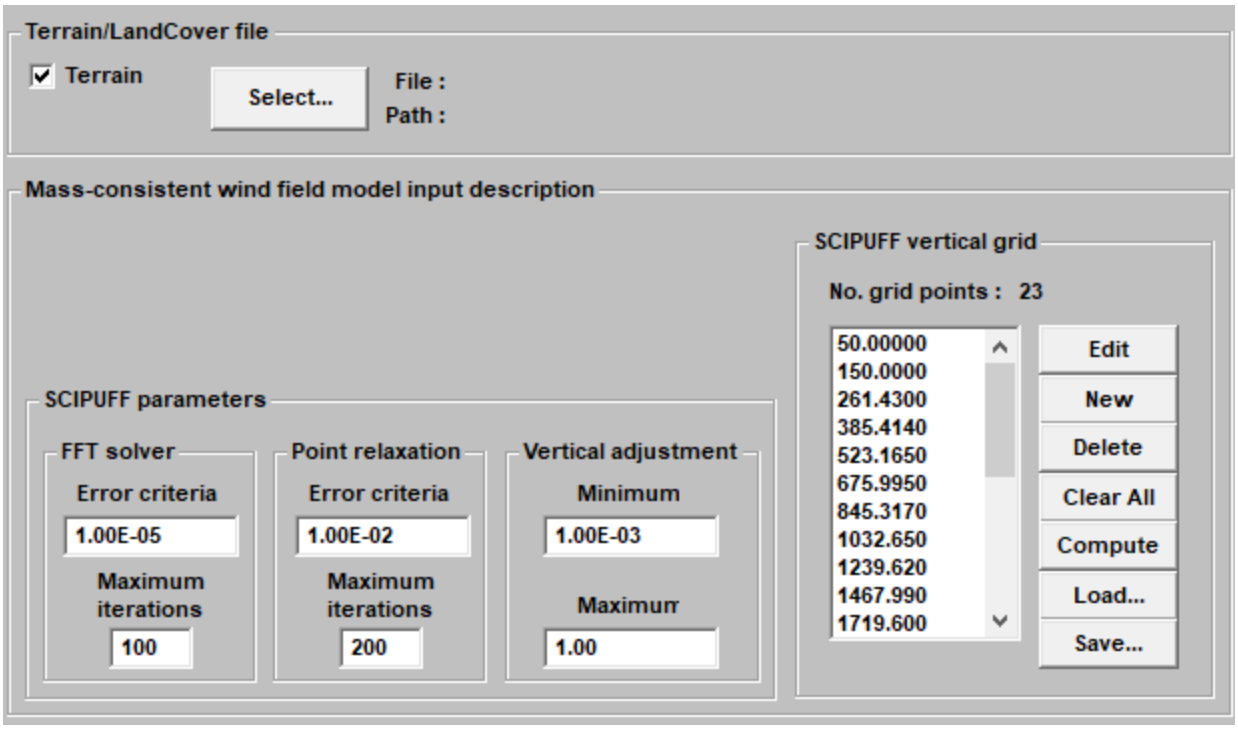

Figure B-31
Terrain/LandCover File Window

Terrain

Select

This brings up an Open File dialog box, which allows the user to specify a previously defined terrain file. See Section 4.5.4 for more information on the terrain file format.

FFT Solver

Error Criteria

The FFT solver error criterion is based on the ratio of the maximum change in the adjustment potential from the previous iteration to the maximum value of the potential. This ratio should decrease with increasing iterations, and the computation ceases once it falls below the specified value. A value of 1.0E-5 will normally be adequate; smaller values will result in greater computation time.

Default: 1.0E-5

Maximum Iterations

If the error criterion is not satisfied, the computation will cease after the specified maximum number of iterations. The calculation should normally take no more than 20 iterations.

Default: 100

Point Relaxation

Error Criteria

The point relaxation error criterion is based on the ratio of the maximum divergence in the adjusted wind field to a tenth of the maximum velocity gradient in the initial, unadjusted field. This ratio should decrease with increasing iterations, and the computation ceases once it falls below the specified value. A value of 0.01 will normally be adequate; smaller values will result in greater computation time.

Default: 0.01

Maximum Iterations

If the error criterion is not satisfied, the computation will cease after the specified maximum number of iterations. The calculation may take 200 to 300 iterations depending on the problem and the error criterion.

Default: 200

Vertical Adjustment

Minimum/Maximum

The vertical adjustment parameter accounts for atmospheric stability and is a function of temperature gradient and wind speed. Large positive temperature gradients and low wind speeds are associated with stable conditions, resulting in a small value of this parameter and relatively small adjustments in the vertical velocity. A value of 0 results in no vertical velocity and forces the wind to flow **around** hills rather than **over** them. A value of 1 corresponds to potential flow. Normally this parameter is computed internally based on temperature and wind speed, but setting maximum and minimum values can force certain flows such as purely horizontal or potential flow.

Default: 1e-3 and 1

SCIPUFF Vertical Grid

Grid Points

A vertical grid for the mass-consistent wind field must be specified. A default grid is provided for typical atmospheric applications. Higher vertical resolution, particularly near the surface of topography with large slopes, can result in excessive computational effort.

Default: A generic grid created with a compromise among vertical extent, resolution, and size.

B.7 Audit Editor

The Audit Editor is used to save additional project information, such as the project title. When the user clicks Audit from the New Project Editor, the Audit Editor window (shown in Figure B-32) will appear.

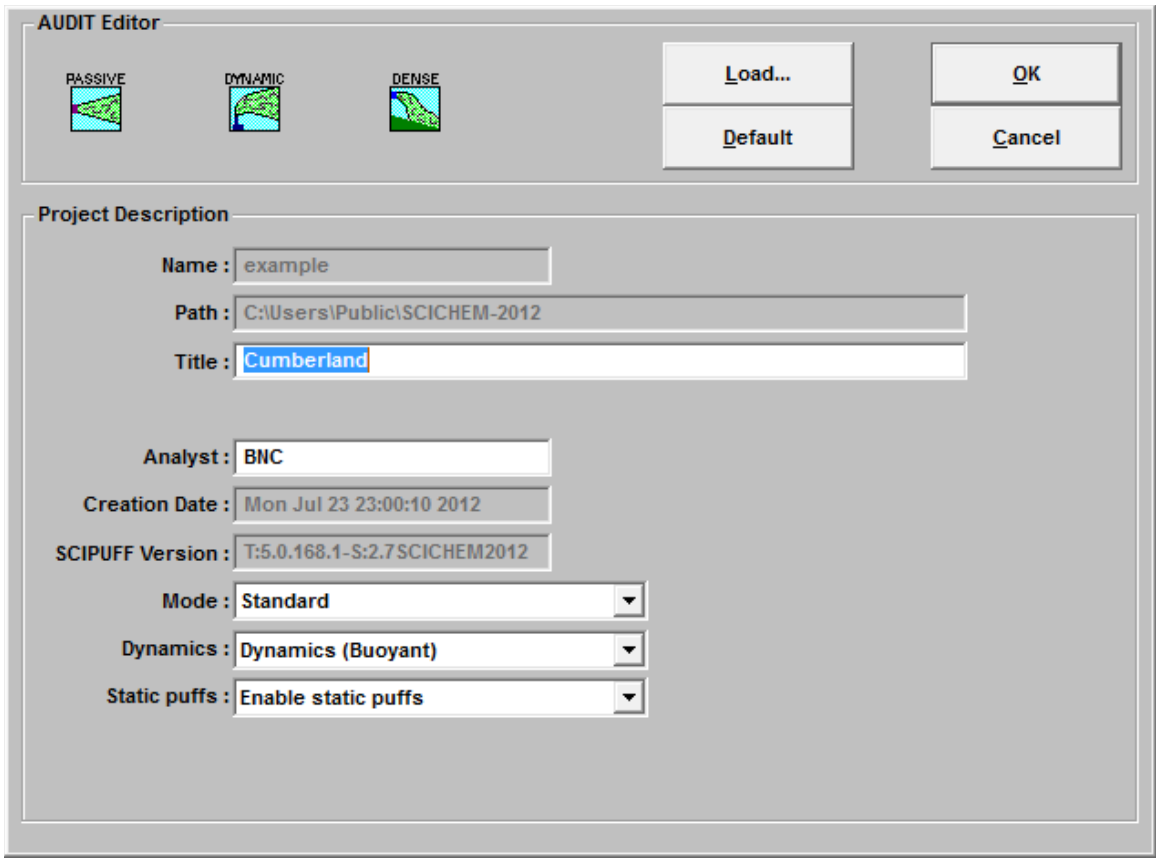

Figure B-32
Audit Editor Window

The icons displayed in the upper left-hand corner determine if the project is Passive, Dynamic, or Dense. Dynamic effects treated are buoyant and momentum plume rise and gases that have densities different from that of air. The following input parameters are displayed in this window:

Name
This specifies the project name. This parameter cannot be edited from this screen.

Path

This specifies the path where the project is stored. This parameter cannot be edited from this screen.

Title

This specifies the project title.

Default: Blank (no title)

Analyst

This specifies the name of the person creating the project.

Default: Blank (no analyst)

Creation Date

This specifies the date that the project is created. This parameter cannot be edited from this screen.

SCIPUFF Version

This specifies the SCIPUFF version number used in the current SCICHEM. This parameter cannot be edited from this screen.

The user may also specify additional project options. They include the following:

Mode

This specifies whether to run SCICHEM in Standard or Fast mode.

See Section B.1.1 for a description of the two modes.

Dynamics

This specifies whether to treat dynamics. It is controlled by the icons at the top left-hand corner of this window.

Static Puffs

This specifies whether to use static puffs in the calculation. Static puffs significantly speed up the calculation; therefore, it is the default to use them.

B.8 Options Editor

The Options Editor is used to define the project options. When the user clicks Options from the New Project Editor, the Options Editor window (shown in Figure B-33) will appear.

Figure B-33
Options Editor Window

The input parameters are defined as follows.

B.8.1 Resolution

Puff Split Grid Level (MGRD)

This specifies the grid resolution parameter that limits the horizontal growth of a puff. The actual resolution used for limiting the horizontal growth of a puff is $\Delta H \times 2^{MGRD}$, where ΔH is the horizontal resolution described in the Horizontal Domain (see Section B.5.2). For example, if ΔH is 1 degree and *MGRD* is 2, the horizontal spacing that limits puff growth is 4 degrees.

The recommended (default) setting of *MGRD* = 2 assumes a smoothly varying wind field. The puff moment calculation accounts for linear velocity gradients, so puffs can usually be allowed to grow larger than the meteorological grid size. Smaller values of *MGRD* give more detailed resolution of the concentration field at the expense of more puffs and longer execution time.

Default: 2

Surface Resolution (DELMIN)

This specifies the minimum grid size (m) for the adaptive grids. SCICHEM uses adaptive grids for surface dose and deposition output and for internal puff interaction calculations. Under some circumstances, the adaptive grid may exhaust its storage allocation unless a limit is imposed on

the minimum grid size. However, setting a limit may result in the loss of small-scale information in the output fields. (It will affect the efficiency of the internal puff interaction calculation—not the result.)

Default: 0

Boundary Layer Resolution (NZBL)

This specifies the number of grid points used in the vertical direction to represent the turbulence profiles in the boundary layer. Not generally modified by the user.

Default: 11

B.8.2 Stable Atmosphere

Turbulence (WWTROP)

This specifies the tropospheric vertical velocity variance (m^2s^{-2}) This value is used in the stable atmosphere above the planetary boundary layer. It also provides a lower bound on the vertical velocity variance within the boundary layer. Not generally modified by the user.

Default: 0.01

Scale (SLTROP)

This specifies the tropospheric vertical length scale (m) used in the stable atmosphere above the planetary boundary layer.

Default: 10

Dissipation (EPSTROP)

This specifies the average tropospheric energy dissipation rate (m^2s^{-3}) used in the large-scale variability model (described in Section 4.7.3) to characterize the mesoscale velocity variance. Not generally modified by the user.

Default: 4.0E-4

B.8.3 Parameters

Surface Dose Height (ZDOS)

This specifies the height (m) above the surface where the surface dose is calculated.

Default: 1.E-20

Minimum Puff Mass (CMIN)

This specifies the minimum puff mass (material mass units). A puff with mass less than this value does not split or distort due to velocity gradients, but it may merge with other puffs. Setting this minimum value may help decrease execution time.

Default: 0

Conditional Averaging (TAVG)

This specifies the averaging time for defining the diffusive component of turbulence. This parameter is used to scale the velocity variances that determine puff diffusion. To obtain a quasi-deterministic prediction of dispersion by neglecting the "meandering" component of turbulence (length scales greater than the plume or cloud size), TAVG should be set to the smaller of the release duration and the sampling period of interest. This is most useful when attempting to compare sampler output with actual data measurements.

Default: Use the full turbulence spectrum for the diffusion calculation (equivalent to a very large TAVG).

B.8.4 Calm Conditions

Turbulence (UUCALM)

This specifies the turbulence value (m^2s^{-2}) used under light wind conditions.

Default: 0.25

Scale (SLCALM)

This specifies the turbulence scale (m) used under light wind conditions.

Default: 1000

B.8.5 Substrate

This specifies the substrate type for secondary evaporation.

Default: Impermeable

B.8.6 Sampler Output

Sampler (receptor) output provides a time history of point concentration values for the locations specified in the sampler input file. The output file contains the concentration time series (in ASCII format) for the locations specified in the sampler input file. This file can then be read with other plotting software to obtain a graphical representation of the sampler time history. Concentration values are written at the maximum time step interval, as defined in the Time Editor (see Section B.4). The maximum number of sampler locations is 500. For details on the sampler location file format, see Section 4.3.6. For the format of the resulting output file (*ProjectName*.SMP), see Section 4.3. A sampler input file can be selected by checking the Add box. The minimum output interval(s) specifies the output interval in seconds for the sampler output.

B.9 Starting a Run

Once a project has been created and the user clicks Continue, the Run Control window will appear, as shown in Figure B-34.

The parameters displayed are those that have previously been defined in the Time Editor (Section B.4). These parameters can be edited prior to commencing the calculation. The parameters are defined in Sections 5.4.3 and 5.4.4.

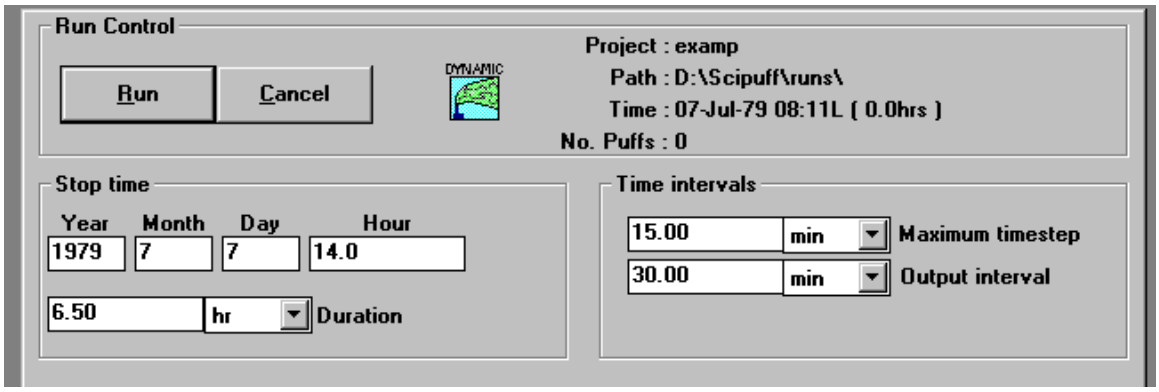

Figure B-34
Run Control window

When the user clicks the Run button, the run will start. A control box appears, which displays the progress of the run, as shown in Figure B-35.

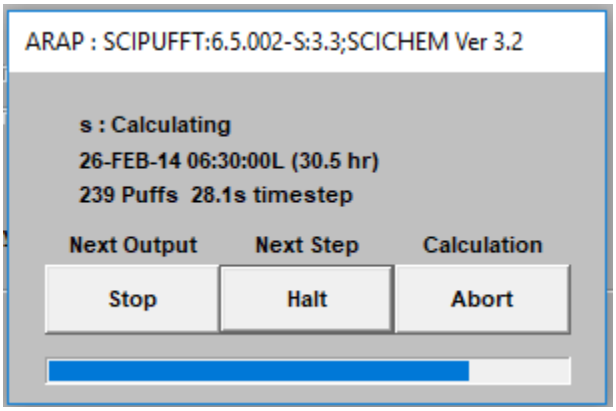

Figure B-35
Control Box Window

The window displays the current run time, the minimum time step, and the number of puffs. From this secondary window, the run can be stopped with either the Stop, Halt, or Abort push buttons. When the Stop button is used, the run is stopped at the next output interval when all the output files are updated. When the Halt button is used, the run is stopped at the next complete time step, and all the output files are forced to be updated. If the Abort button is used, the run is stopped as soon as possible, and the output files are not updated beyond the previous complete time step.

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