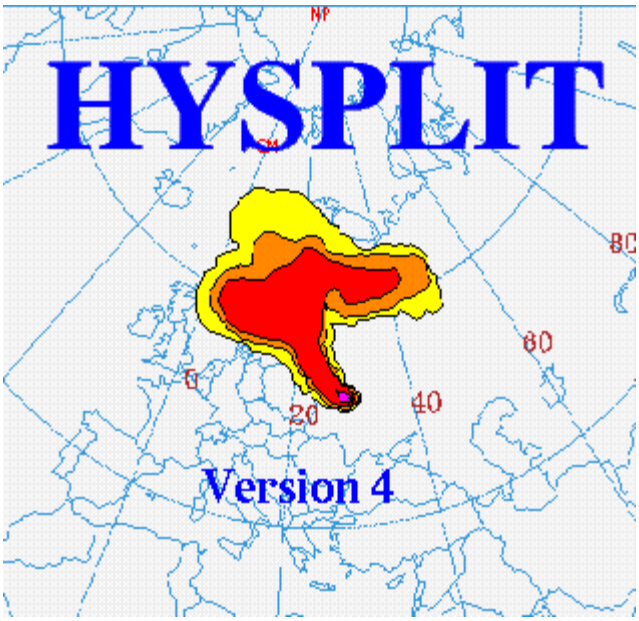
HYSPLIT4 User's Guide



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HYSPLIT4 USER's GUIDE

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Abstract The HYSPLIT_4 (Hybrid Single-Particle Lagrangian Integrated Trajectory) Model installation, configuration, and operating procedures are reviewed. Examples are given for setting up the model for trajectory and concentration simulations, graphical displays, and creating publication quality illustrations. The model requires specially preformatted meteorological data. Programs that can be used to create the model's meteorological input data are described. The User's Guide has been restructured so that the section titles match the GUI help menu tabs. Although this guide is designed to support the PC and UNIX versions of the program, the executable of the on-line web version is identical. The only differences are the options available through the interface.

Features

The HYsplit_4 (HYbrid Single-Particle Lagrangian Integrated Trajectory) model is a complete system for computing trajectories complex dispersion and deposition simulations using either puff or particle approaches.[2] It consists of a modular library structure with main programs for each primary application: trajectories and air concentrations.

Gridded meteorological data, on a latitude-longitude grid or one of three conformal (Polar, Lambert, Mercator) map projections, are required at regular time intervals. The input data are interpolated to an internal sub-grid centered to reduce memory requirements and increase computational speed. Calculations may be performed sequentially or concurrently on multiple meteorological grids, usually specified from fine to coarse resolution.

Air concentration calculations require the definition of the pollutant's emissions and physical characteristics (if deposition is required). When multiple pollutant species are defined, an emission would consist of one particle or puff associated with each pollutant type. Alternately, the mass associated with a single puff may contain several species. The latter approach is used for calculation of chemical transformations when all the species follow the same transport pathway. Some simple chemical transformation routines are provided with the standard model distribution.

The dispersion of a pollutant is calculated by assuming either a Gaussian or Top-Hat horizontal distribution within a puff or from the dispersal of a fixed number of particles. A single released puff will expand until its size exceeds the meteorological grid cell spacing and then it will split into several puffs. An alternate approach combines both puff and particle methods by assuming a puff distribution in the horizontal and particle dispersion in the vertical direction. The resulting calculation may be started with a single particle. As its horizontal distribution expands beyond the meteorological grid size, it will split into multiple particle-puffs, each with their respective fraction of the pollutant mass. In this way, the greater accuracy of the vertical dispersion parameterization of the particle model is combined with the advantage of having an expanding number of particles represent the pollutant distribution as the spatial coverage of the pollutant increases and therefore a single particle can represent increasingly lower concentrations.

Air concentrations are calculated at a specific grid point for puffs and as cell-average concentrations for particles. A

concentration grid is defined by latitude-longitude intersections. Simultaneous multiple grids with different horizontal resolutions and temporal averaging periods can be defined for each simulation. Each pollutant species is summed independently on each grid.

The routine meteorological data fields required for the calculations may be obtained from existing archives or from forecast model outputs already formatted for input to HYSPLIT. In addition, several different pre-processor programs are provided to convert NOAA, NCAR (National Center for Atmospheric Research) re-analysis, or ECMWF (European Centre for Medium-range Weather Forecasts) model output fields to a format compatible for direct input to the model. The model's meteorological data structure is compressed and in "direct-access" format. Each time period within the data file contains an index record that includes grid definitions to locate the spatial domain, check-sums for each record to ensure data integrity, variable identification, and level information. These data files require no conversion between computing platforms.

The modeling system includes a Graphical User Interface (GUI) to set up a trajectory, air concentration, or deposition simulation. The post-processing part of the model package incorporates graphical programs to generate multi-color or black and white publication quality Postscript printer graphics.

A complete description of all the equations and model calculation methods for trajectories and air concentrations has been published[3] and it is also available on-line. The on-line and the version included with the PC installation contains all the most recent corrections and updates.

Pre-Installation Preparation

There are two installation programs that can be downloaded. The trial version (*HYSPLIT_win{32|64}U.exe ~ 70 Mb*) available to anyone and a fully functional version (*HYSPLIT_win{32|64}R.exe ~ 70 Mb*) that requires a user registration through the web site. Both versions identical, except the trial version will not work with forecast meteorological data files. In addition, several supplemental programs (Ghostview and Tcl/Tk) are packaged with the trial version for convenience. It is assumed that these would have already been installed when the registered version is installed on top of the trial version.

The self-installing executable contains only HYSPLIT related programs. No additional software is required to run a simulation if the command line interface is sufficient. To enable the model's GUI, the computer should have Tcl/Tk script language installed. The most recent version can be obtained over the Internet from or an older version is packaged with some of the other programs on the HYSPLIT web site. The installation of Tcl/Tk will result in the association of the *.tcl* suffix with the *Wish* executable and all Hysplit GUI scripts will then show the Tk icon. The HYSPLIT GUI has been tested with Tcl/Tk version 8.5.4.

The primary HYSPLIT graphical display programs convert the trajectory and concentration model output files to Postscript format. The Postscript files can also be viewed directly through the GUI if Ghostscript and Ghostview have been installed. See for more information on the Postscript file viewer. The HYSPLIT code and GUI have been tested with Ghostscript 8.63 and Ghostview 4.9. Installation to different default drives, directories, or other versions might require editing the main GUI script's directory pointers (edit file: */guicode/hysplit4.tcl* or the directory entry in the Advanced-Configuration-Directories menu tab.

The third optional GUI feature is the ability to convert the Postscript output file to a different graphical formats using ImageMagick. More information on this software can be found at The HYSPLIT code and GUI have been tested with ImageMagick 6.4. Similar to Ghostscript, installation to a different default drives or directories as suggested by the installation process may require editing the main GUI script's directory pointers. Proper functioning of the conversion software with Postscript files requires the installation of Ghostscript. Although the setup script tests for the default language, it is possible that installation to non-English default windows operating systems might require additional editing of the directory pointers.

Windows Installation (all operating systems)

HYSPLIT installation to a computer running Windows is provided through a self-installing file. Executables are

installed in various directories for trajectories, dispersion, display and manipulation of results, and the creation of input meteorological data files. The trajectory and dispersion model source code is not provided. However all the Fortran source code to create meteorological data files in a format that the model can read are provided in the */data2arl* directory. Each subdirectory contains a *@readme.txt* file with more complete information about the contents of that directory.

During the installation you will be prompted as to the directory location. It is suggested you select a simple default location (such as *C:/hysplit4*). The installation program installs all code and executables to your selected directory, and creates a shortcut on the desktop to /guicode/hysplit4.tcl with the "Start In" directory as your selected default. You may have one of two versions of the installation program: HYSPLIT_win{32|64}{R|U}.exe. The suffixes R and U refer to the Registered or Unregistered versions. The two versions are almost identical, except that the unregistered version does not permit calculations with current forecast meteorological data.

HYSPLIT and all the related programs are available for either 32 bit or 64 bit operating systems. The 32 bit version can be installed on either OS, while the 64 bit programs can only be installed on a 64 bit OS. An Apple MAC version is also available (HYSPLIT_mac.dmg).

Installing on top of an old version will bring up a "Continue" or "Cancel" prompt. It is not possible to rename the installation directory at this stage. Rename your old installation prior to installing the new code if you wish to keep the original version.

The installation will contain several sub-directories, some of which are required for model execution, and some of which provide additional documentation and other information. For instance ...

- *bdyfiles* - This directory contains an ASCII version of gridded land use, roughness length, and terrain data. The current file resolution is 360 x 180 at 1 degree. The upper left corner starts at 180W 90N. The files are read by both HYSPLIT executables, *hyts_std* (trajectory model) and *hycs_std* (concentration model), from this directory. If not found, the model uses default constant values for land use and roughness length. The data structure of these files is defined in the file ASCDATA.CFG, which should be located in either the model's startup or */bdyfiles* directory. This file defines the grid system and gives an optional directory location for the landuse and roughness length files. These files may be replaced by higher resolution customized user-created files. However, regardless of their resolution, the model will only apply the data from these files at the same resolution as the input meteorological data grid. More information on the structure of these files can be found in the local *@readme.txt* file.

- *data2arl* - Current forecast or archive meteorological data can be obtained from the ARL ftp server*: ftp://gus.arlhq.noaa.gov /pub/archives (or /forecasts)*. Older archive data can be ordered from the NCDC (National Climatic Data Center). However if you have access to your own meteorological data or data formatted as GRIB (Gridded Binary), this directory contains various example decoder programs to convert meteorological data in various formats to the format (ARL packed) that HYSPLIT can read. Sample programs include GRIB decoders for ECMWF model fields, NCAR/NCEP (National Centers for Environmental Prediction) re-analysis data, and NOAA Aviation, ETA, and Regional Spectral Model files. All the required packing and unpacking subroutines can be found in the */source* subdirectories. Sample compilation scripts for Compaq Visual Fortran 6.6 are in some of the decoder directories. More information on how to run these programs can be found in the Meteorology section.

- *examples* - The directory contains several example scripts and batch files that can be used to create automated simulations.

- *html* - Contains all the HELP files in HTML format. These files can be displayed with any browser or interactively through the GUI. The files that are opened in the GUI depend upon the context from which HELP is invoked.

- *document* - This directory contains PDF (Adobe Portable Document Format) versions of the User's Guide (all the HTML help files put together in one document) and other documentation such as ARL-224, the principal ARL

Technical Memorandum describing the model and equations. This User's Guide (this document) provides detailed instructions in setting up the model, modifications to the *Control* file to perform various simulations and output interpretation. The *@readme.txt* file contains additional information about compilation, typical CPU times, and a summary of recent model updates.

- *exec* - Is the directory that contains all the executable programs. The GUI looks for all programs in this directory. When running examples from the command prompt in certain directories, the relative path should be included prior to the executable: "../exec/program.exe"

- *graphics* - There are two types of graphical plotting programs provided in the ../exec directory. Publication quality graphics can be created using the postscript conversion programs, *concplot* and *trajplot*, which use a Fortran Postscript library created by Kevin Kohler[4]. All graphical routines use the map background file *arlmap* in this directory. The map background file uses a simple ASCII format and contains the world's coastal and political boundaries at relatively coarse resolution. Other higher resolution map background files are available in the */graphics/mapfiles* directory or from the HYSPLIT download web page. All graphical programs search the startup directory first for *arlmap* before going to */graphics*, therefore customized maps can be created without changing the HYSPLIT installation structure.

- *guicode* - This directory contains a Tcl/Tk GUI interface source code script for HYSPLIT. The interface is used to set up the input *Control* file as well as run the graphical output display programs. To use the interface you must first install Tcl/Tk. The upper-level Tcl script is called *hysplit4.tcl*, which calls all other Tcl scripts. Executing this script starts the HYSPLIT GUI. The Desktop shortcut as well as the Start Menu options should point to this script. If the installation program did not properly setup the Desktop, you can manually create a shortcut to the script and edit its properties such that the "Start In" directory is */hysplit4*. You should also select the HYSPLIT icon from the */icons* directory.

- *working* - This is the *Hysplit4 root directory*, which contains sample CONTROL files that can be used for initial guidance to set up more complex simulations. These should be loaded into the GUI from the approprate "Retrieve" menu tab. Examples include:

  sample_conc - concentration simulation example from users guide

  sample_traj - trajectory simulation example from users guide

  The "plants.txt" file contains a sample listing of starting locations that can be opened in the GUI to select from a list of previously determined starting locations. This file can easily be customized. The "tilelist.txt" file contains the approximate coordinates of NCEP's NAM (North America Mesoscale model) tile domains.

Problems

If Tcl/Tk does not exist on your system or there are other problems with the GUI interface, it is very easy to run the sample cases directly in the */working* directory by running the batch file "run_{model}.bat" If the sample simulation works well, then it is only necessary to manually edit the *CONTROL* file to try out different simulation variations. The *CONTROL* file options are explained in more detail in the individual Trajectory and Concentration Setup sections.

In general, premature termination during the model initialization phase will result in messages to standard output. However after the model has started, fatal, diagnostic, and progress notification messages are written to a file called *Message*. If the model output is not what you expected, first check the *Control* file to determine if the input setup is what is desired, then check the *Message* file for indication of abnormal performance. These files are always written to the model's startup directory - */Hysplit4* if the model is run from the GUI. At times error messages may be lost in the display buffer after premature termination. In this case the model should be rerun from the command line window for proper display of all standard output messages. The *"Advanced*" menu contains a the View MESSAGES tab that displays the last MESSAGE file for viewing. Other features of the advanced menu are used to modify the model's configuration file and are explained in more detail in that section. Modifications to these parameters require a complete

understanding of the model's design and operation.

References

[1]Draxler, R.R., 1999, HYSPLIT_4 User's Guide, NOAA Technical Memorandum ERL ARL-230, June, 35 pp.

[2]Draxler, R.R., and G.D. Hess, 1998, An overview of the Hysplit_4 modelling system for trajectories, dispersion, and deposition, *Australian Meteorological Magazine, 47, 295-308*.

[3]Draxler, R.R., and G.D. Hess, 1997, Description of the Hysplit_4 modeling system, NOAA Technical Memorandum ERL ARL-224, December, 24p.

[4]Stein, A.F., R.R. Draxler, G.D. Rolph, B.J.B. Stunder, M.D. Cohen, and F. Ngan , 2015. NOAA’s HYSPLIT atmospheric transport and dispersion modeling system, Bulletin of the American Meteorological Society. 96, 2059–2077. doi: http://dx.doi.org/10.1175/BAMS-D-14-00110.1

[5]PSPLOT libraries can be found at www.nova.edu/ocean/psplot.html and were created by Kevin Kohler (kevin@ocean.nova.edu).

HYSPLIT4 User's Guide Help File Index

Model Overview

GUI Overview

METEOROLOGY - Data Overview

ARL Data FTP - External sources of data

- Forecast and appended ARL archives for the last two days
- Archive of long-term ARL formatted data
- Reanalysis data archive from the ARL server
- Set Server changes the name and directory of the FTP server

Convert to ARL - Convert data on local computer to ARL format

- WRF-ARW Advanced Research WRF NetCDF
- NARR archive North America Regional Reanalysis GRIB1
- Global Lat-Lon European Centre or NOAA global lat-lon grids
- ECMWF ERA ECMWF Reanalysis ERA-40 or Interim GRIB1 files
- MM5V3 Regional Version 3 binary output files
- MCIP IOAPI formatted files
- User entered single station and level user data entry

Display Data - Viewing HYSPLIT formatted meteorological data

- Check File all the records in a meteorological file
- Contour Map of a single meteorological variable
- Text Profile of all variables at a single location
- Grid Domain shows a map of meteorological grid locations

Utility Programs - Meteorology / Trajectory / Concentration Menus

- GIS to Shapefile converts text GIS output to ESRI Shapefile
- Postscript to Image converts to another graphic format

Meteorology Help

- Data Format description of the packed meteorological data format
- Sample Programs to read ARL and GRIB1 data files

TRAJECTORY - Menu Overview

- Quick Start for automatic configuration and execution
- Setup Run creates the trajectory simulation CONTROL file
- Save / Retrieve Options for custom simulations for future use
- Run Model menu tab to execute the trajectory model

Display Options

- Trajectory converts the endpoints file to a graphic
- Frequency converts multiple trajectory files to a graphic

Utility Programs

- Endpoints to IOAPI converts the endpoints file to IOAPI

Special Simulations - Trajectory simulations with special requirements

- Run Ensemble by varying location on meteorology grid
- Run Matrix defines a grid of multiple source locations
- Multi-time starts at trajectories regular intervals
- Multi-space starts new trajectories along a trajectory
- Run daily invokes script to do multiple simulations in time
- Run Cluster Analysis to find which trajectories belong together
- GeoLocation back trajectory analysis from sampling locations
- Control File Format line-by-line description
- Endpoints File Format description

CONCENTRATION - Menu Overview

- Quick Start for automatic configuration and execution
- Concentration Setup of the simulation CONTROL file
- Pollutant, Deposition, and Grid menu to select items below:
- Pollutant definition of the emission characteristics
- Grid Definition or the air concentration sampling grid
- Deposition definition of the pollutant deposition parameters
- Run Model to start the concentration model

Display Options

- Concentration Contours converts the binary model file to a graphic
- Grid Values uses colorfill to show values on the concentration grid
- Pointer Select uses mouse to extract concentration values to a file
- Global Grid graphic optimized to plot global concentration grids
- Particle displays horizontal and vertical particle distributions
- Plume Arrival uses colorfill to show first arrival times after start
- Source-Receptor View create graphic from a source-receptor matrix file
- Source-Receptor Stats creates a statistics map for multi-source simulations
- Ensemble View Map creates probability maps from multiple simulations
- Ensemble Box Plot shows the probability distribution at one location
- Ensemble Statistics computes ensemble statistical performance

Utility Programs

- Binary File Merge adds or masks concentration binary files
- Binary File Extract creates a temporal or spatial concentration file extract
- Binary File Average adds or masks concentration binary files
- Binary File Apply Source multiplies time-varying dispersion factors by source term
- Convert to ASCII converts the binary concentration file to an ASCII format file
- Convert to DATEM convert to DATEM format and compute verification statistics
- Convert to Dose convert a binary file to dose using a dose factor data file

Convert to IOAPI converts the concentration binary file to IOAPI
- Convert to Station extracts the concentrations at a station and writes to a file
- Convert PARDUMP converts PARDUMP file to binary concentration file
- Particle Adjustment adjust particle positions for improved initialization
- Transfer Coefficient using measurements to solve for the emissions vector

Special Simulations - Concentration simulations with special requirements

- Run daily invokes a script for multiple simulations in time
- Run Matrix configures and runs dispersion for an array of locations
- GeoLocate from measurements determine the emissions location
- Ensemble Meteorology for simulations using meteorology grid offsets
- Ensemble Turbulence for multiple turbulence simulations
- Ensemble Physics for multiple physical parameterizations
- Global runs a simulation with particle mass transfer to Eulerian global grid
- Run Dust Storm for PM10 emissions from dust storms
- Daughter Products from nuclear decay from nuclide

Related Concentration Help

- Multi-Processor special simulations in multi-processor environment
- Concentration File Format line-by-line description
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- Configuration Setup to edit the SETUP.CFG namelist file
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- Concentration edit menu for for concentration simulations
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- Emissions File configuration of the point source file
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- Meteorology Along the Trajectory
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- Concentration Packing and Output Units
- Input and Output Particle Files
- In-Line Conversion Modules
- Puff-Split-Merge Issues
- Variables Not Set in GUI

Satellite Data - access to selected satellite data archives

- NASA TOMS FTP Aerosol Index (AI)
- TOMS Viewer for AI and model concentration and particle positions

Advanced Help

- Special Topics for complex simulation scenarios
- PARDUMP file format for particle displays or model restarts
- MESSAGE file format to evaluate simulation details
- ASCDATA.CFG file format for terrain, land-use, and roughness

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VERIFICATION - Model statistics with experimental data

GUI Overview

Although the model can be configured and run manually from the command line, it is usually much quicker to use the GUI. A summary of the main features in each of the primary GUI menus is reviewed below. More detailed help information can be found with the help button associated with each specific menu.

Meteorology / ARL Data FTP

Forecasts - Links to only the most recent forecast data for a variety of different meteorological models available on the ARL FTP server. The data have already processed to a HYSPLIT compatible format. Appended data are defined as a combination of analysis and short forecasts (e.g. 0h and +3h appended with each new 6h cycle) that are operationally maintained as a rolling archive valid for 48 hours prior to the most recent forecast cycle.

ARL Archive - Provides access to the long-term data archives at ARL for the GFS/GDAS (formerly FNL) and the NAM/NDAS (formerly EDAS) archives. Unless otherwise noted, some of the archives go back to about 1995.

NOAA Reanalysis - The NCAR/NCEP reanalysis data archived has been reformatted for HYSPLIT and placed on the ARL ftp server. These data are available from 1948 through the end of the last year. The files are updated once-a-year.

Set Server - A generic menu that can be customized to open different backup or user defined FTP servers to download pre-formatted HYSPLIT compatible meteorological forecasts.

Meteorology / Convert to ARL

Many of the scripts linked in this menu will convert various data file formats into the data format used by HYSPLIT. GRIB version 2 is not yet supported. However, conversion software from GRIB-2 to GRIB-1 can be obtained from several different sources (NOAA-NCEP, ECMWF, WMO). All files must be on the local computer. FTP is no longer supported through these menus.

WRF-ARW - Processes fields from NCARs Advanced Research WRF model into the ARL format. The data conversion routines require NetCDF routines currently supported only on UNIX or LINUX platforms.

NARR Archive - Archived GRIB-1 fields from the North American Regional Reanalysis model (32 km resolution, 3-hr intervals). The GRIB files must be independently downloaded from the NCDC NOMADS web site. The downloaded files need to be renamed to end with the day-hour {DDHH}. The script is designed only to work with archive data to create a multi-day file as long as one month.

Global Lat-Lon - Archived GRIB-1 fields from the global model of ECMWF or NOAA may be processed locally into ARL format. The procedure is designed only to work with archive data from their current operational model, where the last four digits of the file name represent the day.

ERA-40 - Archive GRIB-1 fields from the ECMWF ERA-40 reanalysis may be processed locally into ARL format. These files must already be present. The procedure is designed only to work with the ERA-40 data files. Three different file types must be downloaded for this conversion: 3-d fields, 2-d surface fields, and one invariant field.

MM5V3 format - Output files from MM5V3 can be converted to ARL format. The script automatically processes all domains (MMOUT_DOMAIN{X}) found in the selected directory.

MCIP IOAPI - Meteorological output files from MM5 converted to the CMAQ IOAPI format. Available only under UNIX systems with NetCDF installed.

User Entered - This menu tab is intended to convert user entered meteorological data to the ARL packed

HYSPLIT compatible format. The conversion program will create a data file with one or more time periods containing a uniform field in space and height but varying in time. The grid is centered over the location specified in the main menu and covers a 50 by 50 km domain.

Meteorology / Display Data

Check File - A program to list the information in the meteorology file index record as well as the ASCII header portion of each data record.

Contour Map - A simple postscript contouring program that can be used to view the data fields in any ARL packed meteorological data set. The output is always written to a file called contour.ps. Multiple time periods may be processed.

Text Profile - This program is used to extract the meteorological data profile interpolated to a user selected latitude-longitude position. The raw data values at the surface and each level are output on the left while temperature converted to potential temperature and winds rotated from grid orientation to true are shown on the right. Output is shown on the screen and is also written to a file called profile.txt.

Grid Domain - Program to generate a map showing the domain of the meteorological data grid with marks at each selected data grid point. Output is written to the file showgrid.ps.

Utilities

Convert Postscript - Converts any Postscript file to another format using ImageMagick. Enter the name of the Postscsript file and the desired name of the output file, with the file suffix indicating the desired conversion.

GIS to Shapefile - When the GIS output option is selected in selected display programs an ASCII text file (in generate format) is created that contains the latitude-longitude values of each contour. This GIS text file can be converted to an ERSI Arc View shapefile. This menu tab is available from three different points. From the meteorology tab the conversion is "line", from the trajectory tab the conversion is "points", and from the concentration tab the conversion is "polygon".

Trajectory

Quick Start - menu tab can be used to run any simulation in one-step. The last configuration will be used for the simulation. The menu brings up a global map with the current source location shown as a blue dot which can be moved to a new location. The *Run Example* menu tab resets the control and namelist files and reruns the example case. This can be used as a starting point for configurations that have been corrupted.

Setup Run - This menu is used to write the CONTROL file that defines all the model simulation parameters. Note that once a simulation has been defined it can be "Saved As" and later " Retrieved." Note that the setup must be "Saved" before proceeding to the "Run Model" step.

Run Model - The selection opens the window for standard output and starts the execution of "hyts_std.exe". Incremental progress is reported on WinNT and later systems, however on LINUX the display remains frozen until the calculation has completed (a beep will sound).

Display - Display options are available to label the time increment along the trajectory and the amount of white space surrounding the trajectory on the map. The HIRES option limits the domain to just fit the trajectory. Output is written to the file trajplot.ps. The plot title can be defined in a file called labels.cfg which should be placed in the \working directory. The special frequency display can be used to plot the spatial frequency distribution of multiple trajectory simulations.

Special Runs - The Ensemble option invokes a special executable that will run multiple trajectories from the same location, with each trajectory using meteorological data slightly offset from the origin point. The Matrix option

simultaneously runs a regular grid of trajectory starting locations. Also available are multiple trajectory options in both time and space as well as a menu to run a series of automated daily trajectories for as long as one month per execution. Multiple trajectories can also be clustered.

Concentration

Quick Start - menu tab can be used to run any simulation in one-step or rerun the example simulation. It's functionality is similar to the trajectory quick start menu.

Setup Run - The menu is almost identical to the Trajectory Setup menu except for the added tab for "Pollutant, Deposition, and Grids", which is used to customize the concentration computation. Unlike trajectories, which are terminated at the top of the model domain, pollutant particles reflect at the model top.

Run Model - Similar in function to trajectory run menu, executes "hycs_std.exe".

Display - Output is written to concplot.ps. Options on the menu permit concentration contours to be dynamically scaled to the maximum for each map (default) or fixed for all maps based upon the highest value on any one map. Other display programs are available for the color fill of uncontoured gridded data or the horizontal or vertical display of the particle distributions and the computation of plume arrival times. Note that the units label as well as the plot title can be defined in a file called LABELS.CFG which should be placed in the \working directory. Special display programs are available for a source-receptor matrix, ensemble, and statistical simulation outputs.

Utilities

Convert to ASCII - Writes an ASCII file for each time period of concentration output with one record for every grid point that has a non-zero concentration value. Each record is identified by the ending date and time of the sample and the latitude and longitude of each grid point. The output file name is constructed from the name of the [input file]_[julian day]_[output hour]. Some other output options are available.

Grid to Station - This program is used to extract the time- series of concentration values for a specific location. That location may be specified by a single latitude-longitude through the GUI or multiple stations may be defined by entering the name of a file that contains an integer station number, latitude, and longitude on each record. The output is written to con2stn.txt which can be read by the time series plotting program to produce the file timeplot.ps. Note that the time series plot is always in integer units and therefore may require the specification of a units multiplication factor.

Convert to DATEM - Conceptually similar to Grid-to-Station, this menu is used to convert a binary file to the DATEM format and then compute model performance statistics. A data file with measurement data in DATEM format must already exist, and the conversion program will match each model calculated concentration with a measurement, compute performance statistics, and display a scatter diagram of measured and calculated values.

Merge Binary Files - Multiple binary concentration files may be added together for a sum, or the maximum value is retained at each grid, or one of the input files may be used as a zero mask, resulting in zero concentrations in the other file when the mask file shows a non-zero value.

Special Runs

Daily - Runs a script to rerun the last dispersion model configuration each time with a different starting day and time for one month. Output files are labeled with the starting time.

Matrix - Runs the matrix pre-processor to create a *CONTROL* file with a grid of starting locations. The source-receptor conversion option needs to be selected in the advanced menu to create the coefficient matrix required for source attribution applications.

Geolocation - Runs a special pre-processor that reads a file of measured sampling data to automatically configure

a *CONTROL* file for each sample which is then run in a script to create a source attribution function for each measured sample.

Ensemble / Meteorology - An application similar to the trajectory ensemble, in that multiple simulations are run each with a different offset in the meteorological data to create an ensemble showing the sensitivity of the simulation to gradients in the meteorological data fields.

Ensemble / Turbulence - Instead of starting each simulation with the same random number seed, multiple simulations are run, each with a different seed, which then shows the concentration sensitivity to the turbulence.

Ensemble / Physics - The physics ensemble varies different turbulence and dispersion namelist parameters from the base simulation to develop an ensemble showing the sensitivity of the calculation to various model physics assumptions.

Global - The global special run invokes an executable that contains a global Eulerian module to permit particle mass to be transferred to the global model at a specified age. A concentration output grid for each computation is created. One representing local/regional scale plumes, the other the contribution to global background concentrations.

Dust Storm - Invokes a pre-processor that creates a *CONTROL* file with each location within the selected computational domain that contains a desert land-use designation. This option should be used in conjunction with the advanced menu option to turn on the dust emission module.

Daughter Products - Invokes a pre-processor that creates a DAUGHTER.TXT file containing the daughter nuclides produced by a parent nuclide along with the half-life and branching fractions. In addition a *CONTROL* file is modified to include the daughter product information. This option should be used in conjunction with the advanced menu option to turn on the daughter product module and set MAXDIM to the number of daughters.

Advanced Topics

Contains several menus for custom model configurations that can be used to change the nature of the simulation and the way the model interprets various input parameters. These menus would be used to configure matrix, ensemble, global, pollutant transformations, and model initialization options.

Trajectory Configuration - Creates the *SETUP.CFG* namelist file for trajectory calculations.

Concentration Configuration - Creates the *SETUP.CFG* namelist file for concentration-dispersion calculations.

Global Configuration - Creates the *GEMPARM.CFG* namelist file to configure the global Eulerian model subroutines.

Dynamic Sampling - Creates a virtual sampler that can fly through the computational domain, either passively with the wind or with a pre-defined velocity vector.

Emissions File - Opens a simple editor to create a special emission file that can define point sources that vary in space, time, and intensity.

Satellite Data / TOMS and Particle Viewer - Permits the download of TOMS aerosol index data and plots those data with particle positions or model generated concentration fields.

Center Reset Button

This will cause any changes to the GUI variables to be set back to the sample trajectory and concentration simulation case which uses the oct1618.BIN sample meteorological file. This button loads the sample_conc and sample_traj control files from the working directory.

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Advanced / Special Topics / ASCDATA.CFG

The *bdyfiles* subdirectory contains ASCII files for gridded land-use, terrain, and roughness length data for HYSPLIT. The terrain file is used by some of the programs in *data2arl* if the terrain is not provided with the other meteorological fields. The resolution for these files is one-degree covering the globe: 360 by 180 grid points. The upper left corner starts at 180W - 90N. If these files are not found, the model uses default constant values for land-use and roughness length.

The structure of these files is given in the *ASCDATA.CFG* file, which defines the grid system and gives the directory location of the land-use, terrain, and roughness length files. The *ASCDATA.CFG* file should be located in the model's startup or root directory. The last line in the file should be modified to reflect the path to the *bdyfiles* directory.

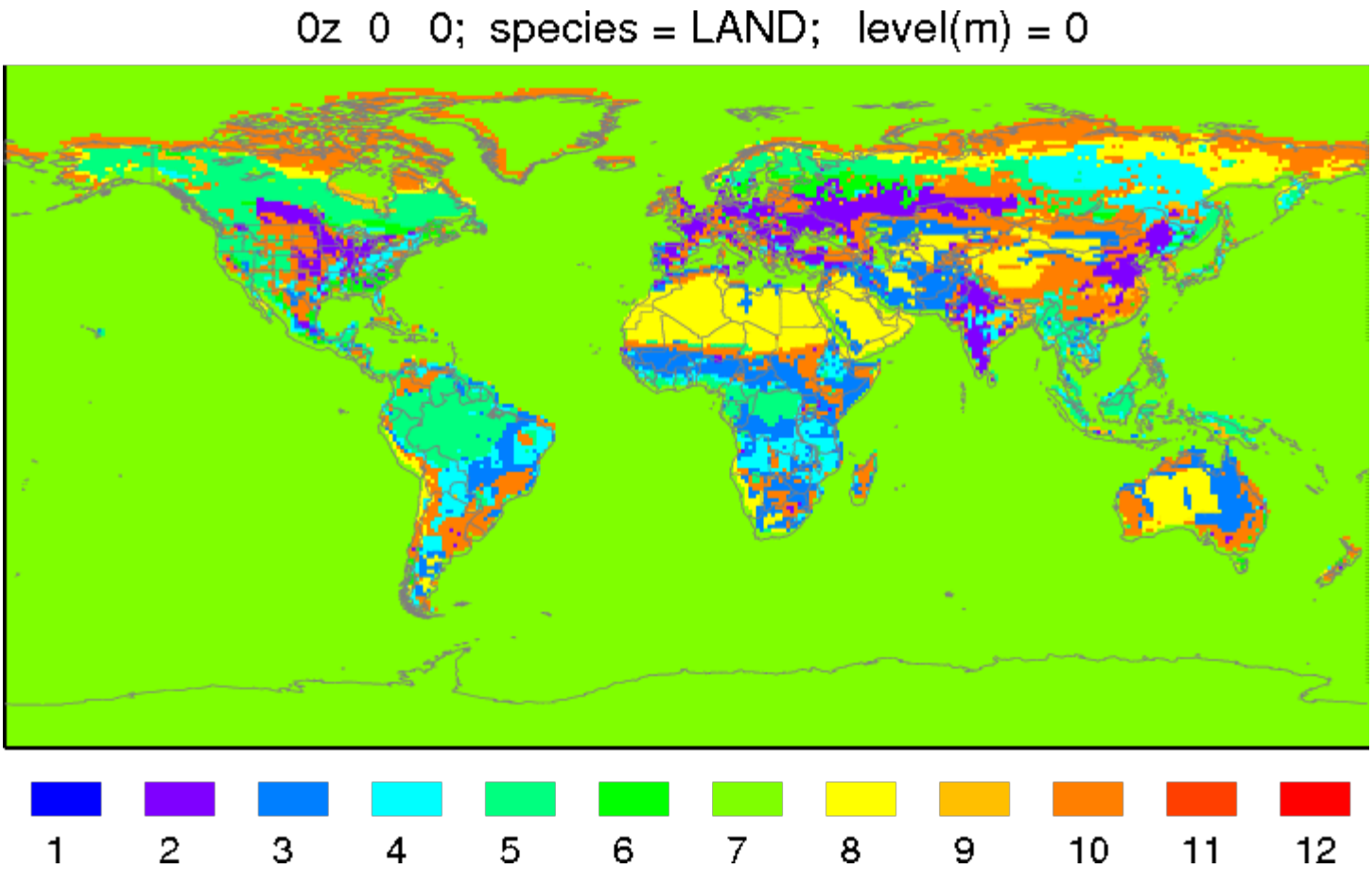
File Format

The ASCDATA.CFG file contains the following six records:

- -90.0 -180.0 lat/lon of lower left corner (last record in file)
- 1.0 1.0 lat/lon spacing in degrees between data points
- 180 360 lat/lon number of data points
- 2 default land use category
- 0.2 default roughness length (meters)
- '../bdyfiles/' directory location of data files

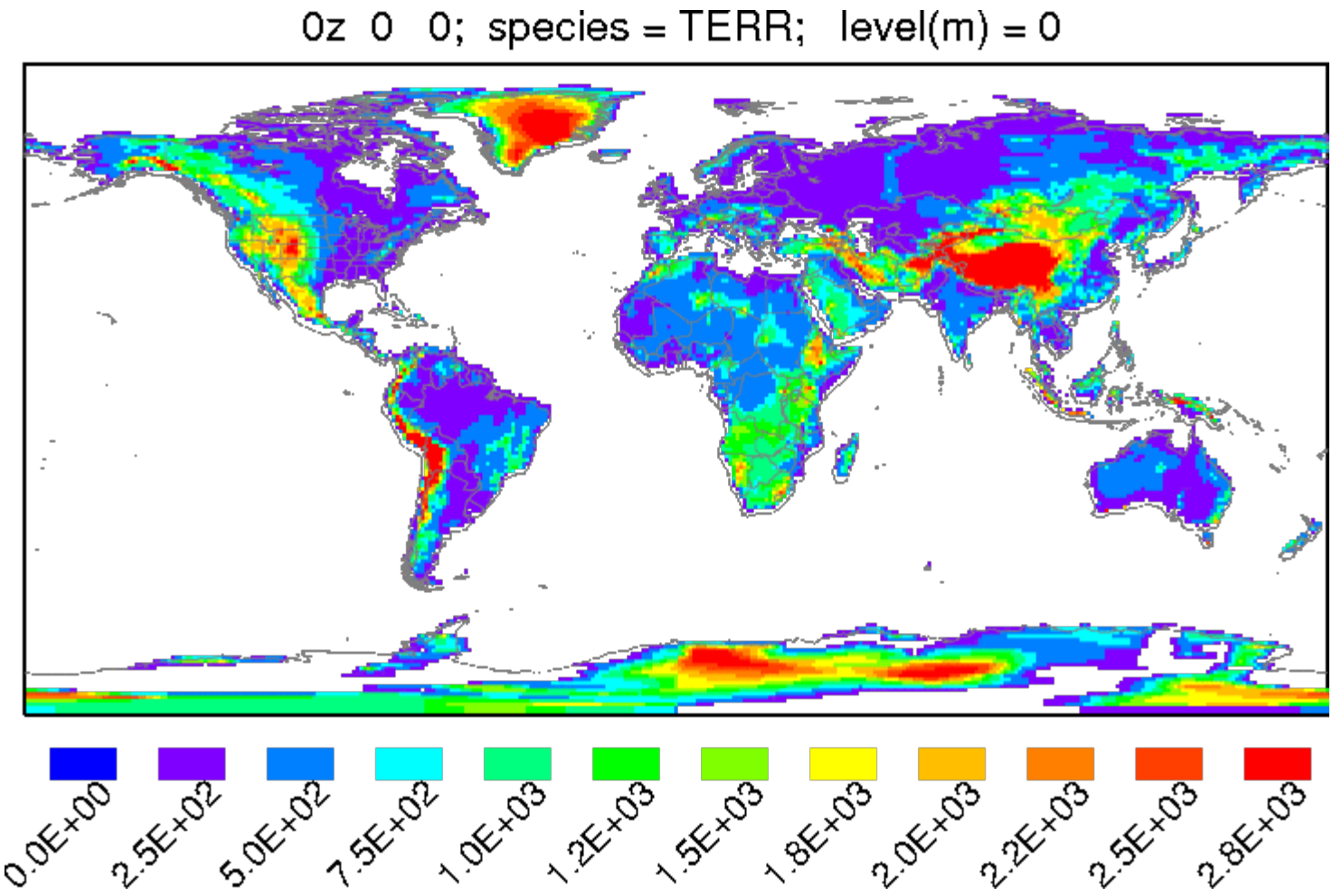
These files may be replaced by higher resolution user created files. Note that the first data point on the first record is assumed to be centered at 179.5W and 89.5N, so that from the northwest corner the the data goes eastward and then southward. User supplied files should define roughness length (cm - F4) and the following land use-categories (I4). The record length of the file should be the number of longitude values times four bytes plus one additional byte for CR.

The 11 Land-Use Categories



1. -urban
2. -agricultural
3. -dry range
4. -deciduous
5. -coniferous
6. -mixed forest
7. -water
8. -desert
9. -wetlands
10. -mixed range
11. -rocky

The One-Degree Terrain



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Meteorology / Help / Sample Programs

The source code for many different meteorological data applications can be found in the *data2arl* directory. A summary of these programs and some others where only the executable is provided are given below. Some of these are available for execution through the GUI, others must be run from the command line. All executables can be found in the *exec* directory.

GRIB records

The various programs and library routines that are required to convert GRIB formatted meteorological data files to ARL HYSPLIT compatible format can be found in the *data2arl* directory. Some of these are summarized below:

content - decodes individual GRIB sections in a record for diagnostic purposes. This program does not unpack the data but only lists the contents of the GRIB file.

inventory - decodes all the records within a GRIB file (without unpacking) providing file content information.

unpacker - decodes GRIB records in a data file to a real data array.

sample - creates a packed meteorological file using dummy fields hardwired into the program. The input meteorological data subroutines should be replaced by routines reading user supplied meteorological data files.

grib2arl - a generic program to convert ECMWF or NOAA global data from ECMWF or NOAA in GRIB1 format on a global latitude longitude grid to the ARL format. ECMWF data may be on the native hybrid sigma or pressure surfaces. For computational purposes, HYSPLIT requires either surface pressure or terrain height as a surface field in the meteorological data file. The default is that surface pressure is assumed to be available in the input GRIB file, otherwise the terrain height is required. This option is set using the "-p" flag. ECMWF GRIB files may contain upper-level variables in one file, surface variables in another file, and invariant data in a third file. In this situation, the upper-level data are considered the primary file "-i" and the surface data are the supplemental file "-s", and the invariant data are the constant file "-c".

- -i[primary grib data: file name {required}]
- -s[supplemental grib data: file name {optional}]
- -c[constant grib data: file name {optional}]
- -x[subgrid extract center longitude {-80.0}]
- -y[subgrid extract center latitude {60.0}]
- -g[output projection {3}]
  - 0 :conformal extract
  - 1 :fixed northern hemisphere polar
  - 2 :fixed southern hemisphere polar
  - 3 :lat-lon global grid (as input)
  - 4 :lat-lon extract grid
- -n[number of (x:y) extract grid points {100}]
- -k[number of output levels including sfc {16}]
- -p[surface defined by {1}:pressure or 0:terrain height]
- -q[analyze grib file {0} or use saved configuration: 1]
- -r[rain fall accumulation time hours: {6}]
- -t[the number of time periods to process: {744}]
- -z[zero initialization of output file 0:no {1}:yes]

fcsubs - library routines required for direct access to variable length records

cmapf - library routines to convert from latitude-longitude to a conformal map projection

w3arl - library routines of the ARL version of the NCEP w3lib GRIB record decoder.

ARL Packed Format

The various programs and library routines that are required to manipulate or display meteorological data already in the ARL packed format can be found in the *exec* directory. Note that when these programs are run from the command line there will be a typical two line prompt, the first for the directory and second for the file name. A directory name should always have the proper terminator (/ or \). The following programs can be found:

chk_rec - program to dump the first 50 bytes of each meteorological data record. Those bytes contain ASCII data describing the packing.

chk_file - program to examine header and data records of an ARL packed meteorological data file. The program uses the same I/O subroutines common to HYSPLIT code. If this program does not work with a data file, neither will HYSPLIT.

chk_data - a simple program that shows how to read and unpack the ARL format packed meteorological data.

contour - creates postscript file of meteorological data contoured and color filled for a single variable at a specified time. The output written to *contour.ps*

display - creates postscript file of meteorological data contoured and color filled for a single variable at a specified time. The output written to *display.ps.* This program is prompted interactive version of the command line program *contour*.

edit_miss - a simple missing data interpolation program to fill in data gaps.

profile - creates text file of the profile of meteorological variables at a specified location and time. The output is written to the screen and to the file *profile.txt*.

showgrid - shows the extent of the meteorological grid domain with a "+" symbol at the intersection of each node. The output is written to *showgrid.ps*

xtrct_grid - extracts a subgrid from the full grid meteorological data file. It permits selection by lat-lon corners and number of levels from the ground. Creates output file called *extract.bin*

xtrct_time - extracts data between two selected time periods from the designated meteorological file. Creates an output file called *extract.bin*

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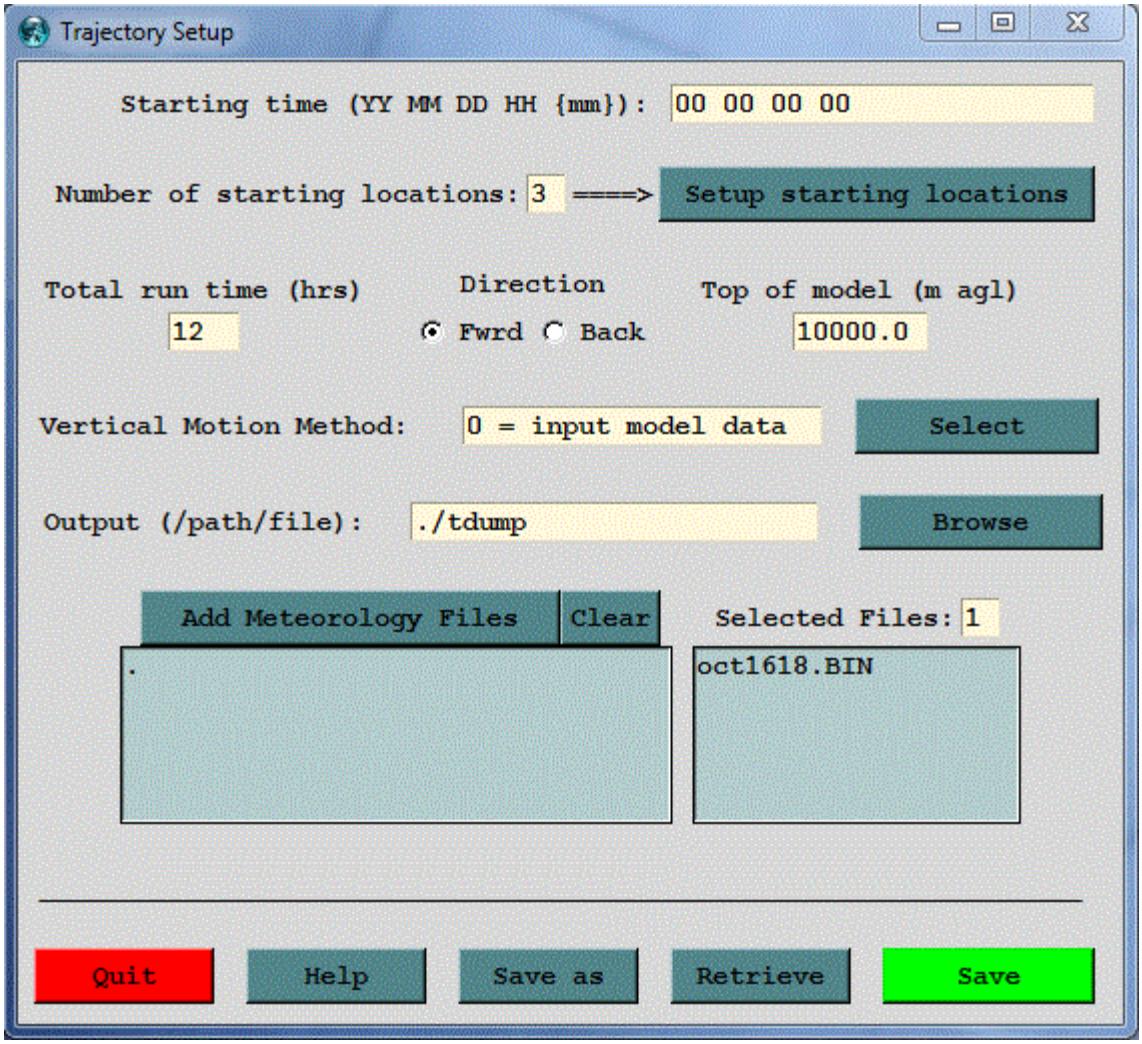
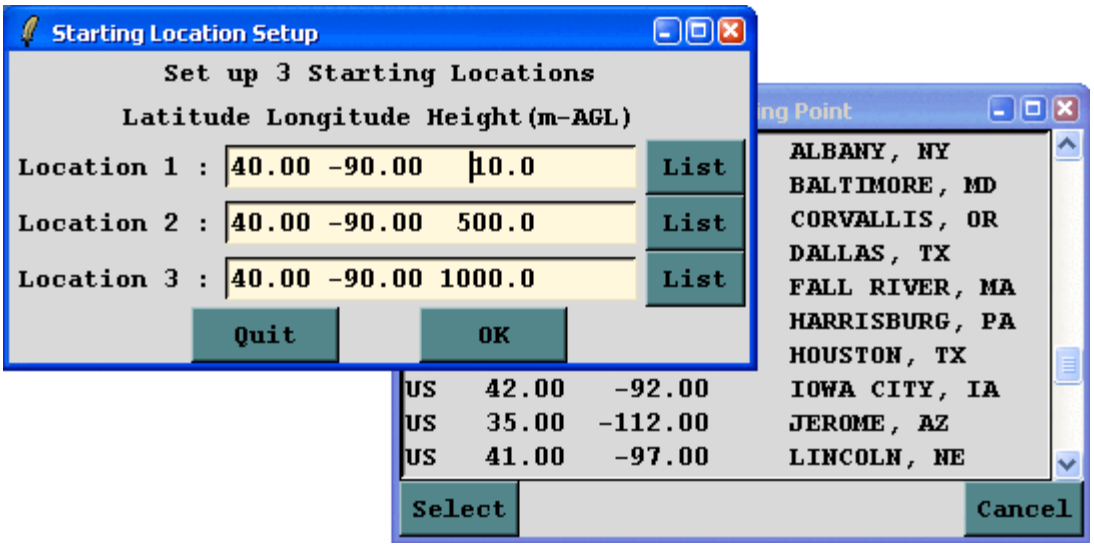
Trajectory / Setup Run

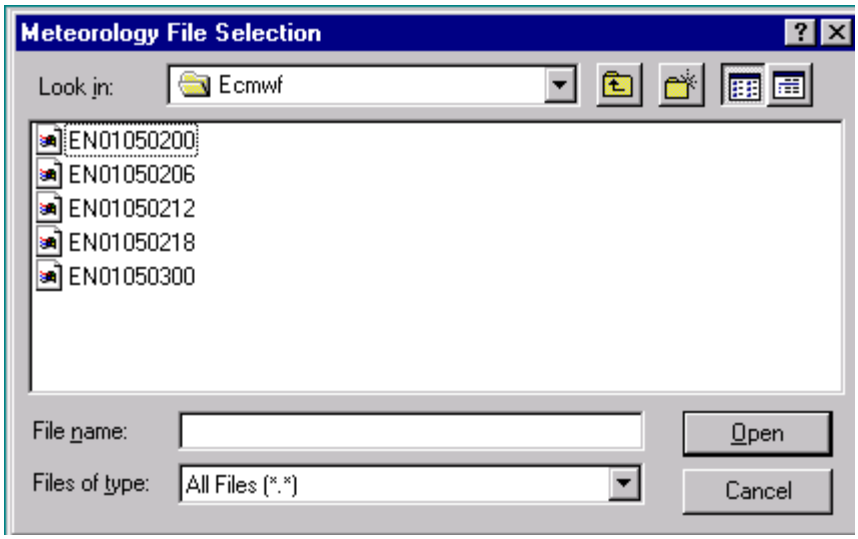
When the *Setup Run* tab is executed, the *default_traj* file is read and the current parameter values are loaded. The menu for the example simulation (*sample_traj*) is shown below. The options shown on the menu correspond with the various lines in the CONTROL file. See the discussion of the control file format for a more detailed description for each of these parameters. However there are some features of the GUI that require additional explanation.



Clicking the *Setup Starting Locations* tab brings up the menu shown below. If the number of starting locations were to have been changed from the default value of three on the main menu, then there would be that number of starting location lines set on the menu, all with the same latitude and longitude. These could then be manually edited for different locations or starting heights. The starting height is by default defined to be above-ground-level (AGL) unless this is changed in the Advanced/Configuration/Trajectory menu. Another possibility would be to click on the *List* tab, which brings up a list of pre-selected starting locations from a file called *plants.txt*, which can be found in the *../hysplit4/working* directory. This file can be edited to reflect starting locations of interest to the user.



Another important feature of the main menu is how to select or add meteorological data files. The *Clear* button will erase all file selections, then pressing the *Add Meteorology Files* tab brings up the file selection dialog shown below. Select a file and click *Open* and the file will be added to the main menu. For each additional file, it is necessary to click again on the *Add Meteorology Files* tab. With each new file the selected files number is incremented by one.



Once the simulation is configured as required, click the *Save* menu tab. This causes the GUI menu to over-write the values in *default_traj*. Note that the format of *default_traj* is identical to the *CONTROL* file. Clicking on *Save* closes the menu and then when the Run Model tab is executed, *default_traj* is first copied to *CONTROL*, and then the trajectory model is run.

When the GUI menu system is restarted, it loads the last values stored in *default_traj*. The *default_traj* file may also be saved to another name to permit future similar simulations to be set up more quickly. This option is available through the Save As and Retrieve menu tab of the setup menu.

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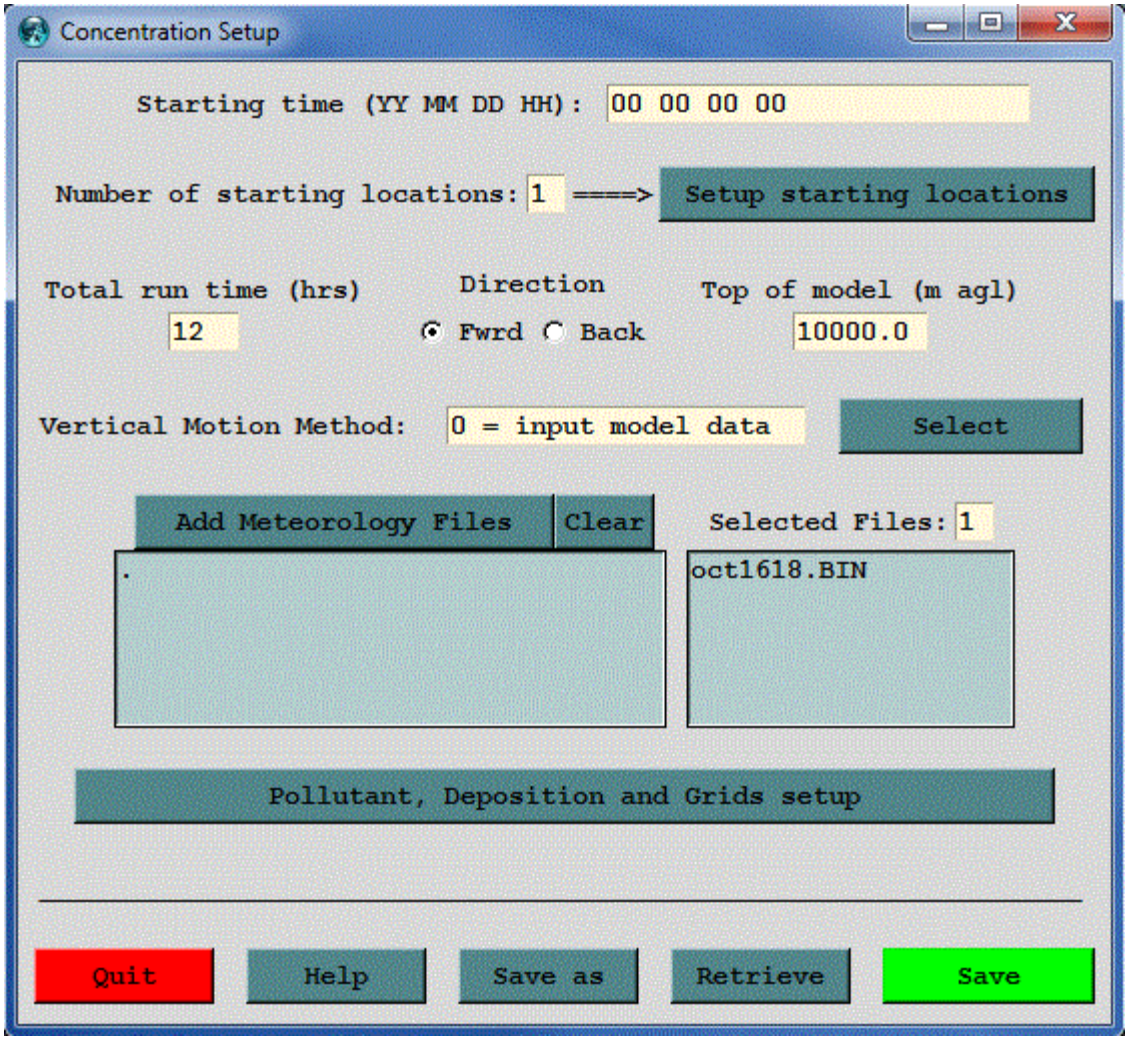
Concentration / Setup Run

The initial setup menu for the concentration model is identical to the trajectory setup run menu in terms of starting time, location, and meteorology. These items will not be discussed again except to note the differences when applied to a dispersion simulation. The meaning of the entries in the *CONTROL* file that correspond to this setup menu are discussed in more detail below and should be reviewed to appreciate how the change in the simulation type (from trajectory to concentration) changes the meaning and context of the same input parameters. These parameters consist of the initial entries of the *CONTROL* file. The initial concentration setup menu is shown in the illustration below.



The entries in the *Control* file for air concentration simulations consist of four groups of input data. The first data group is almost identical to the trajectory simulation and is described in the next section. The other three groups define the pollutant emission characteristics, the concentration grid in terms of spacing and integration interval, and the pollutant characteristics relevant to computing deposition and removal processes. These latter three entries are accessed through the "Pollutant, Deposition, and Grids Setup" tab. Each of the these sections contains a more detailed description of the input parameters as well as the corresponding *CONTROL* file values that need to be set for command line simulations.

Initial *CONTROL* File Section

The concentration model input control file can be created using any text editor. However if the GUI is not being used, it would be easier to let the model create the initial file based upon standard output prompts. These are described in more detail below. When data entry is through the keyboard (a file named *CONTROL* is not found), a *STARTUP* file is created. This contains a copy of the input, and which later may be renamed to *Control* to permit direct editing and model execution without data entry. If you are unsure as to a value required in an input field, just enter the forward

slash (/) character, and the indicated default value will be used. This default procedure is valid for all input fields except directory and file names. An automatic default selection procedure is also available for certain input fields of the *CONTROL* file when they are set to zero. Those options are discussed in more detail below. Each input line is numbered (only in this text) according to the order it appears in the file. A number in parenthesis after the line number indicates that there is an input loop and multiple entry lines may be required depending upon the value of the previous entry.

1- Enter starting time (year, month, day, hour)

Default: 0 0 0 0

Enter the two digit values for the UTC time that the calculation is to start. Use 0's to start at the beginning (or end) of the file according to the direction of the calculation. All zero values in this field will force the calculation to use the time of the first (or last) record of the meteorological data file. In the special case where year and month are zero, day and hour are treated as relative to the start or end of the file. For example, the first record of the meteorological data file usually starts at 0000 UTC. An entry of "00 00 01 12" would start the calculation 36 hours from the start of the data file.

2- Number of starting locations

Default: 1

Single or multiple pollutant sources may be simultaneously tracked. The emission rate that is specified in the pollutant menu is assigned to each source. If multiple sources are defined at the same location, the emissions are distributed vertically in a layer between the current emission height and the previous source emission height. The effective source will be a vertical line source between the two heights. When multiple sources are in different locations, the pollutant is emitted as a point source from each location at the height specified. Point and vertical line sources can be mixed in the same simulation. The GUI menu can accommodate multiple simultaneous starting locations, the number depending upon the screen resolution. Specification of additional locations requires manual editing of the *CONTROL* file. Area source emissions can be specified from an input file: *emission.txt*. When this file is present in the root directory, the emission parameters in the *CONTROL* file are superseded by the emission rates specified in the file. More information on this file structure can be found in the advanced help section.

3(1)- Enter starting location (lat, lon, meters, Opt-4, Opt-5)

Default: 40.0 -90.0 50.0

Position in degrees and decimal (West and South are negative). Height is entered as meters above ground level unless the mean-sea-level flag has been set.

The optional 4th (emission rate - units per hour) and 5th (emission area - square meters) columns on this input line can be used to supersede the value of the emission rate (line 12-2) when multiple sources are defined, otherwise all sources have the same rate as specified on line 12-2. The 5th column defines the virtual size of the source: point sources default to "0".

4- Enter total run time (hours)

Default: 48

Sets the duration of the calculation in hours. Backward calculations are configured by setting the run time to a negative value. See the discussion in the advanced help section on backward "dispersion" calculations.

5- Vertical motion option (0:data 1:isob 2:isen 3:dens 4:sigma 5:diverg 6:msl2agl 7:average 8:damped)

Default: 0

Indicates the vertical motion calculation method. The default "data" selection will use the meteorological model's vertical velocity fields; other options include isobaric, isentropic, constant density, constant internal sigma coordinate, computed from the velocity divergence, a special transformation to correct the vertical velocities when mapped from quasi-horizontal surfaces (such as relative to MSL) to HYSPLIT's internal terrain following sigma coordinate, and a special option (7) to spatially average the vertical velocity. The averaging distance is automatically computed from the ratio of the temporal frequency of the data to the horizontal grid resolution.

6- Top of model domain (internal coordinates m-agl)

Default: 10000.0

Sets the vertical limit of the internal meteorological grid. If calculations are not required above a certain level, fewer meteorological data are processed thus speeding up the computation. Trajectories will terminate when they reach this level. A secondary use of this parameter is to set the model's internal scaling height - the height at which the internal sigma surfaces go flat relative to terrain. The default internal scaling height is set to 25 km but it is set to the top of the model domain if the entry exceeds 25 km. Further, when meteorological data are provided on terrain sigma surfaces it is assumed that the input data were scaled to a height of 20 km (RAMS) or 34.8 km (COAMPS). If a different height is required to decode the input data, it should be entered on this line as the negative of the height. HYSPLIT's internal scaling height remains at 25 km unless the absolute value of the domain top exceeds 25 km.

7- Number of input data grids

Default: 1

Number of simultaneous input meteorological files. The following two entries (directory and name) will be repeated this number of times. A simulation will terminate when the computation is off all of the grids in either space or time. Calculations will check the grid each time step and use the finest resolution input data available at that location at that time. When multiple meteorological grids have different resolution, there is an additional restriction that there should be some overlap between the grids in time, otherwise it is not possible to transfer a particle position from one grid to another. If multiple grids are defined and the model has trouble automatically transferring the calculation from one grid to another, the sub-grid size may need to be increased to its maximum value.

8(1)- Meteorological data grid # 1 directory

Default: (\main\sub\data\ )

Directory location of the meteorological file on the grid specified. Always terminate with the appropriate slash (\ or /).

9(2)- Meteorological data grid # 1 file name

Default: file_name

Name of the file containing meteorological data. Located in the previous directory.

Next Section of the CONTROL file

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Advanced / Special Topics / Message File Format

A MESSAGE file is created during each simulation. The file contains information from certain key subroutines that can be used for diagnostic purposes if a simulation were to fail. An example file is shown below in the left column from the test concentration simulation. A trajectory MESSAGE file would be similar but without the particle number and mass information. In the right column, in red, a more detailed description of each item is provided.

Start Namelist configuration

Internal grid parameters (nlvl,aa,bb,cc): 19 30.0 -25.0 5.0
&SETUP INITD = 4, KHMAX = 9999, NUMPAR = 500, MAXPAR = 10000, MAXDIM = 1,
QCYCLE = 0.0000E+00,
FRME = 0.10000000,
FRMR = 0.0000E+00,
KRND = 6,
DELT = 0.0000E+00,
ISOT = 0,
TKER = 0.50000000,
NDUMP = 0,
NCYCL = 0,
TRATIO = 0.75000000,
MGMIN = 10,
KMSL = 0,
NSTR = 0,
CPACK = 1,
ICHEM = 0,
NOUT = 0, TM_PRES = 0, TM_TPOT = 0, TM_TAMB = 0, TM_RAIN = 0, TM_MIXD = 0,
DXF = 1.0000000,
DYF = 1.0000000,
DZF = 9.9998E-03,
NINIT = 1,
PINPF = PARINIT,
POUTF = PARDUMP
-- End Namelist configuration ---
NOTICE main: pollutant initialization flags
Gas pollutant - T
Current version and release date
Tabulates value of namelist variables

Number of internal model sigma levels and the polynomial parameters used to describe the vertical grid. These are configured automatically based upon the meteorological input data files defined for this simulation.

The value of all variables that can be defined by the SETUP.CFG namelist file are listed. If no SETUP.CFG file was defined for this simulation, then the default values for these variables are listed.

The settings of all internal deposition flags are shown here. In this case the simulation is for a gas.

NOTICE metpos: (mtime,ftime) - 50379840 0
NOTICE metpos: (mtime,ftime) - 50379960 0
NOTICE advpnt: (kg,nx,ny,nz) - 1 10 10 19
NOTICE sfcinp: reading ASCDATA.CFG
NOTICE metgrd: (kg, xyr,xy1) - 1 10 10 17 9
NOTICE metinp: NGM 1 1 10 10 17 9 50379840 95 10 16 0

```
##################################
WARNING prfsig: extrapolation from level (k,m): 16 7159.121
Input data levels: 10
Internal Sigma levels: 19
##################################
NOTICE metinp: NGM 1 63 10 10 17 9 50379960 95 10 16 2
NOTICE main: Initial time step (min) 20
NOTICE main: 1 50379860166 0.33333320
NOTICE main: 1 50379880332 0.6666647
NOTICE main: 1 50379900498 0.9999961
NOTICE main: 2 50379930498 0.9999961
NOTICE main: 2 50379960498 0.9999961
NOTICE metpos: (mtime,ftime) - 50380080 50379840
NOTICE metinp: NGM 1 125 10 10 17 9 50380080 95 10 16 4
```

The subroutine that determines which meteorological data are required is called for the first time. Data for times 840 and 960 are requested. The zeros for the second field indicate no data are in memory. Times are always in relative minutes.

The first advection entry sets sub-grid #11 to 10x10 with 19 levels.

The surface boundary files are opened.

The lower left corner of sub-grid #1 is set at position 17,9 of the main meteorological data grid.

The NGM data for the first computational hour are read starting at record #1, loaded into a 10x10 sub-grid, corner 17,9, at time [x]840 for the date: 95 10 16 0

When these data are interpolated to the internal grid, it is determined that there are no input data records above 7159 m, therefore data for those levels are extrapolated.

Computations for the first hour require data at two time periods for interpolation (hours 0 and 2).

The initial time step was set to 20 minutes. Subsequent time steps may change.

The time, number of particles, and the total mass is shown for the three time steps of the first hour. After one hour the emission stops.

During hour two, no further emissions (or particles) are released. The time step is now 30 minutes.

After the hour 2, new NGM data are required. The data in memory at 0 UTC (time 840) are replaced with data at 4 UTC (time 080).

The new data are input into the same sub-grid location.

```
NOTICE main: 3 50379990498 0.9999961
NOTICE main: 3 50380020498 0.9999961
NOTICE main: 4 50380050498 0.9999961
NOTICE main: 4 50380080498 0.9999961
NOTICE metpos: (mtime,ftime) - 50380200 50379960
NOTICE metinp: NGM 1 187 10 10 17 9 50380200 95 10 16 6
NOTICE main: 5 50380110498 0.9999961
NOTICE main: 5 50380140498 0.9999961
NOTICE main: 6 50380170498 0.9999961
NOTICE main: 6 50380200498 0.9999961
```

- Index Height %Mass
- 6 935.0 1.41
- 5 630.0 10.84
- 4 385.0 31.33
- 3 200.0 29.72
- 2 75.0 20.48
- 1 10.0 6.22

Computations proceed as before for computational hours 3 and 4. Particle number remains the same because no particles have moved off the computational domain. The mass remains the same because deposition is not turned on for this simulation.

At the end of hour 4, data are required for 6 UTC (time 200) to proceed with the calculation. These data replace the 2 UTC (time 960) in memory.

Every 6 hours, the model prints out the vertical mass distribution of all the particles within the computational domain. This is the mass distribution relative to the model's internal sigma levels and there is no relation to the levels that may be specified for the concentration output file. Only non-zero levels are shown. The internal levels are defined by the polynomial parameters given at the beginning of the MESSAGE file.

At this point the computation will continue for the number of hours specified in the CONTROL file. Vertical profiles are shown every 6 hours. As the particles move across the computational domain, the sub-grid position may be moved (from position 17,9) or expanded larger than 10x10) to match the spatial extent of the particle distribution. This may occur at any time during the computation or even multiple times during the same computational hour.

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Advanced / Help

This section provides some guidance in configuring the model to perform certain specialized calculations. These include deciding between particle or puff releases, dealing with continuous emissions, creating an file with time variations of the emission rate, unit-source simulations with time-varying emissions, area source emissions, multiple pollutants, pollutant transformations, atmospheric chemistry, deposition and decay, compilation limits, scripting for automation applications, backward dispersion for source attribution, configuring the time or spatial variation of the emission rate using an input file, and how to compute deposited pollutant transport on ocean water surfaces. The Advanced menu is composed of four sections.

1. The **Configuration Setup** menu permits the creation and modification of the *SETUP.CFG* namelist file for either Trajectory or Air Concentration calculations. The namelist file is a variable length file that is used to set additional parameters that can be used to modify the nature of the simulation. The namelist file is not required because all the namelist variables take on default values when the *SETUP.CFG* file is not found. The same namelist file can be used for either trajectory or air concentration simulations but only certain variables are applicable to each simulation. Supplemental plot labeling options are available, a menu to configure a dynamic sampler that can move in space and time for use with the concentration simulation, and a menu to configure the default directory structure and location of executable programs used by the GUI. More complex point source emissions scenarios can be defined by creating the EMITIMES emissions file.

2. The **Satellite Data** menu opens two special menus that deal with downloading and displaying TOMS satellite data. The **FTP NASA TOMS** satellite data menu opens up an anonymous FTP window to access the current satellite archives for the TOMS aerosol index (AI). These data can then be displayed through the **TOMS Viewer**. In addition to AI, the viewing program will also display the pollutant particle positions. The particle position file, called PARDUMP by default, is a snapshot of all the pollutant particles at a given time. Its creation is controlled through the configuration menu.

3. The **View MESSAGES** menu is used to display the diagnostic message file. For all trajectory or concentration simulations, diagnostic information is written to standard output until the initialization process has completed. At that point the *MESSAGE* file is opened and subsequent diagnostic and certain error messages are written to this file. If the model does not complete properly, some additional diagnostic information may be obtained from this file.

4. The **Scan for Updates** menu can be used to make small updates to a limited number of executables and scripts for the same HYSPLIT release version. Updates to executables and scripts may be posted to the ARL web server. This menu compares the dates of those updates with the installed versions. If newer programs are available, you will be prompted to replace each with the update. Older programs are copied to the updates directory and the update can be reversed if desired. The update process only changes programs in the ./exec directory and scripts in the ./guicode directory. Once a significant number of updates have accumulated, the entire release version will be updated and a new installation must be manually downloaded from the ARL server. Only updates to the same version number are permitted.

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Meteorology / Help

Meteorological data fields to run the model are usually already available or can be created from routine analysis archives or forecast model outputs. More complete descriptions of the different data sets are available on-line. The meteorological data available through the menu system are summarized in the following sections.

The meteorology menu is divided into four sections: data FTP, data conversion, data display, and utility programs.

- The FTP section provides access to various data files that may be FTP'd from the ARL server compatible for immediate input to HYSPLIT. These files include current and appended forecasts as well as various regional and global analysis archives and longer term archives such as the NCAR/NCEP reanalysis data. All data files have already been converted for HYSPLIT applications.
- The convert menu gives data processing options for files that are stored on the local computer. Processing of forecast or analysis files are available for archive, forecast, and regional or global data files in various formats. Processing for GRIB1 formatted input files is available for NARR, Global ECMWF/NOAA, and ERA-40. In addition native formatted files from MM5V3 can be converted locally. NetCDF is supported on UNIX systems permitting conversion of WRF-ARW and MCIP IOAPI data files. In addition, a simple interface has been created to permit the entry of user generated time-varying data at a single location.
- The display data menu tab provides some simple tools that can be used to examine the data already in ARL packed format. The most basic is the check file listing of the individual data records. The contour map program will display a contour plot of any variable at any one time in the file. Multiple time periods may be processed. The profile program returns a text file of the profile of meteorological parameters at a pre-selected point. The grid domain menu shows the extent of the meteorological grid with a mark at each point.
- The utility menu permits conversion of Postscript files to any other graphical format and the creation of shapfiles.

More detailed information about the format of the ARL packed data is available. In addition, various library routines and utility programs are provided to manipulate both the GRIB and ARL packed data files.

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Meteorology / ARL Data FTP

The ARL web server contains several meteorological model data sets already converted into a HYSPLIT compatible format in the public directories. Direct access via FTP to these data files is "hardwired" into the GUI. The data files are automatically updated on the server with each new forecast cycle. Only an email address is required for the password to access the server. The "FTP menu" is locked until the FTP process is completed, at which point a message box will appear indicating the file name that was just transferred. Alternatively, there is an option to download the files directly from the NOAA nomads website via HTTP (http://http://nomads.ncep.noaa.gov/pub/data/nccf/com/hysplit/prod/).

Note that the NOAA models run by NCEP may be at higher spatial resolution than what is archived in a HYSPLIT compatible format on the ARL server. If calculations using higher resolution data are required, then the original GRIB encoded files must be obtained and converted as described in the data conversion section. GRIB decoding can be difficult. Although the required software is provided through the GUI, the large file size downloads may limit the practical application of these real-time data files.

Meteorology / Data FTP / Current Forecast

Forecast data are available for NOAA's North America Model (NAM), the Global Forecast System (GFS), and the Rapid Update Cycle (RUC) at various resolutions, projections, and forecast time durations. The files are updated at two to four hours after the cycle time. Forecast files are available for the last several days depending upon the server and not all files are on all FTP servers. All forecast files follow the same file naming convention of hysplit.t{cycle}z.{name}, where cycle represents the initial UTC time of the forecast (00,06,12,18) and the names are as follows:

- gfsf :: 1-deg 3P +192h (0.7 Gb) global forecast at one-degree resolution at 3 hour intervals at pressure levels out to +84 hours
- gfslrf :: 2.5d 12P +360h (0.03 Gb) long-range global forecast at two and half degree resolution at 12 hour intervals at pressure levels and from forecast hours +192 to +360.
- gfs0p5f :: 0.5-deg 3S +84h (2.6 Gb) global forecast at one-half degree resolution at 3 hour intervals at hybrid levels out to +84 hours
- namf :: 12-km 3P +84h (1.6 Gb) regional forecast for the entire domain at 12 km resolution every three hours on pressure levels out to a +84 hours.
- namsf :: 12-km 1S +48h (2.7 Gb) regional forecast extracted for CONUS at 12 km resolution at hour intervals on sigma surfaces out to +48 hours.
- namsf.AK :: 12-km 1S +48h (1.5 Gb) regional forecast extracted for Alaska at 12 km resolution at hour intervals on sigma surfaces out to +48 hours.
- namsf.HI :: 12-km 1S +48h (1.4 Gb) regional forecast Hawaii nest at 2 km resolution at hour intervals on sigma surfaces out to +48 hours.
- namsf.FW :: 1-km 1S +36h (2.2 Gb) regional forecast Fire-Weather nest at 2 km resolution at hour intervals on sigma surfaces out to +48 hours (location varies from cycle to cycle)
- namsf.{XX}tile :: 12-km 1s +48h (0.3 Gb) regional forecast extracted for the XX quadrant of the US at 12 km resolution at hour intervals only for sigma surfaces below 0.6777 out to +48 hours. Quadrants are available for the northeast (NE), southeast (SE), southwest (SW), and northwest (NW).
- namsf{HH}.CONUS :: 4-km 1S +6h (2.0 Gb) regional forecast CONUS nest for forecast hour beginning at HH+1h at 4 km resolution at hour intervals on sigma surfaces out to +6, +12, +18, +24 hours for files f00,f06,f12,f18, respectively.
- rap :: 20-km 1P +12h (0.2 Gb) for the CONUS is at 20 km resolution at hourly intervals on pressure surfaces out to +18. Updated every three hours.

Additional information about the forecast data on the ARL server can be found at the ARL web page.

Meteorology / Data FTP / Appended Forecast

The appended forecast files consist of a special time extraction of the previous seven (-48 hr) forecast cycle files to create a series of pseudo-analysis (0-hour initialization) and short-time (+3 h or +1,+2,+3,+4,+5) forecasts that have been appended to each other to create a continuous data time series for the previous 48 hours in a single file. These special time extracts are only available for the following files.

- gfsa :: 1-deg 3P -48h (160 Mb)
- nama :: 12-km 3P -48h (829 Mb)
- ruca :: 20-km 1P -48h (60 Mb)

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Meteorology / ARL Data FTP / Archive

The ARL web server contains several meteorological model data sets already converted into a HYSPLIT compatible format on the public directories. Direct access via FTP to these data files is "hardwired" into the GUI. Only an email address is required for the password to access the server. The "FTP menu" is locked until the FTP process is completed, at which point a message box will appear indicating the file name that was just transferred.

The ARL analysis data archive consists of output from the Global Data Analysis System (GDAS) and the NAM Data Analysis System (NDAS - previously called EDAS) covering much of North America. Both data archives are available from 1997 in semi-monthly files (SM). The EDAS was saved at 80-km resolution every 3-h through 2003, and then at 40-km resolution (AWIPS 212 grid) starting in 2004. The GDAS (every 6-h) was saved on a hemispheric projection at 191-km resolution through the end of 2006. The new 1-degree and half-degree GDAS archive is available every three hours. See notes below for a more detailed discussion of each file.

- EDAS :: 80 km 3P (<=2003 SM 82 Mb) Semi-Monthly data files at three hour intervals on pressure surfaces
- EDAS :: 40 km 3P (>=2004 SM 600 Mb) Semi-Monthly data files at three hour intervals on pressure surfaces
- GDAS :: 1-deg 3P (>=2005 WK 600 Mb) Weekly files (W1=1-7; W2=8-14; W3=15-21; W4=22-28; W5=29-end) every three hours on pressure surfaces
- GDAS :: 0.5-deg 3S (>=2010 DA 468 Mb) Daily files every three hours on the native GFS hybrid sigma coordinate system. Beginning July 28, 2010.
- NAM12 :: 12-km 3P (>=2007 DA 395 Mb) Composite archive 0 to +6 hour forecasts appended into daily files for the CONUS at three hour intervals on pressure surfaces
- NAMs :: 12 km 1S (>=2008 DA 994 Mb) Composite archive 0 to +6 hour forecasts appended into daily files for the CONUS at one hour intervals on sigma surfaces

From the GUI it is necessary to enter the year, month, and data file period. Semi-monthly files are designated by 001 (1st through the 15th) and 002 (16th through the end of the month). Weekly files by the week number and the two-digit day for the daily files. The file names are created automatically.

For earlier global archive data see Meteorology - ARL Data FTP - Reanalysis.

Additional information about the data archives on the ARL server can be found at the ARL web page.

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Meteorology / ARL Data FTP / Reanalysis

Global NOAA-NCEP/NCAR pressure level reanalysis data archives were reprocessed into the HYSPLIT compatible format and are available on ARL's web site for 1948 through the end of the previous year. Data for each additional year are updated annually. The global data are on a latitude-longitude grid (2.5 degree) and are archived as one file (122 Mb) per month. The GUI menu tab accesses the correct directory with the proper file name using anonymous ftp after the desired year and month have been selected.

The NCEP/NCAR Reanalysis Project is a joint project between the National Centers for Environmental Prediction (NCEP, formerly "NMC") and the National Center for Atmospheric Research (NCAR). The goal of this joint effort is to produce new atmospheric analyses using historical data (1948 onwards) and as well to produce analyses of the current atmospheric state (Climate Data Assimilation System, CDAS). Until recently, the meteorological community has had to use analyses that supported the real-time weather forecasting. More information about the reanalysis project and data can be found at the CDC web site.

A subset of this data (global pressure level only) is available from ARL in a format suitable for transport and dispersion calculations using HYSPLIT through the GUI. Data files are named according to the following syntax: RP{YEAR}{MONTH}.gbl, where R indicates "Reanalysis", P indicates that the data are on pressure surfaces, YEAR is a four digit year, and MONTH is a two digit month. The file suffix identifies the projection as the 2.5 degree global latitude-longitude projection (gbl). The projection details are encoded in the file's index record and are processed by HYSPLIT during trajectory or dispersion computations.

A comparable data set is also available from ECMWF's 40 year reanalysis project. The GRIB files must be downloaded independently from the GUI through a web browser. Although cost free, registration with ECMWF is required. The downloaded ECMWF GRIB data files may be converted through the GUI to the ARL format.

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Meteorology / ARL Data FTP / Set Server

Meteorological data files formatted for use by HYSPLIT are available from several different FTP servers. The GUI currently supports the definition of three different servers for forecast and analysis data. The default server locations and their root data directories are written to the file default_ftp when the GUI is started for the first time. The FTP application will only search for data at one location as shown in the text box. One may select either the default, alternate, or backup sites. Not all data files are available at all sites. After selecting a new server, it is only necessary to exit the GUI and the location in the text box will be used for all subsequent FTP commands.

It is possible to edit both the server location and root data directory and the exiting the GUI will cause subsequent FTPs to use the edited location. However, if the edits are desired to be saved, then there are two save options. In the first, Save Changes, just updates the internal array so that the edited text is saved in either the default, alternate, or backup locations, so that pressing the radiobutton will bring up the edited locations rather than the original values for those entries. In the Save to File option, the changes are saved to the internal array as well as the default_ftp file, so that when the GUI is closed and reopened, the new values will be available.

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Meteorology / Convert to ARL / WRF-ARW

This menu tab is intended to convert WRF-ARW NetCDF output files to the ARL packed HYSPLIT compatible format. Input files can have any name. The reformatted output files are named by default to ARWDATA.BIN. The output file can be renamed through the GUI menu. Multiple time periods from a single file can be processed into one output file. However, if single-time multiple files are to be processed, then each time period should be given a unique name and then the files can be "cat" or "type" together into a single file if that is desired. Also note that the HYSPLIT NetCDF decoder library is not available under Windows and this program will only work in a UNIX or MAC environment.

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METEOROLOGY / Convert to ARL / NARR Archive

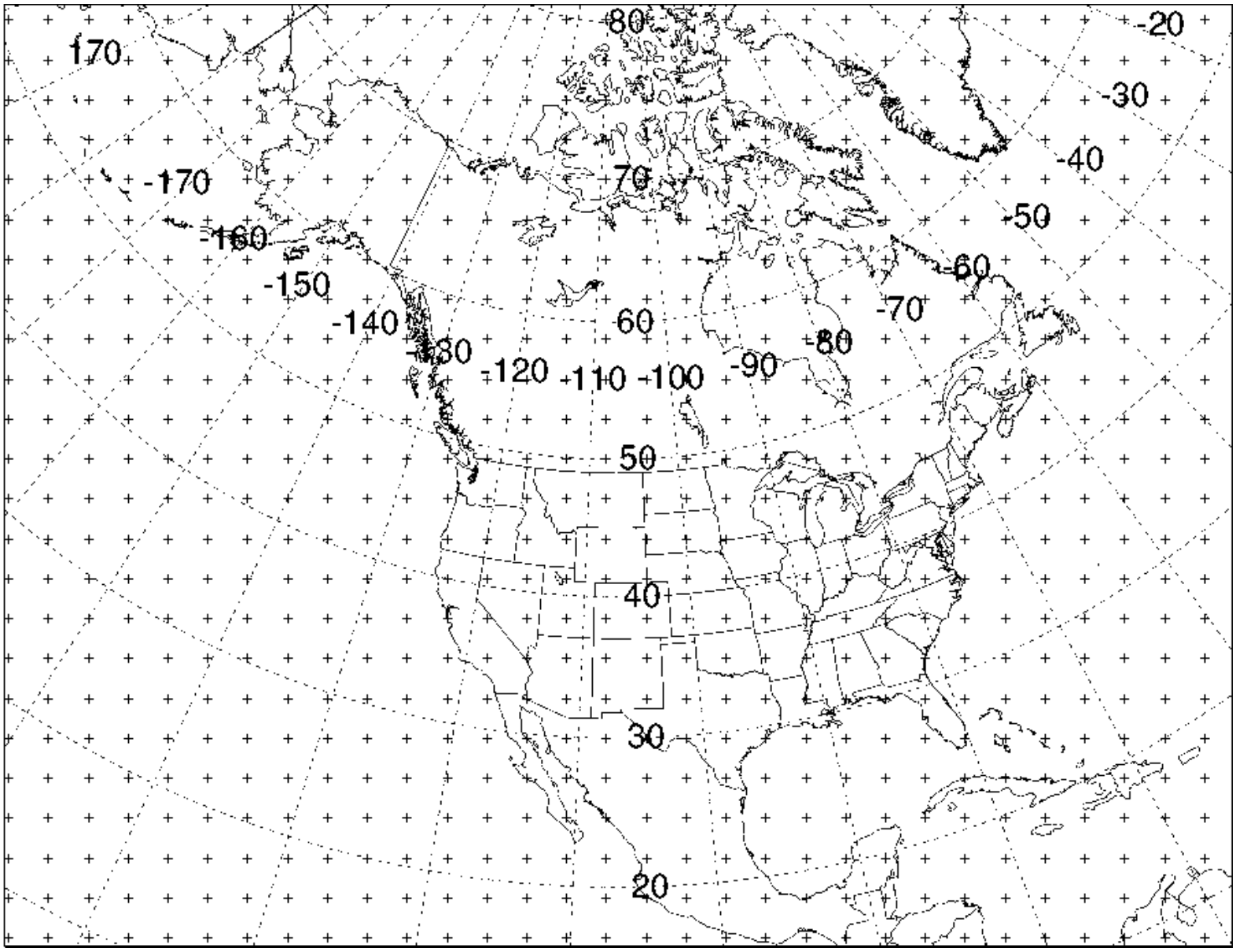
This menu item is intended to convert existing NARR GRIB-1 files to the ARL packed format. The data files to process are determined by selecting any file in the GRIB data directory. Subsequent file names will be constructed automatically between the starting and ending day at the hour interval set by the radio-button. Day (DD) and hour (HH) must be embedded the within the GRIB file name according to the following NOMADS archive convention: narr-a_221_{YYYY}{MM}{DD}_{HH}00_000.grb. Year (YYYY) and month (MM) are fixed according to the file name' selected to set the base file name. Time intervals of 12 hours or more should be avoided in transport and dispersion calculations. Only one month of data or less should be processed into one output file.

The GRIB files for the North American Regional Reanalysis (NARR) can be downloaded from the NOMADS web page. When selecting data to download, all variables and cycles should be obtained. The simplest approach is to use an FTP client and go to the directories of the desired data and download all the narr-a_221_{YYYY}{MM}{DD}_{HH}00_000.grb files for the desired period.

However, the NARR GRIB files are bit mapped, meaning some of the corners do not have data defined due to differences in the internal grid projection of the model vesus the output grid. HYSPLIT does not support projections with a bit map and when running the data converter a message will be generated:

WARNING w3fi63: BMS detected in GRIB file
Insure final grid does not intersect BMS
Full domain grid: 349 277
Bitmap reduction: 309 237

which indicates the the grid has been slightly reduced to insure that all data points within the domain have valid data. The reduced domain is shown below with the + indicating every 10th data point.



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Meteorology / Convert to ARL / Global Lat-Lon

This menu tab is intended to convert existing ECMWF or NOAA GRIB-1 files to the ARL packed HYSPLIT compatible format. Subsequent file names will be constructed automatically between the starting and ending day at the hour interval set by the radio-button. Day and hour are assumed to be the last four digits of the file name: {base}{DD}{HH}. Input files could consist of multiple time period forecasts or single-time period archives. Time intervals of 12 hours or more should be avoided in transport and dispersion calculations. Only one month of data or less should be processed into one output file. HYSPLIT cannot properly position to the correct starting data record if there is a month transition included within a data file.

The input data may be on pressure surfaces or the native hybrid coordinate system. The "number of levels", counted from the surface upwards, can be used to restrict the size of the output file. This may be particularly useful when the input file consists of 60 or more hybrid levels.

Four different grid conversions are available through the menu. The "Extract" option interpolates the data to a conformal map projection of 100x100 grid points at 100 km resolution at the center of the latitude and longitude selection of the slider bar. The Northern- or Southern Hemisphere options create a 95-km resolution polar stereo-graphic grid centered about the pole. The "Input" option results in no interpolation and the program just converts the original latitude-longitude data (global or regional) to the ARL packed format.

The conversions from this menu are intended for data sets created by the operational ECMWF or NOAA forecast models. These may be forecast or analysis data. Conversion of ECMWF reanalysis data is done through a different menu.

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Meteorology / Convert to ARL / ECMWF ERA

This menu tab is intended to convert ECMWF reanalysis data archives (ERA-40) GRIB1 files to the ARL packed HYSPLIT compatible format. Data files must first be downloaded from the ECMWF web page . The user can select which fields and time periods to extract. A GRIB file may contain multiple time periods. No more than one month's data should be included in a GRIB file if it is to be converted to ARL format. All the time periods from one input file will be processed into one output file. The ECMWF download menu permits copying all the data on the global grid or extracting regional sub-grids. The ARL conversion program can handle either option.

The conversion menu is designed to select three different GRIB file types: upper air data, surface data, and time invariant data. The upper air and surface data files should contain data for the same time periods. To be able to run HYSPLIT, the upper air data file must contain at a minimum the following variables: geopotential, temperature, u-velocity, v-velocity, w-velocity, and relative humidity. The surface variable file should contain the 2m temperature, the 10m u- and v- velocity components, and the total precipitation field, if wet removal calculations are required. The invariant file should contain the surface geopotential field (terrain height). Terrain height or surface pressure is required for HYSPLIT to be able to interpolate pressure level data to its internal terrain following coordinate system.

The ECMWF input data may be on pressure surfaces or its native hybrid coordinate system. The "number of levels", counted from the surface upwards, can be used to restrict the size of the output file. This may be particularly useful when the input file consists of 60 or more hybrid levels. The rainfall summation time is the interval in hours at which the rain "bucket" is emptied. For a pure forecast, the bucket is never emptied, for the interim data, the bucket is emptied every 12 hours.

Four different grid conversions are available through the menu. The "Extract" option interpolates the data to a conformal map projection of 100x100 grid points at 100 km resolution at the center of the latitude and longitude selection of the slider bar. The Northern- or Southern Hemisphere options create a 95-km resolution polar stereo-graphic grid centered about the pole. The "Input" option results in no interpolation and the program just converts the original latitude-longitude data (global or regional) to the ARL packed format. The "Input" option must be used for latitude-longitude sub-grids because interpolation from input data sub-grids is not supported.

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Meteorology / Convert to ARL / MM5V3 format

This menu tab is intended to convert MM5 Version 3 output files, usually named MMOUT_DOMAIN{X}, to the ARL packed HYSPLIT compatible format. Input files can have any name. The reformatted output files are named by default to DATA{X}.ARL, where "X" is the domain number. The output file can be renamed through the menu. Multiple time periods can be contained in one file. Note that the conversion program rounds the output times to the nearest 15 minutes. This is required because when MM5 is run on a multiprocessor system, output times may differ be a few minutes for each output cycle.

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Meteorology / Convert to ARL / MCIP IOAPI

This menu calls a utility program to convert meteorological data files created by MCIP for the CMAQ model. The data files follow a specific naming convention and may contain multiple variables and time periods. They are in the IOAPI format. The conversion program is currently only available on UNIX or LINUX systems and will convert all the required fields in one pass for all available time periods. The data from multiple input files, say each file contains one day, may be appended automatically by setting the append file name to a non-null string. If there are time period overlaps between input files, it is best not to append them, but to select multiple input files when running HYSPLIT.

There are three required MCIP input meteorological data files: METCRO3D_, METDOT3D_, METCRO2D_, and one file, GRIDDOT2D_ that gives the grid information. All data values are interpolated to the dot grid. In the GUI, only one input file needs to be selected and the conversion program uses the file suffix and the standard naming convention to determine the names of the other files to open. Due to file name character length restrictions, the directory information is removed and all the input files should be in the local working directory.

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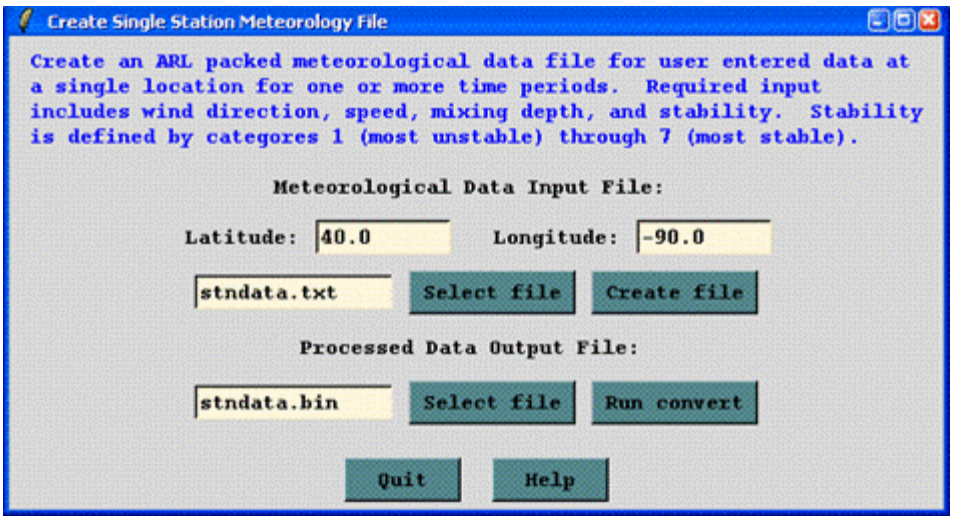
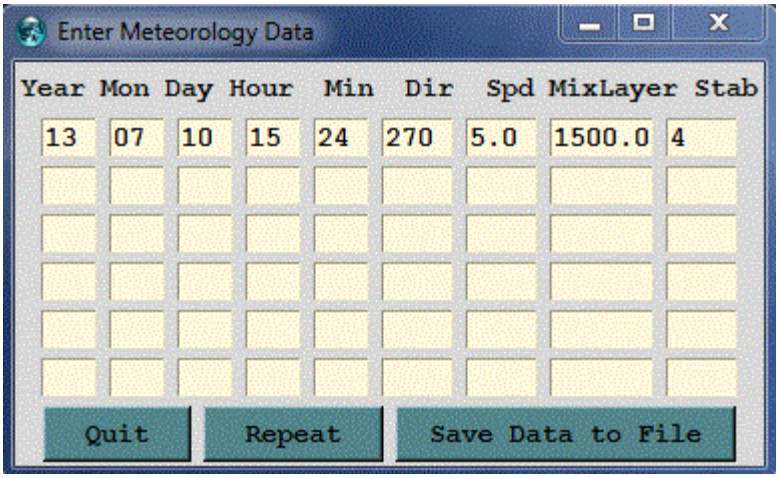
Meteorology / Convert to ARL / User entered

This menu tab is intended to convert user entered meteorological data to the ARL packed HYSPLIT compatible format. The conversion program will create a data file with one or more time periods containing a uniform field in space and height but varying in time. The grid is centered over the location specified in the main menu and covers a 250 by 250 km domain at a horizontal resolution of 10 km. It is intended to be used for very short-range simulations. The main menu permits the selection of an existing text input file (space delimited format), or the creation of a file through the menu shown below. After the meteorological data have been entered and saved to a file, the conversion program is run from the "Run convert" menu button.



The data entry widget contains five time fields and four data fields. The output file time interval is computed automatically from the input data. No interpolation is performed and the input data nearest in time to the output time are used for the conversion. The maximum output interval is one hour. Note that the date-time field defaults to the current system clock time. The meteorological variables are wind direction, speed (m/s), mixed layer depth (m), and Pasquill stability category (1=A to 7=G). After filling in the data for the first line, use the *Repeat* button the fill the remaining table entries and then edit the time and data fileds as required.



The conversion program computes the component turbulent velocity variances based upon the stability category and wind speed and assumes those values are constant with height within the mixed layer. Above the mixed layer top the variances are set to the model's minimum value. Using these data for input the model should be configured in the Advanced menu to use the variances for the dispersion. Otherwise the diffusion calculation will default to the "deformation" method and with a spatially constant wind field; the dispersion will always be at its minimum value.

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Meteorology / Display Data / Check File

The program called through this menu is used to show the details of the meteorological data file contained in the index record as well as a listing of the header portion (first 50 bytes) of each data record. The output is written to a text file called chkfile.txt. More detailed information about the structure of a meteorological data file is available. The check file program uses the same library routines as HYSPLIT. Therefore if this program does not work with the meteorological data file, neither will HYSPLIT.

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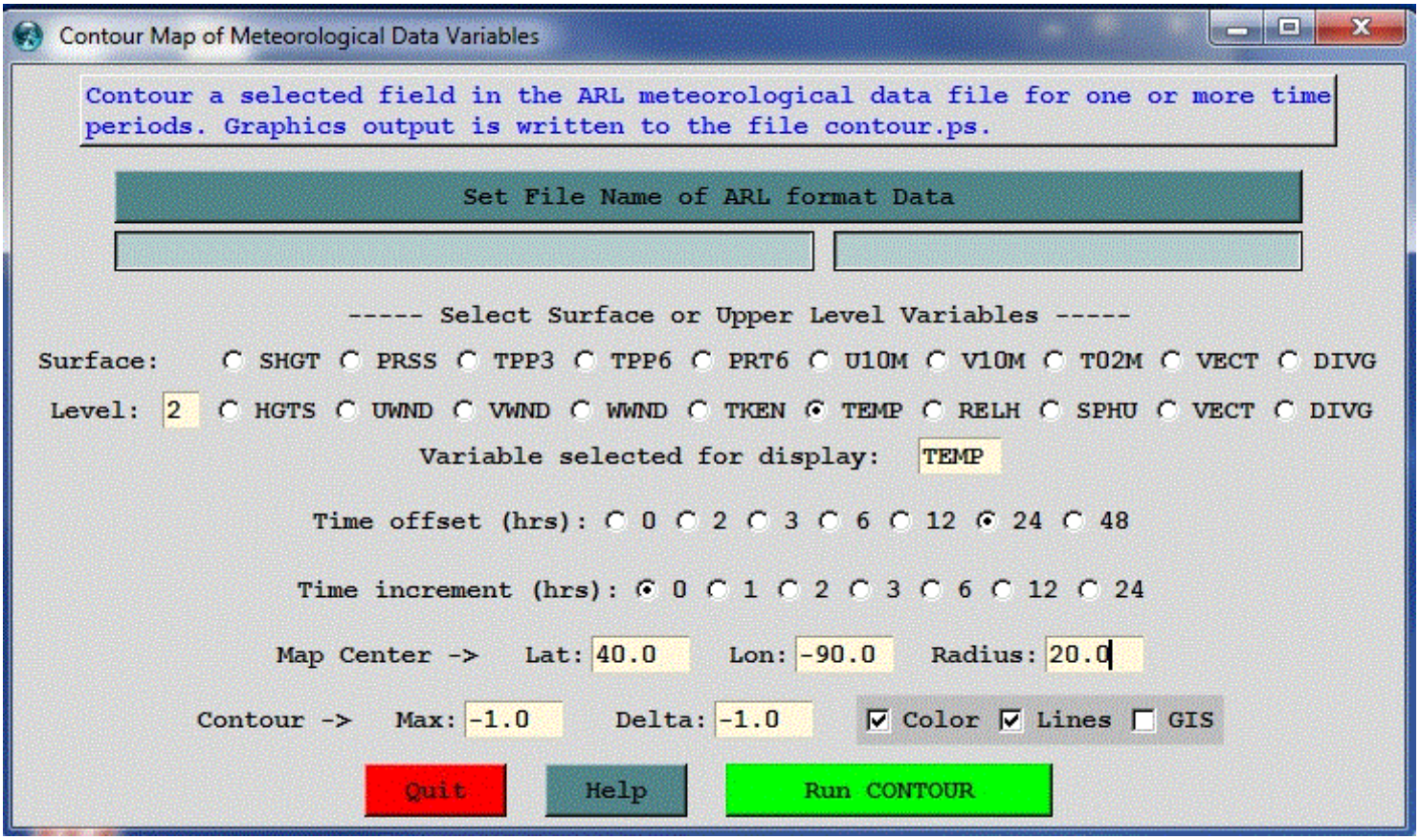
Meteorology / Display data / Contour Map

The contour display program, run from this menu, provides a simple tool to create a contour map for any variable at any time period in any ARL packed format meteorological data file. A simple configuration is available through the menu shown below. More options are available if the program is run through the command line.



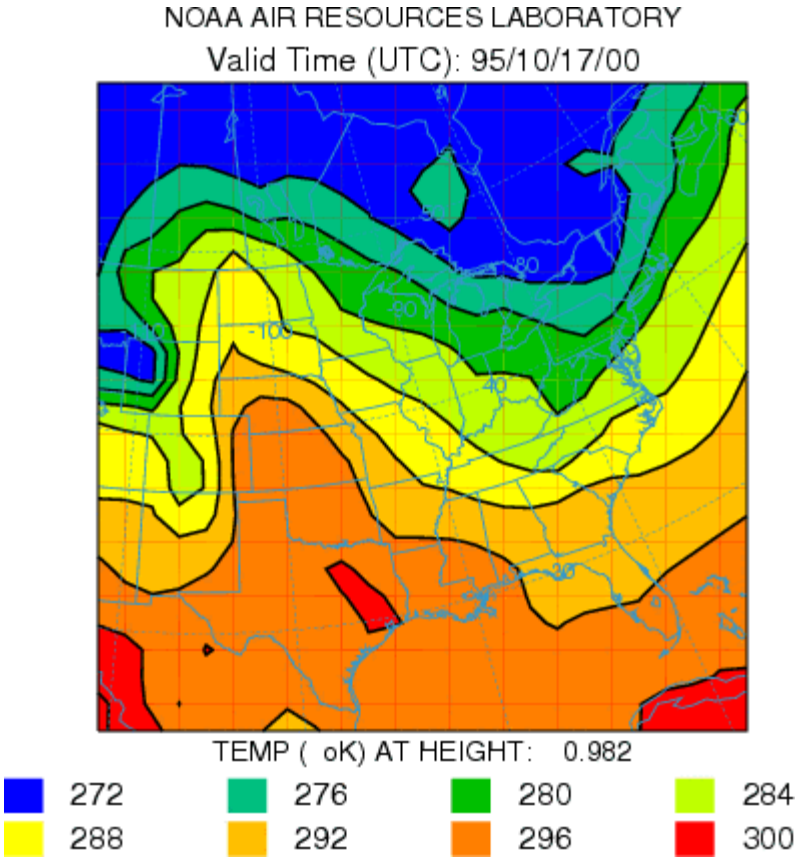
In the example shown above, the sample meteorological data file has been selected to display the temperature (TEMP) variable on model level #2. The time period to be shown is offset 24 hours from the first time period in the file. No additional time periods are shown when the increment is set to zero. The map will be centered about 40N 90W with a radius of 20 degrees latitude. The maximum contour value and the temperature difference (Delta) between contours will be determined automatically (-1.0). The radiobuttton default is to draw contour lines on top of the color fill.

For a latitude-longitude grid, the full grid cannot be plotted. Instead a sub-grid not centered at 0 deg latitude, 0 deg longitude must be set.

There are two additional derived display options available. Selecting the variable "VECT" will produce a wind vector plot and selecting "DIVG" will produce a plot of the wind field divergence. Both of these options require the U and V velocity fields at the selected level in the order of U followed by V.

The radio buttons show only the most common set of variables found in the meteorological data files. The menu does not know which variables are available in the selected file. The check file program can be used to examine the variables contained in each file. The variable selected for display using the radio-button may be superseded by replacing the text entry with the desired variable identification.

The output file *contour.ps* is created in Postscript format. It is shown below, as displayed by the Ghostscript viewer, and may be converted to GIF through the Convert Postscript menu tab.



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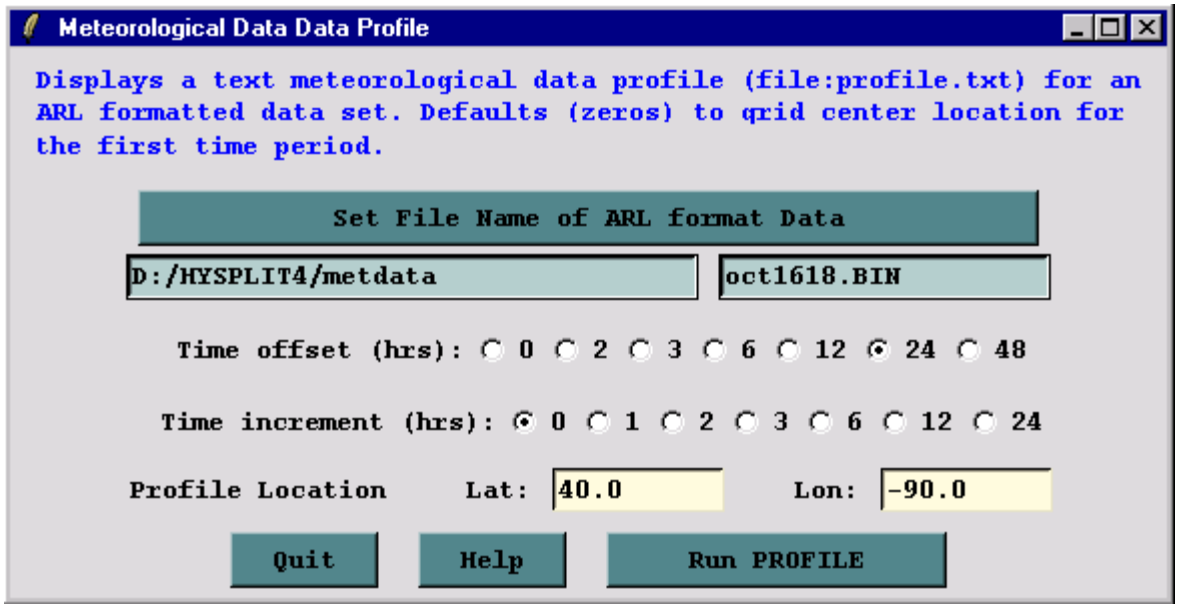
Meteorology / Display Data / Text Profile

The profile program is used to create a profile at a specific location of the meteorological variables in an ARL format packed data file. Output is written to the ASCII text file *profile.txt*. Note that the program does not interpolate to the selected point, but processes the data at the grid point nearest to the location selected. In the example shown below the sample meteorological data file has been selected to display the profile at 40N 90W. The time period to be shown is offset 24 hours from the first time period in the file. No additional time periods are shown when the increment is set to zero.



The output is written to a file called *profile.txt* and the following would be shown in the GUI's display window. The U & V wind components shown on the left side are relative to the grid, while those on the right side are with respect to north-south and east-west. They would be the same for a latitude-longitude grid.

```
METEOROLOGICAL PROFILE LISTING ...
 Meteorological Profile: oct1618.BIN
 File start time : 95 10 16  0  0
 File ending time: 95 10 18  0  0


 Profile Time:  95 10 17  0  0
 Profile Location:   40.00 -90.00  ( 21, 13)

        TPPT  EXCO  HFLX  PRSS  ICWT  SNOW  SHGT  MXLR  WFLX  CPPT  MSLP
          mm                hPa
   998     0  1E-3  -5.6   998     0     0   184  1.00  1E-6     0  1020

        UWND  VWND  WWND  SPHU  TEMP                          TPOT  UWND  VWND
         m/s   m/s  mb/h  g/kg    oC                            oK  W->E  S->N
   981  -1.5   5.0  -2.3   3.9  16.3                         291.1  -0.2   5.3
   942 -0.42   5.1 -0.19   3.8  13.3                         291.5   0.9   5.1
   895   2.3   4.4   1.6   2.8  10.6                         292.9   3.3   3.6
   842   6.7   1.7   1.4   2.7  10.6                         298.0   6.9  -0.1
   784  11.9  -1.5  0.15   4.3   8.4                         301.9  11.1  -4.5
   720  16.2  -5.7     0   4.8   5.6                         306.2  14.2  -9.7
   652  16.2  -8.8   2.5   3.1  0.77                         309.6  13.4 -12.7
   581  14.9  -8.3   4.3   1.5  -5.9                         312.2  12.2 -11.9
   508  16.3  -7.7   2.4  0.63 -13.2                         315.5  13.7 -11.6
   433  21.3  -6.2  -4.2  0.20 -20.0                         321.5  21.3  -6.2
```

Exit

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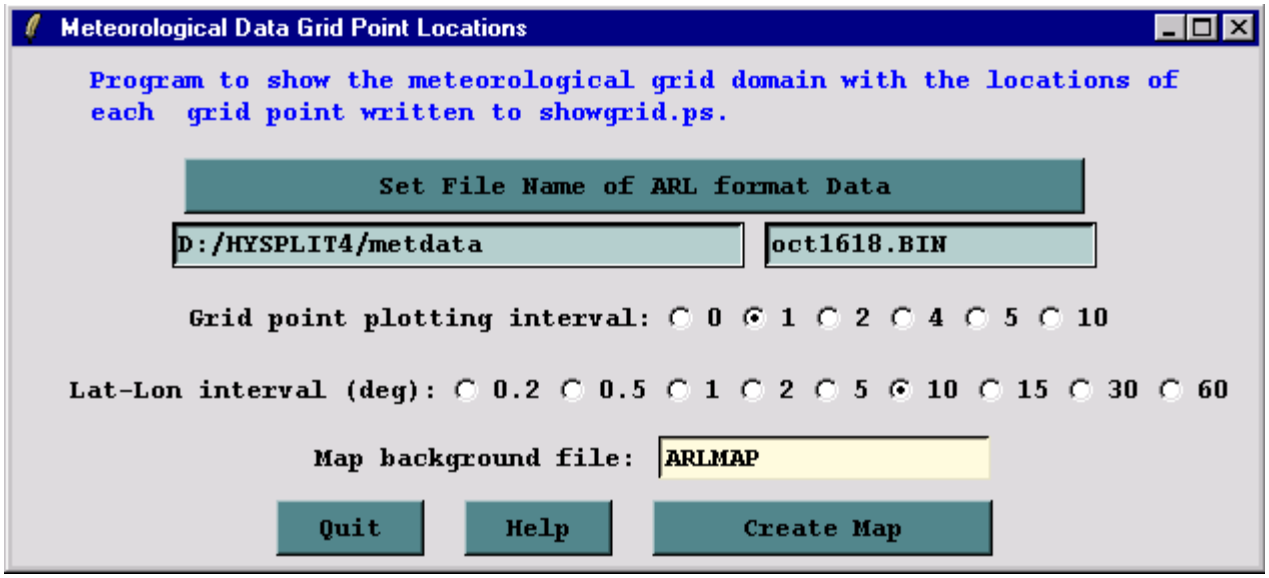
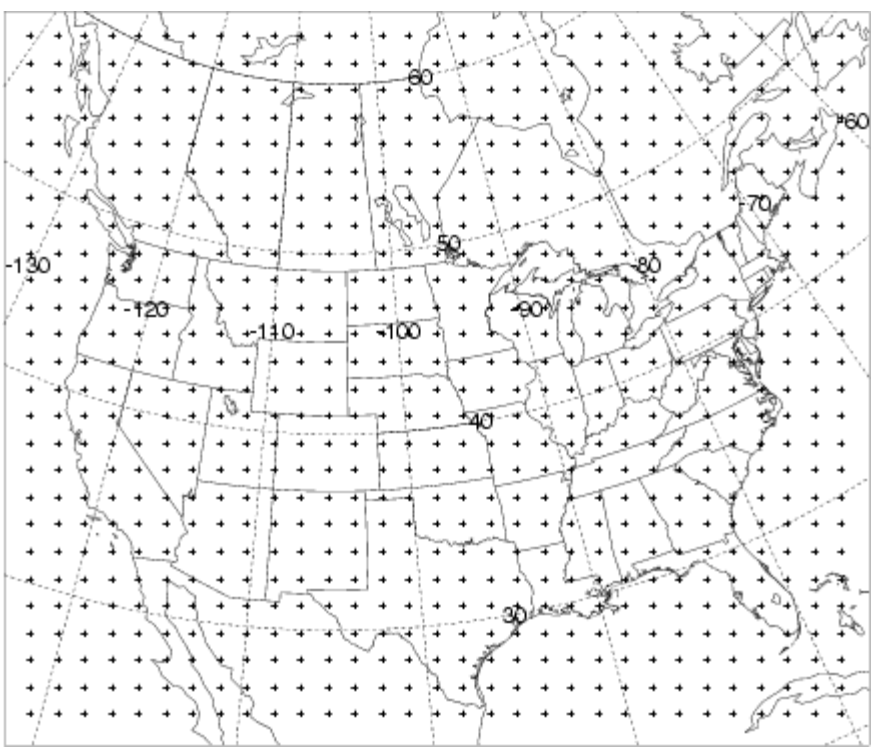
Meteorology / Display Data / Grid Domain

The *showgrid* program is used to show the domain of the ARL packed format meteorological grid file. Output is to a Postscript file and contains a plus symbol at every grid point intersection as selected by the integer plotting increment. A non-zero value for the Lat-Lon interval draws latitude-longitude lines at that interval over the map background. The example below is shown for the sample meteorological data file.



The following graphic is produced:



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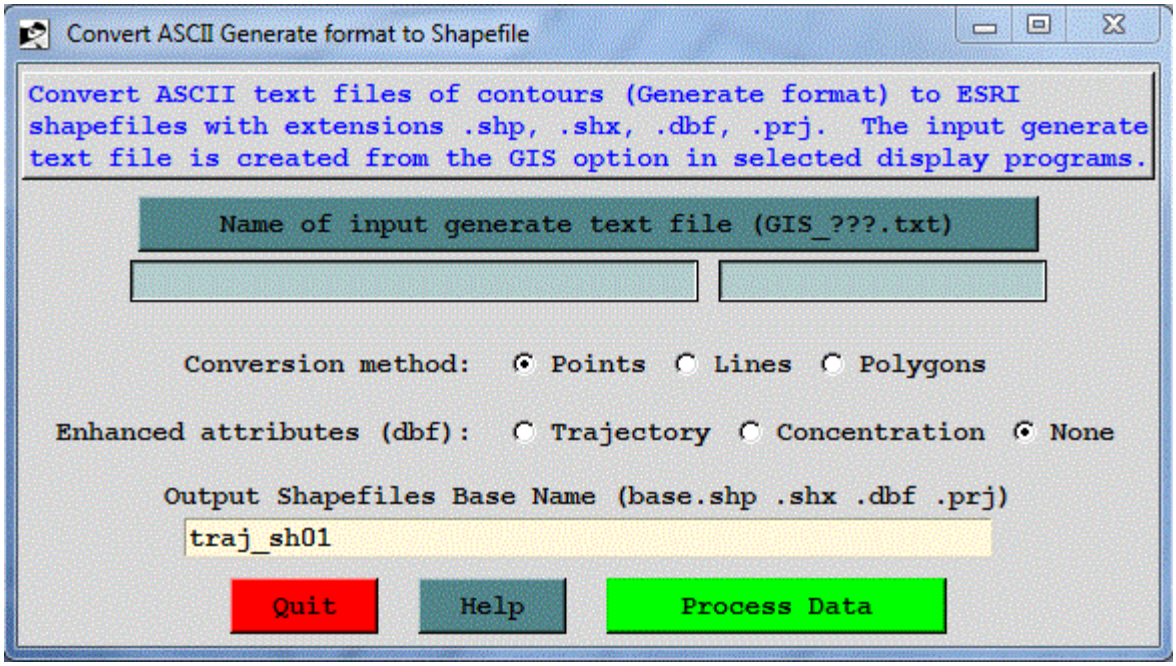
Meteorology / Utilities / GIS to Shapefile

A utility tab is provided in the meteorology, trajectory, and concentration menus that will convert an ESRI generate format text file to a Shapefile for import into ArcView or comparable GIS applications. The "ascii2shp" conversion software is available under the GNU license from the Free Software foundation. The conversion can be run from the command line or the GUI menu shown below.



Normally the fields will be blank when the menu is first invoked. Prior to creating the shapefiles it is necessary to create the "*Generate*" text file which contains the latitude-longitude points of each contour as created by the contouring programs available through the display menus. Checking the GIS box in the menu (-a1 option on the command line) creates these files. All generate format files start with *GIS* and end with *.txt*. The remainder of the file name depends upon the application from which it was created. However in all applications, the two-digit string prior to the *.txt* identifies the frame number. There is one GIS output file per frame. Use the upper browse button to set the generate format input file name.

The generate files can be converted to shapefiles consisting of points or lines (for trajectories), and lines or polygons (for concentrations). Polygons are closed lines. A polygon that runs off the map display is becomes a line and may not be displayed correctly if treated as a polygon.

Normally the *base.dbf* file will contain only the minimum amount of information. However, the trajectory and concentration plotting programs automatically create an enhanced attributes file (GIS_???.att). To add this information to *base.dbf*, check one of the enhanced attributes options.

In the lower text entry box enter the base name of the output shapefiles. All output files will be created in the working directory. Note that depending upon the upper level menu from which the conversion was called, the shapefile conversion will be either for lines (meteorology), points (trajectory), or polygons (concentration), although the option can be superseded by the checkbox selection.

What is a Shapefile?

The Shapefile format is a working and interchange format promulgated by ESRI for simple vector data with attributes. It is apparently the only file format that can be edited in ARCView 2/3, and can also be exported and imported in Arc/Info. An excellent white paper on the shapefile format is available from ESRI, but it is .pdf format, so you will need Adobe Acrobat to browse it. The file format actually consists of four files.

- XXX.shp - holds the actual vertices.
- XXX.shx - hold index data pointing to the structures in the .shp file.
- XXX.dbf - holds the attributes in xBase (dBase) format.
- XXX.prj - holds the projection information.

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Meteorology / Utilities / Convert Postscript

A utility tab is provided in the meteorology, trajectory, and concentration menu's that will convert the Postscript graphic to another format. The menu shows the name of the last Postscript file that was created. If that is not the file desired, it should be replaced with the appropriate file name. All output files are assumed to reside in the working directory and therefore a file from any menu can be converted from any of the conversion menu tabs. The file suffix represents the conversion format. The slider bar determines the size of the output graphic in pixels per inch. The default value of 70 will produce an output frame of comparable size to the input graphic. The checkboxes permit the creation of a multiframe animation in one file or multiple output files if the "Frames" option has been checked. The "Crop" option eliminates the white space around the graphic. However, the crop option may produce inconsistent results when used in conjunction with the animation feature.

The conversion process uses Ghostscript to read the Postscript file and ImageMagick to convert that file to a variety of other supported graphical formats. These programs can be stand-alone, but they have been linked through the Tcl/Tk GUI menu. Conversion to GIF is the default. Proper installation of all the previously mentioned 3rd party software is critical in the correct operation of the conversion process. This software is included with the HYSPLIT trial version but not with the registered installation executable. Links to these programs are also available through the HYSPLIT utilities web page.

If non-default directories were selected during the installation of *Ghostscript* and *ImageMagick*, it may be necessary to manually edit directory locations. The directory pointers can be changed from the "Advanced-Configuration-Directories" menu tab, which modifies the file default_exec. In the rare situation when this file cannot be edited or does not exist because the GUI did not load because of problems with Tcl/Tk, then the appropriate lines in the upper-level Tcl/Tk file ..*guicode\hysplit4.tcl* need to be changed. For instance, the lines that might require editing would be similar to the following:

```
set magick_dir "c:/Program Files (x86)/ImageMagick-6.4.4-Q8/convert.exe"
set gsc_dir "c:/Program Files (x86)/gs/gs8.63/bin/gswin32.exe"
set gsv_dir "c:/Program Files/Ghostgum/gsview/gsview32.exe"
```

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Meteorology / Help / ARL Data Format

The following sections describe the ARL packed data format in a little more detail to permit the development of customized applications. Library routines are provided to simplify the task of creating a model compatible data file. A meteorological data file is composed of one or more time periods. Each time period begins with one or more ASCII index records that summarize the valid time, the grid definition, the variables, and level information. Each subsequent record contains one horizontal data field, consisting of 50 ASCII bytes of time, variable, and level information for that record, followed by X times Y bytes of data, where X and Y are the number of data points in the horizontal and vertical directions, respectively. Floating point or integer data are packed as one byte per variable. Precision is maintained by packing the differences between adjacent grid points rather than packing the absolute values. In any time period, although not required, the surface data precede the upper-level data fields. All records are of the same length to permit the model to read the file in a "direct access" mode. Data files can be read on most computing platforms without any transformation and appended to each other using routine operating system commands such as "cat" or "type". Only binary transfers or copies are permitted. All the routines discussed in this section can be found in the *source* directory.

Valid Meteorological Data Types

Meteorological variables are identified to the model by a unique four-character identification field that is written to the first 50-byte header portion of each data record. Some of the variables that can be decoded by the model and their units are identified below.

Sample Surface Level Parameters

Description	Units	Identification
Pressure at surface	hPa	PRSS
Pressure at mean sea level	hPa	MSLP
Temperature at surface	K	TMPS
Total precipitation (6-h)	m	TPP6
U-Momentum flux	N/m^2	UMOF
V-Momentum flux	N/m^2	VMOF
Sfc sensible heat flux	W/m^2	SHTF
Latent heat flux	W/m^2	LTHF
Downward short wave flux	W/m^2	DSWF
Temperature at 2 m	K	T02M
Relative humidity at 2 m	%	RH2M
U-component of wind at 10 m	m/s	U10M
V-component of wind at 10 m	m/s	V10M
Total cloud cover	%	TCLD

Sample Upper-Level Parameters

Description	Units	Identification
U wind component (respect to grid)	m/s	UWND
V wind component (respect to grid)	m/s	VWND
Geopotential height	gpm*	HGTS
Temperature	K	TEMP
Pressure vertical velocity	hPa/s	WWND

Data may be obtained from any source, however there are certain minimum data requirements to run the model: surface pressure or terrain height, u-v wind components, temperature, and moisture. In addition, precipitation is required for wet removal calculations. Not required, but certainly necessary to improve vertical mixing calculations, would be some measure of low-level stability. This may take the form of a near-surface wind and temperature or the fluxes of heat and momentum.

It is also important to have sufficient vertical resolution in the meteorological data. Some of the NOAA higher resolution data files have five or more levels in the boundary layer (<850 hPa) in addition to wind and temperatures near the surface, usually at 2 and 10 m agl. These surface values are especially important when the data are only available on absolute pressure surfaces, rather than terrain following sigma surfaces, to avoid interpolation to the surface between data levels when the local terrain is well above sea-level.

Starting with HYSPLIT (Revision 596) the optional field DIFF is recognized as the difference between the original data and the packed data: DIFF=ORIGINAL-PACKED. The effect of this is to increase the precision of variables that have this additional field. When the DIFF field is read by HYSPLIT, the values are added to the data field resulting in values closer to the original data. Currently only DIFW and DIFR (vertical velocity and precipitation) are recognized as valid DIFF fields.

Creation of a Meteorological Input Data File

One may prepare meteorological data from any number of different sources to be in a suitable format for the model using a series of routines described in this section. In general it is assumed one has access to a meteorological data source, either the data fields are already on a grid, such as those output from a meteorological model, or perhaps from observations that have been interpolated to a grid. Some example conversion programs are provided within the GUI to convert from either NOAA or ECMWF GRIB format data files to the HYSPLIT format.

The meteorological data are processed in time-sequence, calling the subroutines provided, to create a HYSPLIT compatible output file. These subroutines will pack the data and write the index record. The index record, which precedes the data records for each time period, can only be written after the data records are processed. The packing routines must first be initialized by setting the appropriate grid parameters and defining all the meteorological variables that will be written to the file. Multiple output grids may be defined and written simultaneously by invoking the *PAKSET* routine with a different unit number for each grid. The grid parameters are all defined in a configuration file, which should be in the directory from which the procedure is invoked:

CALL PAKSET (kunit,fname,krec,nx,ny,nz)

Kunit is the Fortran unit number to which the data records will be written. *Fname* is the character string of the name of the configuration file. It can be any name, but it will default to *metdata.cfg*. The file is opened internally on *kunit* to read the configuration file. This routine needs to be called once for each grid. *Krec* is the starting record number (of the index record) to which output will be written. It is normally set to 1 unless you want to start writing in the middle of a

file. The remaining parameters (*nx, ny, nz*) are returned by the subroutine and define the horizontal and vertical grid dimensions. These values can be used to set variable dimensions. It is your responsibility to open *kunit* for output after having completed the *pakset* calls:

*OPEN(file=myfile, unit=kunit, form='unformatted', access='direct', recl={50+nx*ny})*

The individual data records are packed and written by a call to *PAKREC*, once for each variable at each level. The routine calculates the record offset from the index record according to the variable and level information provided in the arguments and writes the record according to the order specified in *metdata.cfg*. The data can be supplied in any order. Note that although the level indicator (LL) goes from 1 to the number of levels, one is subtracted before it is written to the 50 byte header to be consistent with the definition of surface data to be at level "0". All the records in a time period may be initialized according to the value of the *kini* flag. Initialization fills in the time variable for all records and assigns the variable identification field as *null*.

CALL PAKREC (kunit,rvar,cvar,nx,ny,nxy,kvar,iy,im,id,ih,mn,ic,ll,kini)

kunit - integer unit number of the defined file
rvar - input array of real*4 data values
cvar - character*1 array of packed data values
nx,ny - integer horizontal grid dimensions
nxy - integer product nx*ny and length of cvar
kvar - character*4 descriptor of variable being written
iy,im - integer year and month
id,ih - integer day and hour
mn - integer minutes (usually 0)
ic - integer forecast hour (hours from initialization)
ll - integer level indicator (1 to NZ)
kini - integer initialization flag (0-no; 1-yes)

When all the data records for a time period have been written, it is necessary to close that time period by writing its index record:

CALL PAKNDX(kunit)

At this point your program can return to *PAKREC* if data records for additional time periods are to be added to the file.

The key to the process is creating the proper configuration file for the data set you want to create. Some of the sample data decoders provided dynamically configure the packing configuration file based upon the command line input information. A sample *metdata.cfg* file for NOAA's global model output is shown below. An extract of the global one-degree latitude-longitude GRIB model data have been interpolated to a 100 km resolution Lambert Conformal projection 100x100 point grid centered about 45N 90W. The configuration file format is such that the first 20 characters are a dummy identification field followed by the data.

Example Meteorological Packing Configuration File

<u>Col 1 (A20) .... Col 21 (A4,2I4,12F10,3I4)</u>
Data Source..... GFSX
Grid Number..... 99
Z-Coordinate..... 2
Pole Latitude..... 45.0
Pole Longitude..... -90.0
Reference Latitude. 45.0
Reference Longitude -90.0
Reference grid size 100.0
Orientation..... 0.0

```
Tangent Latitude... 45.0
Synch point X...... 50.5
Synch point Y...... 50.5
Synch Latitude..... 45.0
Synch Longitude.... -90.0
Reserved........... 0.0
Number X points.... 100
Number Y points.... 100
Number of Levels... 16

Format: F6.,I3,(1X,A4)

Level 01:.0000 6 PRSS MSLP TPP6 U10M V10M T02M
Level 02:1000. 6 HGTS TEMP UWND VWND WWND RELH
Level 03: 975. 6 HGTS TEMP UWND VWND WWND RELH
Level 04: 950. 6 HGTS TEMP UWND VWND WWND RELH
Level 05: 925. 6 HGTS TEMP UWND VWND WWND RELH
Level 06: 900. 6 HGTS TEMP UWND VWND WWND RELH
Level 07: 850. 6 HGTS TEMP UWND VWND WWND RELH
Level 08: 800. 6 HGTS TEMP UWND VWND WWND RELH
Level 09: 750. 6 HGTS TEMP UWND VWND WWND RELH
Level 10: 700. 6 HGTS TEMP UWND VWND WWND RELH
Level 11: 600. 6 HGTS TEMP UWND VWND WWND RELH
Level 12: 500. 6 HGTS TEMP UWND VWND WWND RELH
Level 13: 400. 6 HGTS TEMP UWND VWND WWND RELH
Level 14: 300. 6 HGTS TEMP UWND VWND WWND RELH
Level 15: 200. 6 HGTS TEMP UWND VWND WWND RELH
Level 16: 100. 6 HGTS TEMP UWND VWND WWND RELH
```

It is important that the information contained in this file is correct because it not only controls the writing of the packed meteorological data file, but much of the information is written into the index record of each time period. The model decodes this information to set up the internal processing of the meteorological data. Starting with HYSPLIT V4.5, the model is also capable of using meteorological data on a latitude-longitude grid. Previous versions were limited to data on a conformal map projection. Data on a regular latitude-longitude grid still need to be converted to the ARL packed format. Modifications to the packing configuration file required to support a latitude-longitude grid are noted below. A complete description of *metdata.cfg* format follows:

Description of the Meteorological Packing Configuration File

Record 1 consists of a four-character string that identifies the source of the meteorological data. This string will be passed through to many of the output graphics.

Record 2 is an optional integer identification of the meteorological data grid. It was used extensively in previous meteorological data file formats. It is not used in Hysplit4 applications.

Record 3 is an integer number that identifies the vertical coordinate system. Only four coordinate types are recognized: 1-pressure sigma; 2-pressure absolute; 3-terrain sigma; 4-hybrid sigma.

Records 4 & 5 identifies the pole position of the grid projection. Most projections will either be defined at +90 or -90 depending upon the hemisphere. The longitude would be the point 180 degrees from which the projection is cut. Lat-Lon Grids only: contains the latitude and longitude of the grid point with the maximum grid point value. Note that lat-lon grids grids should be defined with reference to the dateline.

Records 6 & 7 is the reference position at which the grid spacing is defined. Lat-Lon Grids only: contains the grid spacing in degrees latitude and longitude.

Record 8 is the grid spacing in km at the reference position. Lat-Lon Grids only: a value of zero signals that the grid is a lat-lon grid.

Record 9 is the grid orientation or the angle at the reference point made by the y-axis and the local direction of north. Lat-Lon Grids only: value always = 0.

Record 10 is the angle between the axis and the surface of the cone. For regular projections it is equal to the latitude at which the grid is tangent to the earth's surface. A polar stereo-graphic grid would be tangent at either 90 or -90, while a Mercator projection is tangent at 0 latitude. A Lambert Conformal projection would be in between the two limits. An oblique stereo-graphic projection would have a cone angle of 90. Lat-Lon Grids only: value always = 0

Records 11 & 12 are used to equate a position on the grid with a position on the earth as given in the following two records:

Records 13 & 14. In this example, the position indicated is the center of the grid located over the North Pole. Any position is acceptable. It need not even be on the grid. Lat-Lon Grids only: contains the latitude and longitude of the 1,1 position grid point.

Record 15 is not currently used.

Records 16 & 17 identify the number of grid points in each direction.

Record 18 is the number of levels in the vertical, including the surface level.

Record 19, through the number of levels, identifies the height of each level in appropriate units according the definition of the vertical coordinate, the number of variables at that level, and the four character identification string for each variable. The height units are as follows for each coordinate:

1-sigma (fraction)
2-pressure (mb)
3-terrain (fraction)
4-hybrid (mb: offset.fraction)

Decoding Meteorological Data Files

One may want to develop other applications for HYSPLIT compatible meteorological data files. For these situations, some lower-level routines are provided in the source code library. The key to reading the meteorological files is decoding the index record. The format for this record is given below. Complete descriptions are similar to the variables in the discussion above.

FORMAT DESCRIPTION

- (A4) Data Source
- (I3) Forecast hour (>99 the header forecast hr = 99)
- (I2) Minutes associated with data time
- (12F7) 1- Pole Lat, 2- Pole Lon, 3- Tangent Lat, 4- Tangent Lon, 5- Grid Size, 6- Orientation, 7- Cone Angle, 8- Xsynch point, 9- Ysynch point, 10- Synch point lat, 11- Synch point long, 12) Reserved
- (3I3) 1) Number x points, 2) Number y points, 3) Number levels
- (I2) Vertical coordinate system flag
- (I4) Length in bytes of the index record, excluding the first 50 bytes

LOOP through the number of data levels

- (F6) height of the first level

(I2) number of variables at that level

LOOP through the number of variables

- (A4) variable identification
- (I3) rotating checksum of the packed data
- (1X) Reserved space for future use

Once the index record has been read and decoded you have sufficient information to read and decode the data records. A data un-packer is provided to convert the packed character*1 array to a real*4 array. It can also be used to extract a sub-grid from the full domain through specification of the sub-grid lower left corner:

CALL PAKINP (rvar,cvar,nx,ny,nx0,ny0,lx,ly,prec,nexp,var1,ksum)

rvar - real output array of integer dimensions lx,ly
cvar - character*1 packed input array of length nx*ny
nx,ny- integer dimensions of the full grid
nx0 - integer sub-grid position of left edge in nx units
ny0 - integer sub-grid position of lower edge in ny units
lx - integer first dimension of sub-grid length
ly - integer second dimension of sub-grid length
prec - real precision of packed data array
nexp - integer scaling exponent of packed data array
var1 - real value of array at position (1,1)
ksum - integer rotating checksum of packed data array

If the entire grid is to be unpacked then *nx0=ny0=1* and *nx=lx*, *ny=ly*. The checksum (*ksum*) that is returned should be compared with the corresponding value in a table generated from reading the index record. If you are not going to compare the checksum, set *ksum = -1*, this will save a little computer time. Due to the sub-grid option the checksum cannot be computed in the regular unpacking loop, but requires a second pass through the data. The checksum pass is enabled when *ksum=0*. It will then return a non-zero value. If you don't reset it to zero, no further checksums will be computed.

If you want to create your own packed data by converting a real*4 array to the character*1 packed data array use the following:

CALL PAKOUT(rvar,cvar,nx,ny,nxy,prec,nexp,var1,ksum)

Although the structure of the packed data may seem complex, unpacking is a very simple process, the basic elements of which are summarized in the Fortran code shown below. The value of each element is the sum of the initial value and the difference stored in that element location.

```
SUBROUTINE UNPACK(CPACK,RVAR,NX,NY,NXY,NEXP,VAR1)

      CHARACTER*1 CPACK(NXY)
      REAL*4 RVAR(NX,NY)
      SCALE=2.0**(7-NEXP)
      VOLD=VAR1
      INDX=0
      DO J=1,NY
      DO I=1,NX
      INDX=INDX+1
      RVAR(I,J)=(ICHAR(CPACK(INDX))-127.)/SCALE+VOLD
      VOLD=RVAR(I,J)
      END DO
```

```
VOLD=RVAR(1,J)
END DO
RETURN
```

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Trajectory / Help

The trajectory menu tab is composed of five main sections: setting up the simulation, executing the model, displaying the trajectory, converting the graphic to other formats, and running special simulations. The model is configured and executed through the menu and results displayed. However for experienced users, each component could be run independently from the command line and the CONTROL file could be created using any text editor.

In the Trajectory Setup menu the entire purpose of the GUI is to configure the model's input *CONTROL* file. This is a text file that configures the simulation parameters. Once the input parameters are set to their desired value, the model is executed from the Run Model menu tab. When complete, the output window is closed and the Trajectory Display menu is used to draw and display the trajectory from the endpoints output file. The Special Runs menu is used to configure several different customized simultaneous multiple trajectory simulations.

For inexperienced users, a review of the Quick Start Help is highly suggested, which goes through the trajectory computation step-by-step using the example meteorological data file.

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Trajectory / Quick Start Help

After the initial installation, the model will be configured to run the example case discussed in more detail below. The "Quick Start" menu tab can be used to run any simulation in one-step. The last configuration will be used for the simulation. The "Quick Start" menu brings up a global map with the current source location shown as a blue dot. A "right-click" of the mouse button will write that source location to the control file, click **Yes** to exit the window, which will close the map, run the model simulation, create the output file, and display the graphics. A "left-click" of the mouse button will set a new source location. A "left-click-hold-drag-release" will define a new "zoomed" domain and the map will be redrawn. An "exit" from the window's menu bar will close the map without updating the control file or running the model. For more detailed simulation configurations, follow the steps below.

The easiest way to run the model is to use the GUI menu to create the model's input *CONTROL* file. For the purposes of this demonstration appropriate meteorological files are provided. If for some reason the menu system is not available, perhaps because Tcl/Tk was not installed, the Control file can be created manually

Step 1 - start the GUI menu system using *\working\hysplit4.tcl* or the desktop shortcut to *Hysplit4*. A widget will appear with the *HYSPLIT* graphic and three button options: *Menu, Help* and *Exit*.**Click on *Menu* tab.**

Step 2 - The four main menus of the Hysplit4 GUI will appear: Meteorology, Trajectory, Concentration, and Advanced. An additional small widget underneath the main menu gives the current Hysplit4 version information. Do not delete this widget as it will terminate the GUI. It provides the reference frame for the model's standard output and messages. **Click on the *Trajectory* tab**.

Step 3 - Five options appear under this item: Setup Run, Run Model, Display, Utilities, and Special Runs. Normally these are run in sequence, however any item can be selected and run if the appropriate input files were created during a previous simulation. **Click on the *Setup* tab**.

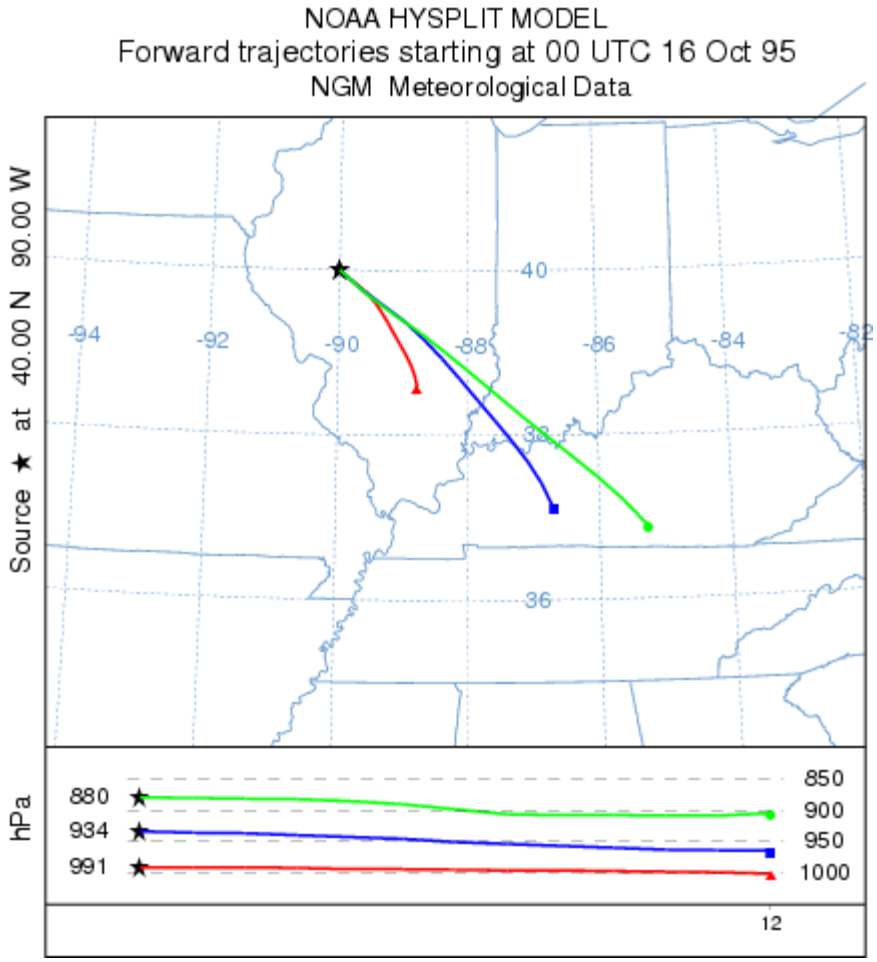
Step 4 - *Setup Run* is used to enter the basic model simulation parameters: the starting time of the calculation; starting location in terms of latitude, longitude, and height; the run-time or duration of the trajectory calculation; and the names and locations of all required files. When modifications to this menu are complete, click on *Save*. However for this example, you will use the Retrieve option for predefined configurations, so do nothing here and **go on to Step 5**.

Step 5 - The example calculation is configured by **clicking on *Retrieve*** and then ***entering the text: sample_traj***, which is the name of the example simulation control file that was created for this demonstration. Then **click on *OK*. A**fter the data entry widget is closed, **click on *Save*** and the setup menu will close.

Step 6 - Click on **Run Model**, which first copies the setup configuration (default_traj) saved in the previous step, to the model's input *CONTROL* file. The model calculation is then started. A series of messages will appear on standard output text window showing the progress of the calculation. When the simulation is completed, the trajectory end-points output file is ready to be converted for graphical display. Under some operating systems, the standard output widget will not show any output until the end of the calculation and the *Trajectory* menu items will be locked until the calculation completes.

After completion **click on Exit** to close the window.

Step 7 - Selecting Display will run a special program that converts the text file of trajectory end-point positions into a high quality Postscript file (*trajplot.ps*) suitable for printing. The conversion widget provides options for the frequency of the labels on the trajectory, a variable zoom factor, and color or black and white graphics options. If the Postscript viewer (Ghostscript) has been installed and associated with the .ps file suffix, then it will be invoked by the GUI. If the viewer does not automatically open, it may be necessary to manually edit *../guicode/hysplit4.tcl* to change the directory location associated with the program *gsview32.exe*. After **clicking on Execute Display**, the following graphic will appear in the *Ghostview* window:



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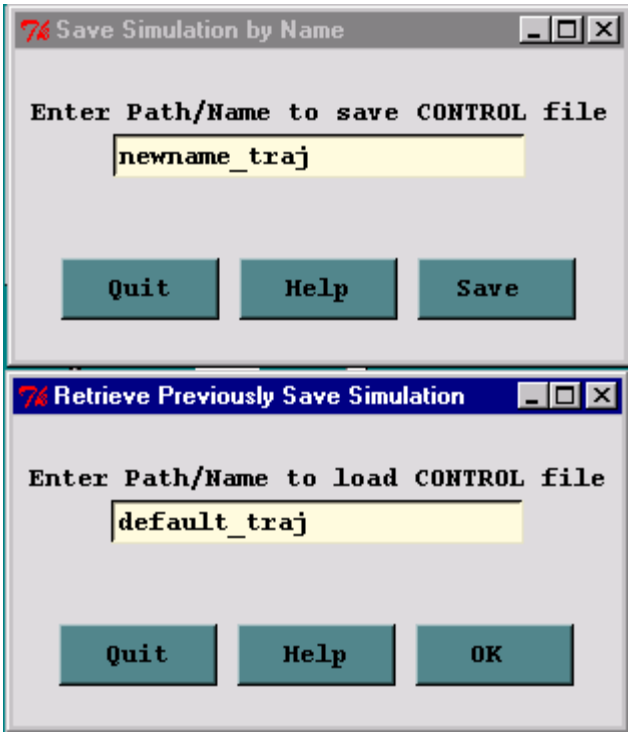
Trajectory / Saving and Retrieving

The trajectory and concentration setup menus for the *CONTROL* file permit a *Save As* or *Retrieve* option. Each of these menus is shown in the panel below. After a simulation has been configured, run, displayed, and assuming that the results are satisfactory and no more changes are required, then go back to the setup menu tab and *Save As* the control file by giving it a unique name, such as *newname_traj* in the example below. There are no restrictions on the naming convention. If the simulation is to be rerun, perhaps with some minor variation, the *Retrieve* option is used to load those values back into the setup menu.



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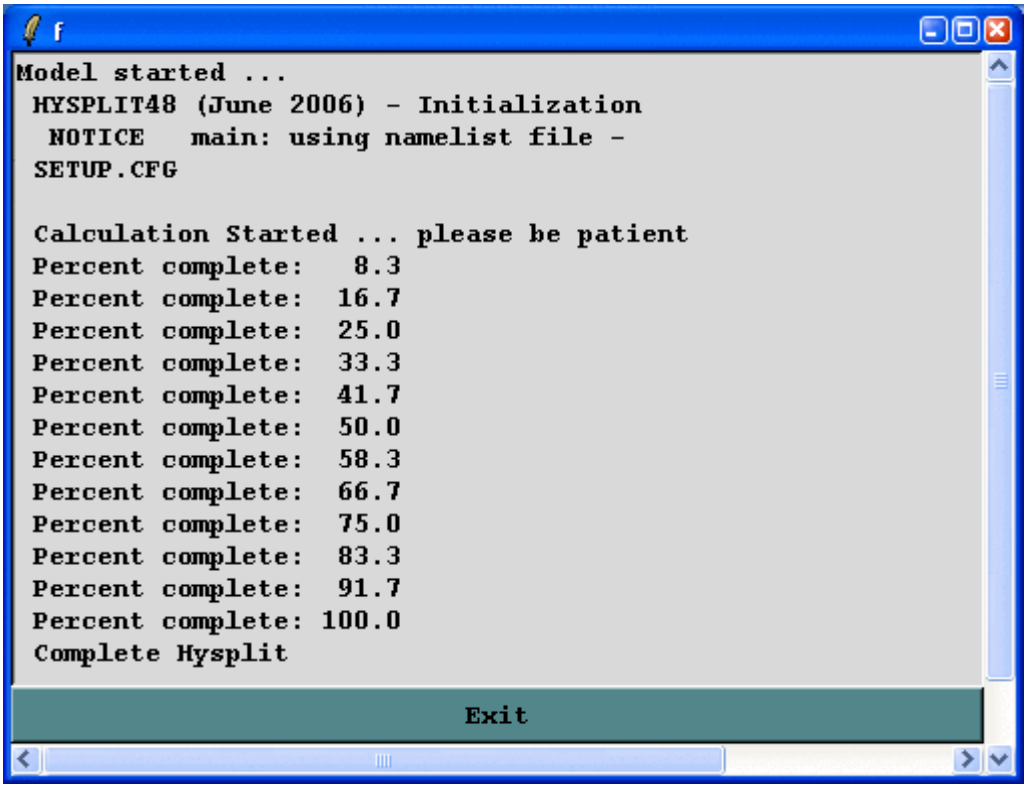
Trajectory / Run Model

Once the Trajectory Setup menu has been closed with the *Save* button, the changes to the simulation parameters are copied to *default_traj*. Clicking on the *Run Model* menu tab first copies *default_traj* to *CONTROL* and then runs the trajectory model executable, *hyts_std{.exe}*. The executable, by default, attempts to open a file named *CONTROL* to read all the required input parameters. If not found, the model will prompt to standard output for values from standard input. This condition should not occur running the model through the GUI. When the model execution starts, output messages are written to a special window, an example of which is shown in the illustration below:



Successful completion of a simulation will show a similar message. Additional run-time diagnostic messages and other error messages are always written to a file called *MESSAGE*. This file may be viewed through one of the Advanced Menu tabs. Depending upon the nature of the error message, perhaps a failure in the model initialization process, error messages may also appear in above window. Once the model has completed, **press Exit** to close the window.

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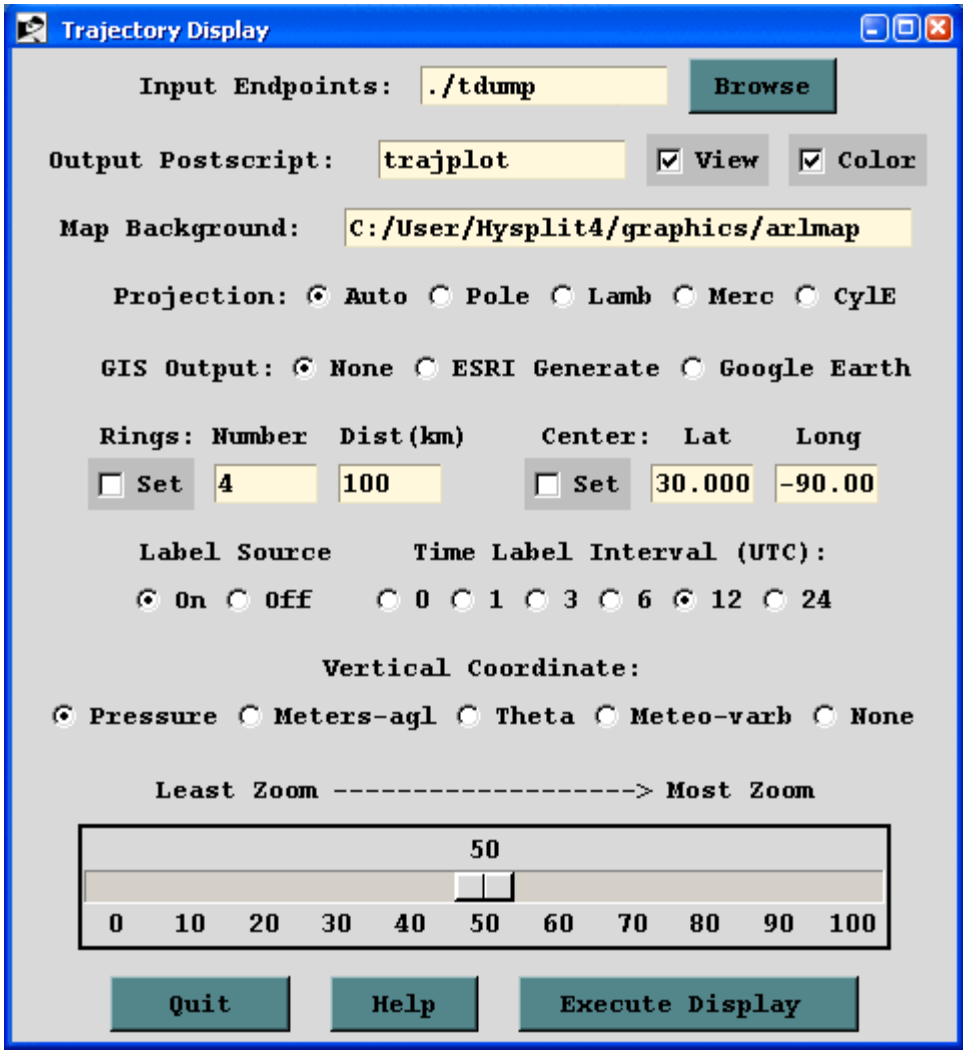
Trajectory / Display / Trajectory

The trajectory model generates a text output file of end-point positions. The end-point position file is processed by *trajplot* to produce the Postscript display file. *Trajplot* can be accessed through the GUI or run directly from the command line. The display program has a variety of command line options, most of which are available through the GUI. There is a one-to-one relationship between GUI options, an example of which is shown below, and the command line options. There are several features particular to the GUI. First the *Trajectory Display* menu will not open unless the *Trajectory Setup* menu was first opened and *Saved*. This procedure sets all the GUI parameters to their *default_traj* values. These are the values shown in the *Display* menu. Normally the map projection is computed automatically based upon the location and length of the trajectory. However some trajectory combinations may give no maps or improperly scaled maps. In these situations one would want to over-ride the default projection and try forcing a selection.



Trajplot Command Line Options

The Postscript conversion program *trajplot* reads the trajectory endpoints output file, calculates the most optimum map for display, and creates the output file - *trajplot.ps*. When executed from the command line, there are several Unix style command line options. There should be no space between the option and any arguments: trajplot -[options (default)]

-a[GIS Output: 0-none, 1-ESRI Generate, 3-Google Earth]

Selecting the ESRI Generate format output creates an ASCII text file for each output time period that consists of

the value and latitude-longitude points along each trajectory. This file can be converted to an ESRI Shapefile or converted for other GIS applications through the utility menu "GIS to Shapefile. The view checkbox would be disabled to do just the GIS conversion without opening the Postscript viewer. Selecting Google Earth will create a compressed file (*.kmz) for use in **Google Earth**; a free software package to display geo-referenced information in 3-dimensions. You must have the free **Info-Zip** file compression software installed to compress the Google Earth file and associated graphics.

-e[End hour to plot: #, (all hours)]

-f[Frames: (0)-all frames in one file 1-one frame per file]

= 0 - all files plotted on one frame
= 1 - one input file per output frame

-g [Circle overlay: ( )-auto, #circ (4), #circ:dist(km)]

= {blank} - draws four distance rings about source point, automatically scaled
= {#} - draws the indicated number of rings about the source point
= {#1}:{#2} - draws the number {#1} of rings about the source point each {#2} kilometers apart. In the special case where #1 is zero, the rings are not drawn, but the size of the plot is scaled as if one ring of radius {#2} is to be drawn.

-h [Hold map at center lat-lon: (source point), lat:lon]

= latitude:longitude - forces the map center to be at the selected location instead of the source point. In conjunction with the -g0:{km} option it is possible to create a constant map projection for each execution.

-i[Input files: name1+name2+name3+... or +listfile or (tdump)]

= tdump - default file name when the -i option is undefined.
= {user defined file name}
= {name1+name2+...} - to overlay multiple tdump files on the same plot based upon file name1 plot limits.
= +filename - filename is a file of filenames to be plotted following the same convention as the previous argument (limit <=5000 files).

-j[Map background file: (arlmap) or shapefiles.(txt|suffix)]

= arlmap - default ASCII file
= shapefiles.(txt|suffix) - file of shapefile names

-k[Kolor: 0-B&W (1)-Color, N:colortraj#1,...colortraj#N]

= 0 - for black and white output
= 1 - for color differentiation of multiple trajectories
= N - 1=red,2=blue,3=green,4=cyan,5=magenta,6=yellow,7=olive

-l[Label interval: -12, -6, 0, (6), 12, ... hrs]

= 0 - for no labels along the trajectory
= 6 - for labels every 6 hours
= 12 - for labels every 12 hours
= {X} - positive at synoptic times
= {-X} - negative with respect to traj start

-L[LatLonLineLabels]

= 0 - none
= 1 - auto
= 2:tenths - at interval specified

-m[Map projection: (0)-auto 1-polar 2-lambert 3-mercator 4-CylEqu]

-o[Output file name: (trajplot.ps)]

= trajplot.ps is the default Postscript output file name, otherwise it may be {user defined}.

-p[Process file name suffix: (ps) or process ID}

-s[Symbol at trajectory origin: 0-no (1)-yes]

-v[Vertical: 0-pressure (1)-agl 2-isentropic 3-meteorology 4-none]

= 0 - The vertical trajectory plot coordinate is in hPa (absolute pressure units).
= 1 - The vertical trajectory plot coordinate is meters above ground level.
= 2 - An isentropic coordinate display requires the trajectory to have been run in those coordinates.
= 3 - Forces the display of one of the selected meteorological variables along the trajectory rather than a trajectory vertical position coordinate. The meteorological variable is selected in the "Trajectory" tab of the Advanced Configuration menu. Only one meteorological variable can be selected for display. If multiple variables are selected, then only the last variable will be plotted.
= 4 - No vertical projection drawn.

-z[Zoom factor: 0-least zoom, (50), 100-most zoom]

= 50 - for standard resolution maps.
= 100 - for high resolution maps (maximum zoom)

Additional Map Label Customization

Many of the Postscript graphics programs have label information that can be customized to some extent. This is accomplished by placing a file called *Labels.cfg* in the startup directory which contains the following valid entries (all in single quotes terminated by &) replacing the new string with the desired text. A sample file called *Labels.bak* may be found in the relevant directory. Not all label strings are valid with every plotting program. For instance with *trajplot*, only the title entry would be used to replace the top label line of the plot.

'TITLE&','NATIONAL WEATHER SERVICE&'
'MAPID&','PROBABILITY&'
'LAYER&','BOUNDARY LAYER AVERAGE&'
'UNITS&','BQ&'
'VOLUM&','/M3&'

Additional supplemental text may be added at the bottom of the graphic by creating a file called *MAPTEXT.CFG*, also to be located in the startup directory. This is a generic file used by all plotting programs but each program will used different lines in its display. The file can be created and edited through the Advanced menu tab.

Standard ASCII Map Background File

By default, all mapping programs use the same text map background file, *arlmap*, which normally would be located in the *../graphics* directory. However, all graphics programs first search the local start directory (*../working* if running the GUI), then the *../graphics* directory. Customized map background files can be read instead of the default file for specialized applications. Some higher resolution map background files are available from the HYSPLIT download web page. These different map files may be accessed implicitly by putting them in the "../working (the startup directory), or

explicitly through the GUI by entering the name of the customized map background file. The map background file format consists of three or more records per graphic line with the following format:

2I5 - line number, number of latitude-longitude points in the line
10F6.2 - latitude points in line
10F7.2 - longitude points in line

ESRI Shapefile Map Background Files

Another mapping option would be to specify a special pointer file (origianlly called *shapefiles.txt*, but now a suffix other than "txt" is permitted) to replace the map background file arlmap in the -j command line option (see above). Note -jshapefiles... rather than -j./shapefiles... is required. This file would contain the name of one or more shapefiles that can be used to create the map background. The line characteristics (spacing, thickness, color) can be specified for each shapefile following the format specified below:

Record format: 'file.shp' dash thick red green blue
file.shp = /dir/name of input shapefile in quotes
dash = {0} for solid; {dashes}/in; <0 color fill
thick = line thickness in inches (default = 0.0)
Red Green Blue = RGB values (0.0 0.0 0.0 is black)
Record example for default: 'arlmap.shp' 0 0.005 0.4 0.6 0.8

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Trajectory / Display / Frequency

Multiple trajectory files can be displayed by creating an arbitrary grid over the computational domain and then counting the number of trajectory intersections over each grid cell and normalizing by the total number of trajectories (or endpoints, as discussed in the following). A trajectory may intersect a grid cell once or multiple times (with residence time options 1, 2, or 3). With the default residence time (RT) option (0), the number of trajectories that intersect each grid cell are divided by the total number of trajectories. With RT=1, the number of endpoints in each grid cell are divided by the total number of trajectories (in this case, there can be values over 100%). With RT=2, the number of endpoints in each grid cell are divided by the total number of endpoints. With RT=3, the number of endpoints in each grid cell are divided by the maximum number of endpoints in any cell. Each trajectory is defined by one output file which is only permitted to contain one trajectory. Trajectory output file names begin with the base name defined in the setup menu *tdump* and are then followed by some arbitrary identification text (such as the date) that is created by the Run Daily menu option. The trajectory endpoint files should reside in the working directory. The first step in the processes is to create a file of trajectory file names which will always be called *INFILE*. The text entry box defines the trajectory base name which is treated as a wildcard string when the filenames are searched and added to the contents of *INFILE*. This file may be manually edited to remove any trajectory files that are not required for the frequency analysis. Then select the grid resolution according to the scale of the desired result. Too fine a grid with too few trajectories can result in poorly contoured display. The gridded binary output file is in the HYSPLIT concentration format. The concentration plotting routine is used to display the trajectory frequency results and hence some of the label options are inconsistent with this particular application. The trajectory frequency results could be exported to an ASCII file using one of the concentration convert utility options or displayed using one of the GIS formats.

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Trajectory / Utilities / Endpoints to IOAPI

This menu calls a utility program to convert the HYSPLIT ASCII trajectory endpoint file to the IOAPI ID_referenced data format. Multiple trajectories and meteorological data values along the trajectory are supported. The conversion program is currently only available on UNIX or LINUX systems and will convert all the endpoints for one or more trajectories in a file in one pass. The maximum number of trajectories and variables per trajectory are subject to compilation limits. The data files follow no specific naming convention and any input or output file name may be selected in the menu.

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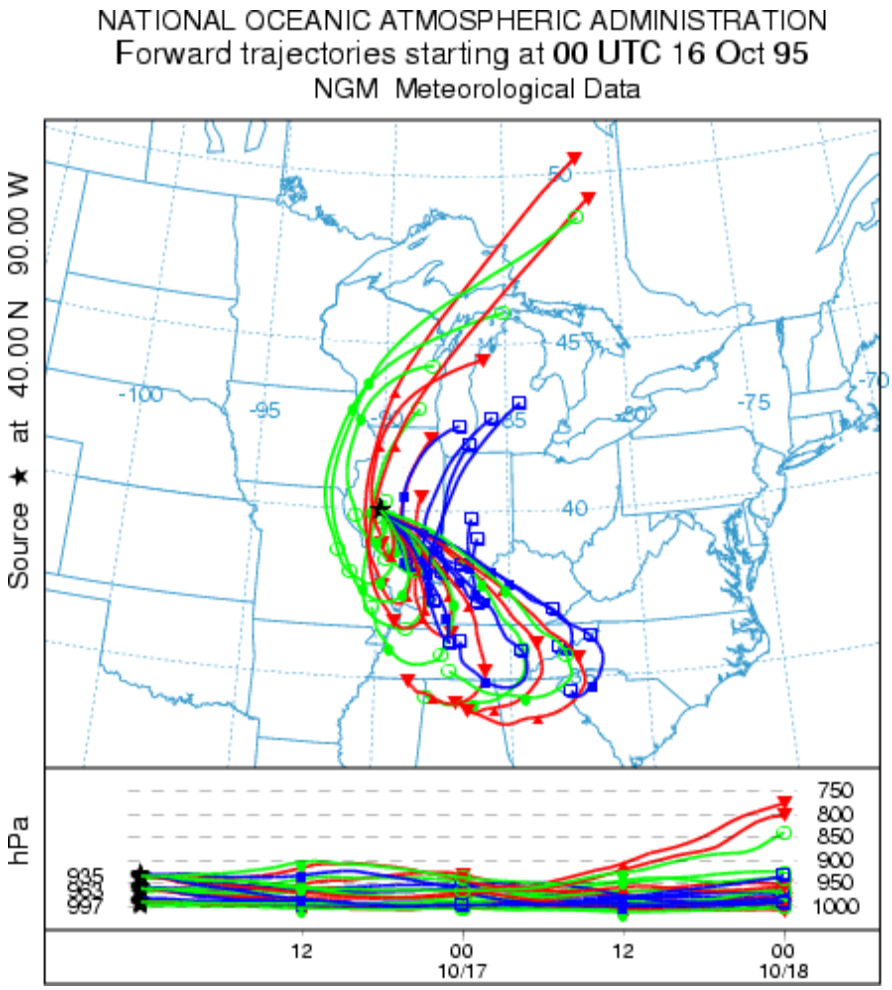
Trajectory / Special Runs

The *Special simulations* menu tab is required because certain options may require a different executable file, modifications to the Control file that are not supported by the GUI, or interactions with other items under the Advanced Menu tab. More information is provided below for each special simulation. Some *Special Simulations* may not be available for all operating systems.

Ensemble

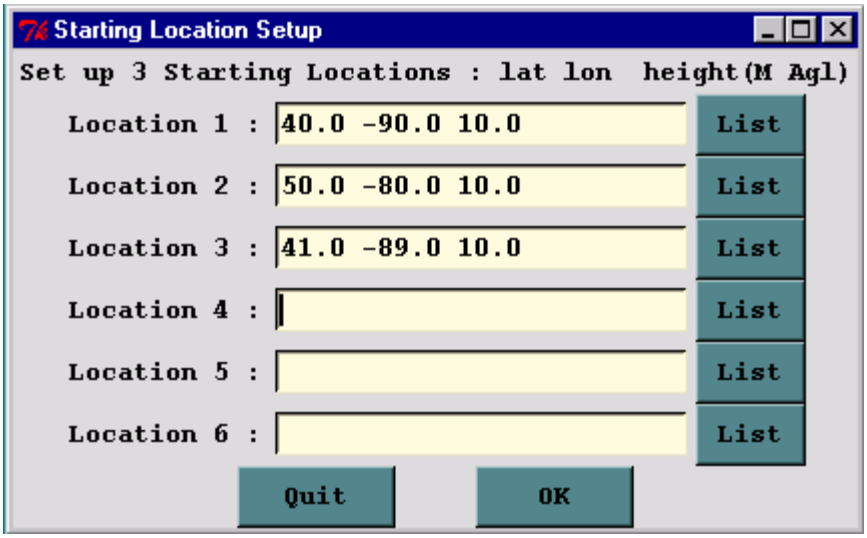
The ensemble form of the model automatically starts multiple trajectories from the selected starting point. Each member of the trajectory ensemble is calculated by offsetting the meteorological data by a fixed grid factor as defined in the Advanced Trajectory Configuration tab. The default offset is one meteorological grid point in the horizontal and 0.01 sigma units in the vertical. This results in 27 members for all-possible offsets in X, Y, and Z. After the model calculation has completed, use the normal Trajectory Display tab to view the results. Because the offset is computed in both directions in the vertical from the starting location, a starting location at the ground would not provide an optimal configuration for this type of simulation. The default vertical offset is about 250 m. Therefore this should be the minimum starting height for ensemble trajectories, unless the default offset is changed in the namelist file. An example of the ensemble trajectory using the example meteorological data is shown in the illustration below.



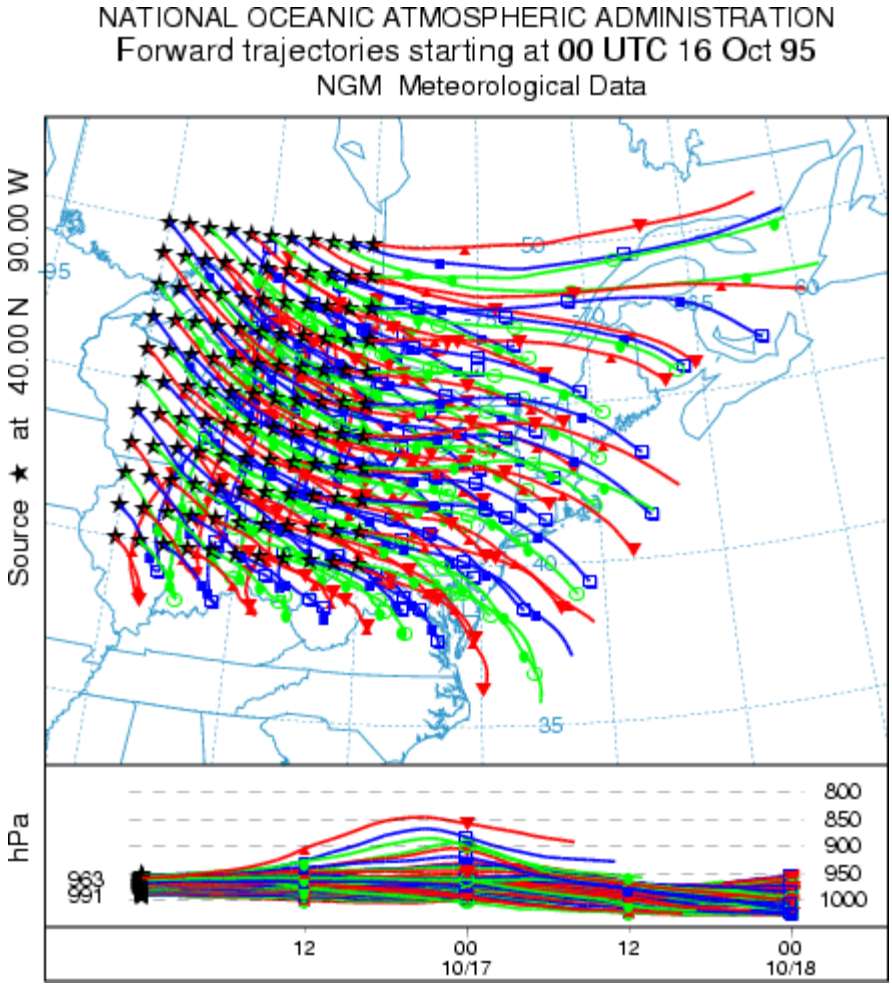
Matrix

The matrix calculation is a way to set up the *CONTROL* file for multiple starting locations that may exceed the GUI limit of 6 under the Trajectory Setup tab. Hundreds or thousands of starting points may be specified. The *Run Matrix* tab just executes the model using a *CONTROL* file that is dynamically created from the *default_traj* file using a special program called *latlon* that is called from within the GUI. The program reads a *CONTROL* file that is required to have

three starting locations and then re-writes the same file with multiple locations. The multiple starting locations are computed by the *latlon* program based upon the number of starting points that fall in the domain between starting point 1 and starting point 2. Each new location is offset by an amount equal to the difference between starting locations 1 and 3. An example would be more illustrative. If the original control file has three starting locations: #1 at 40N, 90W, #2 at 50N, 80W, and #3 at 41N, 89W; then the matrix processing results in a CONTROL file with 121 starting locations, all one degree apart, all between 40N 90W and 50N 80W.

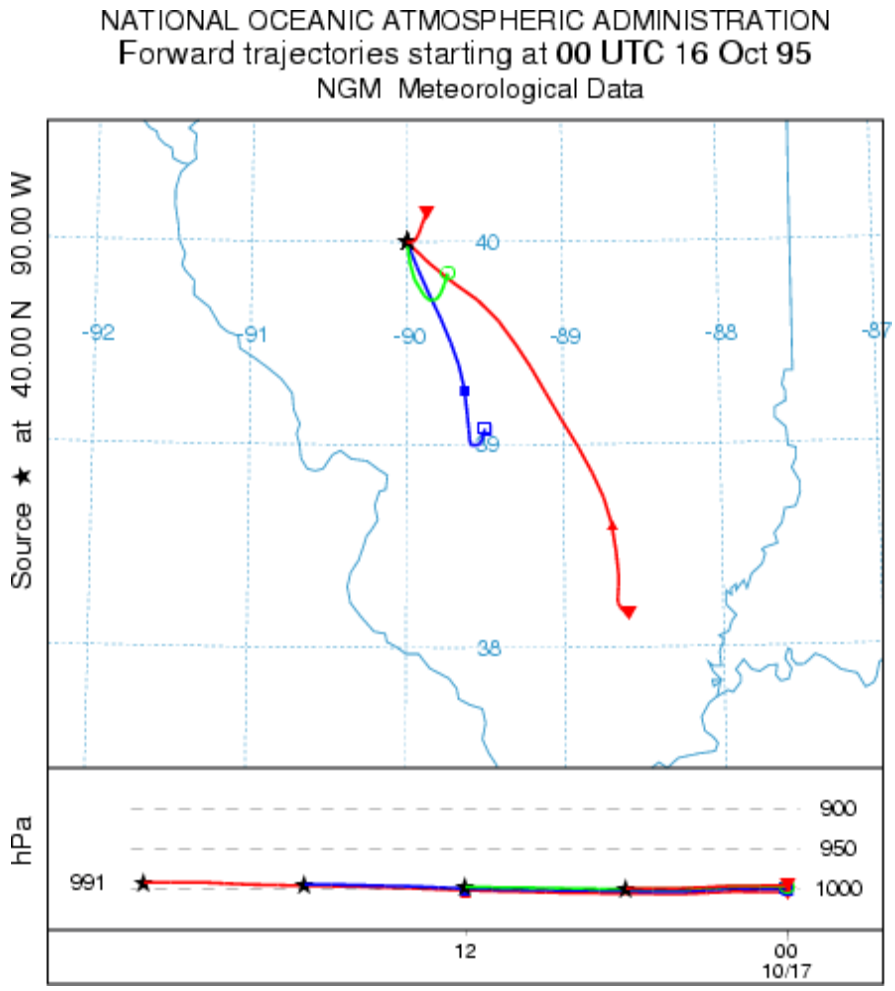


The reason for this approach is that only the *CONTROL* file is modified and not *default_traj*. The GUI never reads *CONTROL*, therefore the file does not need to conform to the GUI limits. The final matrix trajectory using the example meteorological data for this configuration is shown in the illustration below.



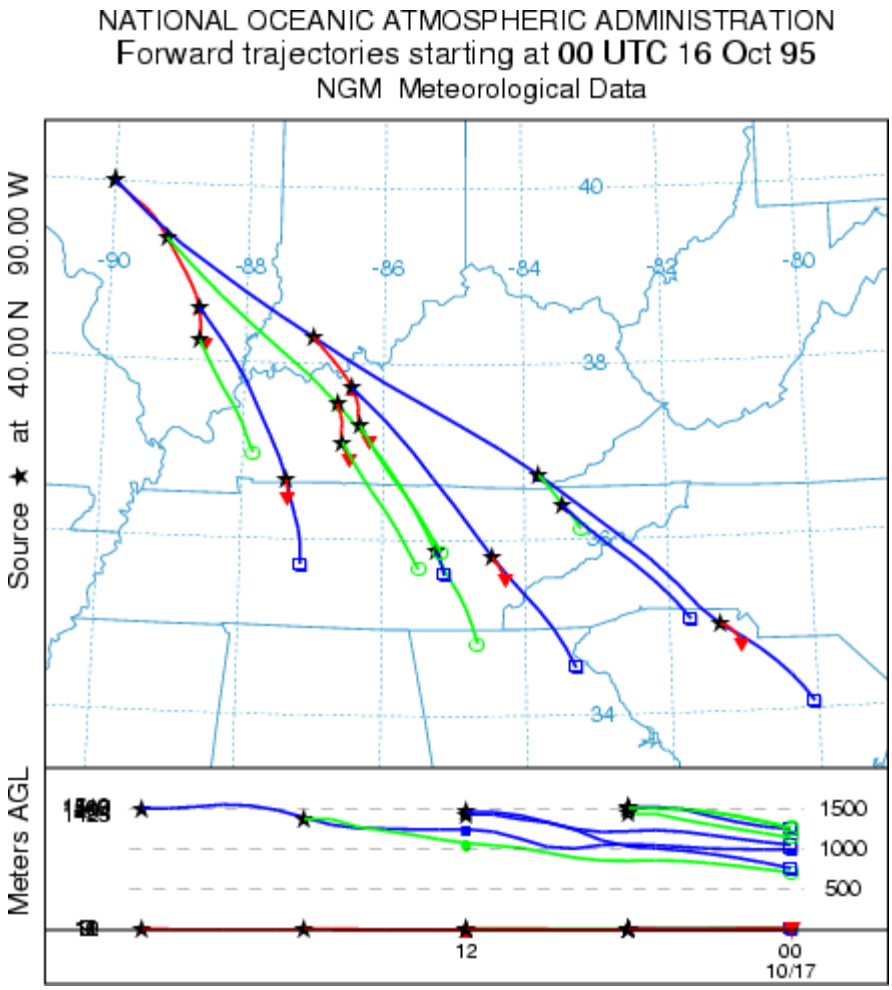
Multiple Trajectories in Time

In the normal simulation configuration, all trajectories start at time that was defined in the first line of the Trajectory Setup menu. Trajectories starting at a different time would require an independent simulation. However, there is shortcut to permit the calculation of multiple trajectories in time from the same starting location. Setup the simulation for a single trajectory then go to the Advanced Trajectory configuration menu. Under the *Temporal Trajectory Restart* line, edit the temporal interval in hours from the default of zero (no restarts) to the desired value. For example, if this value is set to 6 hours (corresponding to *NSTR=6* in the namelist file *SETUP.CFG*), then in addition to the normal trajectory that starts at the initial time, new trajectories would be started every six hours for the duration of the simulation. The result of this simulation, using the example meteorological data, is shown in the illustration below.



Multiple Trajectories in Space and Time

The standard setup options of the GUI permit the calculation of multiple trajectories in space or height by simply specifying new locations in the *CONTROL* file. A variation of that procedure was shown above with respect to setting up a matrix of starting locations. The model also permits the start of new trajectories at different locations along an existing trajectory. This can be considered a special case of multiple trajectories-in-time because when starting a new trajectory along an existing trajectory, the new starting location differs in time and space from the original trajectory. In this variation, new trajectories are started at multiple levels at the temporal restart interval. The multiple restart levels are assumed to be the same multiple starting heights specified in the original setup and therefore the number of restart heights must equal the number of starting locations. Go the Advanced Configuration menu and setup the example as in the previous case to restart trajectories every 6 hours. Then change the *Number of Levels* parameter from its default value of zero (no new trajectories) to the number of new trajectories will be started. For example, set the number of levels to 2 (sets the *NVER*=2 parameter in the *SETUP.CFG* namelist file). The number of starting locations should also be set to two, at the same location, but with release heights of 10 and 1500 m. Two trajectories, at 10 and 1500 m, will start every 6 hours. The result is shown in the illustration below.



Daily

Another way to generate multiple trajectories in time is to use the automated daily trajectory menu option to create an endpoints file for each starting time. This differs from the previous approach where all trajectory endpoints were written to one output file. Using this menu the model is executed in a script with a unique output file name for each simulation. This method is required for trajectory clustering.

Clustering

Multiple trajectories may be aggregated into groups to minimize the difference between trajectories in that group using clustering methods. The use of the clustering program requires one endpoints file for each trajectory. Normally a minimum of 30 trajectories is recommended for clustering.

Geo-Location

Multiple trajectories can be run from sampling data to determine the highest frequency of upwind directions associated with the non-zero measurements. The geo-location menu automatically configures the trajectory control file and runs the model based upon a data file of measured values such that a trajectory is started from each location every hour that there is a non-zero measurement.

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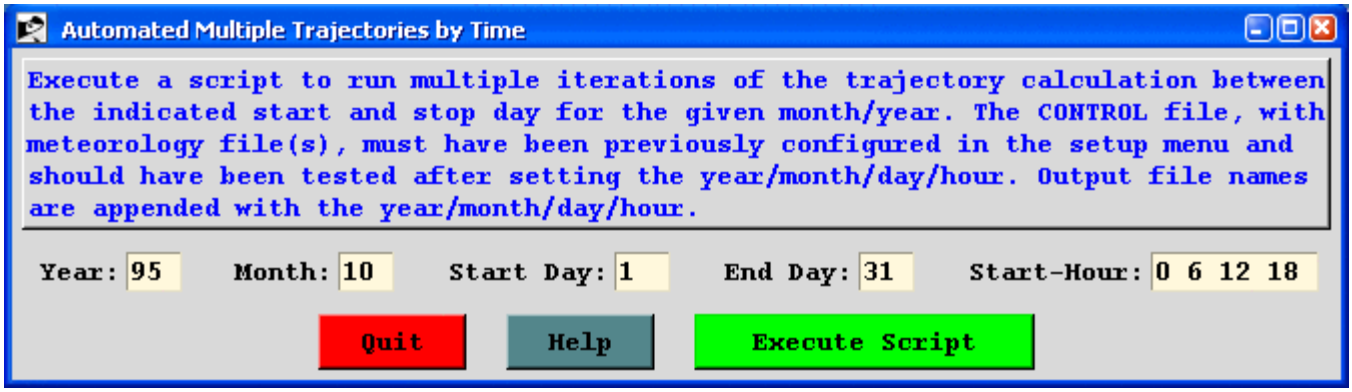
Trajectory / Special Runs / Daily

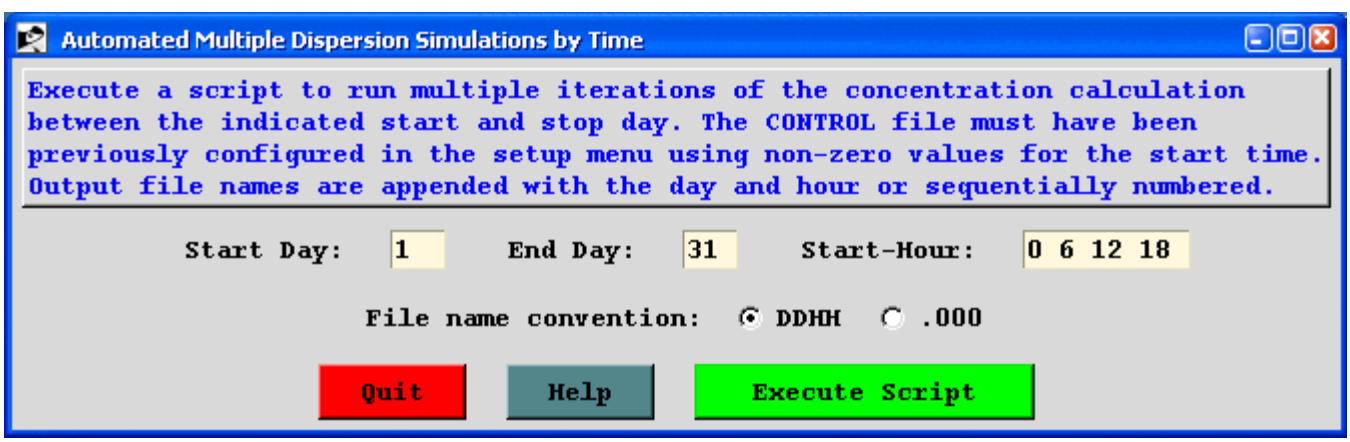
This special menu can be used for either trajectory or concentration simulations to run automated multiple simulations for one month. The script will replace the starting day and hour in the CONTROL file with values generated in the script from the menu shown below. In this example the model will be run four times a day (at 0, 6, 12, and 18 UTC) for each day from 1 through 31. Note that the start-hour field is just treated as a string and can be replaced with any sequence of starting hours. The model output files are named according to the fields set in the control file and namelist file menus, but are appended with the four digit day and hour field. This approach differs from a single simulation with multiple starting times in that each simulation is independent and a new output file is created for each run.



The model should be configured and run for the first simulation time through the standard run menu to insure that the simulation is configured correctly. If part of the simulation requires meteorological data from the previous month or the next month, these should be included in the base simulation test.

At first it will appear that after pressing the *Execute Script* button that nothing is happening. However, as each day's simulation is completed, the *Start Day* entry box increases in value until its value matches the *End Day*, at which time the script is completed. Note that concentration simulations are much slower than trajectories and it may take a while before the start day field is updated.

The dispersion daily run menu contains an additional entry shown below that determines how the file name is calculated for each run. The default approach is the same as with the trajectory calculation, where the day and hour is appended to the base name. Another option is to name the files sequentially using a three digit number. Using sequential numbering, the output files can be processed by the probability display programs used in conjunction with the ensemble calculation.



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Trajectory / Special Runs / Clustering

The *Trajectory Cluster Analysis* window has the series of tasks necessary for running a trajectory cluster analysis. This differs from most, if not all, other HYSPLIT GUI windows that only run one program or do one task. Given a set of trajectories beginning at one location, the cluster analysis will objectively result in sub-sets of trajectories, called clusters, that are each different from the other sub-sets. The program will usually produce at least one possible outcome set of clusters. If more than one outcome is given, the user must then subjectively choose one for the final result.

Description of clustering process:

Initially, total spatial variance is zero. Each trajectory is defined to be a cluster, in other words, there are N trajectories and N clusters. For the first iteration, which two clusters (trajectories) are paired? For every combination of trajectory pairs, the cluster spatial variance (SPVAR) is calculated. SPVAR is the sum of the squared distances between the endpoints of the cluster's component trajectories and the mean of the trajectories in that cluster. Then the total spatial variance (TSV), the sum of all the cluster spatial variances, is calculated. The pair of clusters combined are the ones with the lowest increase in total spatial variance. After the first iteration, the number of clusters is N-1. Clusters paired always stay together.

D = distance between a trajectory endpoint and the corresponding cluster-mean endpoint

SPVAR = SUM(all trajectories in cluster) [SUM(all trajectory endpoints) {D*D}]

TSV = SUM(all SPVAR)

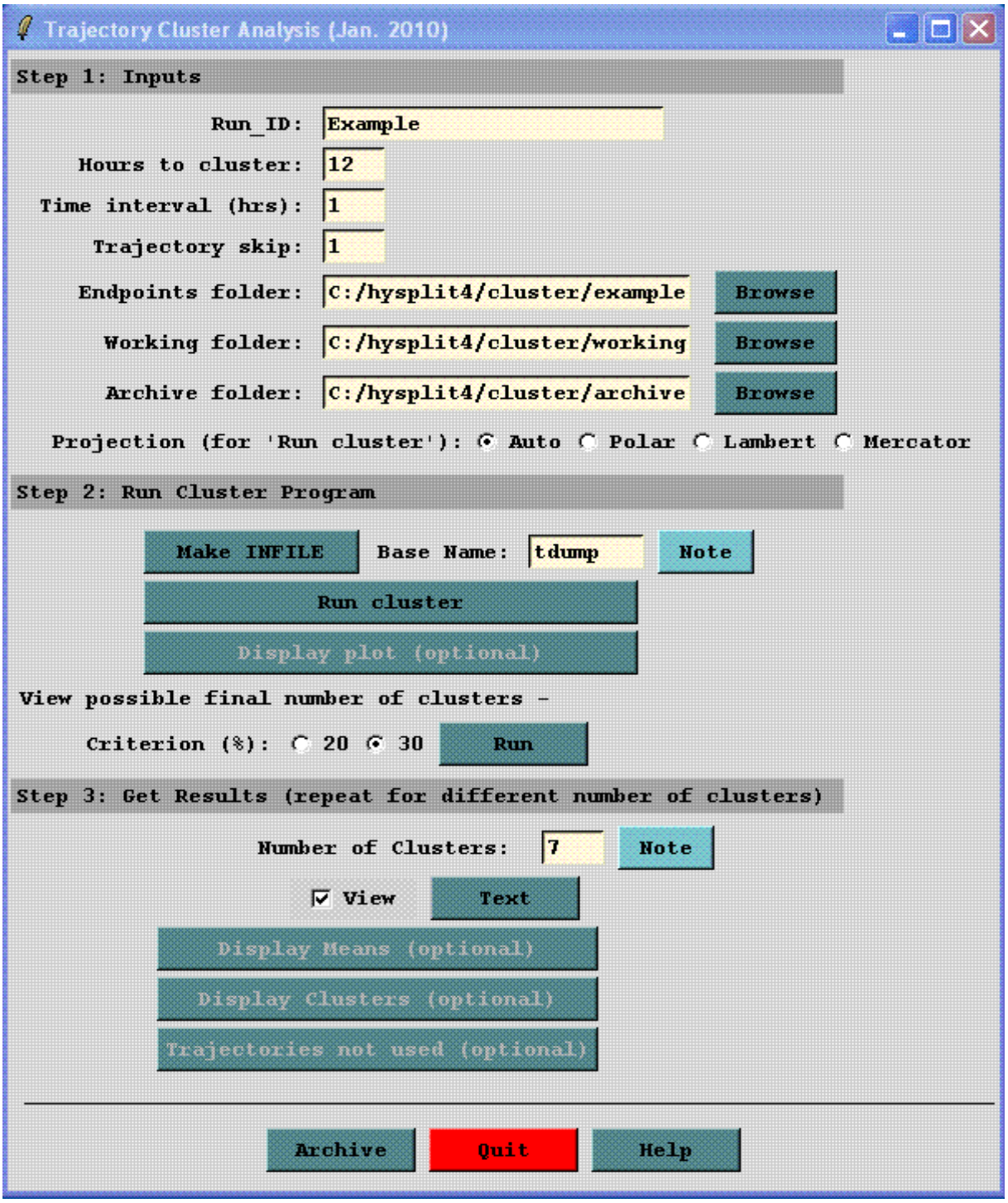
For the second iteration, which two clusters are paired? The clusters are either individual trajectories or the cluster of two trajectories that were initially paired. Again every combination is tried, and the SPVAR, and TSV for each is calculated. The two clusters combined are the ones that result in the lowest increase in TSV. The percent change in TSV and number of clusters (N-2) are written to a file.

The iterations continue until the last two clusters are combined, resulting in N trajectories in one cluster.

In the first several clustering iterations the TSV increases greatly, then for much of the clustering it typically increases at a small, generally constant rate, but at some point it again increases rapidly, indicating that the clusters being combined are not very similar. This latter increase suggests where to stop the clustering and is clearly seen in a plot of percent change in TSV vs. number of clusters, where the number of clusters are decreasing to the right on the plot. The iterative step just before (to the left of on the plot) the large increase in the change of TSV gives the final number of clusters. Typically there are a few "large" increases.

How to run the cluster analysis:

The window shown is from the *Run Example* case. For *Run Standard*, the *Run_ID* is "Standard", *Hours to cluster* is "36", the Endpoints folder (directory) is "c:/hysplit4/cluster/endpts", and the *Number of clusters* is set to "1". *Run Example* performs cluster analysis on the example set of 12-h duration forward trajectories. Note one of the trajectories has a duration less than 12 hours and so it is not clustered. The number of trajectories in the example set is small to keep the cluster section of the HYSPLIT PC package a reasonable size.



Step 1. Inputs.

Run ID - A label to identify each run. The label ends at the first blank space. The other numeric inputs may be part of the label. For instance if trajectories during 2004 from Ohio were clustered, the Run_ID could be Ohio_2004. If you used 48-h trajectories, hourly endpoints, and every other trajectory, a label of Ohio_2004_48_1_2 could be used. If you later decided to only use the first 36-h of the trajectory Ohio_2004_36_1_2 might be used.

Hours to cluster - Trajectory durations up to the given hour are used. Must be a positive number. Time is from trajectory origin whether backward or forward. Trajectories terminating before the given hour will NOT be included in the clustering. Premature terminations commonly result from missing meteorology data or the trajectory reaching the meteorological grid horizontal or top edge. 36 hours is typical.

Time interval - Identifies which endpoints along a trajectory to use. Typically every hourly endpoint is used (1). For long trajectories, skipping endpoints will save computational time.

Trajectory skip - Identifies which trajectories in a folder to use. A value of 1 means every trajectory will be used; 2 means every other trajectory; 5 every 5th trajectory, etc. Useful with very large sets of trajectories.

Endpoints folder - All trajectory endpoints files containing 'tdump' in their name in this folder will be used for clustering.

Working folder - Cluster files are written to this folder.

Archive folder - All cluster files may be moved to this folder for archiving or to remove the files from the working directory. For permanent archiving, the files need to be moved or renamed since they will be overwritten by files from subsequent runs.

Projection - Trajectory endpoint latitudes and longitudes are converted to grid points using the specified map projection in the main cluster program "Run cluster". The projection for the plots is specified separately in Step 3.

Step 2. **Run Cluster Program**. Possible solutions to the cluster analysis will be available at the end of this step.

Make INFILE. Trajectories must have been run previously, such as via *TRAJECTORY-Special Simulations – Run Daily*. All the trajectory endpoints files need to be in one folder and each must have the name “tdump” within its filename. In this step, a file, *INFILE*, listing all the “tdump” files will be created in the working folder.

Note on endpoints files - There can be only one trajectory per file. At least 16 trajectories are needed after trajectories are skipped, if specified.

Run Cluster The cluster analysis program is run here given the *INFILE* file, the trajectory endpoints files, and the above inputs. On a typical PC, a cluster run with 365 trajectories, 36-h duration, and using every hourly endpoint, will take a couple minutes. Going beyond several years of trajectories will result in a run that will take a long time and/or use much memory. A warning message is given for “larger” runs, but there can be hard to tell if a "large" job fails due to lack of memory and/or is feasible.

For example with 1100 trajectories it may appear not to be running. Try some intermediate runs - 600 trajectories, 900 trajectories - and note the run time. Add to the number of trajectories as reasonable. Let it run overnight. If it takes "too long", increase the "time interval" to say 2 to use every other trajectory endpoint and/or set the "trajectory skip" to say 3 to use every third trajectory. Another option to bypass possible GUI errors is to run cluster.exe from the command line. To do this, open the "Command Prompt" (for Windows, Start, All Programs, Accessories), cd to your cluster working directory (e.g. cd \hysplit4\cluster\working), and run \hysplit4\exec\cluster.exe. If the file with the input values CCLUSTER exists in the cluster working directory, cluster.exe will start running, otherwise you will be prompted for the input values. When done, "exit" the Command Prompt, and return to the GUI for the subsequent processing.

The cluster program produces these output files:

CLUSTER – trajectory start date/time and endpoints (tdump) filename for all the trajectories in *INFILE*; then for each pass, a listing of the trajectories in each cluster.

DELPCT – the change in total spatial variance of all the clusters from one pass to the next.

CLUSTERno – the filename and trajectory start date/time of trajectories, if any, not clustered; used to create cluster results (*CLUSLIST*)

CMESSAGE – diagnostics output file

Display plot (optional) shows the percent change in total spatial variance (TSV) for the final 30 iterations. This data is from the file *DELPCT*. Generally there can be seen at least one time when there is a large increase in the change of TSV, indicating that “different”, rather than “similar”, clusters are being paired and that the cluster process should stop before that occurs.

View possible final number of clusters. Typically a pairing of "different" clusters is indicated by a 30% change in the percent change in total spatial variance (see *Step 2, Display plot*). *Run* lists the possible final cluster numbers. If the 30% criterion does not identify any, the 20% criterion may be chosen. The maximum is arbitrarily set to 20 clusters.

Step 3 Get Results. This step may be repeated using different numbers of clusters. If you exit the GUI, but have not archived your results, enter the Run_ID and the Working folder again from Step 1, then continue with Step 3. If you have already archived the results, but want to try a different number of clusters, manually copy everything from the archive folder to the cluster working folder, enter the *Run_ID* and the Archive and working folders, then enter the number of clusters, etc.

Number of clusters Enter the final number of clusters, one of the values listed in *Step 2, Run*. In general, this will be a value where the plot from *Step 2,Display plot* shows a sharp upward turn.

Assign trajectories to clusters "Run" creates a text file listing the trajectory start date/times and filenames in each cluster (*CLUSLIST_NF*, where NF is the final number of clusters). Note Cluster #0 is for trajectories not clustered. Depending on the application, this text file may be the outcome and the plots below may not be needed.

Display Means produces one map with the mean trajectory for each cluster (1-NF), given the final number of clusters, NF. The arbitrary cluster number and percent of trajectories in each cluster are given.

Display Clusters produces one map for each cluster, showing the trajectories in each cluster.

Trajectories not used are those input to the cluster program, i.e. in the endpoints directory, and at the given skip interval, that terminate before the trajectory duration equal to the *Step 1, Hours to cluster*. This occurs when the trajectory reaches the meteorology grid edge or when there is missing meteorology. *Trajectories not used* immediately displays a plot showing the trajectories not used and opens the Trajectory Cluster Display window, from which the cluster-mean trajectories for the trajectories not used (cluster #0) and all the other clusters may be displayed. Note the plot showing the trajectories not used must have been previously created in *Step 3, Display Clusters*, though it is not displayed there.

Archive All files are moved, not copied, to the given directory. Files created in Step 3 contain the final number of clusters (NF) in their filename; hence output using various values of NF may be readily archived.

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Trajectory / Special Runs / Geo-Location

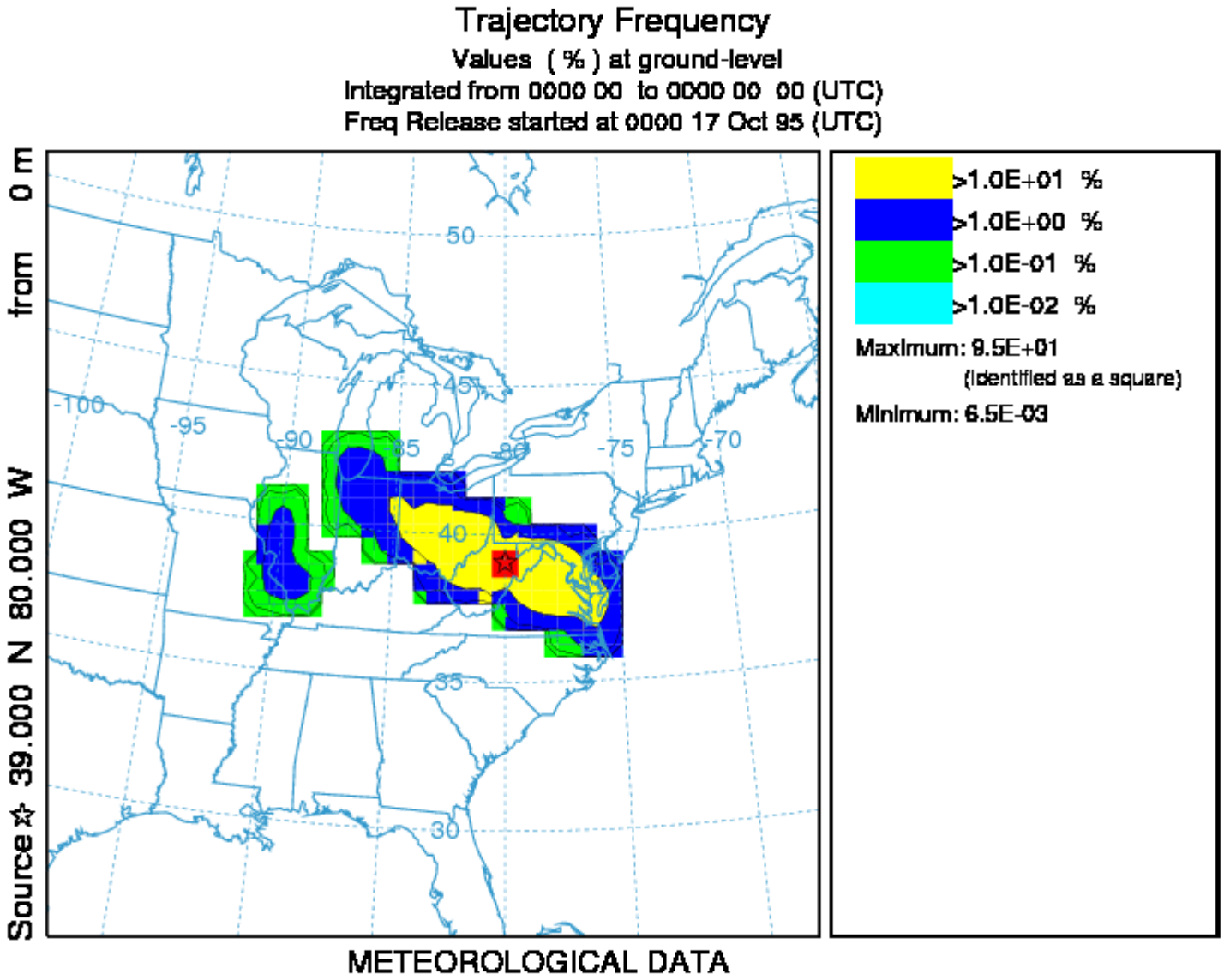
Summary: This menu is used to configure the model to execute a script to run multiple iterations of the backward trajectory calculation for periods that correspond with individual measured sampling data. The trajectory results can then be overlaid using the frequency plot menu option to indicate the most probable source regions. The CONTROL file should have been previously defined for a forward calculation that corresponds to the sampling period of the measured data. The measured data file must be in the DATEM format. The configuration process is very similar to that described for dispersion simulations.

Step 1: defines the measured data input used in this series of calculations. The trajectory model is run backward, from each of the sampling locations, with a trajectory started (at the beginning, middle, end) for each sampling period with a non-zero measurement. Measured values less than or equal to the value in the text entry box are considered to be zero. Sampling data files are in the ASCII text DATEM format. The first record provides some general information, the second record identifies all the variables that then follow on all subsequent records. There is one data record for each sample collected. All times are given in UTC.

An example measured data file can be used with the sample meteorological data to configure multiple trajectory simulations starting on 95 10 16 00. Note that the sampling data run from 0600 on the 16th through 1200 on the 17th, suggesting at least a 30 h if not 36 h trajectory is required to span the measurement data domain. First create a CONTROL file by running a forward simulation for one trajectory that spans the computational period.

Step 2: creates three CONTROL.{xxx} files for each sampling location with a non-zero measurement at the beginning, middle, and end of the sampling period using the *dat2cntl* program. The CONTROL files are numbered sequentially from 001 to a maximum of 999. The trajectory output files are labeled using the base name from the CONTROL file followed by the sampler ID number and the starting date and time of the trajectory. A sampler collecting two contiguous in-time samples will have the same trajectory computed at the end of one sampling period and the beginning of the next sampling period because there will be two different CONTROL files for each. However, the output file name will be the same and hence the results will not be double counted in any statistical analysis. Using the sample data, running step two creates 45 CONTROL files from 15 non-zero measurements.

Step 3: sequentially runs the trajectory simulations starting with CONTROL.001 through the last available control file. Each simulation uses the same namelist configuration. Once the calculation has completed, the individual trajectories can be gridded and displayed using the trajectory frequency menu, the results of which are shown below.



In this case the measurement data were created using a forward dispersion simulation from 40N 80W which is near the maximum point of the trajectory frequency plot, the position of the maximum is also indicated along the left edge plot label.

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Trajectory / Setup Run / Control File Format

The trajectory model input control file can be created using any text editor. However if the GUI is not being used, it would be easier to let the model create the initial file based upon standard output prompts. These are described in more detail below. When data entry is through the keyboard (a file named *CONTROL* is not found), a *STARTUP* file is created. This contains a copy of the input, and which later may be renamed to *CONTROL* to permit direct editing and model execution without data entry. If you are unsure as to a value required in an input field, just enter the forward slash (/) character, and the indicated default value will be used. This default procedure is valid for all input fields except directory and file names. An automatic default selection procedure is also available for certain input fields of the *CONTROL* file when they are set to zero. Those options are discussed in more detail below. Each input line is numbered (only in this text) according to the order it appears in the file. A number in parenthesis after the line number indicates that there is an input loop and multiple entry lines may be required depending upon the value of the previous entry.

1- Enter starting time (year, month, day, hour, {minutes optional})

Default: 00 00 00 00 {00}

Enter the two digit values for the UTC time that the calculation is to start. Use 0's to start at the beginning (or end) of the file according to the direction of the calculation. All zero values in this field will force the calculation to use the time of the first (or last) record of the meteorological data file. In the special case where year and month are zero, day and hour are treated as relative to the start or end of the file. For example, the first record of the meteorological data file usually starts at 0000 UTC. An entry of "00 00 01 12" would start the calculation 36 hours from the start of the data file. The minutes field is optional but should only be used when the start time is explicitly set to a value.

2- Enter number of starting locations

Default: 1

Simultaneous trajectories can be calculated at multiple levels or starting locations. Specification of additional locations for certain types of simulations can also be accomplished through the Special Simulations menu tab, or through manual editing of the *CONTROL* file and running the model outside of the GUI. When multiple starting locations are specified, all trajectories start at the same time. A multiple trajectory in time option is available through the Advanced menu through a namelist file parameter setting.

3(1)- Enter starting location (lat, lon, meters)

Default: 40.0 -90.0 50.0

Trajectory starting position in degrees and decimal (West and South are negative). Height is entered as meters above ground-level. An option to treat starting heights as relative to mean-sea-level is available through the Advanced menu through a namelist file parameter setting.

4- Enter total run time (hours)

Default: 48

Specifies the duration of the calculation in hours. Backward calculations are entered as negative hours. A backward trajectory starts from the trajectory termination point and proceeds upwind. Meteorological data are processed in reverse-time order.

5- Vertical motion option (0:data 1:isob 2:isen 3:dens 4:sigma 5:diverg 6:msl2agl 7:average)

Default: 0

Indicates the vertical motion calculation method. The default "data" selection will use the meteorological model's vertical velocity fields; other options include {isob}aric, {isen}tropic, constant {dens}ity, constant internal {sigma} coordinate, computed from the velocity {diverg}ence, vertical coordinate remapping from MSL to AGL, and a special option (7) to spatially average the vertical velocity. The averaging distance is automatically computed from the ratio of the temporal frequency of the data to the horizontal grid resolution.

6- Top of model domain (internal coordinates m-agl)

Default: 10000.0

Sets the vertical limit of the internal meteorological grid. If calculations are not required above a certain level, fewer meteorological data are processed thus speeding up the computation. Trajectories will terminate when they reach this level. A secondary use of this parameter is to set the model's internal scaling height - the height at which the internal sigma surfaces go flat relative to terrain. The default internal scaling height is set to 25 km but it is set to the top of the model domain if the entry exceeds 25 km. Further, when meteorological data are provided on terrain sigma surfaces it is assumed that the input data were scaled to a height of 20 km (RAMS) or 34.8 km (COAMPS). If a different height is required to decode the input data, it should be entered on this line as the negative of the height. HYSPLIT's internal scaling height remains at 25 km unless the absolute value of the domain top exceeds 25 km.

7- Number of input data grids

Default: 1

Number of simultaneous input meteorological files. The following two entries (directory and name) will be repeated this number of times. A simulation will terminate when the computation is off all of the grids in either space or time. Trajectory calculations will check the grid each time step and use the finest resolution input data available at that location at that time. When multiple meteorological grids have different resolution, there is an additional restriction that there should be some overlap between the grids in time, otherwise it is not possible to transfer a trajectory position from one grid to another. If multiple grids are defined and the model has trouble automatically transferring the calculation from one grid to another, the sub-grid size may need to be increased to its maximum value.

8(1)- Meteorological data grid # 1 directory

Default: (\main\sub\data\ )

Directory location of the meteorological file on the grid specified. Always terminate with the appropriate slash (\ or /).

9(2)- Meteorological data grid # 1 file name

Default: file_name

Name of the file containing meteorological data. Located in the previous directory.

10- Directory of trajectory output file

Default: (\main\trajectory\output\ )

Directory location to which the text trajectory end-points file will be written. Always terminate with the appropriate slash (\ or /).

11- Name of the trajectory endpoints file

Default: file_name

The trajectory end-points output file is named in this entry line.

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Trajectory / Display / Endpoint File Format

The trajectory model generates its own text output file of ASCII end-point positions. The trajectory display program processes the end-point file. The format of the file is given below:

Record #1

I6 - Number of meteorological grids used in calculation

Records Loop #2 through the number of grids

A8 - Meteorological Model identification
5I6 - Data file starting Year, Month, Day, Hour, Forecast Hour

Record #3

I6 - number of different trajectories in file
1X,A8 - direction of trajectory calculation (FORWARD, BACKWARD)
1X,A8 - vertical motion calculation method (OMEGA, THETA, ...)

Record Loop #4 through the number of different trajectories in file

4I6 - starting year, month, day, hour
2F9.3 - starting latitude, longitude
F8.1 - starting level above ground (meters)

Record #5

I6 - number (n) of diagnostic output variables
n(1X,A8) - label identification of each variable (PRESSURE, THETA, ...)

Record Loop #6 through the number of hours in the simulation

I6 - trajectory number
I6 - meteorological grid number or antecedent trajectory number
5I6 - year month day hour minute of the point
I6 - forecast hour at point
F8.1 - age of the trajectory in hours
2F9.3 - position latitude and longitude
1X,F8.1 - position height in meters above ground
n(1X,F8.1) - n diagnostic output variables (1st to be output is always pressure)

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Concentration / Help

The concentration menu tab is composed of six main sections: setting up the simulation, executing the model, displaying the concentrations, various utility programs for converting the output to other formats, configuring special simulations, and simulations in a multi-processor environment. The model can be entirely configured and executed through the menu. However for experienced users, each component may be run independently from the command line.

In the Concentration Setup menu, the entire purpose of the GUI is to configure the model's input *CONTROL* file. This is a text file that configures the simulation parameters. Once the input parameters are set to their desired value, the model is executed from the Run Standard Model menu tab. When complete, the output window is closed and Display Options menu is used to draw and display the concentration contours from the model's binary concentration output file. The Special Simulations menu is used to configure several different customized simultaneous for ensemble applications, source-receptor matrices, and some simple chemistry simulations. The Multi-processor tab invokes some of the same special simulations but will only run under a multi-processor- computing environment. Normally this is not an option available under MS Windows.

For inexperienced users, a review of the Quick Start Help menu is highly suggested, which goes through a concentration computation step-by-step using the example meteorological data file.

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Concentration / Quick Start Help

Upon installation the first time the model will be configured to run the example case discussed in more detail below. The "Quick Start" menu tab can be used to run any simulation in one-step. The last configuration will be used for the simulation. The "Quick Start" menu brings up a global map with the current source location shown as a blue dot. A "right-click" of the mouse button will write that source location to the control file, close the map, run the model simulation, create the output file, and display the graphics. A "left-click" of the mouse button will set a new source location. A "left-click-hold-drag-release" will define a new "zoomed" domain and the map will be redrawn. An "exit" from the window's menu bar will close the map without updating the control file or running the model. For more detailed simulation configurations, follow the steps below.

The easiest way to run the model is to use the GUI menu to edit the model's input *CONTROL* file. For the purposes of this demonstration appropriate meteorological files are provided. If for some reason the menu system is not available, the *CONTROL* file can be created manually.

Step 1 - start the GUI menu system using the desktop shortcut *Hysplit4* to *\working\hysplit4.tcl*. A widget will appear with the *HYSPLIT* graphic and three button options: *Menu*, *Help Exit*. **Click on *Menu*.**

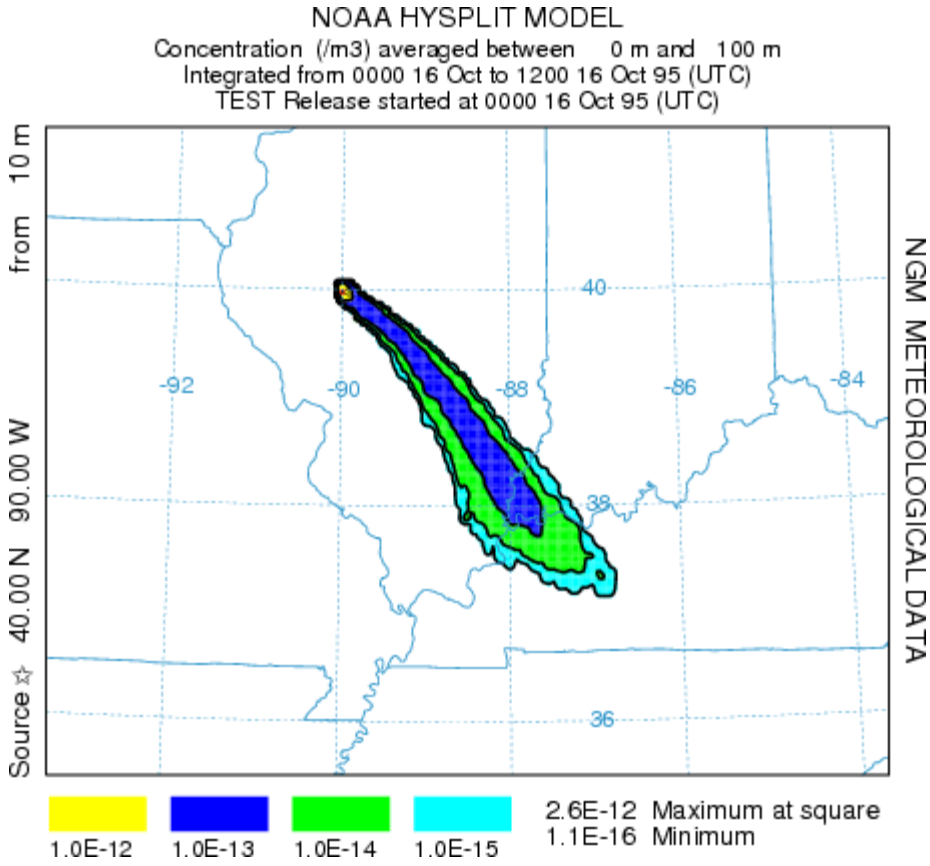
Step 2 - The four main menus of Hysplit4 will appear: Meteorology, Trajectory, Concentration, and the optional Advanced menu. An additional small widget underneath the main menu gives the current Hysplit4 version information. Do not delete this widget as it will terminate the GUI. It provides the reference frame for the model's standard output and messages and the version number required for updates. **Click on *Concentration*.**

Step 3 - Under the concentration menu there are also five options: concentration setup, run standard model, concentration display, utility programs, and special simulations. In general, they should be executed in sequential order. **Click on *Setup Run*.**

Step 4 - The *Setup Run* menu brings up similar starting information requirements as with the trajectory menu. There are three additional sub-menus: Pollutant - that can be used set the emission rate, duration, and start time of the emission; Grids - to set the location, resolution, levels, and averaging times of the concentration output grid; and Deposition - to set the characteristics of each pollutant. **Click on *Retrieve***, enter name of sample pre-configured control file: ***sample_conc***, then **click on *OK***. After the data entry widget is closed, **click on *Save*** and the setup menu will close.

Step 5 - From the main concentration menu tab **select** Run Model, which copies the setup configuration to the model's input *CONTROL* file and starts the model simulation. Messages will appear on standard output showing the progress of the calculation or after the calculation has completed. Be patient as concentration calculations may take considerably longer than trajectory calculations. **Click on Exit** to close the message window. At that point the binary concentration output file is ready to be converted to a graphical display.

Step 6 - **Click on *Display / Concentration*** and then **select** Contours to run a special program that converts the binary concentration file to the Postscript file *concplot.ps*, suitable for printing. The display widget contains multiple options for different pollutants (if defined), data grids, levels, and contour options. These are discussed in more detail in the graphics section. For this example, accept the defaults and just click **on *Execute Display***. If the Ghostview Postscript viewer has been installed and properly associated with .ps files, then it will be automatically invoked by the GUI. If the viewer does not open, it may be necessary to manually edit the file *hysplit4.tcl* for the directory entry associated with the program *gsview32.exe*. The output file can be printed directly on any Postscript device or printed through *Ghostscript/Ghostview*. The 12 hour average air concentration for a one hour release is shown in the illustration below.



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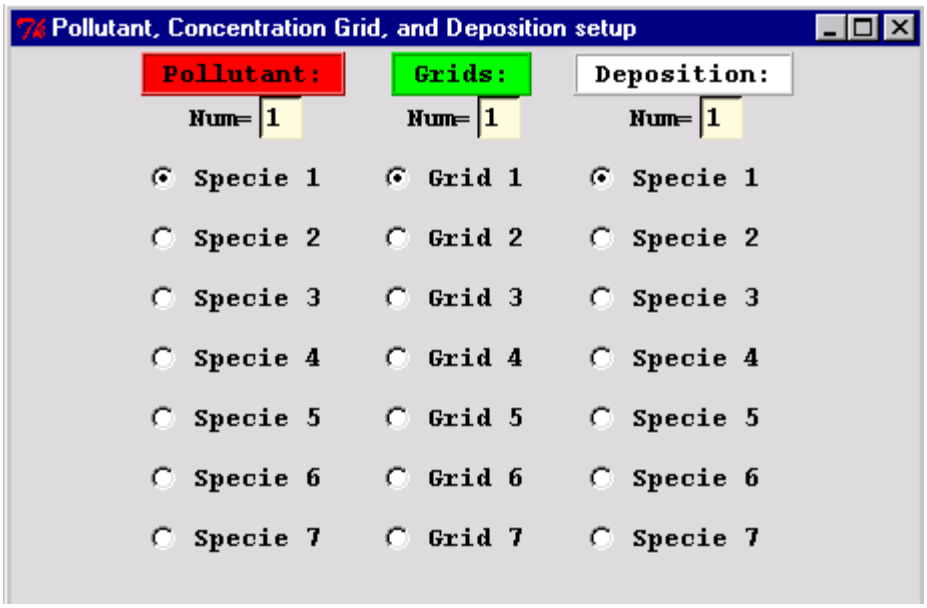
Concentration / Setup Run / Pollutant, Deposition, Grids

There are three menu choices under this tab: Pollutant, Grid, and Deposition. The first permits editing of the emission rate parameters, the second defines the concentration output grid, and the third the deposition characteristics of the pollutant, if that feature is enabled. This menu is illustrated below. To edit the parameters for a specific species entry just select the appropriate checkbox.



Note that up to 7 pollutant species may be defined by changing the *Num* parameter. However, in the current version, the pollutant and deposition menus must both reference the same number of species. Multiple species simulations are calculated independently, hence there is no computational benefit by doing two different simulations or combining both species in one simulation. The multiple species option is primarily used for chemical transformation simulations. A simple example is available from the configuration menu checkbox of "10% per hour", which transforms species #1 to species #2 at a rate of 10% per hour. The transformation occurs on the same particle and is discussed in more detail in the Advanced Applications section. More complex transformations require a linkage with compatible external modules. None are available at this time for public distribution.

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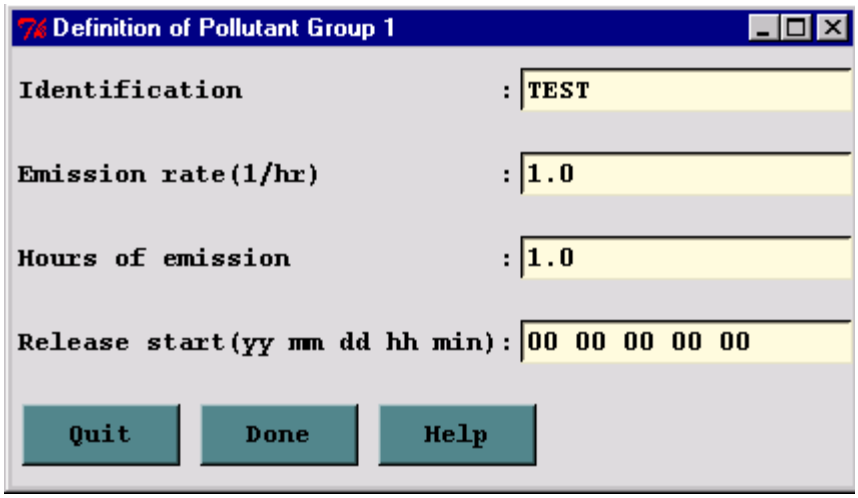
Concentration / Setup Run / Pollutant Definition

There are four *CONTROL* file entries, lines 11(1) through 14(4), that correspond with each line of the pollutant menu shown in the illustration below.



10- Number of different pollutants

Default: 1

Multiple pollutant species may be defined for emissions. Each pollutant is assigned to its own particle or puff and therefore may behave differently due to deposition or other pollutant specific characteristics. Each will be tracked on its own concentration grid. The following four entries are repeated for each pollutant defined.

11(1)- Pollutant four Character Identification

Default: TEST

Provides a four-character label that can be used to identify the pollutant. The label is written with the concentration output grid to identify output records associated with that pollutant and will appear in display labels. Additional user supplied deposition and chemistry calculations may be keyed to this identification string.

12(2)- Emission rate (per hour)

Default: 1.0

Mass units released each hour. Units are arbitrary except when specific chemical transformation subroutines are associated with the calculation. Output air concentration units will be in the same units as specified on this line. For instance an input of kg/hr results in an output of kg/m^3. When multiple sources are defined this rate is assigned to all sources unless the optional parameters are present on line 3(1).

13(3)- Hours of emission

Default: 1.0

The duration of emission may be defined in fractional hours. An emission duration of less than one time-step will be emitted over one time-step with a total emission that would yield the requested rate over the emission duration.

14(4)- Release start time: year month day hour minute

Default: [simulation start]

The previously specified hours of emission start at this time. An entry of zero's in the field, when input is read from a file, will also result in the selection of the default values that will correspond with the starting time of the meteorological data file. Day and hour are treated as relative to the file start when month is set to zero.

Temporal or Area Emission Variations

This menu is only designed to input point source emission rates. Unless additional input values are provided in the control file after each emission location, the same rate will apply to all defined point sources for the duration of the emission. When more complex emission scenarios are required, emission data can be read in from a file that defines a diurnal emission cycle for any number of pollutants at any number of locations. If the emission rate is to vary in time beyond one diurnal cycle, there is another input file that can be defined to set a new rate with each emission cycle. In this latter scenario the rate as well as the location may be changed.

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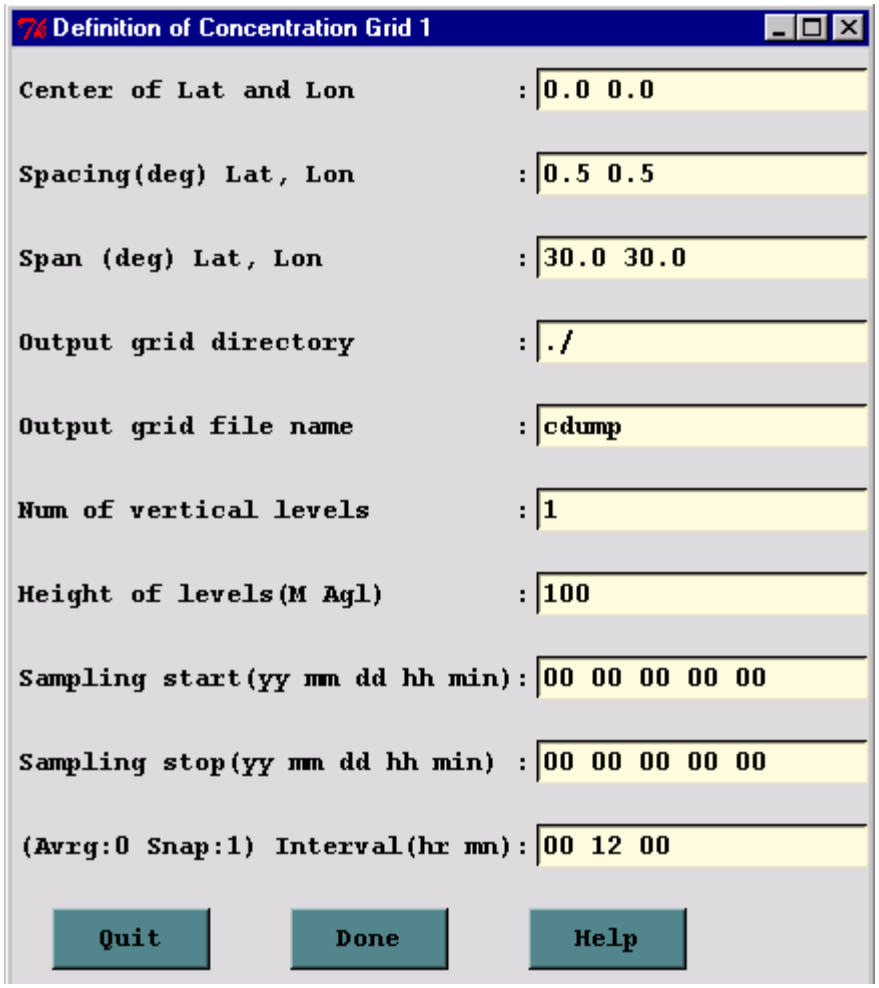
Concentration / Setup Run / Grid Definition

This section is used to define the grid system to which the concentrations are summed during the integration and subsequently for post-processing and display of the model's output. There are 10 entries in the CONTROL file for each concentration grid that has been defined. The lines 16(1) through 25(10) correspond with each of the menu items shown in the illustration below.



Dispersion calculations are performed on the computational (meteorological) grid without regard to the definition or location of any concentration grid. Therefore it is possible to complete a simulation and have no results to view if the concentration grid was in the wrong location. In addition, very small concentration grid spacing will reduce the model's integration time step and may result is substantially longer simulation clock times.

15- <u>Number of simultaneous concentration grids</u>

Default: 1

Multiple or nested grids may be defined. The concentration output grids are treated independently. The following 10 entries will be repeated for each grid defined.

16(1)- <u>Center Latitude, Longitude (degrees)</u>

Default: [source location]

Sets the center position of the concentration sampling grid in degrees and decimal. Input of zero's will result in selection of the default value, the location of the emission source. Sometimes it may be desirable to move the

grid center location downwind near the center of the projected plume position.

17(2)- Grid spacing (degrees) Latitude, Longitude

Default: 1.0 1.0

Sets the interval in degrees between nodes of the sampling grid. Puffs must pass over a node to contribute concentration to that point and therefore if the spacing is too wide, they may pass between intersection points. Particle model calculations represent grid-cell averages, where each cell is centered on a node position, with its dimensions equal to the grid spacing. Finer resolution concentration grids require correspondingly finer integration time-steps. This may be mitigated to some extent by limiting fine resolution grids to only the first few hours of the simulation.

In the special case of a polar (arc,distance) concentration grid, defined when the namelist variable cpack=3, the definition changes such that the latitude grid spacing equals the sector angle in degrees and the longitude grid spacing equals the sector distance spacing in kilometers.

18(3)- Grid span (deg) Latitude, Longitude

Default: [180.0] [360.0]

Sets the total span of the grid in each direction. For instance, a span of 10 degrees would cover 5 degrees on each side of the center grid location. A plume that goes off the grid would have cutoff appearance, which can sometimes be mitigated by moving the grid center further downwind.

In the special case of a polar (arc,distance) concentration grid, defined when the namelist variable cpack=3, the definition changes such that the latitude span always equals 360.0 degrees and the longitude span equals the total downwind distance in kilometers. Note that the number of grid points equals 360/arc-angle or the total-distance divided by the sector-distance.

19(4)- Enter grid # 1 directory

Default: (\main\sub\output\ )

Directory to which the binary concentration output file for this grid is written. As in other directory entries a terminating (\) slash is required.

20(5)- Enter grid # 1 file name

Default: file_name

Name of the concentration output file for each grid. See Section 6 for a description of the format of the concentration output file.

21(6)- Number of vertical concentration levels

Default: 1

The number of vertical levels in the concentration grid including the ground surface level if deposition output is required.

22(7)- Height of each level (m)

Default: 50

Output grid levels may be defined in any order for the puff model as long as the deposition level (0) comes first (a

height of zero indicates deposition output). Air concentrations must have a non-zero height defined. A height for the puff model indicates the concentration at that level. A height for the particle model indicates the average concentration between that level and the previous level (or the ground for the first level). Therefore heights for the particle model need to be defined in ascending order. Note that the default is to treat the levels as above-ground-level (AGL) unless the MSL (above Mean-Sea-Level) flag has been set (see advanced configuration).

23(8)- Sampling start time: year month day hour minute

Default: [simulation start]

Each concentration grid may have a different starting, stopping, and output averaging time. Zero entry will result in setting the default values. "Backward" calculations require that the stop time should come before the start time.

24(9)- Sampling stop time: year month day hour minute

Default: 12 31 24 60

After this time no more concentration records are written. Early termination on a high resolution grid (after the plume has moved away from the source) is an effective way of speeding up the computation for high resolution output near the source because once turned-off that particular grid resolution is no longer used for time-step computations.

25(10)- Sampling interval: type hour minute

Default: 0 24 0

Each grid may have its own sampling or averaging interval. The interval can be of three different types: averaging (type=0), snapshot (type=1), or maximum (type=2). Averaging will produce output averaged over the specified interval. For instance, you may want to define a concentration grid that produces 24-hour average air concentrations for the duration of the simulation, which in the case of a 2-day simulation will result in 2 output maps, one for each day. Each defined grid can have a different output type and interval. Snapshot (or now) will give the instantaneous output at the output interval, and maximum will save the maximum concentration at each grid point over the duration of the output interval. Therefore, when a maximum concentration grid is defined, it is also required to define an identical snapshot or average grid over which the maximum will be computed. There is also the special case when the type value is less than zero. In that case the value represents the averaging time in hours and the output interval time represents the interval at which the average concentration is output. For instance, a setting of {-1 6 0} would output a one-hour average concentration every six hours.

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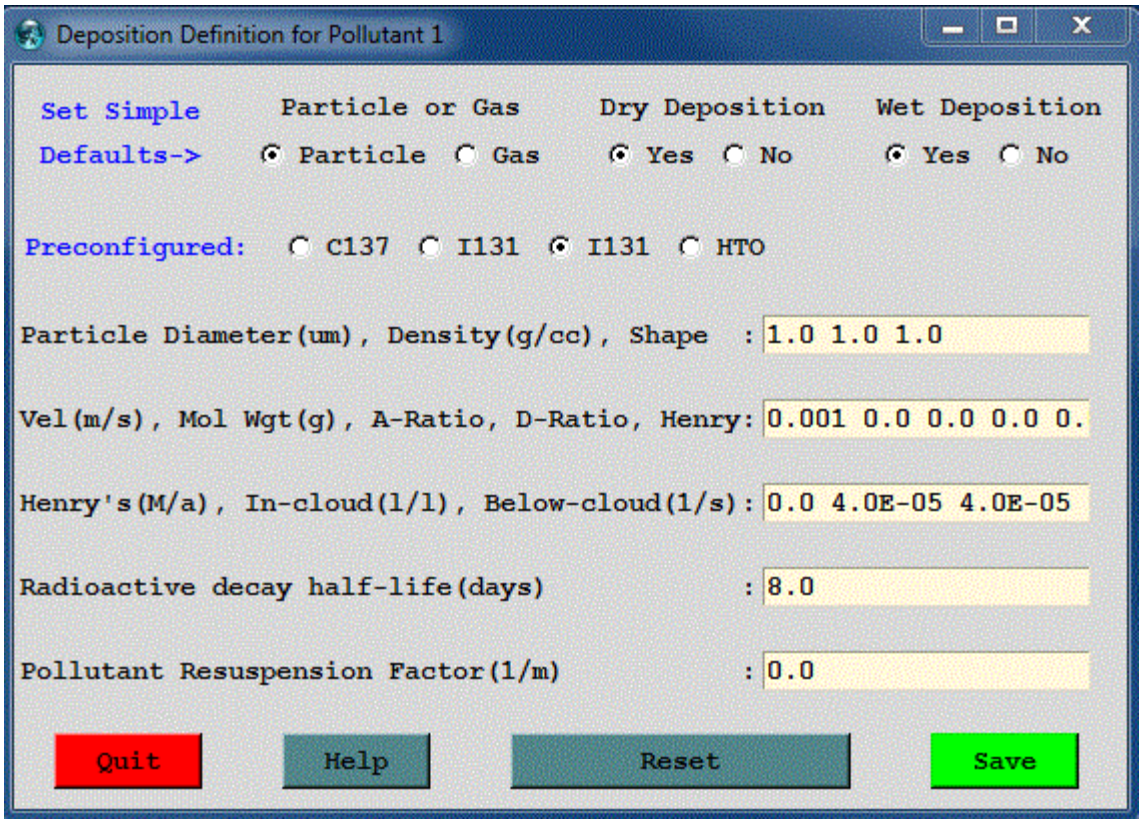
Concentration / Setup Run / Deposition Definitions

This section is used to define the deposition parameters for emitted pollutants. The number of deposition definitions must correspond with the number of pollutants released. There is a one-to-one correspondence. There are 5 entries in the *CONTROL* file for each defined pollutant. The lines 27(1) through 31(5) correspond with each of the menu items shown in the illustration below. The radio-buttons along the top can be used to set default deposition parameters, which can then be edited as required in the text entry section. The second line of radio-buttons define the deposition values for some preconfigured species: Cesium, Iodine (gaseous and particiulate), and Tritium. The reset button sets all deposition parameters back to zero.

Note that turning on deposition will result in the removal of mass and the corresponding reduction in air concentration, the deposition will not be available in any output unless height "0" is defined as one of the concentration grid levels.



26 - Number of pollutants depositing

Default: number of pollutants on line # 10

Deposition parameters must be defined for each pollutant species emitted. Each species may behave differently for deposition calculations. Each will be tracked on its own concentration grid. The following five lines are repeated for each pollutant defined. The number here must be identical to the number on line 10. Deposition is turned off for pollutants by an entry of zero in all fields.

27(1)- Particle: Diameter (µm), Density (g/cc), and Shape

Default: 0.0 0.0 0.0

These three entries are used to define the pollutant as a particle for gravitational settling and wet removal calculations. A value of zero in any field will cause the pollutant to be treated as a gas. All three fields must be defined (>0) for particle deposition calculations. However, these values only need to be correct only if gravitational settling or resistance deposition is to be computed by the model. Otherwise a nominal value of 1.0

may be assigned as the default for each entry to define the pollutant as a particle. If a dry deposition velocity is specified as the first entry in the next line (28), then that value is used as the particle settling velocity rather than the value computed from the particle diameter and density.

If gravitational settling is on and the Shape is set to a negative value then the Ganser (1993) calculation is used to replace Stokes equation for estimating particle fallspeeds. The absolute value of the Shape factor is used for the calculation. The Stokes equation overestimates particle fallspeeds for particles larger than about 20 micron diameter. As this diameter often lies within size distributions of volcanic ash particles, it is desirable to use the Ganser formulation so that particle fallspeeds can be computed accurately. Ganser, G.H., 1993: A rational approach to drag prediction of spherical and nonspherical particles. Powder Technology, 77, 143-152. .

The particle definitions can be used in conjunction with a special namelist parameter NBPTYP that determines if the model will just release the above defined particles or create a continuous particle distribution using the particle definitions as fixed points within the distribution. This option is only valid if the model computes the gravitational settling velocity rather than pre-defining a velocity for each particle size.

28(2)- Deposition velocity (m/s), Pollutant molecular weight (Gram/Mole), Surface Reactivity Ratio, Diffusivity Ratio, Effective Henry's Constant

Default: 0.0 0.0 0.0 0.0 0.0

Dry deposition calculations are performed in the lowest model layer based upon the relation that the deposition flux equals the velocity times the ground-level air concentration. This calculation is available for gases and particles. The dry deposition velocity can be set directly for each pollutant by entering a non-zero value in the first field. In the special case where the dry deposition velocity is set to a value less than zero, the absolute value will be used to compute gravitational settling *but with no mass removal*. The dry deposition velocity can also be calculated by the model using the resistance method which requires setting the remaining four parameters (molecular weight, surface reactivity, diffusivity, and the effective Henry's constant). See the table below for more information.

Table I. Some typical pollutant constants from Wesely (1989) and Walmsley and Wesely (1996).

Chemical	Symbol	D_{rx}	H^* (M/atm) effective	H(M/atm) Actual	f_o
Sulfur dioxide	SO_2	1.9	$1x10^5$	1.24	0.0
Ozone	O_3	1.6	0.01	0.013	1.0
Nitrogen dioxide	NO_2	1.6	0.01	0.01	0.1
Nitric oxide	NO	1.3	$3x10^{-3}$	$1.9x10^{-3}$	0.0
Nitric acid	HNO_3	1.9	$1x10^{14}$	$2.1x10^5$	0.0
Hydrogen peroxide	H_2O_2	1.4	$1x10^5$	$1.0x10^5$	1.0
Ammonia	NH_3	0.97	$2x10^{14}$	62	0.0
Peroxyacetyl nitrate	PAN	2.6	3.6	5	0.1
Nitrous acid	HNO_2	1.6	$1x10^5$	$2.1x10^5$	0

D_{rx} - Diffusivity ratio; H - Henry's constant; f_o - Surface reactivity ratio

Wesely, M.L., 1989, Parameterizations of surface resistances to gaseous dry deposition in regional-scale numerical models, *Atmos. Environ.*, 23, 1293-1304.

Walmsley, J. L., and M.L. Wesely, 1996, Modification of coded parameterizations of surface resistances to gaseous dry deposition, *Atmos. Environ.*, 30, 1181-1188.

29(3)- Wet Removal: Actual Henry's constant, In-cloud (GT 1 =L/L; LT 1 =1/s), Below-cloud (1/s)

Default: 0.0 0.0 0.0

Suggested: 0.0 8.0E-05 8.0E-05

Henry's constant defines the wet removal process for soluble gases. It is defined only as a first-order process by a non-zero value in the field. Wet removal of particles is defined by non-zero values for the in-cloud and below-cloud parameters. In-cloud removal can be defined as a ratio of the pollutant in rain (g/liter) measured at the ground to that in air (g/liter of air in the cloud layer) when the value in the field is greater than one. For within-cloud values less than one, the removal is defined as a time constant. Below-cloud removal is always defined through a removal time constant. The default cloud bottom and top RH values can be changed through the SETUP.CFG namelist file. Wet removal only occurs in grid cells with both a non-zero precipitation value and a defined cloud layer.

30(4)- Radioactive decay half-life (days)

Default: 0.0

A non-zero value in this field initiates the decay process of both airborne and deposited pollutants. The particle mass decays as well as the deposition that has been accumulated on the internal sampling grid. The deposition array (but not air concentration) is decayed until the values are written to the output file. Therefore, the decay is applied only the the end of each output interval. Once the values are written to the output file, the values are fixed. The default is to decay deposited material. This can be turned off so that decay only occurs to the particle mass while airborne by setting the *decay* namelist variable to zero.

31(5)- Pollutant Resuspension (1/m)

Default: 0.0

Suggested: 1.0E-06

A non-zero value for the re-suspension factor causes deposited pollutants to be re-emitted based upon soil conditions, wind velocity, and particle type. Pollutant re-suspension requires the definition of a deposition grid, as the pollutant is re-emitted from previously deposited material. Under most circumstances, the deposition should be accumulated on the grid for the entire duration of the simulation. Note that the air concentration and deposition grids may be defined at different temporal and spatial scales.

Previous Section of the CONTROL file

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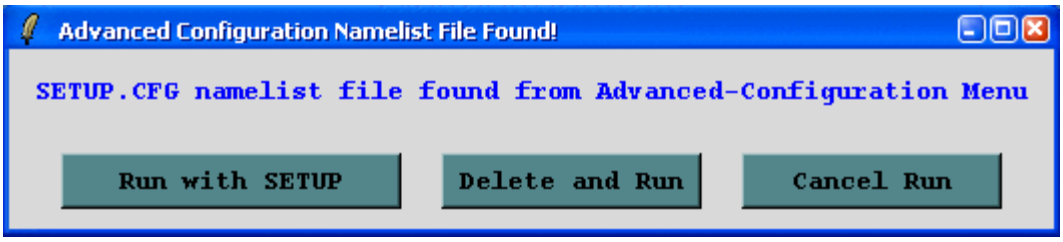
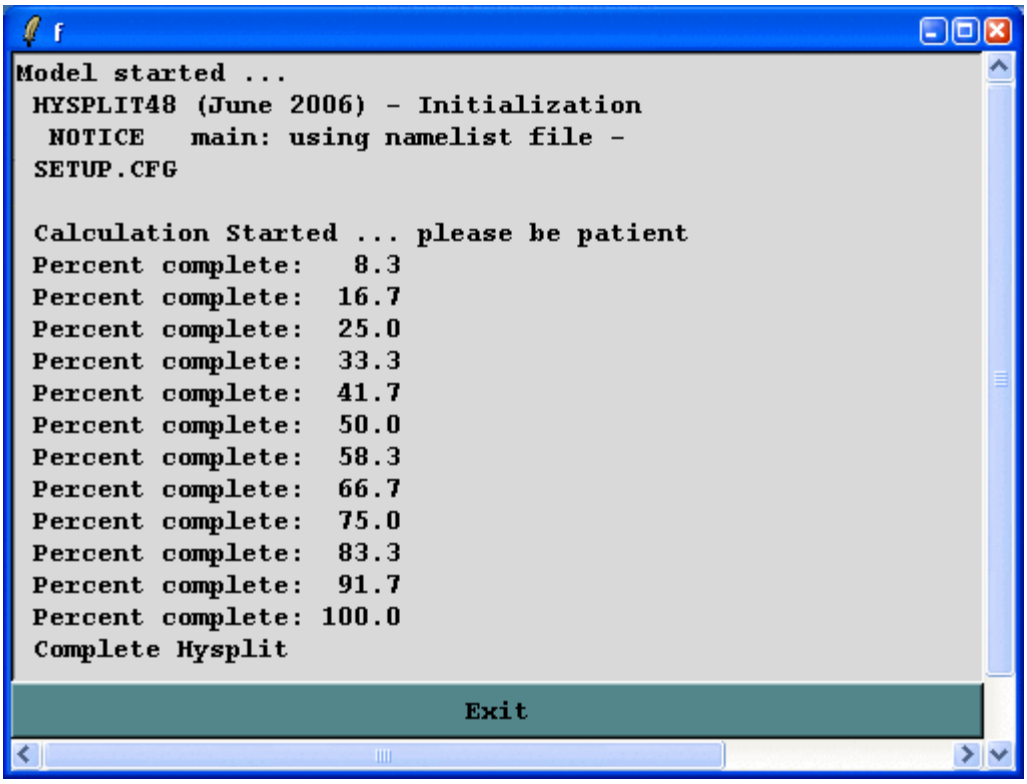
Concentration / Run Model

Once the Concentration Setup menu has been closed with the *Save* button, the changes to the simulation parameters are copied to *default_conc*. Clicking on the *Run Standard Mode*l menu tab first copies *default_conc* to *CONTROL* and then runs the trajectory model executable, *hycs_std*. The executable, by default, attempts to open a file named *CONTROL* to read all the required input parameters. If not found, the model will prompt to standard output for values from standard input. This condition should not occur running the model through the GUI.

In the situation where the namelist file *SETUP.CFG* has been created through the *Advanced/Configuration* menu tab, the message shown below will appear. If the intent was to run using this file, then continue, otherwise one can delete the file and run, or terminate the simulation. The situation may arise that the namelist file was created for a previous simulation and is not needed this time.



When the model execution starts, output messages are written to a special window. Successful completion of a simulation will show a message similar to the example shown in the illustration below:



Additional run-time diagnostic messages and other error messages are always written to a file called *MESSAGE*. This file may be viewed through one of the Advanced Menu tabs. Depending upon the nature of the error message, perhaps a failure in the model initialization process, error messages may also appear in above window. Once the model has completed, **press Exit** to close the window.

Sometimes a configuration (long duration, very fine grid, too many particles) will lead to extremely long run times, perhaps requiring the model to be terminated prematurely. Closing the GUI will not terminate the simulation because it

always runs in background. In this situation it is necessary to use the *cntl-alt-del* key combination (Windows) to find and kill the *hycs_std* executable.

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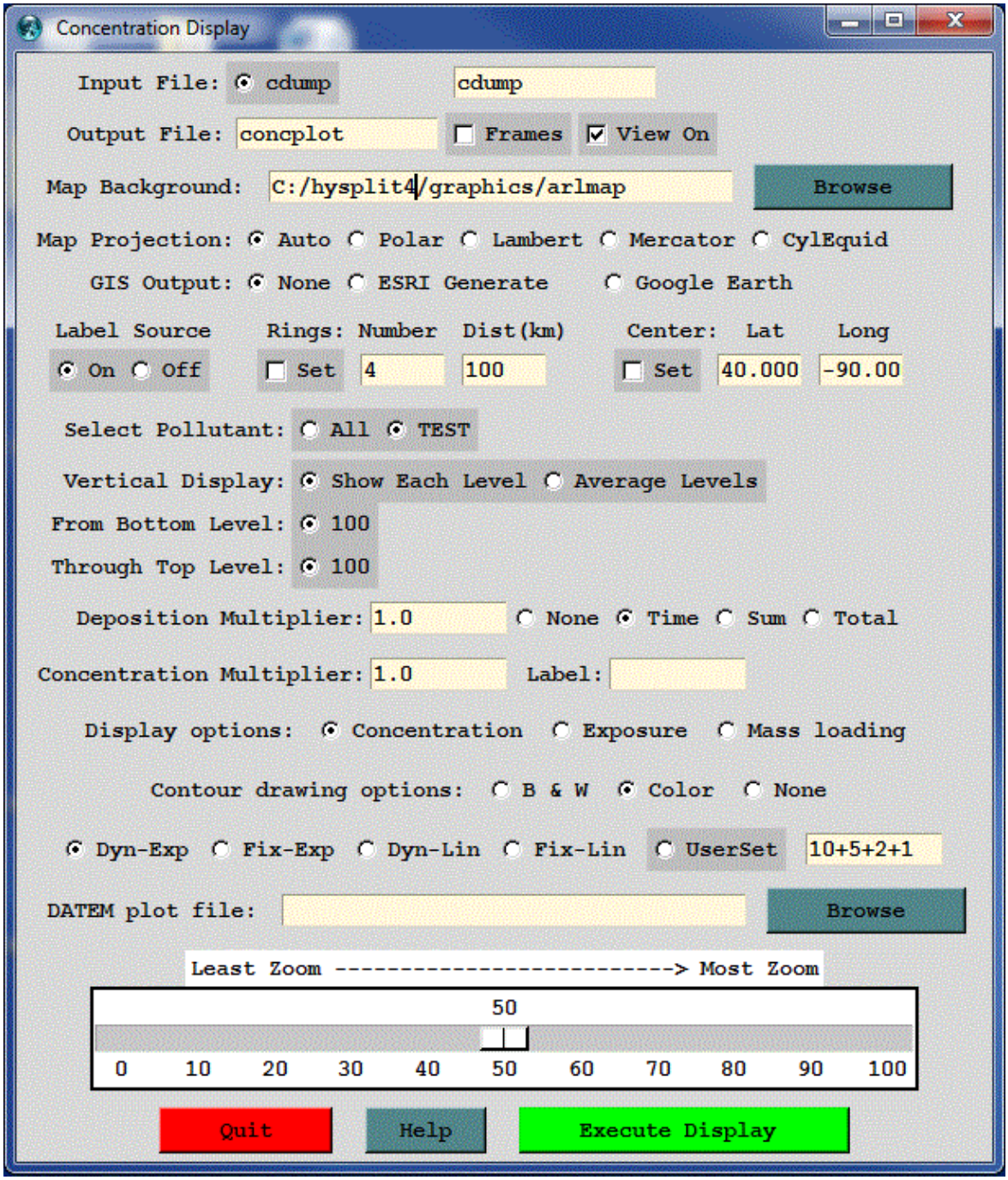
Concentration / Display / Contours

The concentration model generates a binary (big-endian) output file on a regular latitude-longitude grid, which is read by the other programs to produce various displays and other output. The plotting program, *concplot*, can be accessed through the GUI, which is shown in the illustration below, or it can be run directly from the command line. Most, but not all, of the command line options are available through the GUI.



Normally only one input file is shown, unless multiple files have been defined in the Concentration Setup Run menu. The default output file name is shown and unless the box is checked all frames (time periods and/or levels) will be output to that one file. The program uses the map background file, *arlmap*, which by default is located in the *\graphics* directory. Other customized map background files could be defined. Some of these higher resolution map background files are available from the HYSPLIT download web page. This plotting program also supports the use of ESRI formatted shapefiles.

The GIS output option will create an output file of the contour polygons (latitude-longitude vectors) in two different format: the ESRI generate format for import into ArcMap or ArcExplorer, or XML formatted files packaged by Info-Zip for import into Google Earth.

For multiple pollutant files, only one pollutant may be selected for display by individual levels, or averaged between selected levels. These levels must have been predefined in the Concentration Setup menu. Multipliers can be defined for deposition or air concentrations. Normally these values would default to 1.0, unless it is desired to change the output units (for instance, g/m^3 to ug/m^3 would require a multiplier of 10^6).

Contours and color fill can be specified as black and white or color. The none option eliminates the black line defining contours and only leaves the color fill. This option is incompatible with GIS output options, which require computation of the contour vector. Contours can be determined **DYN**amically by the program, changing with each map, or **FIX**ed to be the same for all maps. A user can set the contour scaling (difference between contours) to be computed on an **EXP**onential scale or a **LIN**ear scale.

Concplot Command Line Options

The Postscript conversion program (*concplot*), found in the */exec* directory with all other executables, reads the binary concentration output file, calculates the most optimum map for display, and creates the output file *concplot.ps*. Multiple pollutant species or levels can be accommodated. Most routine variations can be invoked from the GUI. More complicated conversions should be run from the command line using the following optional parameters:

concplot -[options (default)]

- -a[Arcview GIS: (0)-no dump, 1-ESRI (log10), 2-ESRI (decimal), 3-Google Earth]

  Selecting the ESRI Generate Format output creates an ASCII text file for each output time period that consists of the value and latitude-longitude points along each contour. This file can be converted to an ESRI Shapefile or converted for other GIS applications through the utility menu "GIS to Shapefile" ". The view checkbox would be disabled to do just the GIS conversion without opening the Postscript viewer. Selecting Google Earth will create a compressed file (*.kmz) for use in **Google Earth**; a free software package to display geo-referenced information in 3-dimensions. You must have the free **Info-Zip** file compression software installed to compress the Google Earth file and associated graphics.

- +a[KML altitude mode: 0-clampedToGround, 1-relativeToGround]:

  Selecting clampedToGround (0) positions the contoured concentrations flat on the Google Earth terrain, whereas selecting relativeToGround will generate 3D contours be extending the edges of the contours to the ground from the valid height of the concentration data.

- -b[Bottom display level: (0) m]

  = 0 - Represents the height (meters) below which no data will be processed for display. The level information is interpreted according to the display (-d) definition.

- -c[Contours: (0)]

  = 0 - Dynamic contour values (10x intervals) are optimized for each map.
  = 1 - Fixed contour values (10x intervals) are the same for all maps.
  = 2 - Dynamic contour values (constant interval) are optimized for each map.
  = 3 - Fixed contour values (constant interval) are the same for all maps.
  = 4 - The contours are set by the user in conjunction with -v option.
  =50 - Force contour interval x10 and set dynamically for each frame.
  =51 - Force contour interval x10 and set as fixed for all frames.

- -d[Display: (1)-by level, 2-levels averaged]

  = *1* - All output levels that fall between the bottom and top display heights are shown as individual frames. A single level will be displayed if both bottom and top heights equal the calculation level or they bracket that level. Deposition plots are produced if level zero data are available in the concentration file and the display height is set to 0.

  = *2* - The concentrations at all levels between the specified range are averaged to produce one output frame per time period. If deposition data is available and a plot is required in addition to the air concentrations, then the bottom height should be set to 0. Deposition is not averaged with air concentrations.

- -e[Exposure units flag: (0)-concentrations, 1-exposure, 2-threshold, 3-special, 4-mass loading]

  = 1 - A custom output format in which all the air concentrations have been converted to time-integrated units and vertically averaged for all levels between the bottom and top heights.

  = 4 - A custom output format in which all the air concentrations have been converted to mass loading.

- -f[Frames: (0)-all frames one file, 1-one frame per file]

  = 0 - All output frames (one per time period) in one file.
  = 1 - Each time period is written to a file: concplot{frame number}.ps

- -g[Graphic circle overlay: ( )-auto, 0-numb, numb:dist(50) km]

  = ( ) - Auto selection procedure draws four circles with the distance between them determined by the program algorithm.

  = # - Specifies the number of circles with the default (50 km) distance interval.

  = number:distance - specifies the number of circles and the distance interval between circles. For the special case of zero circles with a distance specified (e.g. -0:1500) the program will fix the map with the top and bottom edge at that distance from the center.

- -h[Hold map at center lat-lon: (source point), lat:lon]

  = lat:lon - Forces the center of the map to be at the specific latitude-longitude point rather than the default source location. This is normally used in conjunction with the -g option to get the same map each time or when there are multiple source locations.

- -i[Input file name: (cdump)]

  = Name of the binary concentration file for which the graphics will be produced. Default name {cdump} or user defined}.

- -j[Graphics map background file name: (arlmap)]

  The program first searches the local directory, then the ..\graphics directory for the name of the default map background file (arlmap). Set this parameter to select the directory/name of any map background file of compatible format or specify a special file of shape file file names.

- -k[Kolor: 0-B&W, (1)-Color, 2-No lines Color, 3-No lines B&W]

  = 0 - Uses gray shade patterns for the contour color fill.
  = 1 - Uses the default four color fill pattern.
  = 2 - Default color fill pattern but without black contour lines.

= 3 - Black and white color fill but without black contour lines.

- -l[Label options: ascii code, (73)-open star]

  The default plot symbol over the source location is an open star. This may be changed to any value defined in the psplot ZapfDingbats library. For instance a blank, or no source symbol would be defined as -l32

- -L[LatLonLabels: 0=none, (1)=auto, 2=set:{value tenths}]

  = 0 - No latitude or longitude lines are drawn on the map
  = 1 - Latitude and longitude lines spacing is determined automatically
  = 2:tenths - line spacing is determined by the given value in tenths

- -m[Map projection: (0)-Auto, 1-Polar, 2-Lambert, 3-Mercator, 4-CylEqu]

  Normally the map projection is automatically determined based upon the size and latitude of the concentration pattern. Sometimes this procedure fails to produce an acceptable map and in these situations it may be necessary to force a map projection.

- +m[Max-Min value plotting: 0=none, (1)=both, 2=values, 3=max-square]

  The default (1) prints the maximum and minimum values below the contours and plots a red square, the size of the concentration grid, at the location of the maximum concentration value. These can be turned off individually using this command line option. Note the +m rather than -m prefix.

- -n[Number of time periods: (0)-all, number, min:max,-increment]

  = 0 - All time periods in the input file are processed.
  = # - Sets the number of time periods to be processed starting with the first.
  = #1:#2 - Processes time periods, including and between #1 and #2.
  = [-#] - Sets the increment between time periods to be processed. For instance, -n-6 would only process every 6th time period.

- -o[Output file name: (concplot.ps)]

  The name of the Postscript output file defaults to concplot.ps unless it is set to a {user defined} value.

- -p[Process file name suffix: (ps) or process ID]

  The suffix defines the character string that replaces the default "ps" in the output file name. A different suffix does not change the nature of the file. It remains Postscript. The suffix is used in multi-user environments to maintain multiple independent output streams.

- -q[Quick DATEM plot file: ( )-none, filename]

  By defining the name of a text file in this field where the data values are defined in the DATEM format, the values given in the file will be plotted on each graphic if the starting time of the sample value falls within the averaging period of the graphic.

- -r[Removal: 0-none, (1)-each time, 2-sum, 3-total]

  = 0 - No deposition plots are produced even if the model produced deposition output.
  = 1 - One deposition plot is produced for each time period.
  = 2 - The deposition is summed such that each new time period represents the total accumulation.
  = 3 - Similar to =2, deposition is accumulated to the end of the simulation and but only one plot is produced at

the end.

- -s[Species: 0-Sum (1)-Single Pollutant {N}-Species Number]

  = {Species Number} - Only one pollutant species may be displayed per plot sequence if multiple species were created during a simulation. However, an entry of "0" will cause all species concentrations to be summed for display.

- -t[Top display level: (99999) m]

  = 99999 - Represents the height (m) above which no data will be processed for display. The level is interpreted according to the display definition.

- -u[Units label for mass: (mass), also see "labels.cfg" file]

  Defines the character string for the units label. Can also be modified using the labels.cfg file.

- -v[Values (:labels:colors are optional) for up to 10 fixed contours: val1+val2+...val10]

  If the contour values are user set (-c4), then it is also possible to define up to ten individual contours explicitly through this option. For instance -v4+3+2+1, would define the contours 4, 3, 2, and 1. Optionally, a label and/or color (RGB) can be defined for each contour (e.g. -v4:LBL4:000000255+3:LBL3:000255255+2:LBL2:051051255+1:LBL1:255051255). To specify a color but not a label, two colons must be present (e.g. -v4::000000255).

- -w[Grid point scan for contour smoothing (0)-none 1,2,3, ... grid points]

  Defines if the gridded concentration data are to be smoothed prior to contouring. For instance, a value of 1 means that each grid point value is replaced by the average value of 9 grid points (center point plus 8 surrounding).

- -x[Concentration multiplier: (1.0)]

  = 1.0 - No units conversion.
  = X - where {X} is the multiplier applied to the air concentration input data before graphics processing.

- -y[Deposition multiplier: (1.0)]

  = 1.0 - No units conversion.
  = X - where {X} is the multiplier applied to the deposition input data before processing.

- -z[Zoom factor: 0-least zoom, (50), 100-most zoom]

  = 50 - Standard resolution.
  = 100 - High resolution map (less white space around the concentration pattern)

Additional supplemental text may be added at the bottom of the graphic by creating a file called *MAPTEXT.CFG*, which should be located in the working directory. This is a generic file used by all plotting programs but each program will used different lines in its display. The file can be created and edited through the Advanced / Panel Labels menu tab. Units and title information can be edited by creating a *LABELS.CFG* file which can also be edited manually or through the Advanced / Border Labels menu tab.

ESRI Shapefile Map Background Files

Another mapping option would be to specify a special pointer file, (origianlly called *shapefiles.txt*, but now a suffix other than "txt" is permitted) to replace the map background file arlmap in the -j command line option (see above). Note -jshapefiles... rather than -j./shapefiles... is required. This file would contain the name of one or more shapefiles that can

be used to create the map background. The line characteristics (spacing, thickness, color) can be specified for each shapefile following the format specified below:

Record format: 'file.shp' dash thick red green blue
file.shp = /dir/name of input shapefile in quotes
dash = {0} for solid; {dashes}/in; <0 color fill
thick = line thickness in inches (default = 0.0)
Red Green Blue = RGB values (0.0 0.0 0.0 is black)
Record example for default: 'arlmap.shp' 0 0.005 0.4 0.6 0.8

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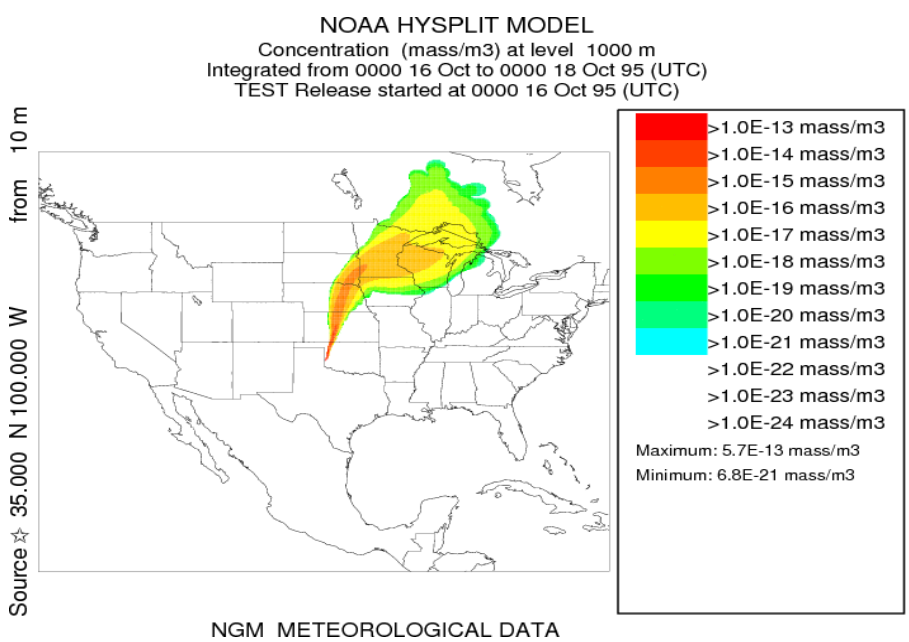
Concentration / Display / Grid Values

A generic Postscript equivalent of the Windows-only concentration grid point data display program is available through this menu. This particular program (*gridplot*) was designed to plot global sized concentration grids, although any sized grid may be displayed. Concentration values over the entire grid (or a zoomed area) will be shown using a color-fill in each grid cell according to its concentration value. The options available through the GUI are setting the input file, output file, lowest contour value, contour interval, species number, linear or logarithmic scaling, and the longitude offset, the center latitude, the zoom factor, the concentration multiplier, and the choice of GIS output. By default, each time period is output to a different file name, gridplot_{???}.ps, where the sequence number {???} is incremented by one for each time period. When called from the *Global Grid* menu tab, the default output file name is gemplot rather than gridplot.

Several other options are available through the command line, which may be needed if multiple levels have been written to the concentration output file. **USAGE: gridplot -[options(default)]**

-i[input file name (cdump.bin)]
-p[Process output file name suffix]
-o[output name (plot.ps)]
-l[lowest interval value (1.0E-36), -1 = use data minimum]
-m[multi frames one file (0=no) 1=yes]
-c[concentration multiplier (1.0)]
-d[delta interval value (1000.0)]
-s[species number to display: (1); 0-sum]
-h[height of level to display (m) (integer): (0 = dep)]
-j[Graphics map background file name: (arlmap)]
-a[scale: 0-linear, (1)-logarithmic]
-x[longitude offset (0), e.g., o--90: U.S. center; o-90: China center]
-y[latitude center (0), e.g., 40.0: U.S. center]
-f[(0), 1-ascii text output files for mapped values]
-g[GIS: 0-none 1-GENERATE(log10) 2-GENERATE(value) 3-KML 4-partial KML]
-k[KML options: 0-none 1-KML with no extra overlays]
-u[mass units(ie, kg, mg, etc); note these are labels only]
-z[zoom: (0)-no zoom, 99-most zoom]



When called from the *Global Grid* menu tab, an additional feature is available through the *Add Plume* checkbox. In this

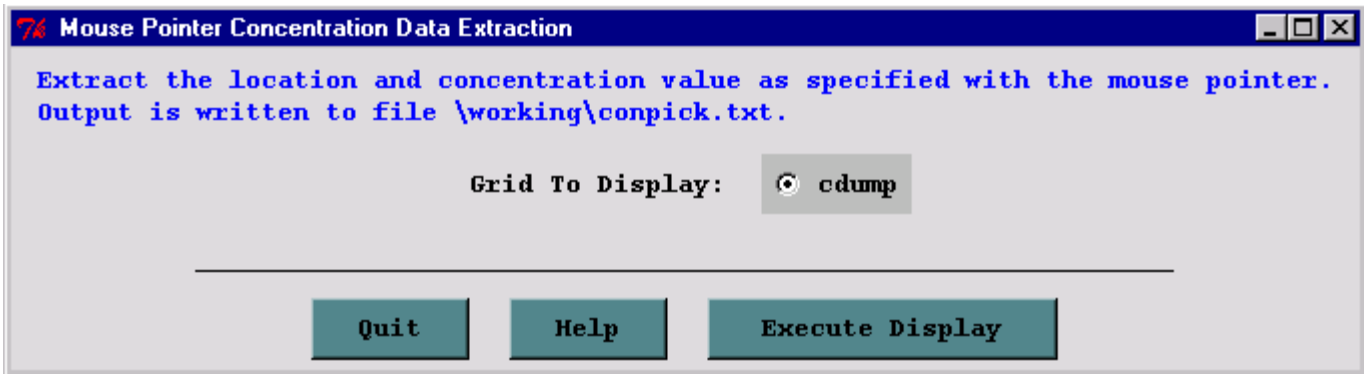
case, the first plume model concentration grid (if more than one is defined) is added to the global model concentration grid as defined in this menu. The merged concentration file is called *concadd.bin* which is then displayed by *gridplot*. The two concentration files that are added must be identical in terms of the number levels and pollutants. However, the spatial grid characteristics may be different. The height of the levels at each index do not have to be identical. If this issue is important, then the heights heights corresponding to the global model heights needs to be set in the CONTROL file setup menu. Note that the global model vertical heights cannot be changed by the user and correspond with the heights of the meteorological data levels. The horizontal characteristics of the output grid always takes the grid dimensions of the second grid (-b).

USAGE: concadd -[options(default)]

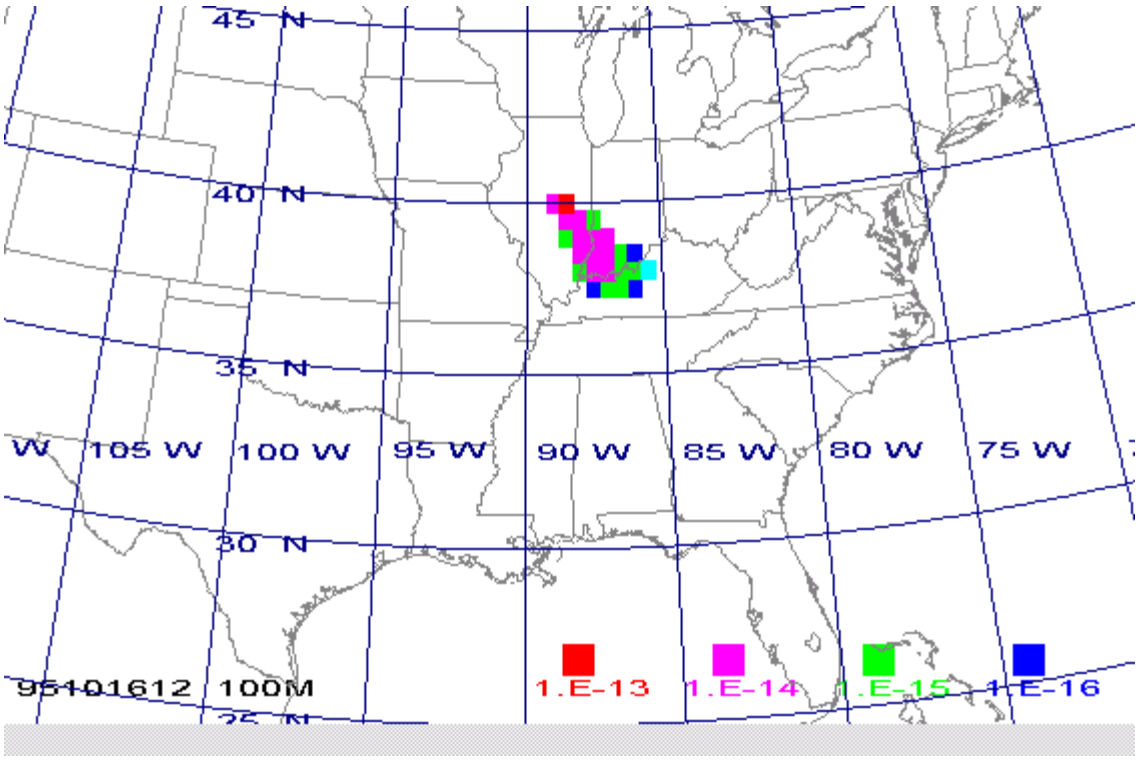
```
-i[input file name (cdump)]
-b[base file name to which input is added (gdump)]
-o[output file name with base format (concadd.bin)]
-g[radius (grid points around center) to exclude; default=0]
-c[concentration conversion factor (1.0)]
-p[sum process (0)=add | 1=max value | 2=zero mask | 3=intersect]
| 4=replace]
-z[zero mask value (base set to zero when input>mask; default=0.0)]
if zero mask value < 0 :
base set to zero when input> zero mask value * base
```

Concentration / Display / Pointer Select

The Windows-only concentration data point registration program is designed to read the binary concentration data file, display the data on the screen, and then use the mouse as a pointer device to pick locations at which the position and concentration data are read and written to the text file: *wincpick.txt*. The concentration data are displayed over the entire grid domain. There are no zoom options. If you want to zoom in on a specific area, then it is necessary to rerun the model with a smaller concentration grid domain. The program is available from the GUI or the command line with the following syntax: *wincpick [input file name]*. The GUI menu, which is shown in the illustration below, only permits selection of the concentration input file name, which must have been previously defined in the Concentration Setup menu.



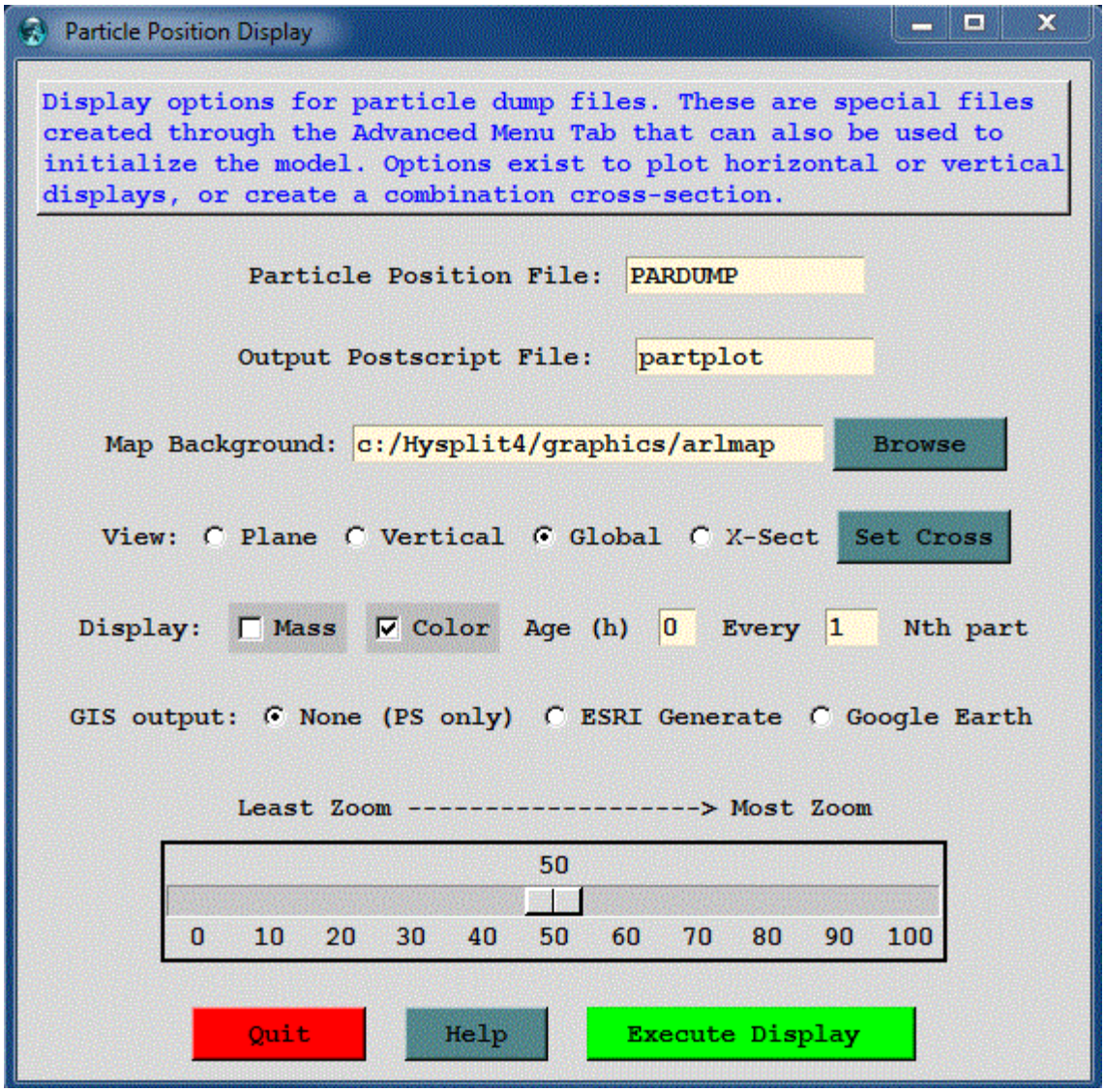
Upon startup, *wincpick* will display the domain background map with a summary of the mouse-based instructions: **left-click** registers the latitude-longitude position of that point to the output file *wincpick.txt*. A **right-click** of the mouse redraws the map for the next time period and at the end of the input file saves and closes all files; and a **CNTL-right-click** closes all files and exits the program before the end of the input file. **Right-click** the mouse to go to the first concentration map. Maps are drawn in sequence of height, pollutant species, and time. **Left-clicks** register the position of the mouse to the output file. If you are interested in only one time period, skip past those times by a **right-click**, register the points of interest, then **CNTL-right-click** to exit. An illustration of the first output period from the sample calculation is shown below.



Concentration / Display / Particle

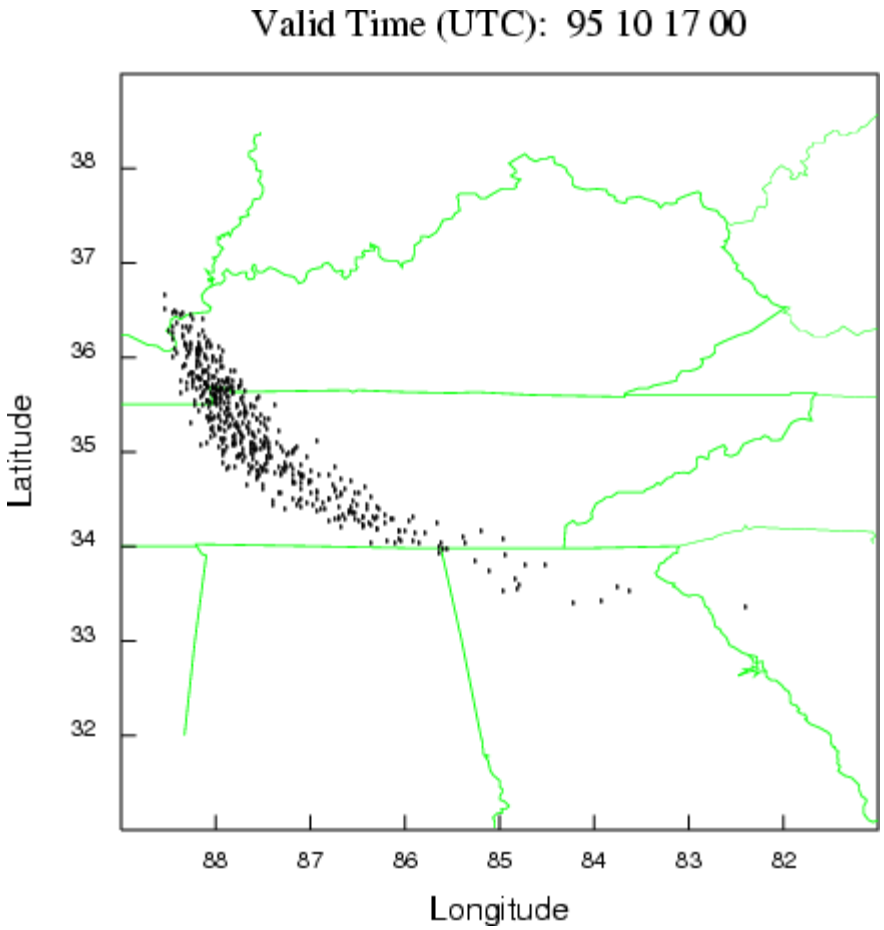
In addition to the normal display programs for air concentrations, which are designed to display and contour the actual values, the particle display programs only show the instantaneous positions of the pollutant particles or puffs that are integrated in time by the model to produce the air concentration fields. To generate the particle position graphics from this menu it is necessary to generate a particle dump file (default name: PARDUMP), which may contain one or more time periods of output. The creation of this file is controlled by the parameters set in the menu tab: "Advanced / Configuration Setup / Concentration."

The particle display menu requires the name of the particle position input file, the base name of the Postscript output file, the type of particle display requested, and some additional options. Setting the mass checkbutton changes the size of the particle display dot according to its mass, the color option sets the dot color rather than just black. The color is set according to the height of the particle or if the age value is non- zero, then the color is set according to the particle age. The GIS option is (*valid only for the horizontal plot*) and it will output either the ESRI generate format file or a Google Earth KML file. If there are too many particles, the density of the display can be reduced by plotting only every Nth particle, the default is 1 to display every particle. The *Set Cross* button permits the specification of the actual cross-section vector, rather than letting the program determine it automatically. Note that similar to the trajectory and concentration plotting programs, shapefiles can also be defined for the map background.

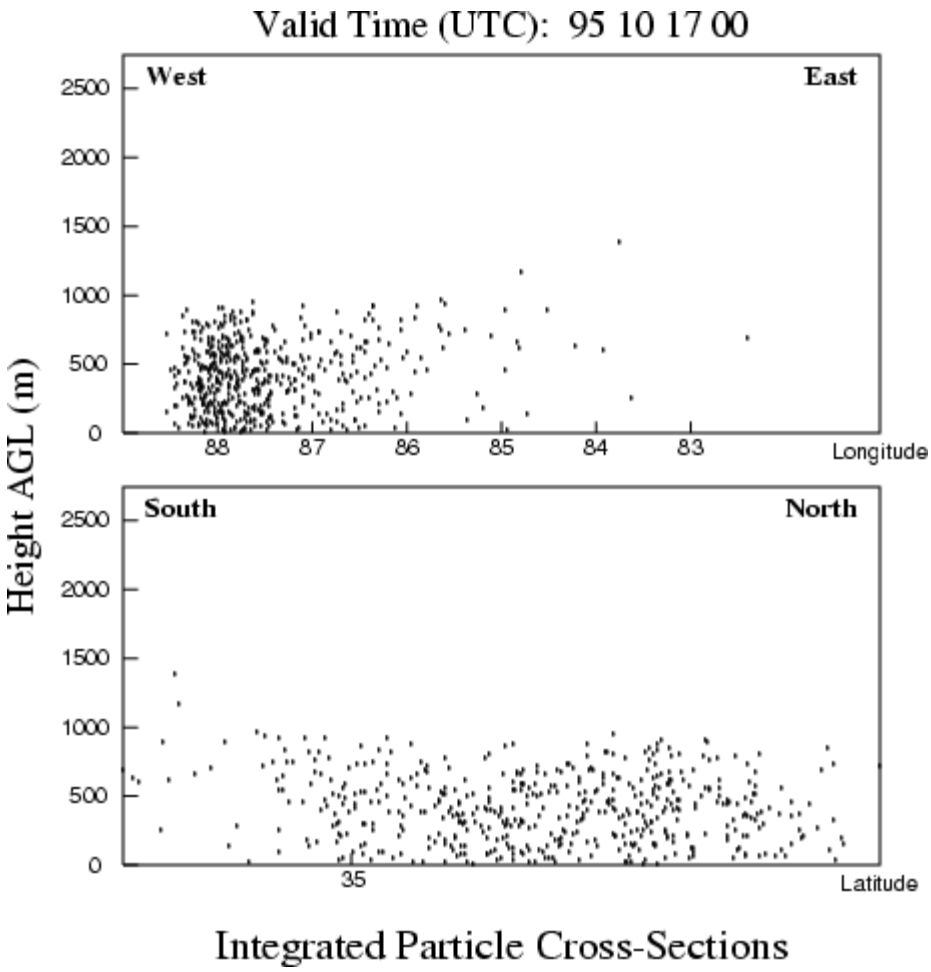


The "Plane" option results in the conventional graphic shown below of the horizonal plane view. There is one black dot for each particle. The size of the dot varies according to the pollutant mass assigned to the particle. All examples are 12

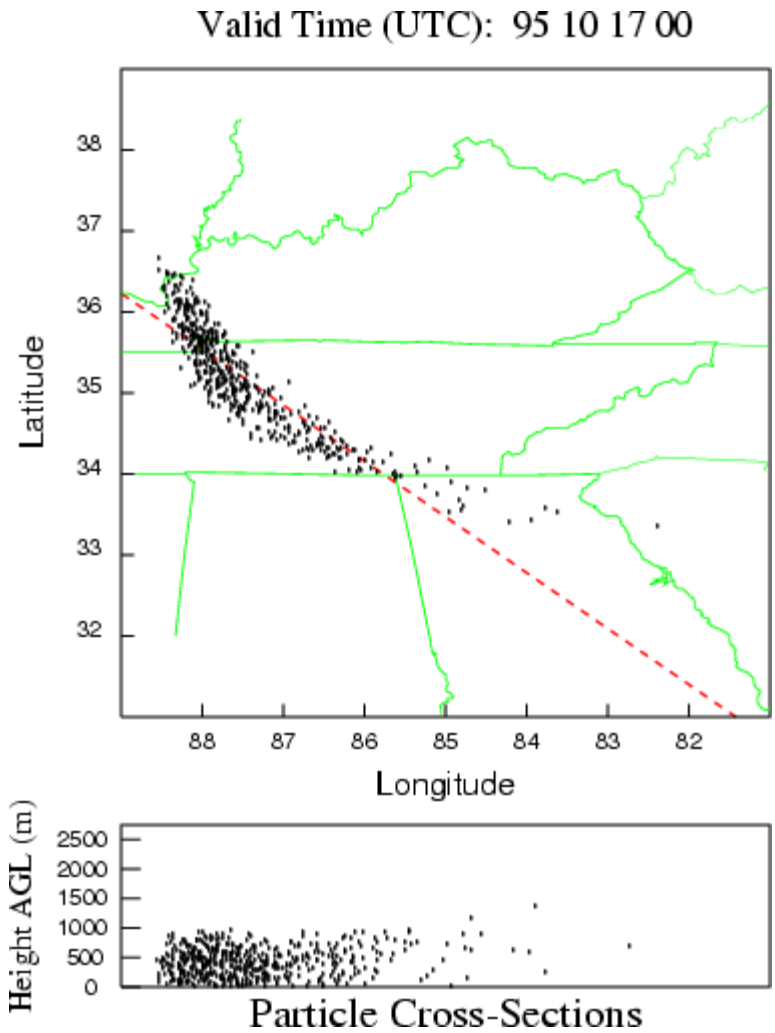
or 24 hours after the start of the test simulation.



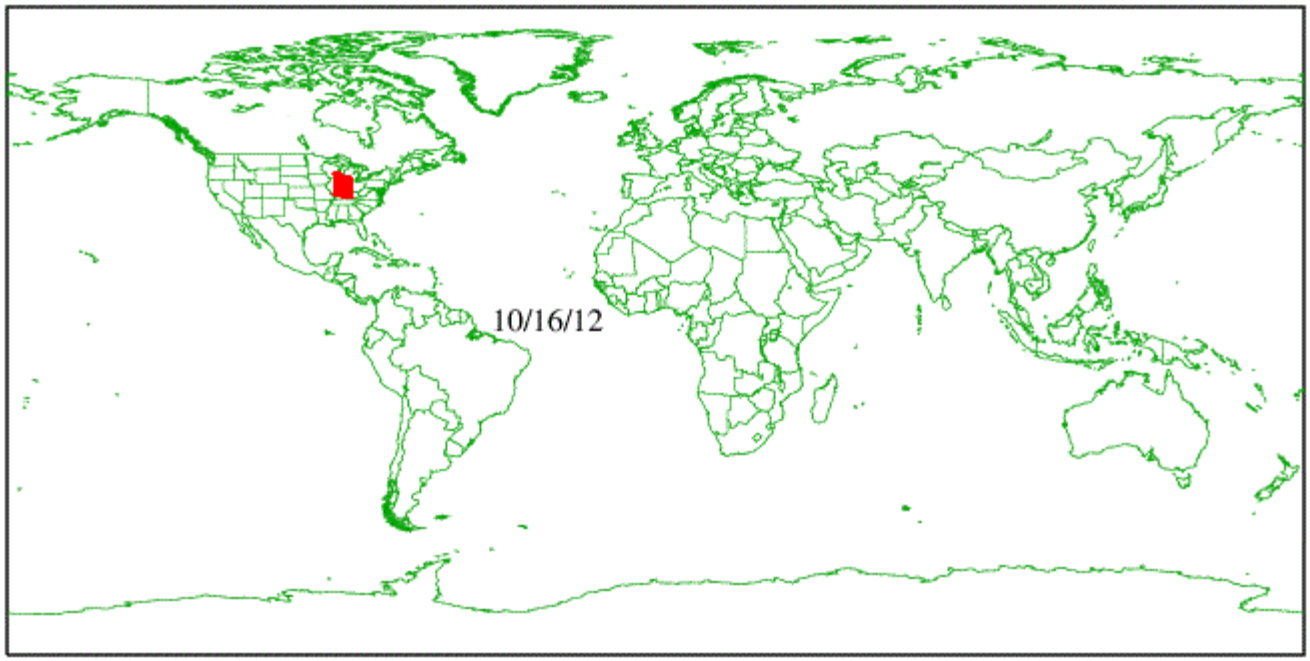
The "vertical" option shows an integrated particle distribution view from the south looking north (top panel) and from the east looking west (bottom panel). All particles in the computational domain are shown.



The "cross-section" view is a combination of the horizontal plane and vertical views. The top panel shows the horizontal particle distribution, while the bottom panel shows the vertical distribution along the red regression line through the plume. Again all particles are shown regardless of their distance from the regression line. The bottom panel view is from left to right in increasing longitude, regardless of the orientation of the regression line.



The global display is a special program that will always map the particles on a global equidistant projection. The other programs try to automatically scale the plots according the to particle distribution, sometimes resulting in distorted plots when the particle coverage becomes global. There are additional command line features in this program (*parsplot*) for particle size and color mapping according to the particle mass that are not available through the GUI.



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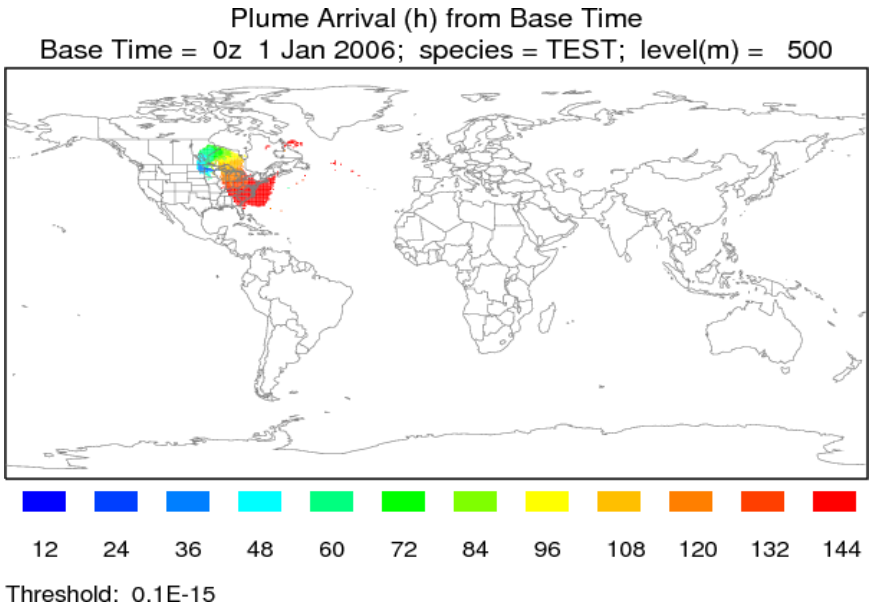
Concentration / Display / Time-of-Arrival

Time of arrival graphic (isochron) shows the time after the start of the simulation that the concentration exceeds the given threshold concentration at each concentration grid cell. The default contour interval (-1) uses the concentration averaging period. Otherwise, the time difference field should be set to hours. A text label with release information may be printed below the threshold through the LABELS.CFG file.

The GUI and the command line options are similar with the command line syntax as follows: **USAGE: isochron -[options(default)]**

-c[color fill no:0 yes:(1)] : the =0 option results in contours
-d[difference in hours between contours (-1)]
-f[frames: (0)-all frames one file, 1-one frame per file] : multiple frames can only be due to multiple levels or species in the input file
-i[input file name (cdump)] : the input file needs to contain multiple time period
-j[graphics map background file (arlmap)] : the shape file option is not available
-n[number of contours (12)] : only 12 contours fit across the display
-o[output name (toa)] : the output file represents all time periods
-p[Process file name suffix: (ps) or process ID] -t[threshold value (1.0E-36)]

In the 144 hour duration example simulation shown below, the concentration field was output every six hours, the contour interval was set to 12 hours, and the threshold to 0.1E-15 . The one hour duration release took about 72 h to reach Hudson's Bay and about 144 h to reach into the Atlantic off the east coast of the U.S.

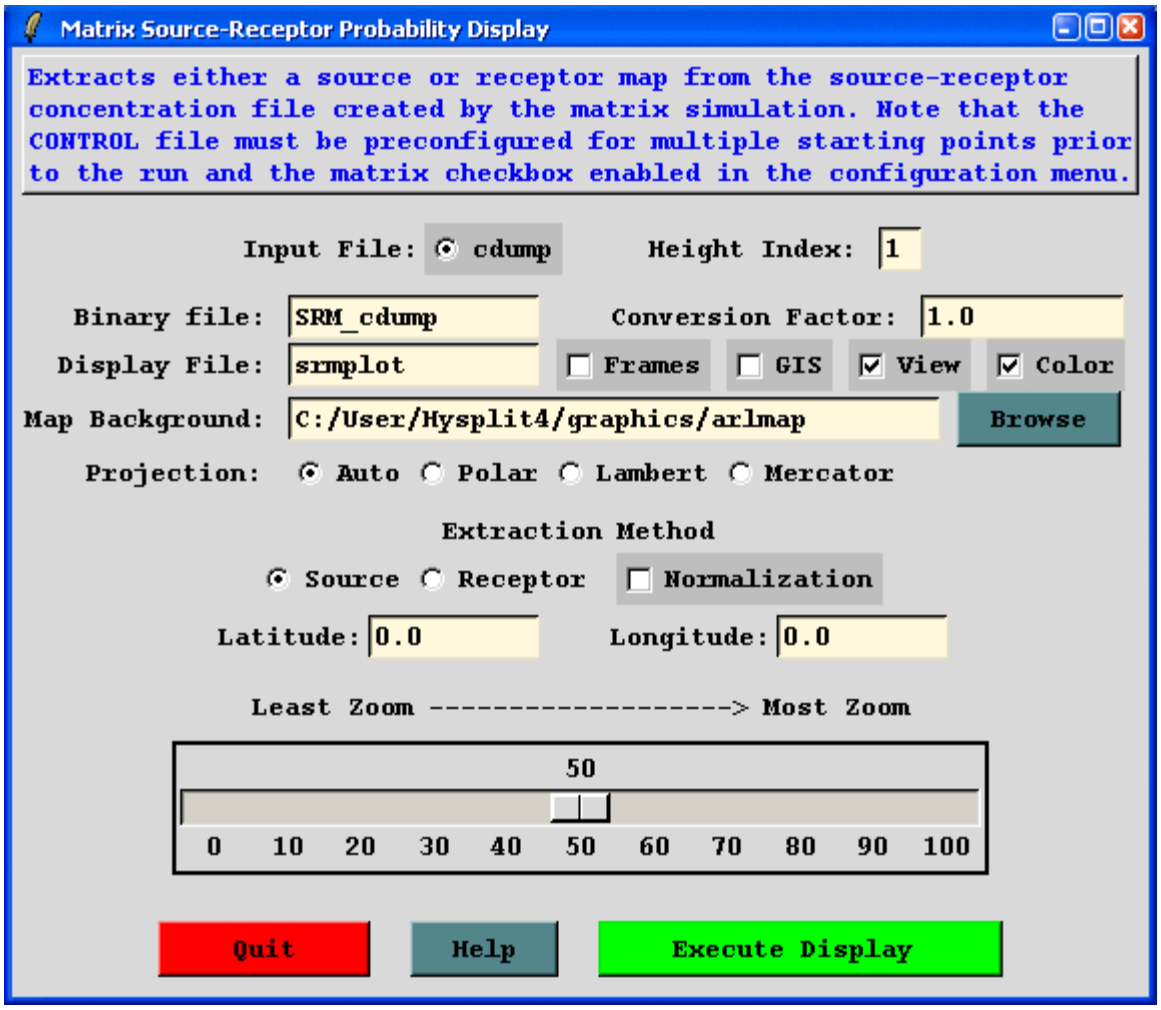


Concentration / Display / Source-Receptor View

This menu option permits the extraction of information for a specific source or receptor if the original model simulation was configured to produce a source-receptor matrix formatted output file. The model should have been run with the matrix option set in the configuration menu. This results in a special concentration output file that may be called a source- receptor matrix, such that each column may be considered a receptor location and each row a pollutant source location. The display program under this menu tab permits the contouring of any row or column.

If the matrix option was not set in the Advanced Concentration configuration tab, then the output file produced is a simple concentration output file, where the concentrations from all the sources of the defined matrix are summed on a single concentration output grid. Source-receptor information cannot be extracted from such a file.

When a location is selected in the menu, a special program is called to extract that location from the concentration matrix output file and then write a standard concentration file for that location. The standard concentration display program is then used to display the information in the extracted file. The source-receptor matrix binary extraction file name will default to *SRM_{original file name}*, but can be changed in the menu. The *Display Matrix* menu, shown in the illustration below, automatically creates the extraction file, calls the standard display program *concplot*, and provides for additional custom label information to identify the plot as a source-receptor concentration matrix.



The menu consists of the standard display options such as the map background file, output file name, zoom factor, and the selection of the extraction method: source or receptor. A latitude and longitude point needs to be entered for all extractions. Selection of the *"source"* extraction method means that the location entered is considered to be the source location and the resulting output is a contour map is just a conventional air concentration simulation showing concentrations from that source. The *"receptor"* extraction method means that the location entered is considered to be

the receptor location and the output is a map of how much air concentration each source contributes to the selected receptor. Note that turning on the "normalization" flag divides all concentrations by the sum of all concentrations at each grid point, resulting in a map that represents a fractional contribution. In addition, a concentration conversion factor can be defined, which will be applied to the binary file before it is contoured.

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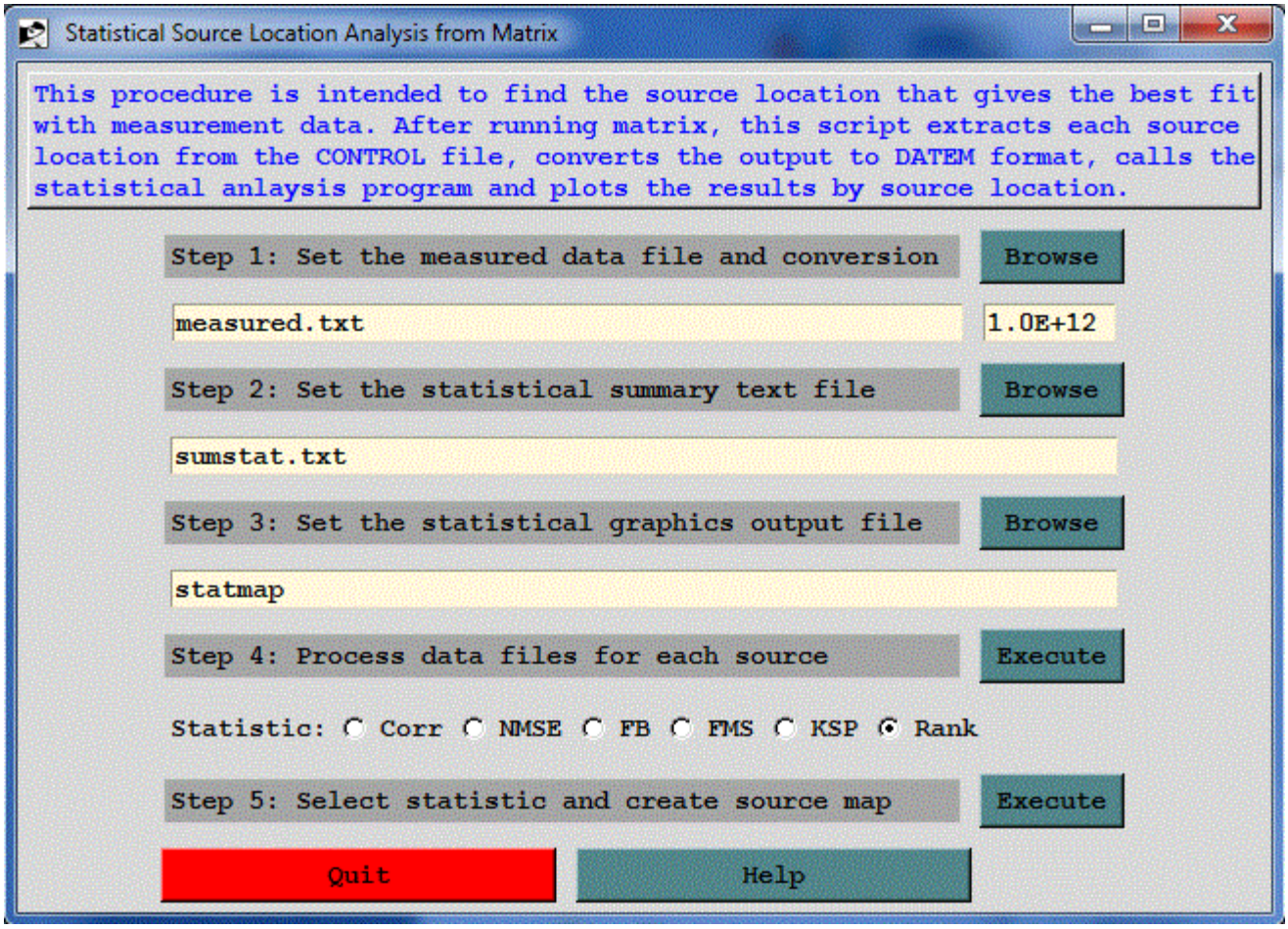
Concentration / Display / Source-Receptor / Stats

Summary: This procedure is intended to find the source location that provides the best fit with measurement data. After running HYSPLIT with the matrix option and ICHEM=1, the script extracts each source location from the CONTROL file, converts the output to the DATEM format, and then calls the statistical anlaysis program which is converted to a gridded binary file which can be plotted by any of the standard concentration plotting programs.



Step 1: defines the DATEM formatted measured data file and unit conversion factor required to convert the HYSPLIT concentration predictions to the same units as given in the measured data file.

Step 2: defines name of the statistical output file that will contain the statistical results from each source location compared with the measured data values. Normally the *statmain* program outputs one results file per execution. In this configuration, the results form each source location are appended to a single file, one record per source.

Step 3: defines the root name of the final output graphics file which will show a plot of the statistical results by source location. The *.ps* suffix is created by default.

Step 4: runs sequentially through all steps of the process, reading each source location from the *CONTROL* file, running *matrix* to extract that location from the HYSPLIT simulation output file, using *c2datem* to convert that binary extract to the DATEM format, and then running *statmain* to append the results to the statistical output file. This step needs only to be run once.

Step 5: defines which statistic will be shown: Corr - correlation coefficient, NMSE - normalized mean square error, FB - fractional bias, FMS - figure of merit in space, KSP - Kolomogorov Smirnoff parameter, and finally the rank, which is a combination of the previous parameters. Once all source locations have been processed, the statistical file is read and

converted to binary gridded format using *stat2grid*. This output file can then be plotted with any of the display programs such as *gridplot*.

Default file names: The following describes the assigned default input and output files names for each processing section, so that they can be identified in the working directory. File names in italics are the ones that can be changed through the menu.

matrix

- *cdump* - binary outfile from a single multi-source simulation using the ICHEM=1 option
- SRM_cdump - binary concentration output file extracted for one source location

c2datem

- SRM_cdump - binary concentration input file from the previous step
- *measured.txt* - measured data file in DATEM format
- hysplit_datem.txt - model prediction output for a single source converted to DATEM format

statmain

- *measured.txt* - measured data input file in DATEM format
- hysplit_datem.txt - model prediction input file for a single source from previous step
- *sumstats.txt* - statistical summary output appended one record per source location

stat2grid

- *sumstats.txt* - statistical summary input file from previous step
- statmap.bin - binary statistical output file gridded in the HYSPLIT concentration format

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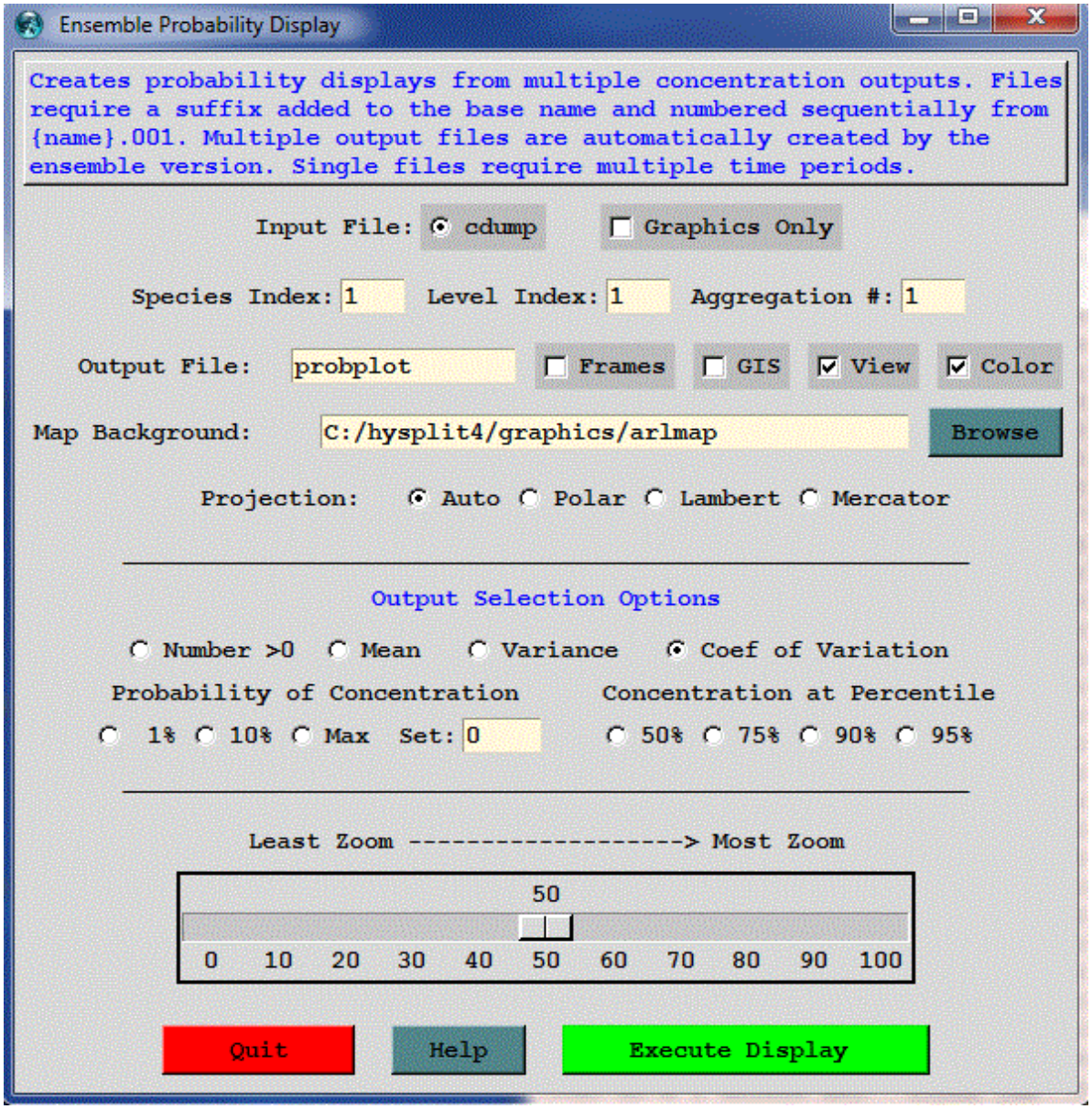
Concentration / Display / Ensemble Map

Multiple concentration output files from the ensemble or variance dispersion simulation can be processed to produce probability displays. The *Ensemble View Map* menu calls a special program *conprob* that reads the concentration files with the ensemble member three-digit suffix (001 to 027) and generates various probability files when the *Graphics Only* box is NOT checked. When this box is checked, then the existing probability files are used to generate all graphics. The appropriate files are then plotted using *concplot* according to the menu selection options. Note that the ensemble display menu can be used to convert multiple concentration output files to probability form, regardless of how they were generated. It is not necessary to use the pre-configured ensemble version of the model to create air concentration probability maps. Any number of multiple simulations can be used as long as the file suffixes end with a numeric three-digit sequence. Menu settings for the output file name should reflect the base name without the numeric suffix. An illustration of the *Ensemble Display* menu is shown below.



The menu includes some of the standard display program (*concplot*) mapping choices, such as background file, output file name, and zoom factor. One critical difference is that there is an option called *Aggregation #*. By default this value is set to one, which means that only the ensemble members for one time period are aggregated together to produce the probability display. Hence there would be an independent probability map for each time period. However, multiple time periods may be combined to produce a single probability plot. The entry represents the number of time periods,

not the actual time span. For instance, if the model output is set to produce a one-hour average and the model is run for 24 hours, then each ensemble member will have 24 time periods of output. By default the probability output will represent the ensemble member variation for each hour, that is 24 frames of output will be produced. However if the aggregation period is set to 24, then all output times will be combined into one output frame and the ensemble result will represent the hourly variations as well as the member variations.

The menu permits a choice of six different ensemble output display options:

1. The **number** of ensemble members at each grid point with concentrations greater than zero shows the spatial distribution of the *Number of Ensemble* members.
2. The **mean** concentration of all ensemble members.
3. The **variance** of all ensemble members (the mean square difference between individual members and the mean).
4. The **coefficient of varition** of all ensemble members (sqrt(variance)*100/mean).
5. The **probability of concentration** produces contours that give the probability of exceeding a fixed concentration value at one of three levels: 1% of the maximum concentration, 10% of the maximum, and the maximum concentration. The maximum is determined to be the first concentration to a power of 10 that is less than the actual maximum value or the value of the maximum set in the data entry box (exponent of 10). The concentration level for the probability display is shown on the graphic with the pollutant identification field set to something like C14, where 14 represents the concentration to the power of 10^{-14}.
6. The **concentration at percentile** levels shows the concentration contours of areas where concentrations will be exceeded only at the given probability level. Although several output levels are computed, the probability level choices through the menu are limited to 50, 90, and 95th percentiles.

The *conprob* extraction program will always produce all the probability variations, one to each output file, for a given aggregation period. If the graphics only checkbox is marked, then the menu skips computing the probability files and uses the existing files in the working directory. The output files may also be plotted individually from the command line using *concplot*. The *conprob* output files contain the following information:

- Cnumb - Number of members
- Cmean - Concentration mean of all members
- Cvarn - Concentration variance of all members
- Ccoev - Concentration coefficient of variation of all members
- Cmax05 - Probability of 5% of the concentration maximum
- Cmax10 - Probability at 10% of the concentration maximum
- Cmax00 - Probability at the maximum concentration level
- Prob10 - Concentrations at the 10th percentile
- Prob25 - Concentrations at the 25th percentile
- Prob50 - Concentrations at the 50th percentile
- Prob75 - Concentrations at the 75th percentile
- Prob90 - Concentrations at the 90th percentile
- Prob95 - Concentrations at the 95th percentile

The command line options for the probability program **conprob [-options]** are as follows:

-b[base] input file name
-c[concentration maximum] value set
-d[diagnostics = true]
-p[pollutant] index number for multi-pollutant files
-t[temporal] aggregation period
-v[value] of concentration below which is assumed to equal zero
-z[level] index number for multi-level files

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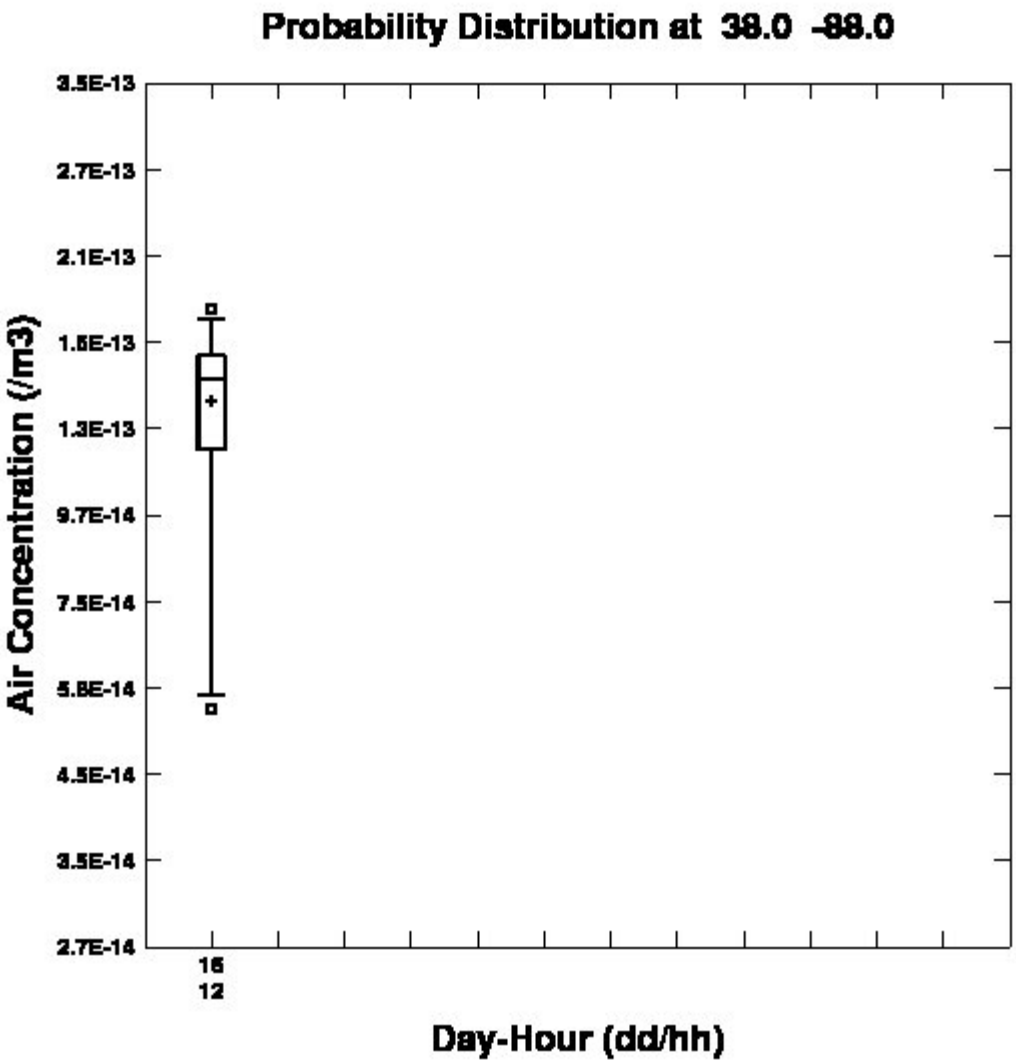
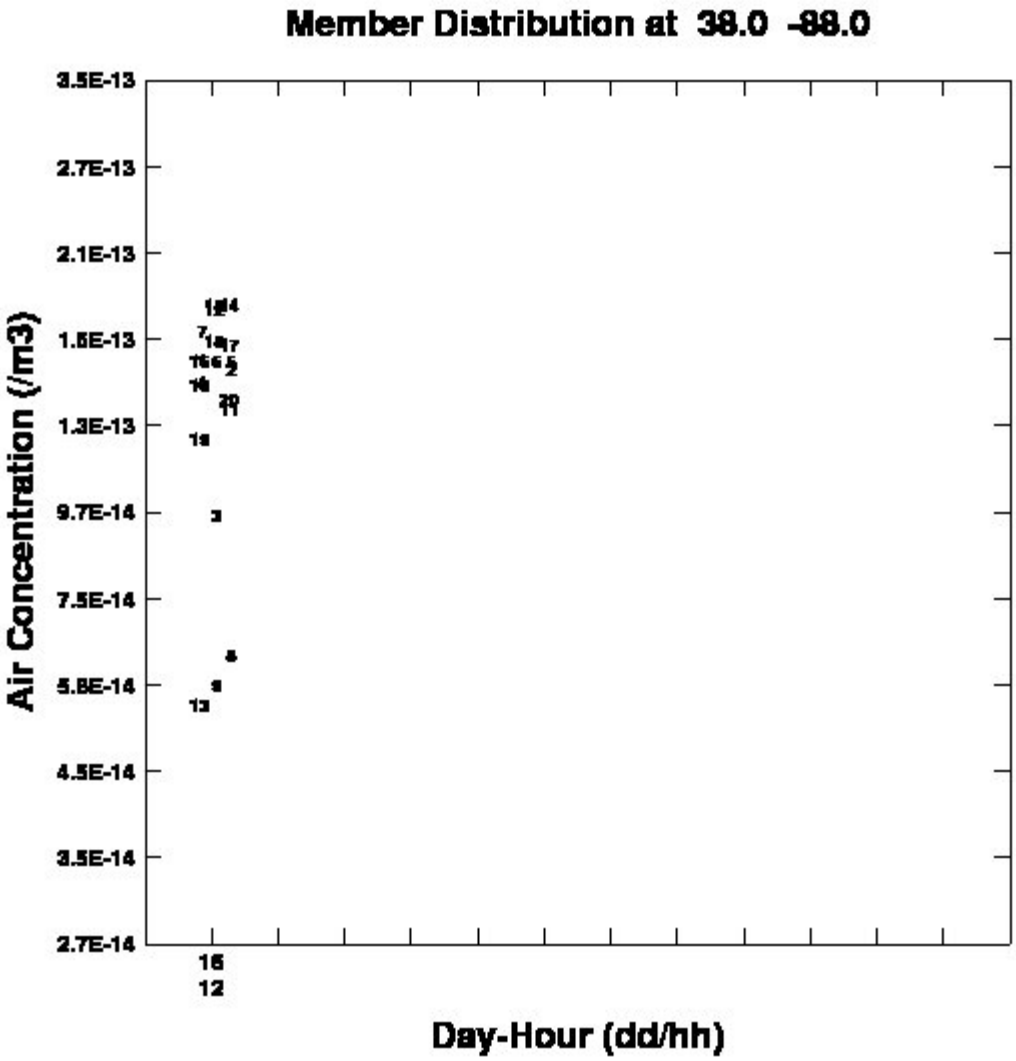
Concentration / Display / Ensemble Box Plot

Multiple concentration output files from the ensemble or variance dispersion simulation can be processed to produce probability displays. The *Ensemble / View Map* menu calls a special program *conprob* that reads the concentration files with the ensemble member three-digit suffix (001 to 027) and generates various probability files. Once these probability files have been created, the concentration distribution at a single location can also be viewed using this menu by entering a latitude-longitude location. The nearest grid point will be selected and the concentration values are retrieved from the prob{xx} files, which represent the various points on the box plot. In the illustration shown below, the limits of the box represent the quartiles (25th and 75th percentiles), the whisker extensions show the 10th and 90th percentiles, and the circles show the 5th and 95th percentiles. The median value is shown by the line through the box, while the mean is shown by the plus symbol. Up to 12 time periods can be shown in one plot. The graphic is always named *boxplots.ps*.



A second graphic called *ensplots.ps* is always produced using the individual ensemble concentration files. The abcissa and ordinate is identical to the boxplot, but the contents show the actual concentration values identified by member number, where the number is the same as the concentration file suffix.



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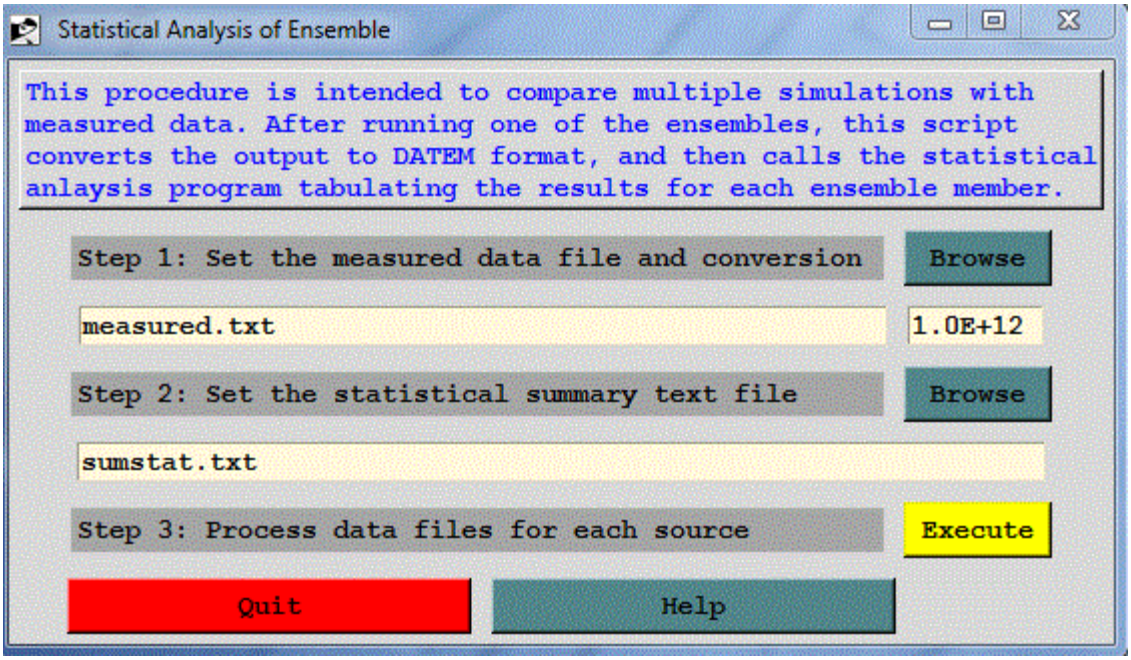
Concentration / Display / Ensemble / Statistics

Summary: This procedure is intended to analyze the binary output files from any of the ensemble simulations. The output file naming convention is such that they are defined by a base name set in the CONTROL file followed by a three digit sequential number suffix (.000). The ensemble simulation needs to be for a case in which experimental data are available for verification. The script converts the output to the DATEM format, and then calls the statistical anlaysis program which appends a statistical summary for each member to a single output file.



Step 1: defines the DATEM formatted measured data file and unit conversion factor required to convert the HYSPLIT concentration predictions to the same units as given in the measured data file.

Step 2: defines name of the statistical output file that will contain the statistical results for each ensemble member compared with the measured data values. Normally the *statmain* program outputs one results file per execution. In this configuration, a subset of the the complete results for each member are appended to a single file. The complete statistics are available in file named *stat_000.txt*.

Step 3: runs sequentially through all steps, processing each ensemble member using *c2datem* to convert that binary concentration data to the DATEM format, and then running *statmain* to append the results to the statistical output file.

Default file names: The following describes the assigned default input and output files names for each processing section, so that they can be identified in the working directory. File names in italics are the ones that can be changed through the menu.

c2datem

- {base name}.{xxx} - binary concentration input file, where xxx = 000 to 999
- *measured.txt* - measured data file in DATEM format
- hysplit_datem.txt - model prediction output for a member converted to DATEM format

statmain

- *measured.txt* - measured data input file in DATEM format
- hysplit_datem.txt - model prediction input file for a single source from previous step
- *sumstats.txt* - statistical summary output appended one record per source location

- stat_{xxx}.txt - complete statistics for each member

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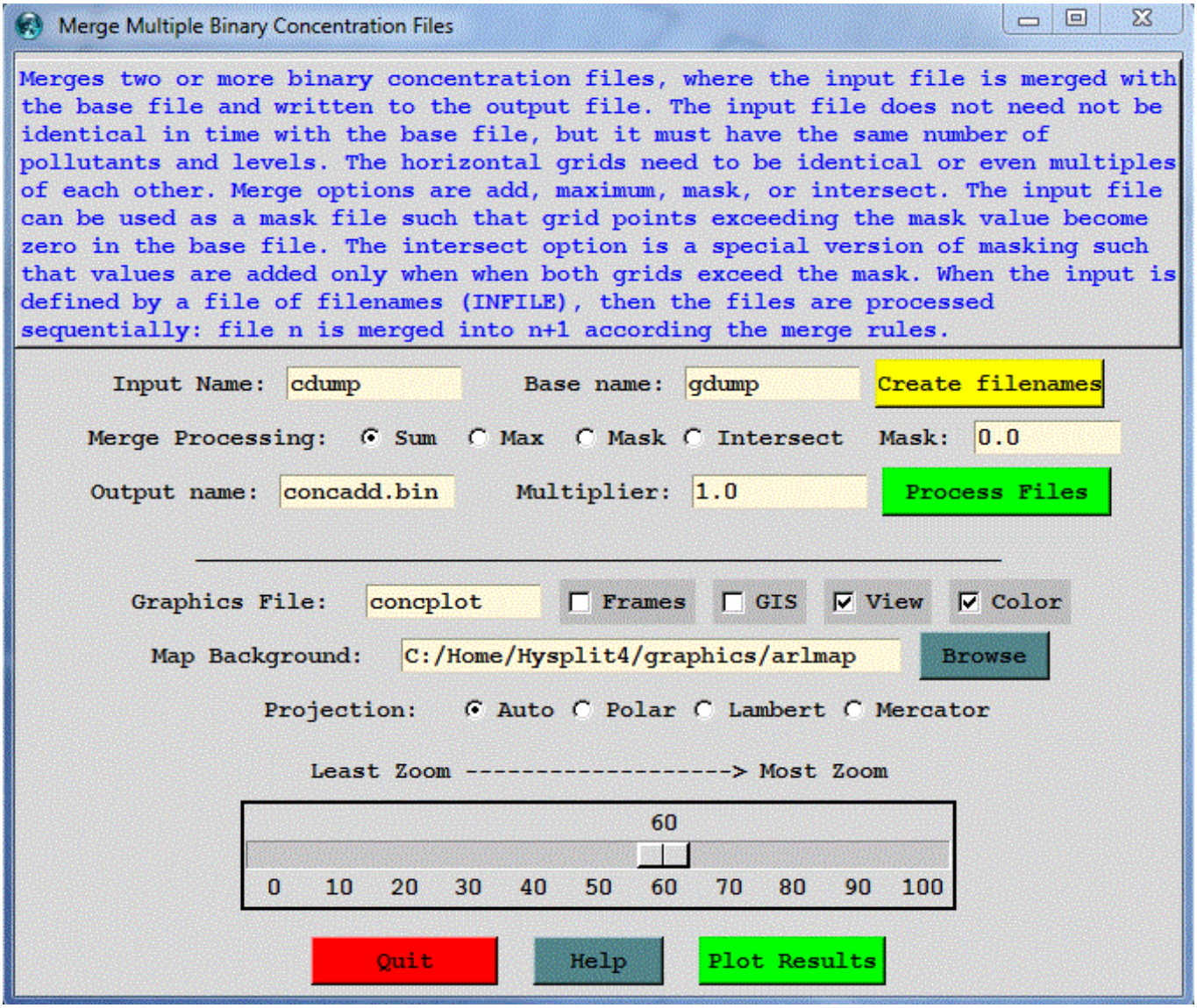
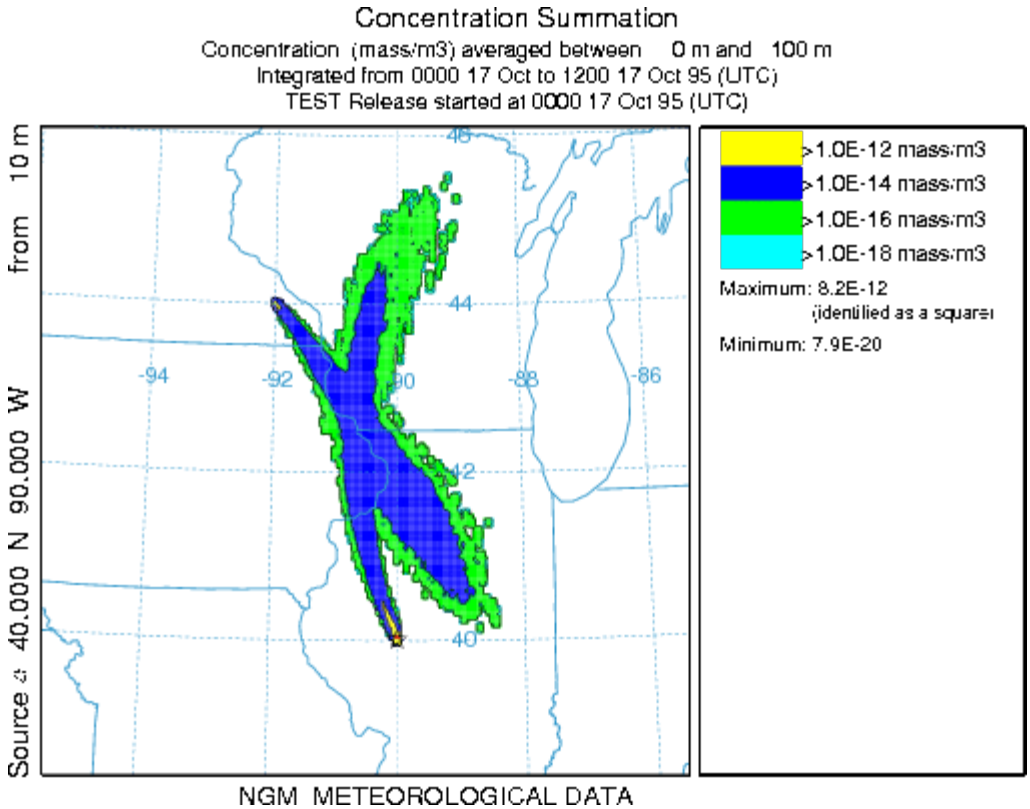
Concentration / Utilities / Binary File Merge

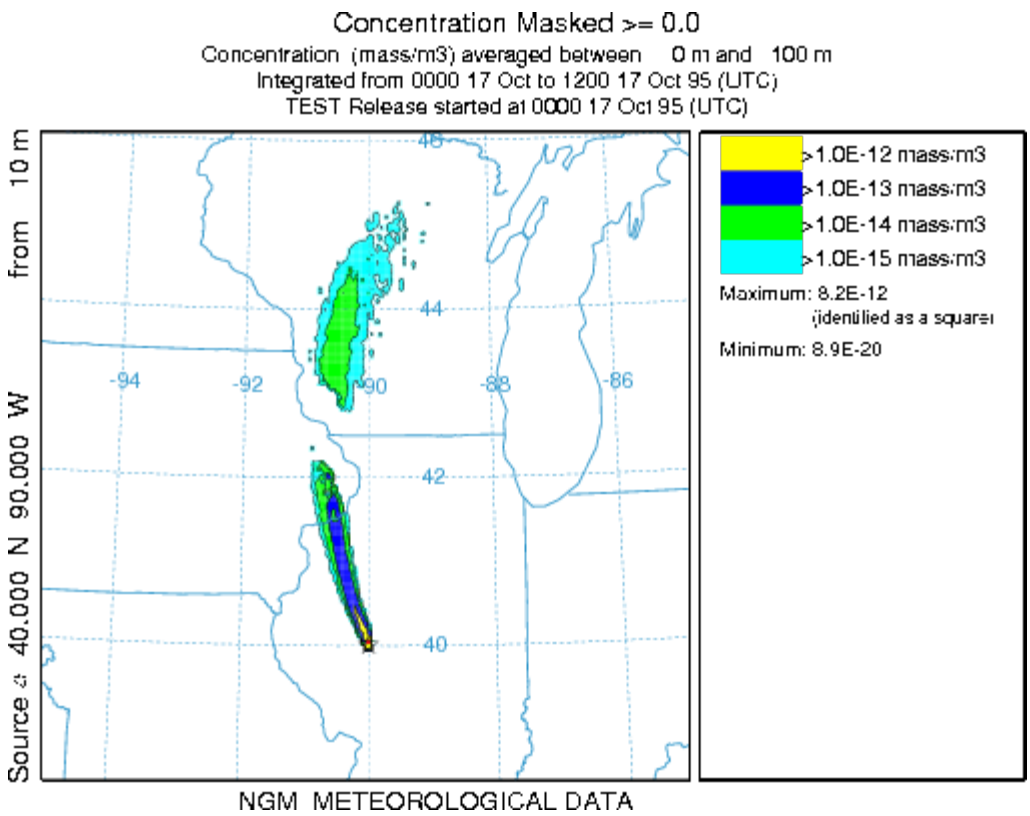
The purpose of the *Binary File Merge* utility menu is to add together two or more gridded HYSPLIT binary concentration files, where the contents of the input file are added to the contents of the base file, the results of which are written to the output file. The input files need not be identical in time, but they must have the same number of pollutants and levels. Levels and pollutants will be matched by index number and not actual height or species. The horizontal grids need to be identical or even multiples of each other. This means that the concentration grid center should be explicitly defined rather than using the default values (0.0). For instance, a half-deg and one-deg concentration grid needs to at least intersect at the corner points. Summations will occur regardless of any grid mismatches. The files are merged at each grid point according to the processing rules: a simple summation, selecting the maximum value, or the sum only at the intersection points. An additional option, called masking, is defined to be such that a concentration value greater than the mask value (normally 0.0) in the input file, will cause the base file to be set to 0.0 at that grid point. The GUI is shown below.



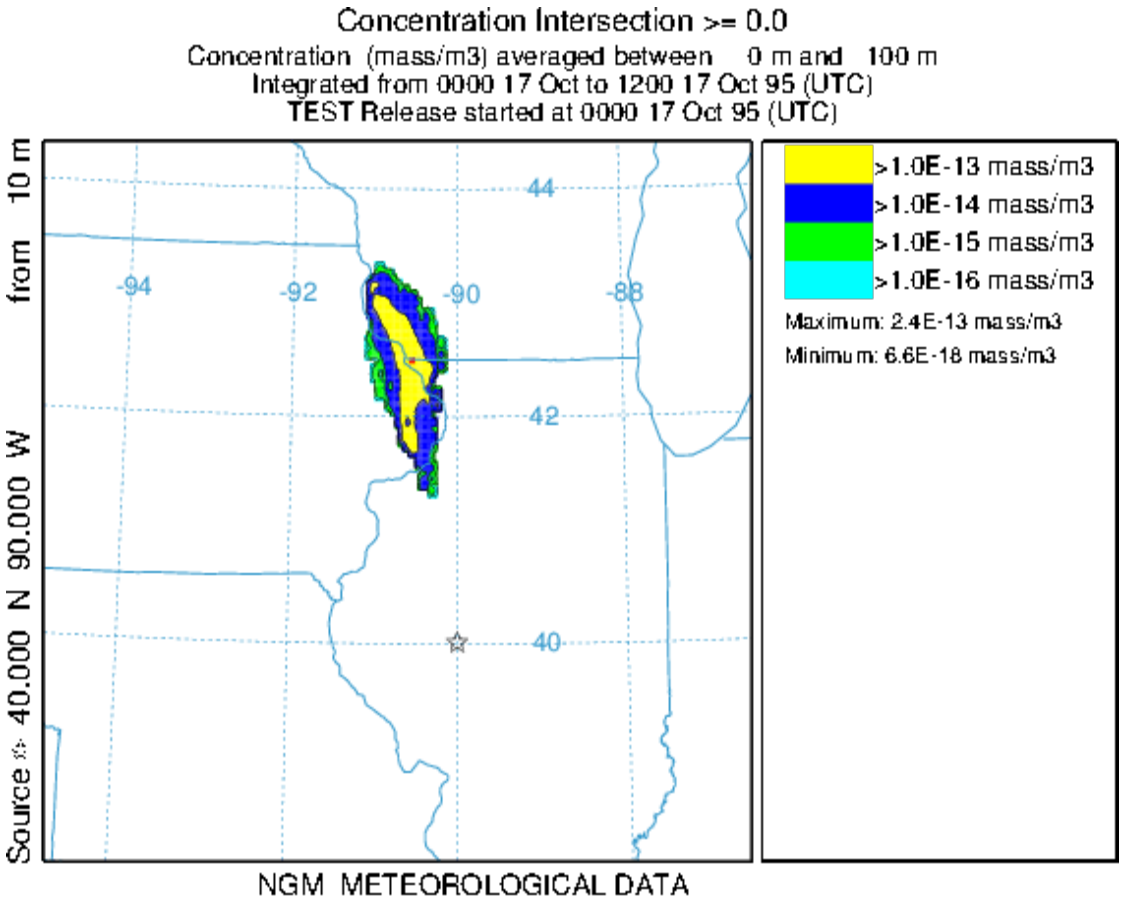
If the *Create Filenames* button is selected, an special file called *INFILE* is created that contains all the file names in the working directory that have the wildcard sequence as defined in the *Input Name* box. These files are then merged sequentially according to the process rules. Note that the concentration multiplier is applied during the writing of the output file and during sequential file processing this conversion is disabled.



The above example shows how two plume simulations have been merged. Each was run for a different day and starting location, however the graphic and its corresponding binary output file, use only the information provided in the base file and the labeling information from the input file has been lost.



In the above example, the input and base files are identical to the previous illustration, but in this example the *mask* checkbox option was selected and the result clearly illustrates the region of the base plume that was intersected by the input plume.



The result from the *intersection* option is shown in the above figure. In this result only the region where the two plumes intersect and both exceed the zero mask value is shown. The region is identical to the missing plume area in the *mask* option.

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Concentration / Utilities / Binary File Extract

Calls the utility program *concrop* to extract a sub-grid from a HYSPLIT binary concentration data file. The new subgrid is written to the file *conxtrct.bin*. The utility program can be used to remove the whitespace by resizing the grid about the non-zero concentration domain or by specifying a sub-grid. Using the -x option will force the extract of the users domain regardless of white space.

```
USAGE: concrop -[options (default)]
-b[latmin:lonmin:latmax:lonmax (all zeroes will produce full grid extract]
-d[process id (txt)]
-f[FCSTHR.TXT: (0)=none 1=output]
-i[Input file name: (cdump)]
-g[Output plume grid limits rather than cropped file: (0)=no; 1=center-radius -1=from{-b}]
-o[Output file name: (ccrop)]
-p[time extract MMDDHH:MMDDHH]
-x[override white space: (0)=no (default) 1=yes]
```

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Concentration / Utilities / Binary File Average

This menu calls the utility program *conhavrg* to spatially average the HYSPLIT binary concentration file and write a new binary file. Each grid cell is replaced by the average value of the center cell and the surrounding cells specified by the scan radius. The default scan radius of 1 means that 9 grid cells will be averaged together.

USAGE: conhavrg [options]
-i[input file name (cdump)]
-o[output file name (cavrg)]
-s[surrounding grid points to average (1)]

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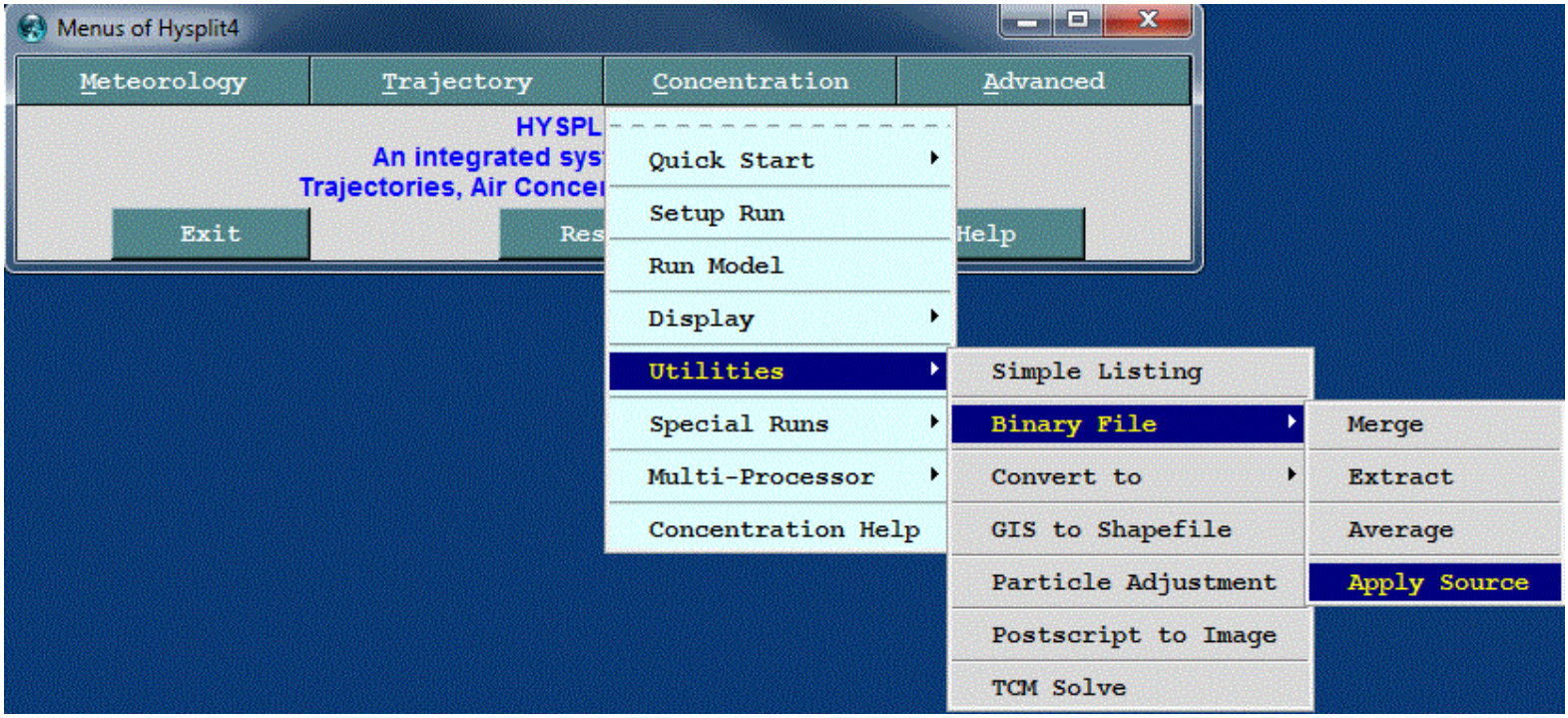
Concentration / Utilities / Binary File / Apply Source

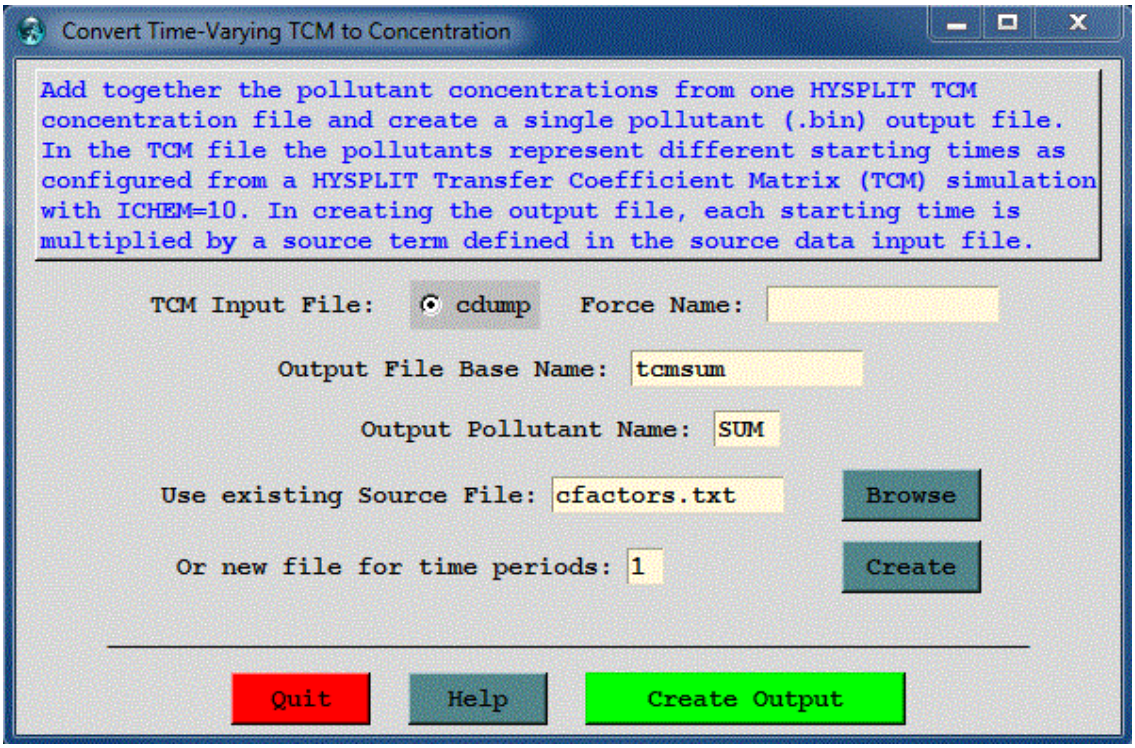
When multiple simulations are conducted, each one representing a different emission, the model results can be analyzed to determine which simulation provides the best fit with any available measurements, or more specifically, what emission rate is required with each simultion to provide the best fit with the measurements. These simulations can each represent a different emission time or location or a combination of both. Currently the code is configured to automatically generate multiple time-varying emissions using the namelist parameters QCYCLE and ICHEM.

As an example, if hourly (the minuimum) resolution is desired over a 24 hour simulation period, then the emission rate needs to be set to emit one one unit for a duration of one hour. The namelist variable *QCYCLE* should also be set to 1.0 hour so that the emissions effectively become continuous at a rate of one unit per hour. This in combination with *ICHEM=10* will result in the creation of 24 concentration arrays with each particle being tagged according to its release hour and those particles will only contribute to concentrations on the grid with the same release-time tag. The pollutant identification field is used and its value corresponds to hours after the start of the simulation. The output concentration grid will appear to be like any other but with 24 pollutants, one for each release period as defined by the *QCYCLE* parameter. Make sure that a sufficient number of particles have been released to provide consistent results for all time periods.

Once the simulation has completed, the unit source simulation can be converted to concentrations by applying an emission rate factor for each release time. This is accomplished by clicking on the Concentration / Utilities / Binary File / Apply Source menu tab. This menu is only intended to work with a single multi-pollutant concentration file created in the manner described previously.



The input required is simply the name of the Transfer Coefficient Matrix (TCM) input file (the previously created multi-pollutant=multi-time-period) input file, the base name of the single pollutant output file which will contain the concentration sum of all the release periods after they are multiplied by the source term, the 4-character pollutant identification field, and the name of the time-varying source term file it it exists, otherwise a new file can be created. An emission rate needs to be defined for each release time, otherwise it is assumed to be zero.



The emissions file format is simply the starting time of the emission given by year, month, day, and hour, and the emission rate in terms of units per hour. The first record of all emissions file should contain the column labels then followed by the data records, one for each release time period. For example, a constant emission rate corresponding to the 12 hour example test simulation (16 October 1995) would appear as follows:

```
YYYY MM DD HH TEST
1996 10 16 00 1.00E+12
1996 10 16 01 1.00E+12
1996 10 16 02 1.00E+12
1996 10 16 03 1.00E+12
1996 10 16 04 1.00E+12
1996 10 16 05 1.00E+12
1996 10 16 06 1.00E+12
1996 10 16 07 1.00E+12
1996 10 16 08 1.00E+12
1996 10 16 09 1.00E+12
1996 10 16 10 1.00E+12
1996 10 16 11 1.00E+12
```

Command Line Options - tcmsum

The underlying binary file conversion program can be run from the command line. As with all other applications, the command line argument syntax is that there should be no space between the switch and options. The command line arguments can appear in any order:

tcmsum -[option {value}]

-c[column number in emissions file (1)]
-i[input file name (cdump)]
-o[output file base name (tcmsum)]
-d[output file name suffix (bin)]
-h[half-life-days (0.0 = none)]
-p[pollutant sum label (SUM)]
-s[source term input file name (cfactors.txt)]
-t[time decay start: MMDDHH (run_start)]

The procedure described in this section is very similiar to the transfer coefficient solution approach with the exeception that here the dispersion coefficients for the individual release times are contained in a single file while in the other approach an input file is required for each release time simulation. The single file created here can be processed through the utility program **conlight** to extract one time period to its own file with each pass through the program. Currently no GUI script application exists to perform this task automatically.

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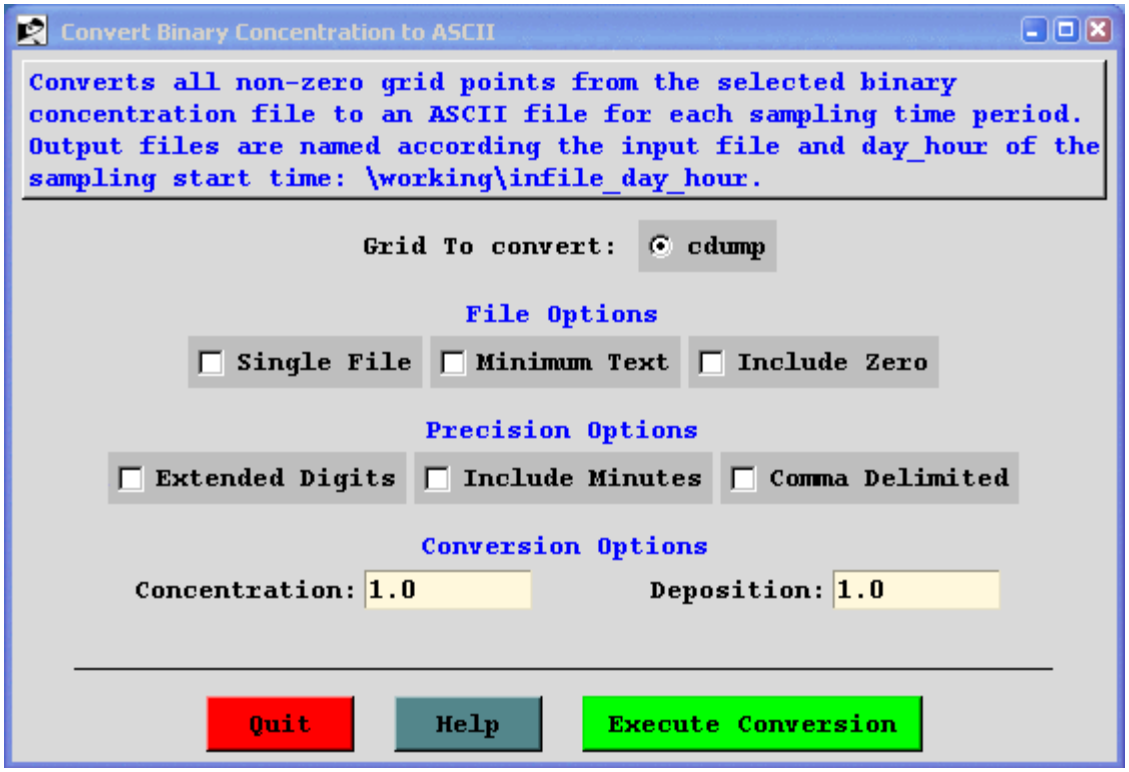
Concentration / Utilities / Convert to ASCII

The Convert to ASCII menu option uses the con2asc program to convert the binary concentration file to a simple ASCII file composed of one record per grid point for all grid points where concentrations at any level are non-zero. Concentrations for multiple levels and pollutant species are all listed on the same record for each grid point. The primary purpose of the conversion is to create a file that can be imported into other applications. An illustration of the GUI menu is shown below for the sample concentration simulation.



The Concentration Setup menu determines the file name selection option on the GUI. There are some additional checkboxes that correspond to various command line conversion options: **con2asc -[options (default)]**

-c[Convert entire file flag]

This option converts the entire binary input file, including all index records, to an ASCII output file with the name {input file}.txt. This option is not available through the GUI (use -s below). Another program, called *conread*, also not available through the GUI, can also be used to dump out the contents of the concentration file. This program can only be run from the command line. For the -c option, the output file format follows the binary file format record-by-record using the following conventions.

Meteorological model and starting time - A4, 6I4
Starting time and locations - 4I4, 2F8.3, F10.1
Concentration grid and spacing - 2I4, 2F8.4, 2F8.2
Vertical grid index record - I4, 20I8
Pollutant identification record - I4, 20A4
Sample start time - 6I4
Sample end time - 6I4
Concentration record - A4, I6, 255(255E10.2)

-d[Delimit output by comma flag (rather than space delimited)]

Set the **Comma Delimited** checkbox.

-i[Input file name (cdump)]

-m[Minimum text output format flag]

Setting this flag turns off the writing of the first output record, which is the column label field: DAY HOUR LAT LON SPECIES-LEVEL. This option corresponds to the **Minimum Text** checkbox of the GUI menu.

-o[Output file name base (Input File Name)]

The default base name for the output file is the input file name. A new output file is created for each sampling period, where the name of the file is composed of the *{base name}_{Julian day}_{hour}* of the sample ending time. If the **Include Minutes** box is checked, then the minutes field of the sample ending time is added to the end of file name. This field is not available through the GUI. The name of each output file is always written to the file named *CON2ASC.OUT* regardless of any other options selected.

-s[Single output file flag]

This option corresponds to the **Single File** checkbox of the GUI menu. The multi-time period ASCII output file is named {input file}.txt.

-t[Time expanded (minutes) file name flag]

-u[Units conversion multiplier for concentration (1.0)]
-U[Units conversion multiplier for deposition (1.0)]

Values other than one in either of these fields will result in the concentration or deposition results to be multiplied by these factors prior to output. Deposition fields are identified by a zero in the level height field.

-x[Extended precision flag]

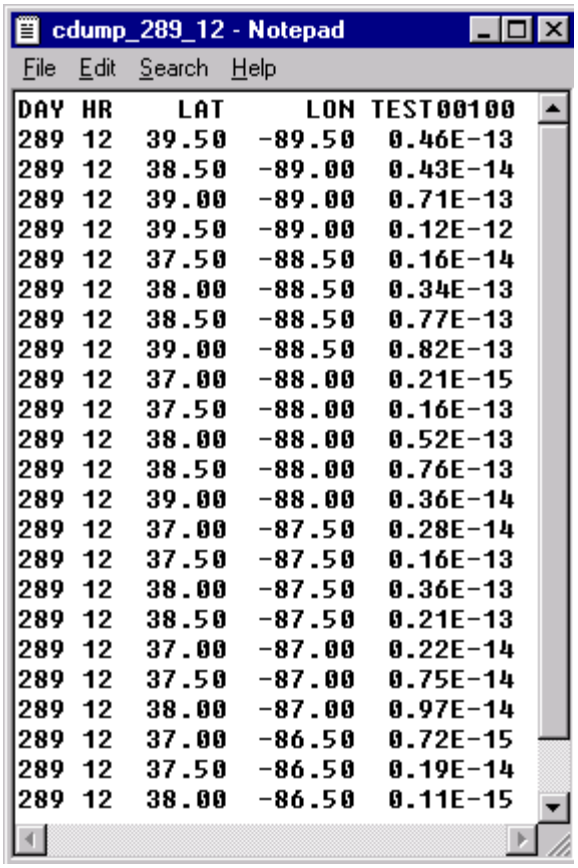
The format of each record in the output file is given by:
2I3 - End of Sample: Julian Day and Hour
F7.2, F8.2 - Latitude and Longitude of grid cell
45E9.2 - Concentration data (by level and pollutant)

If the **Extended Digits** checkbox of the precision options is set, then the latitude and longitudes will be given by four digits after the decimal place.

-z[Zero points output flag]

Setting the zero flag causes the program to output the concentration values all all grid points, including the ones that are zero. This corresponds to the **Include Zero** checkbox of the GUI menu.

Each output record is identified by the day (Julian: 1 to 365) and hour (UTC) of the ending time of each sample. The ASCII conversion of the first file generated by the sample calculation is shown below in the illustration.



cdump_289_12 - Notepad

File Edit Search Help

DAY	HR	LAT	LON	TEST00100
289	12	39.50	-89.50	0.46E-13
289	12	38.50	-89.00	0.43E-14
289	12	39.00	-89.00	0.71E-13
289	12	39.50	-89.00	0.12E-12
289	12	37.50	-88.50	0.16E-14
289	12	38.00	-88.50	0.34E-13
289	12	38.50	-88.50	0.77E-13
289	12	39.00	-88.50	0.82E-13
289	12	37.00	-88.00	0.21E-15
289	12	37.50	-88.00	0.16E-13
289	12	38.00	-88.00	0.52E-13
289	12	38.50	-88.00	0.76E-13
289	12	39.00	-88.00	0.36E-14
289	12	37.00	-87.50	0.28E-14
289	12	37.50	-87.50	0.16E-13
289	12	38.00	-87.50	0.36E-13
289	12	38.50	-87.50	0.21E-13
289	12	37.00	-87.00	0.22E-14
289	12	37.50	-87.00	0.75E-14
289	12	38.00	-87.00	0.97E-14
289	12	37.00	-86.50	0.72E-15
289	12	37.50	-86.50	0.19E-14
289	12	38.00	-86.50	0.11E-15

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Concentration / Utilities / Convert to DATEM

This menu calls a utility program to convert the HYSPLIT binary concentration file to the DATEM data format and compares the model predicted results with the actual measured data. The Data Archive of Tracer Experiments and Meteorology (DATEM) web page contains additional details about each of the experiments, the data formats, and more complete descriptions of each of the programs used to convert the data and generate the statistical results. The on-line repository has links to several different tracer experiments and their associated meterological data. All experimental data have been converted to a common format. The meteorological data are compatible for direct use by HYSPLIT.

To facilitate application of the analysis software, all the experimental data from the second CAPTEX release are provide in the ./hysplit/datem directory. Included are the control, namelist, measured data, and meteorological data files. The meteorological data is taken from the North American Regional Reanalysis. The computational sequence is as follows:

1) Configure and Run HYSPLIT

- Go to the concentration setup run menu and retrieve ./datem/captex.cnt
- Go to the advanced configuaration concentration menu and retrieve ./datem/captex2.cfg
- Save and then Run Model

2) Convert HYSPLIT run results to DATEM format

- Browse to load the measured data file ./datem/captex2.txt
- Create the DATEM file hysplit.txt from the binary file hysplit2.bin
- Compute the Statistics and view the Scatter Plot

In the first section of the menu, a measured data file already in DATEM format should be selected. The input data file represents the HYSPLIT binary concentration output file which is then converted to a DATEM formatted text file using the units conversion factor. The conversion program will match each measurement with a model calculated concentration corresponding to the location and time duration of the measurement. Note that the model temporal output frequency needs to be the same or of finer resolution than the measurement periods, otherwise calculations cannot be matched with the measurements.

The rotation angle entry field (default = 0.0) can be used to test the sensitivity of the model prediction to small changes in wind direction. Setting a non-zero angle will result in the rotation of the calculated plume with respect to the sampling network in the direction specified. The rotation is computed using the first source location specified in the setup menu. The effect of this test is comparable to rotating the transport wind direction by the same amount. However, this sensitivity test only makes sense in the context of plumes that have a relatively homogeneous and stationary structure.

Once the model output file in DATEM format has been created, the statistical evaluation program should be run to compare the model calculations with the measurements in terms of various performance statistics. Two data processing options are available. For verification statistics, all values can be compared, only plume values (both measured and calculated values are greater than zero), or all values but excluding pairs where both measured and calculated values are zero. In terms of averaging, the measured and calculated values can be used directly, temporally averaged resulting in one value for each location, or spatially averaged resulting in one value for each time period. The contingency level is the concentration value required to be exceeded to compute the false alarm rate, probability of detection, and threat-score. The contingency level is also used as the plotting threshold for the measured-calculated scatter diagram which is created by the *Scatter Plot* menu button.

Note that simulations with multiple species and levels are not supported. The concentration data files follow no specific naming convention and any input or output file name may be selected in the menu. Arbitrary input file names can only be set through the *Setup / Grids* menu. The statistical output files are always written to *stat{A|T|S}.txt* where the character A|T|S represents All data, Temporal averaging, or Spatial averaging. An additional output file, *data{A|T|S}.txt* is created for the scatter diagram plot, which is always named *scatter.ps*.

DATEM format description

- Record 1 (ASCII) - file identification information
- Record 2 (ASCII) - column identification information
- Record 3 ... end - individual data records

  Field 1 (I4) - start year of sample
  Field 2 (I3) - start month of sample
  Field 3 (I3) - start day of sample
  Field 4 (I5) - start hour minute of sample (HHMM)
  Field 5 (I7) - sample duration hours minutes (HHHMM)
  Field 6 (F10) - sample location latitude (fractional degrees)
  Field 7 (F10) - sample location longitude (fractional degrees)
  Field 8 (F10) - sample value
  Field 9 (I10) - sample station identification (integer)

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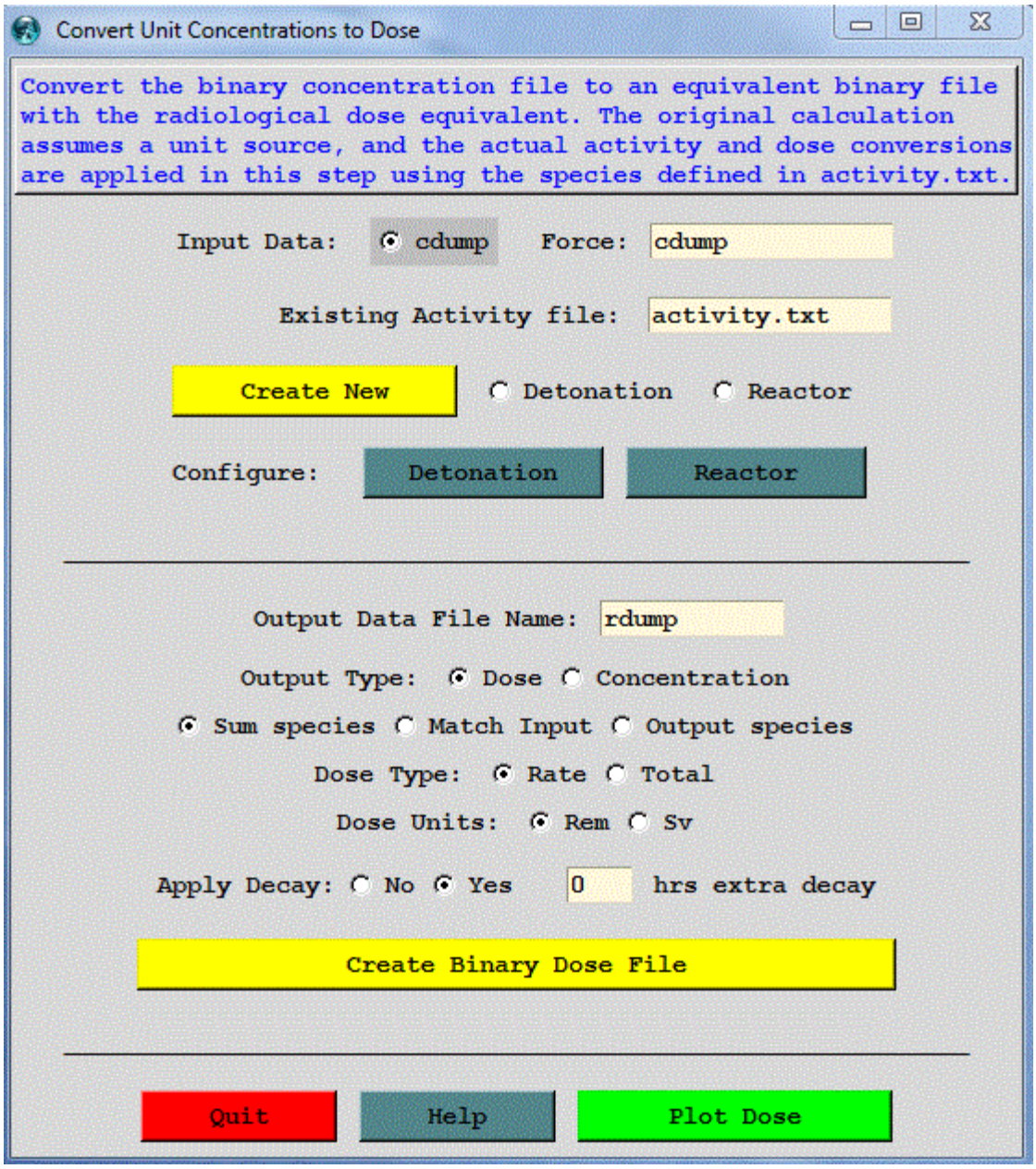
Concentration / Utilities / Convert to Dose

Converts a HYSPLIT binary concentration and deposition file to dose in rem/hr. The HYSPLIT calculation should be done using a unit emission so that the concentration units are m-3 and the deposition units are m-2. This post-processing step reads the file activity.txt which contains the activity (Bq) at time=0 for all the isotope products. Sample activity.txt files can be created by the program for a high-energy nuclear detonation or a thermal fission reaction from a power plant reactor. The file also contains the half-life and cloud- and ground-shine does conversion factors for each radionuclide specified in the file.

For nuclear detonations, the activity.txt file contains columns for either a high-energy or thermal fission reaction assuming a yield of 1 kT. The emission factor can be specified as a multiple of 1 kT. Activation products resulting from the fission are not considered. Two fuel sources (U235 and Pu239) are available for each reaction type. The fission yield data were obtained from T.R. England and B.F. Rider, Los Alamos National Laboratory, LA-UR-94-3106; ENDF-349 (1993). The external dose rate for cloud- and ground-shine is computed from the factors given by Eckerman K.F. and Leggett R.W. (1996) DCFPAK: Dose coefficient data file package for Sandia National Laboratory, Oak Ridge National Laboratory Report ORNL/TM-13347.

During the processing step, the cumulative product of the activity and dose factor is computed for each decay weighted concentration averaging period, independently for noble gases and particles. Command line options exist to turn off the dose calculation but still multiplying the dispersion factors by the activity, resulting in air concentration output. If the dispersion factors input file contains only one pollutant type and level, then an option can be set to output each of the species defined in the activity.txt file. Concentration units may also be converted from Bq to pCi.

For nuclear power plant accidents, the same fission product table can be used by entering the duration of the reactor operation in terms of mega-watt-hours based upon the relation that 3000 MW-hours releases an energy equivalent to 2.58 kT. An alternative approach is to generate an activity.txt file that corresponds with the radionuclide release profile of the reactor accident. The command line option -afdnpp will create a sample activity.txt file that corresponds to the maximum emissions over a 3-hour period during the Fukushima Daiichi Nuclear Power Plant accident for the 10 most critical radionuclides for short-term dose calculations.



Post Processing Program *CON2REM* command line options (default):

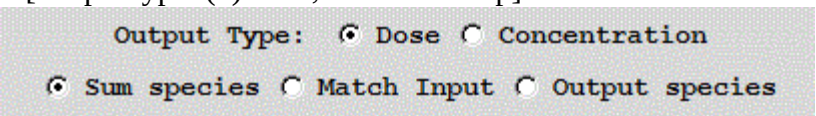
- -a[activity data file name (activity.txt) or {create|fdnpp}]

  Names the input file describing activity associated with each species and the dose conversion factors. The -acreate option will create a sample activity.txt file for a 1kT detonation with just a few species to illustrate the format. The -afdnpp option will create a file with the top ten radionuclides contributing to dose during the Fukushima Daiichi Nuclear Power Plant accident. The activity for those radionuclides represents the

- -b[breathing rate for inhalation dose in m3/h (0.925)

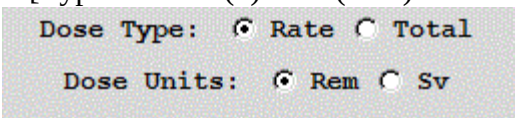
  The breathing rate is used as a multiplier for the calculation of the inhalation dose factor. This is only used for the cloudshine dose calculations.

- -c[Output type: (0)-dose, 1-air conc/dep]



If the flag is set to one, the dose conversion factors are set to one and the output will be concentration,the product of the input air concentration (from a unit emission) times the activity for each radionuclide defined in activity.txt. The values are summed for all species in each pollutant class (NGAS or RNUC).

- -d[Type of dose: (0)=rate (R/hr) 1=summed over the averging period (R)]

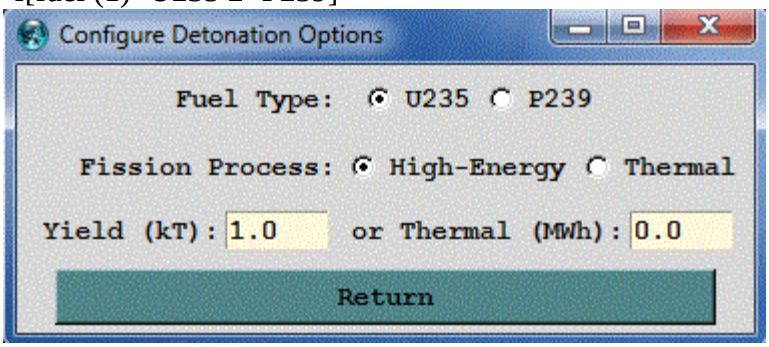


When computing dose, the option is to output a rate or the total dose accumulated over each concentration averaging period. Note that dose from deposition is always summed over the duration of the simulation.

- -e[include the inhalation dose in the calculation (0)=No 1=Yes]'

This is used in conjunction with the -b option. The default is not to include the inhalation dose as part of the cloudshine calculation. If this is turned on, insure that the inhalation dose factors are correctly defined in the last column of activity.txt.

- -f[fuel (1)=U235 2=P239]



This flag selects which column of the activity.txt file will be used to determine the emission amount. The first two columns are for U-235 fission and the last two columns are for Pu-239 fission. There are columns for high-energy or thermal fission (see -p flag). Also see the -y and -w flags to scale the emissions to the event.

- -g[decay type: 0=normal {c=1}, (1)=time averaged decay]

Prior to computing the dose, the activity is time-decayed to either the end of the sampling time (0=normal) or as the time averaged activity between the start and end time of each sampling period (1=time-averaged, the default). Normal decay can only be applied to air concentration calculations. Dose output always requires time-averaged decay.

- -h[help with extended comments]

Provides a short narrative of the functionality of this program with a list of all the command line options.

- -i[input file name (cdump)]

The name of the HYSPLIT air concentration/deposition binary output file. The simulation can contain both air concentrations and deposition field. Proper conversion of the model output fields to dose requires a unit release rate in the HYSPLIT calculation.

- -n[noble gas 4-char ID (NGAS)]

The program searches for this pollutant 4-character identification to use as the dispersion factor for noble gases. All other ID values (RNUC, etc) are assumed to be for particles. All species will be summed to either the NGAS or the other dispersion factor unless species matiching is defined (-s1).

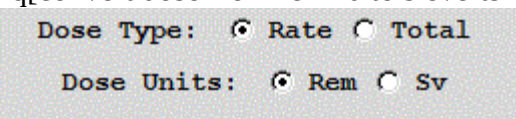
- -o[output file name (rdump)]

  The output file will contain the same number of levels and time periods as the input file but with the dispersion factors (unit concentrations) converted to dose or species concentration according to the settings of the other command line options.

- -p[process (1)=high-energy 2=thermal]

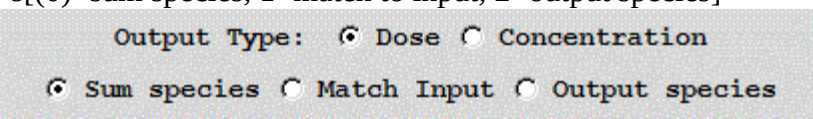
  Defines which column of the activity.txt file to use for a specific fuel type. Option 1 is for high-energy fission (columns 1 or 3) and option 2 is for thermal fission (columns 2 or 4). In the case of the FDNPP activity.txt file, the activity values are the same in all columns. This feature may be used with customized activity.txt files to select different source options. Also see the -f flag for selection the fuel type.

- -q[convert dose from rem=0 to sieverts=(1)]

  The default dose output is in REM because the conversion factors are defined in the activity.txt file in REM/Bq. Setting this value to one converts the dose output from REM to Sieverts (100 REM = 1 Sievert).

- -s[(0)=sum species, 1=match to input, 2=output species]

  The default value (0) sums each species in the the activity.txt file to its corresponding pollutant class (NGAS - noble gas, or RNUC - radionuclide particle). The match to input option (1) just does a one-to-one match of the pollutant ID in the activity.txt file with the pollutant IDs used in the simulation. Pollutant IDs can be 4-digit integer number or character for option (1). In option (2), the output file can be expanded to include a concentration for each species defined in the activity.txt file using the dispersion factors from its pollutant class from the simulation. In this configuration, HYSPLIT can only be run with one level and species.

- -t[0=no decay input decayed, or decay by species half-life (1)]

  The default (1) is for all species to be decayed to the valid time of the concentration output from the start time of the simulation which is assumed to be the time fission ceased. The time of release to the atmosphere can occur much later. The no decay option is only required when decay has already been applied in the dispersion calculation. In general, decay should only be set in the dispersion calculation for short-duration releases which coincide with the termination of fission, otherwise decay may be computed incorrectly. Computing decay within this post-processing step is the most accurate way to approach dose simulations.

- -u[units conversion Bq->pCi, missing: assume input Bq]

  When air concentration output is selected, then the output units can be converted from Bq to pCi.

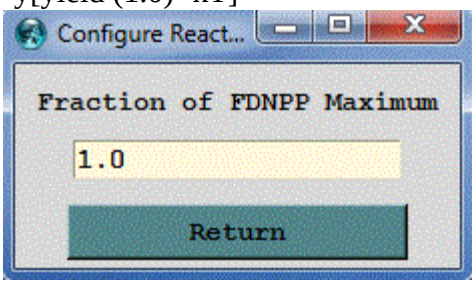
- -w[Fission activity in thermal mega-watt-hours, replaces the -y option value]

  If the activity.txt file represents the number of fissions per kT, and the -w field is non-zero, then the activity is computed with respect to the number of MWh generating the fission products. The assumption is that a 3000 MW reactor creates about 2.58 kT per hour of fission products.

- -x[extended decay time in hours beyond calculation (0)]

Additional decay time can be added using this field to estimate long-term doses. This calculation applies to either -t option but only for deposition doses. This option permits longer-term doses to be computed by adding additional decay to the existing output files.

- -y[yield (1.0)=kT]



The default assumes that the activity levels defined in activity.txt represent the emissions from a 1 kT device. Other values are computed as a multiplier to the values defined in the table. The multiplier can be used in the context of a detonation in terms of kT or a multiple of the 3-hour emission maximum from the Fukushima Daiichi Nuclear Power Plant accident.

- -z[fixed decay time in hours (0)]'

The fixed decay is computed to the end of the sample time in the output file regardless of the actual simulation or release start time. All output periods, regardless of sampling time, will be decayed for these number of hours.

An example of the activity.txt file for a 1 kT detonation:

- Mass Nucl T1/2 U235H U235T Pu239H Pu239T Cloudshine Groundshine Inhalation
- Hr= 0.00 sec Bq Bq Bq Bq rem/h|Bq/m3 rem/h|Bq/m2 rem/Bq
- 85 Kr 3.38613E+08 9.44699E+11 7.53098E+11 5.74803E+11 3.27318E+11 9.18000E-11 0.00000E+00 0.00000E+00
- 90 Sr 9.18326E+08 4.50386E+12 5.67152E+12 2.06059E+12 2.06059E+12 3.53880E-11 5.90400E-13 2.38000E-06
- 131 I 6.94656E+05 5.31842E+15 3.74884E+15 5.64272E+15 5.00710E+15 6.08400E-09 1.31040E-10 7.38000E-07
- 133 Xe 4.52995E+05 1.10002E+16 1.33275E+16 9.66744E+15 1.39641E+16 5.00400E-10 0.00000E+00 0.00000E+00
- 137 Cs 9.52093E+08 4.66591E+12 5.85842E+12 4.21162E+12 6.25592E+12 3.34080E-11 1.07640E-12 4.63000E-07
- 140 Ba 1.10160E+06 3.68093E+15 5.07968E+15 3.02654E+15 4.37621E+15 2.90520E-09 6.84000E-11 1.03000E-07
- 140 La 1.44979E+05 2.81554E+16 3.86593E+16 2.38668E+16 3.33141E+16 3.99600E-08 7.77600E-10 1.07000E-07

An example of the activity.txt file for the Fukushima-Daichii Nuclear Power Plant Accident for the top ten radionuclides important for short-term dose calculations. The activity represents the maximum number of Bq released over a 3 hour period.

- Mass Nucl T1/2 U235H U235T Pu239H Pu239T Cloudshine Groundshine Inhalation
- Hr= 0.00 sec Bq Bq Bq Bq rem/h Bq/m3 rem/h Bq/m2 rem/Bq
- 95 Nb 3.02000E+06 1.62000E+13 1.62000E+13 1.62000E+13 1.62000E+13 1.26000E-08 2.62000E-10 2.38000E-06
- 110 Ag 2.18000E+07 6.48000E+12 6.48000E+12 6.48000E+12 6.48000E+12 4.57000E-08 9.29000E-10 2.38000E-06
- 132 Te 2.82000E+05 1.62000E+16 1.62000E+16 1.62000E+16 1.62000E+16 3.36000E-09 7.63000E-11 7.38000E-07

- 131 I 6.94656E+05 8.10000E+15 8.10000E+15 8.10000E+15 8.10000E+15 6.08400E-09 1.31040E-10 7.38000E-07
- 133 I 7.49000E+04 8.10000E+15 8.10000E+15 8.10000E+15 8.10000E+15 9.94000E-09 2.22000E-10 7.38000E-07
- 133 Xe 4.52995E+05 3.66000E+17 3.66000E+17 3.66000E+17 3.66000E+17 5.00400E-10 0.00000E+00 0.00000E+00
- 134 Cs 6.50000E+07 8.10000E+14 8.10000E+14 8.10000E+14 8.10000E+14 2.54000E-08 5.33000E-10 4.63000E-07
- 137 Cs 9.52093E+08 8.10000E+14 8.10000E+14 8.10000E+14 8.10000E+14 3.34080E-11 1.07640E-12 4.63000E-07
- 140 Ba 1.10160E+06 4.05000E+13 4.05000E+13 4.05000E+13 4.05000E+13 2.90520E-09 6.84000E-11 1.03000E-07
- 140 La 1.44979E+05 4.05000E+13 4.05000E+13 4.05000E+13 4.05000E+13 3.99600E-08 7.77600E-10 1.07000E-07

As an example, a HYSPLIT simulation could be configured with two species, NGAS for the noble gases and RNUC for the radio-nuclide particles. After the emissions stop, the total emissions of both NGAS and RNUC should equal one. Then in the post-processing step, *con2rem* is called and the concentration and deposition fields are multiplied by the total emission and dose conversion factor for each species and added together to get a ground-shine and cloud-shine dose file, which can then be plotted using any of the standard HYSPLIT display programs. Dose results, by species, are decayed to the valid time of the output graphic. An additional time factor can be added for long-term dose estimates.

One aspect of applying the decay in the the post-processing step is that the decay times are referenced to the start of the simulation rather than the start of the release. This means that the radionuclide release rate is valid at the start of the simulation time. This might be the best configuration for a nuclear power plant accident, where the fission is assumed to have stopped at the start of the release (and simulation). However in other situations, where emissions might be occurring in concert with some other process, then starting the decay at the time when the radionuclides are released might be a more appropriate configuration. If the decay is computed during the model calculation for each species released then use the *con2rem* options -s1 -t0 to apply just the emission factors and not decay in the post-processing step.

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Concentration / Utilities / Convert to IOAPI

This menu calls a utility program to convert the HYSPLIT binary concentration file to the IOAPI gridded data format. Multiple species, levels, and time periods are supported. The conversion program is currently only available on UNIX or LINUX systems. The data files follow no specific naming convention and any input or output file name may be selected in the menu. Arbitrary input file names can only be set through the *Setup / Grids* menu.

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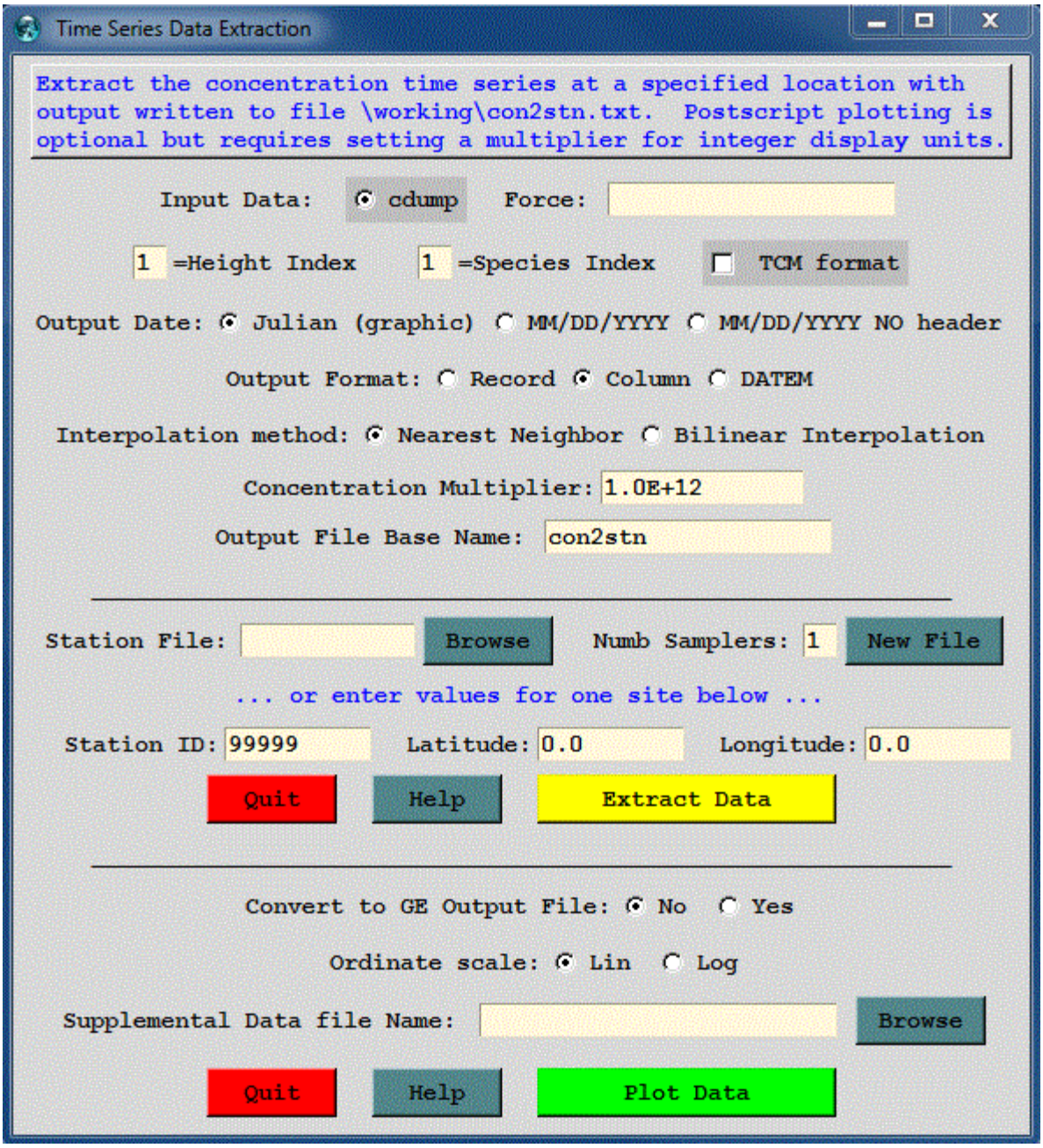
Concentration / Utilities / Convert to Station

The purpose of the *Convert to Station* utility menu (also called time series data extraction) is to list concentrations at specific latitude-longitude locations by extracting that information to a text file. The menu also has an option to produce a time series plot at one or more of the stations or a KML formatted file suitable for display by Google Earth. An illustration of the menu is shown below. The concentration grid names are determined from the *Concentration / Setup Run* menu tabs and therefore the setup menu needs to be called prior to opening this menu. The species and height values are index numbers starting at one. A height index of 1 is the data at the first output level, regardless of its actual height value. The date field can be written as a fractional Julian day (for plotting) or using a MM/DD/YYYY field (for spreadsheets) with or without an index record. The no index record option is used to concatenate multiple files.

The TCM checkbox is used to flag the input file as having been created using the ICHEM=10 namelist option. There is no specific marker in the concentration to indicate that the file is in this format. The file contains multiple pollutants, each associated with a different time of release. The TCM flag also causes the first output time group with each record to be associated with the time of release rather than the time of the sample collection. The second time group of the record becomes the start time of the sample collection.



Similar to the other menus in the utility section, the input concentration file must be defined in the Concentration Setup menu. The menu options correspond to the command line options of the *con2stn* extraction program. There are two options that can be used to define an extraction location. A station location can be defined directly as an entry in the menu, or a list of stations can be defined using an input file. If the input file does not exist, it can be created by using the *New File* button. In this example illustration, a file has been defined with three locations that are within the plume of the example simulation. The file consists of three records, one for each station:

```
001 39.0 -89.0
002 38.0 -88.0
003 37.0 -87.0
```

The extraction program is called *con2stn* and for these three stations, produces the output file shown below, called by default *con2stn.txt*. The base name of the output file (*con2stn*) can be changed in the menu. In contrast to the simulation shown in all the previous examples, in this case the output averaging time was decreased from 12 hours to one hour, to generate a smoother looking graphic.

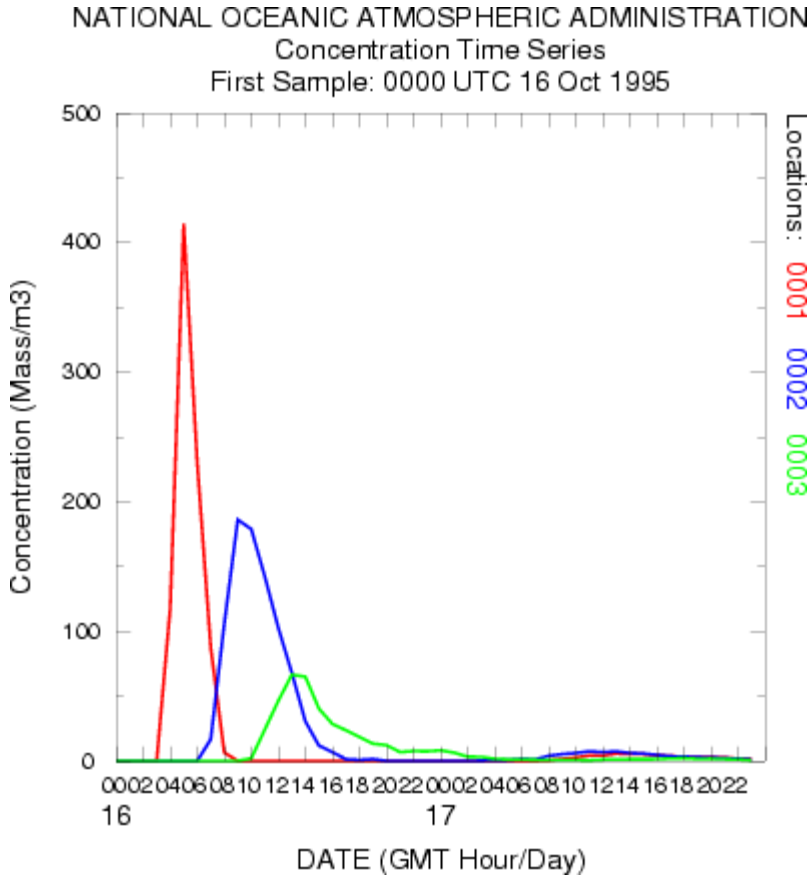
JDAY	YR	MO	DA1	HR1	DA2	HR2	1	2	3
289.000	95	10	16	0	16	1	0.	0.	0.
289.042	95	10	16	1	16	2	0.	0.	0.
289.083	95	10	16	2	16	3	0.	0.	0.
289.125	95	10	16	3	16	4	0.	0.	0.
289.167	95	10	16	4	16	5	117.701	0.	0.
289.208	95	10	16	5	16	6	414.454	0.	0.
289.250	95	10	16	6	16	7	230.186	0.	0.
289.292	95	10	16	7	16	8	87.431	16.723	0.
289.333	95	10	16	8	16	9	6.572	105.681	0.
289.375	95	10	16	9	16	10	0.	186.133	0.
289.417	95	10	16	10	16	11	0.	178.893	2.082
289.458	95	10	16	11	16	12	0.	142.384	24.254
289.500	95	10	16	12	16	13	0.	102.709	46.464
289.542	95	10	16	13	16	14	0.	68.016	66.541
289.583	95	10	16	14	16	15	0.	30.602	65.018
289.625	95	10	16	15	16	16	0.	11.883	40.429
289.667	95	10	16	16	16	17	0.	6.797	28.568
289.708	95	10	16	17	16	18	0.	1.368	23.695
289.750	95	10	16	18	16	19	0.	0.778	18.564
289.792	95	10	16	19	16	20	0.	1.482	13.358
289.833	95	10	16	20	16	21	0.	0.	12.230

The output file shows the Julian day, month, day, and hour of the sample start; day and hour of sample ending time, and the concentrations for each station (location selected by latitude-longitude). The format of each output record is as follows:

F8.3, 6I4 - Starting: Julian day, year, month, day, hour; Ending: day, hour
XF10 - Concentration value at X stations

The lower section of the GUI is used to create a simple time series concentration plot of the concentration time series or an output file (*con2stn.kml*) suitable for display by Google Earth. The *con2stn.txt* file is created first which is then read by the Google Earth conversion program (*stn2ge*).

For time series data, one or more stations may be plotted. The plotting feature is also available through the command line. The option is selected from the **Display Time Series** checkbox. The program, *timeplot*, reads the data file produced by the *con2stn* conversion program and plots the concentration values to the *timeplot.ps* output file. The illustration for the previous text file is shown below.



There are only two plot options supported through the GUI: linear or logarithmic ordinate scaling. If integer ordinate units are desired then it may be necessary to specify a units conversion factor, in this case 10^{15}, to create data in the text file that can be plotted. With the log scaling option, the conversion factor can be set to 1.0, and the ordinate scale will cover the appropriate order-of-magnitude range to plot all the data.

Command Line Options - con2stn

The program can be run from the command line or through interactive prompts from the keyboard. The command line argument syntax is that there should be no space between the switch and options. The command line arguments can appear in any order: **con2stn -[option {value}]**

-a[rotation angle:latitude:longitude]
-c[input to output concentration multiplier]
-d[mm/dd/yyyy format: (0)=no 1=w-Label 2=wo-Label]
The default date format is to write a fractional Julian date in the first output field. This format is required for plotting purposes. However, a more conventional month/day/year format can be selected, which is more compatible with spreadsheet applications. In the first option (=1) an informational header record is written. In the other option (=2) the header record is excluded, which is more convenient when appending multiple files.
-h[half-life-days (one -h entry for each pollutant)]
-i[input concentration file name]
Unspecified file names will result in a standard input prompt.
-m[maximum number of stations (200)]
-o[output concentration file name]
-p[pollutant index (1) or 0 for all pollutants]
Level and pollutant index values can be selected for files with multiple levels and species. Setting zero (0) for either index forces the output to be the record format rather than the column format. Record format contains the index numbers for the pollutant and level.
-r[record format 0=record (1)=column 2=datem]

The default output format is to create multiple columns, one for each station, for a selected pollutant and level. Setting the value to one formats the output as one record for each station, level, and pollutant. A value of two sets the output to the DATEM format.

-s[station list file name (contains: id lat lon)]

The station positions can be read from a file (space or comma delimited) with the first field being an integer that represents the location identification, followed by the decimal location in latitude and longitude.

-t[transfer coefficient processing]

-x[(n)=neighbor or i for interpolation]

The default interpolation method (-xn) is to use the value at nearest grid point to each latitude-longitude position, otherwise bilinear interpolation (-xi) is used.

-z[level index (1) or 0 for all levels]

Command Line Options - stn2ge [option {value}]

-i[input text file name] contains data in the format output from *con2stn*

-s[station list file name] same file used as input to *con2stn*

-o[google earth output filename (less .kml)]

Command Line Options - timeplot [option {value}]

-i[input concentration file name] contains data in the same format as output from *con2stn*

-m[minimum ordinate value (0.0)]

-n[sequential station number]

For files with multiple stations select the station to plot; default for multiple stations is to plot all stations; several stations can be selected to plot by appending station numbers with the plus symbol: hence -n3+5+6 will plot stations 3, 5, and 6.

-p[draw only points, no connecting line]

-y[The default is linear ordinate scaling. The flag sets y-axis log scaling.]

-z[three character time label]

Note that multiple pollutants and levels are not supported. Timeplot labels can also be customized by creating a *LABELS.CFG* file. See the Border Labels discussion for more information on this file format.

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Convert particle position file to concentration file (S350)

This program reads the HYSPLIT binary particle output file (PARDUMP) and recalculates the concentrations using the CONTROL file to determine grid dimensions, times, and output file names. Par2conc is used in conjunction with the namelist variable NDUMP < 0 (input and output of particle files).

The name of the particle positions output file is specified on the command line as follows:

- USAGE: PAR2CONC -[options(default)]
- INPUT PARAMETERS: -i[input file name (PARDUMP)]

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Concentration / Utilities / Particle Adjustment

This menu calls a utility program that can be used to adjust the particle positions prior to restarting the simulation from a saved particle position file. The particle position file needs to be written by setting the appropriate namelist parameter as described in the Advanced/Configuration Setup/Concentration menu tab. Normally observational data should be consulted prior to making any adjustments to the particle positions. Positions are only shifted horizonatally and not vertically. The same horizontal adjustment is applied at all heights. If a height adjustment is required, the model should be re-run with a different initial particle height distribution.

One or more particle files may be processed by a single execution. A standard simulation only generates one particle output file containing positions at one or more time periods. Multiple particle position files, with a three-digit suffix (.001, .002, etc), are automatically generated by the ensemble version of the model. The adjusted output is always written to a new file name, defaulting to *PARINIT*, also the default name for initializing a new simulation.

Regardless of how many time periods are contained in the particle position file, the adjustment is only applied to one time period, normally the initialization time period for the next simulation. If the time field (-t) is not specified, then the adjustment occurs to the first time period in the file, otherwise the adjustment is applied to the MMDDHH designated in the time argument. Only this one time period is written to the output file, regardless of how many time periods are contained within the input file.

A particle position shift can be specified as an angular adjustment in degrees and distance from a fixed location (such as the particle source point). A shift may also be specified as a window translation, where all particles within a given latitude-longitude window are shifted by a specified number of degrees in latitude and longitude. No particles outside of the window or beyond the radius are shifted unless the blending (-b) flag is set. In this case, the shift is applied to each particle in a linearly decreasing fashion to zero adjustment at a distance of two windows.

The spatial adjustment of the particle positions in the HYSPLIT binary particle output file are specified on the command line (or through the GUI) as follows:

- USAGE: parshift -[options (default)]
- -b[blend shifting outside of the window or distance range]
- -i[input base file name particle positions (PARDUMP)]
- -o[output base file name of adjusted partciles (PARINIT)]
- -r[rotation shift (degrees:kilometers:latitude:longitude)]
- -s[search for multiple input files with .000 suffix attached to base name]
- -t[time MMDDHH (missing field then process first time only)]
- -w[window translation corners lat1:lon1:lat2:lon2 (-90.0:-180.0:90.0:180.0)]
- -x[delta longitude for window translation (0.0)]
- -y[delta latitude for window translation (0.0)]

The particle position file may be converted to a binary concentration file through the command line utility program par2conc.

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Concentration / Utilities / Transfer Coefficient

Overview: This menu can be used to solve the transfer coefficient matrix for the source term vector given a measured data vector and where the matrix values are the dilution factors for each source-receptor pair. The measured data vector at multiple receptor locations and/or times is required and it must be defined in the DATEM format. The format of this file is discussed more detail in the GeoLocation menu. Due to model errors and insufficient sampling not all simulations will yield a solution. Results are written to the file *source.txt*.

Theory: Assume that the concentration at receptor R is the linear sum of all the contributing sources S times the dilution factor D between S and R:

- $S_1D_{11} + S_2D_{12} = R_1$
- $S_1D_{21} + S_2D_{22} = R_2$

The dilution factors are defined as the transfer coefficient matrix. The sum of each column product S_iD_{ij} shows the total concentrations contributed by source i to all the receptors. The the sum of the row product S_iD_{ij} for receptor j would show the total concentration contributed by all the sources to that receptor. In this situation it is assumed that S is known for all sources. The dilution factors of the coefficient matrix are normally computed explicitly from each source to all receptors, the traditional forward downwind dispersion calculation.

In the case where measurements are available at receptor R and source S is the unknown quantity, the linear relationship between sources and receptors can be expressed by the relationship:

- $D_{ij}\ S_i = R_j$,

which has a solution if we can compute the inverse of the coefficient matrix:

- $S_i = (D_{ij})^{-1}\ R_j$.

For example, in the case of an unrealistic 2x2 square matrix (the number of sources equals the number of receptors), the inverse of D is given by:

$$\begin{vmatrix} +D_{22} & -D_{12} \\ -D_{21} & +D_{11} \end{vmatrix} 1/(D_{11}D_{22}-D_{12}D_{21})$$

The solution for S_1 (first row) can be written:

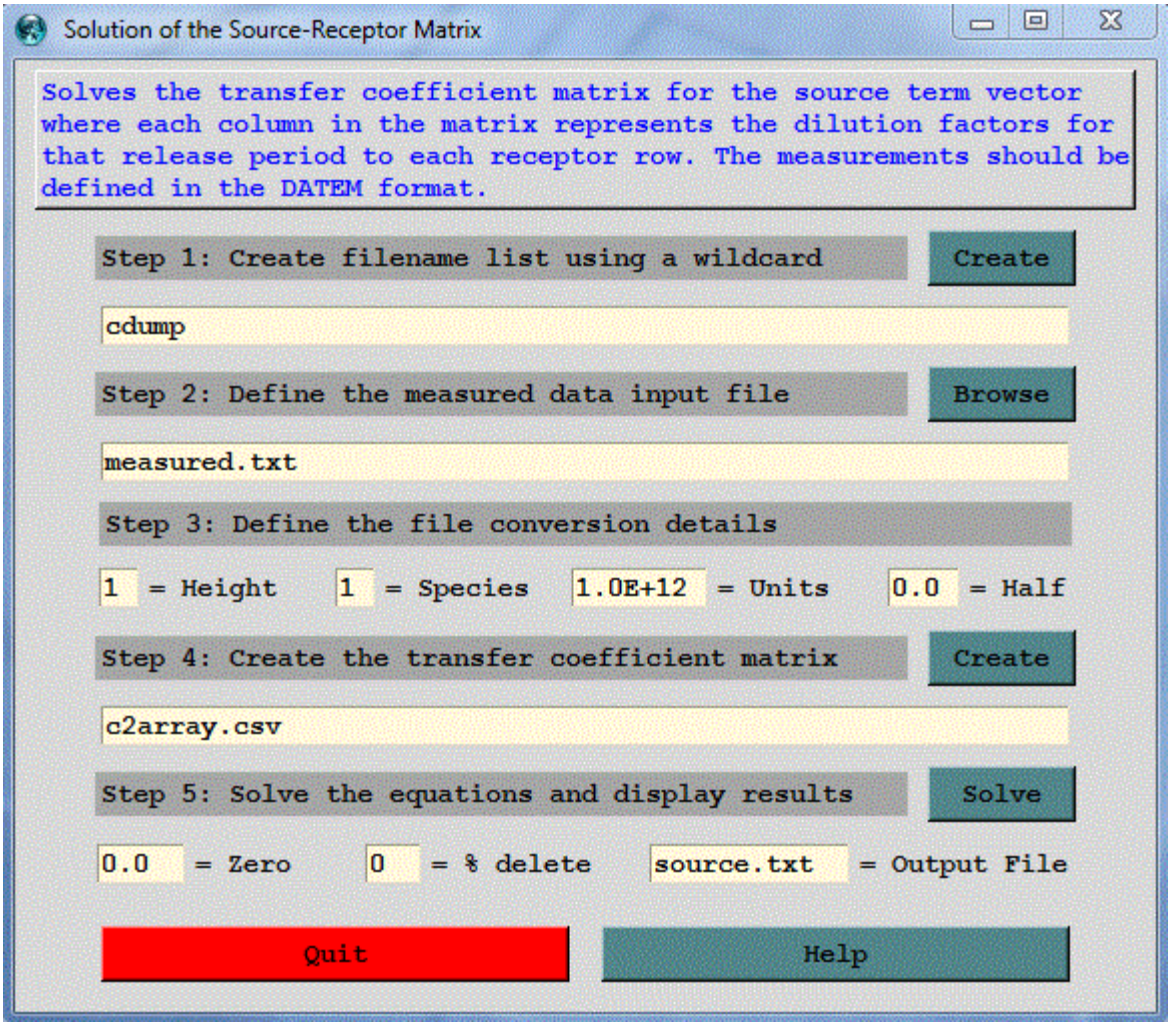
- $D_{22}R_1/(D_{11}D_{22}-D_{12}D_{21}) - D_{12}R_2/(D_{11}D_{22}-D_{12}D_{21})$

As a further simplification, assume that there is no transport between S_1 and $R_2(D_{12} = 0)$, and then the result is the trivial solution that the emission value is just the measured concentration divided by the dilution factor:

- $S_1 = R_1/D_{11}$

The matrix solution has three possibilities. The most common one is that there are too many sources and too few receptors which results in multiple solutions requiring singular value decomposition methods to obtain a solution. The opposite problem is that there are too many receptors and too few unknowns hence an over determined system requiring regression methods to reduce the number of equations. Unfortunately, possibilities for a matrix solution may be limited at times due to various singularities, such as columns with no contribution to any receptor or measured values that have no contribution from any source. The solution to these problems is not always entirely numerical as the underlying modeling or even the measurements can contain errors. Note that large dilution factors (very small predicted

concentrations) at locations with large measured values will lead to large emissions to enable the model prediction to match those measurements. The opposite problem also exists in that negative emission values may be required to balance high predictions with small measurements. The solution to the coefficient matrix is driven by errors, either in the measurements, the dispersion model, or the meteorological data.



Step 1: defines the binary input files which are the output file from the disersion simulations configured to produce output at an interval that can be matched to the measured sampling data. Ideally the model simulation emission rate should be set to a unit value. Each simulation should represent a different discrete emission period. For example, a four day event might be divided into 16 distinct 6-hour duration emission periods. Therefore the matrix would consist of 16 sources (columns) and as many rows as there are sampling data. The entry field in step 1 represents the wild card string *entry* that will be matched to the files in the *working* directory. The file names will be written into a file called *INFILE*. This file should be edited to remove any unwanted entries.

Step 2: defines the measured data input file which is an ASCII text file in the DATEM format. The first record provides some general information, the second record identifies all the variables that then follow on all subsequent records. There is one data record for each sample collected. All times are given in UTC. This file defines the receptor data vector for the matrix solution. It may be necessary to edit this file to remove sampling data that are not required or edit the simulation that produces the coefficient matrix to insure that each receptor is within the modeling domain.

Step 3: defines the file conversion details from sampling units to the emission units. For instance, the default value of 10^{+12} converts the emission rate units pg/hr to g/hr if the sampling data are measured in pg/m^3 (pico = 10^{-12}). The exponent is +12 rather than -12 because it is applied in the denominator. The height and species fields are the index numbers to extract from the concentration file if multiple species and levels were defined in the simulation. The half life (in days) is only required when dealing with radioactive pollutants and the measured data need to be decay

corrected back to the simulation start time.

Step 4: creates the comma delimited input file called *c2array.csv* with the dilution factors in a column for each source and where each row represents a specific receptor location. The last column is the measured value for that receptor. The column title represents the start time of the emission in days from the year 1900. This step calls the program *c2array* which reads each of the measured data values and matches them to the input files to extact the dilution factors from each source to that measured value.

Step 5: solves for the source vector using the SVD (Singular Value Decomposition) methods from Numerical Recipes, The Art of Scientific Computing, Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T., 1986, Cambridge University Press, 818 p. The solution may be controlled to some extent by defining a threshold zero dilution factor, below which the dilution factors are set to zero. An alternative approach is the define a cumulative percentage dilution factor, below which an entire sampling row may be eliminated. For instance, if the % delete field contains 10, then the rows representing the lowest 10% of the dilution factors are removed. In the event the computation fails to produce an adequate solution, it may be necessary to edit *c2array.csv*. The solution results are written to an output file *source.txt* and also displayed throught the GUI. A solution may contain negative values as well as extreme positive emission results. Such values are not realistic and are a result of model errors or other uncertainties. This step calls the program *tcsolve*.

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Concentration / Special Runs

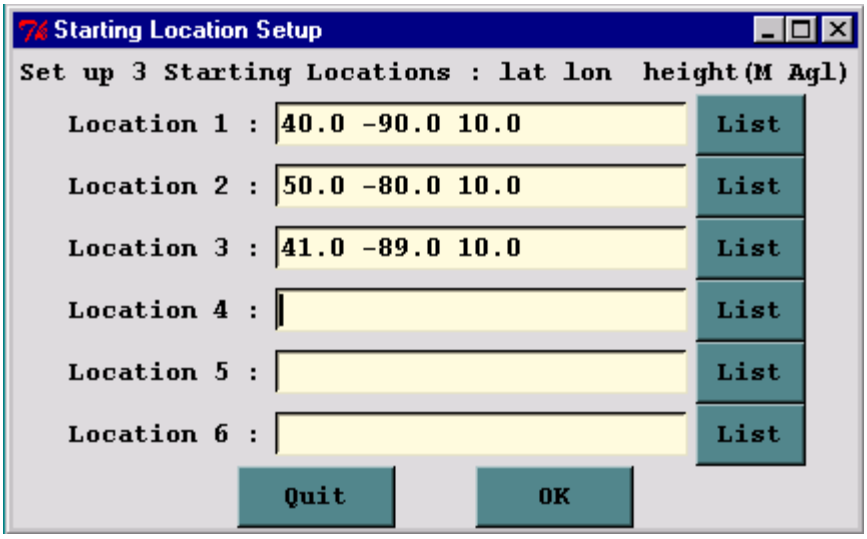
Special simulations may require a different executable file, modifications to the Control file that are not supported by the GUI, or interactions with other items under the Advanced Menu tab. More information is provided below for each special simulation. Special model configurations may not be available for all operating systems. Note that most of the special simulations may be run using a single processor system or multiprocessor system (supporting MPI).

Daily

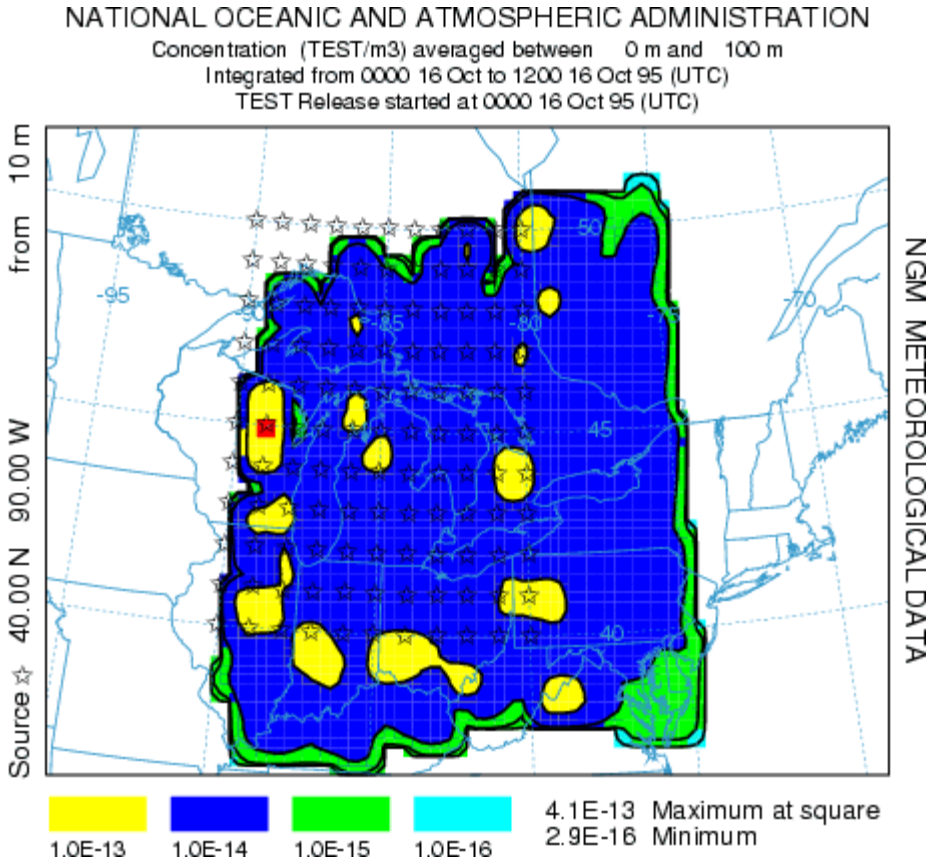
This menu will execute a special script to run the last configured dispersion calculation for multiple starting times, creating an output file for each simulation. More information is available from the daily help menu.

Matrix

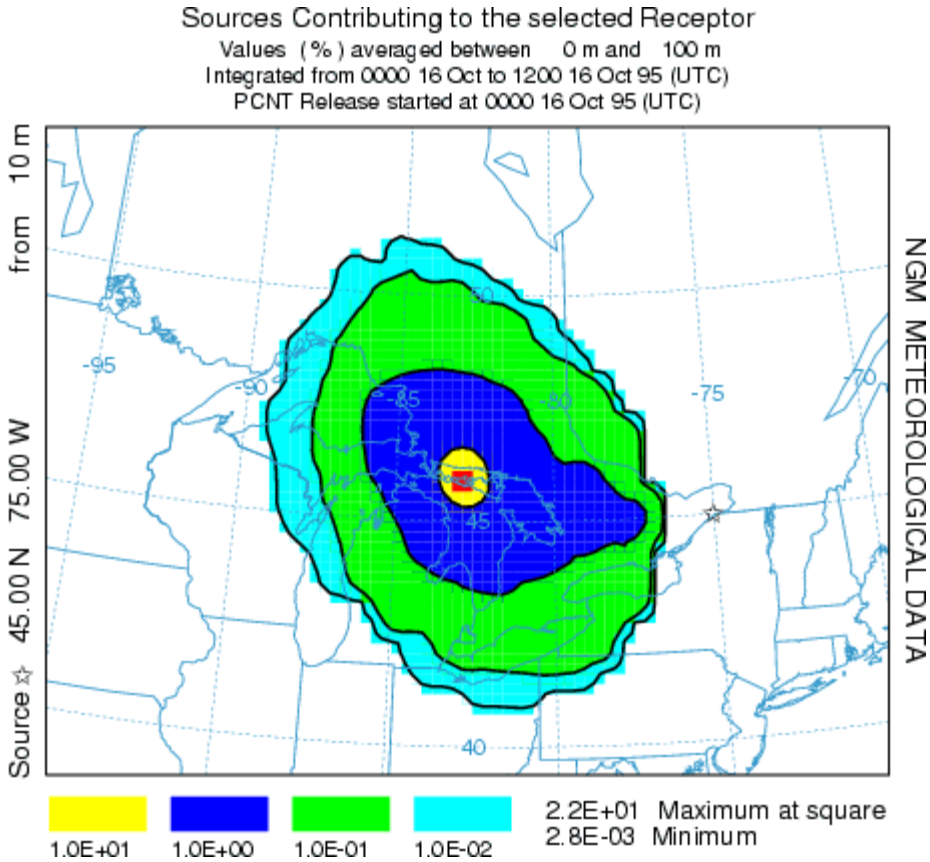
Although the setup of the concentration matrix calculation is similar to that of the trajectory matrix calculation, there is an additional option that can be set in the Advanced Menu configuration tab that changes the nature of the concentration output file to produce a source-receptor matrix. This will be discussed further below. The matrix calculation is a way to set up the *CONTROL* file for multiple starting locations that may exceed the GUI limit under the Concentration Setup menu tab. Hundreds or thousands of starting points may be specified. The *Run Matrix* menu tab first runs a program that reads the *CONTROL* file with three starting locations and then rewrites the same *CONTROL* file with multiple locations. The multiple locations are computed from the number of starting points that fall in the domain between starting point 1 and starting point 2, where each new location is offset is the same as that between starting locations 1 and 3. For instance, if the original control file has three starting locations: #1 at 40N, 90W; #2 at 50N, 80W, and #3 at 41N, 89W; then the matrix processing results in a Control file with 121 starting locations, all one degree apart, all between 40N 90W and 50N 80W.



In the normal model execution mode, the concentration contributions from multiple sources are summed on the concentration grid, hence it is not possible to determine the fraction of the material comes from each source location. This can be seen in the illustration below using the above configuration for the first 12 hours of the sample case.



However, if the "Matrix" conversion module is checked in the Advanced Concentration Configuration menu tab, then the multiple source simulation maintains the identity of each source in the concentration output file. The Display Matrix menu tab permits extraction of information for individual sources or receptors from this special concentration output file. The results of the same simulation are shown in the illustration below. In this case the receptor check-box was set and the receptor location was identified as 45.0,-75.0 with normalization. Therefore the graphic illustrates the fractional contribution of each region to the first 12 hour average concentration at the designated receptor.



The following table illustrates the HYSPLIT matrix configuration. Emissions occur from each of N source locations and the receptors represent the concentration grid of M nodes. A single concentration output file is produced where each source contributes to its own concentration grid of M receptors. When selecting a "source" display, the M columns from the source location (row) represent the downwind concentration pattern for that source. When the receptor location (column) is selected, the contours represent the concentrations (each row of that column) contributing to that receptor from each of the source locations. Source and receptor grids should be of comparable resolution.

	Receptor 1	Receptor 2	Receptor 3	...	Receptor M
Source 1					
Source 2					
Source 3					
...					
...					
...					
...					
...					
Source N					

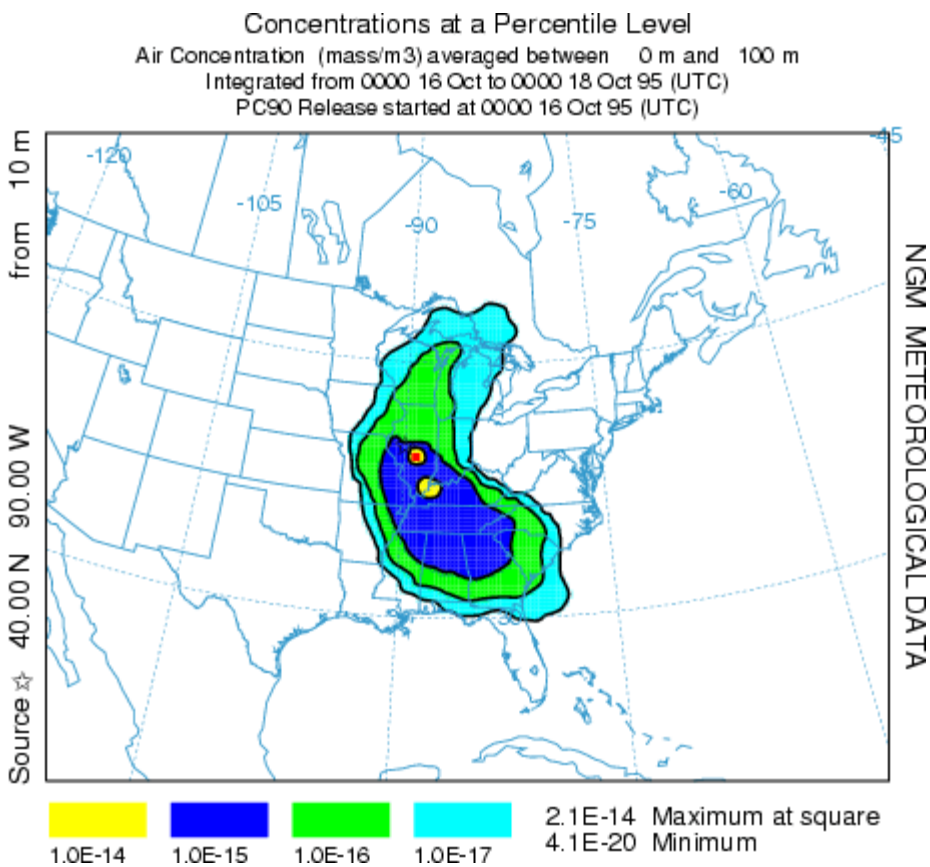
There are two other more quantitative approaches to source-attribution available through the menu and both require the measured sampling data. In the first approach, menu system is used to configure the model to execute a script to run multiple iterations of the upwind dispersion calculation for periods that correspond with individual measured sampling data. The results are then overlaid to determine the most likely source region. In the second approach, the menu system is used to solve the source-receptor coefficient matrix for the source term vector given a measured data vector and where the matrix values are the dilution factors for each source-receptor pair as described above.

Geolocation

In a manner similar to the daily menu, the dispersion model can be run for multiple simulations in time but where each simulation is configured as an adjoint calculation (backward in time) from measured concentration data points. More information on this procedure can be found in the geolocation help menu.

Ensemble-Meteorology

The ensemble form of the model, an independent executable, is similar to the trajectory version of the ensemble. The meteorological grid is offset in either X, Y, and Z for each member of the ensemble. The model automatically starts each member on a single processor in a multi-processor environment or cycles through the simulations on one processor. The calculation offset for each member of the ensemble is determined by the grid factor as defined in the Advanced Concentration Configuration Tab. The default offset is one meteorological grid point in the horizontal and 0.01 sigma units in the vertical. The result is 27 ensemble members for all offsets. The normal Setup Menu tab is used to configure the *CONTROL* file. Note that if fewer than 27 processors are available, the ensemble configuration menu permits starting the calculation at any ensemble member number within the valid range. Because the ensemble calculation offsets the starting point, it is suggested that for ground-level sources, the starting point height should be at least 0.01 sigma (about 250 m) above ground. The model simulation will result in 27 concentration output files named according the file name setting in the control file "{cdump}.{001 to 027}" with a suffix equivalent to the ensemble member number. On a single processor system, the calculation may take some time to cycle through all the memberes. The menu will be locked until the simulation has completed. A message file window will open after termination. Computational progress may be monitored by noting the generation of new concentration output and message files with the ensemble number suffix in the /working directory. The concentration output from each member can be displayed through the concentration display menu tab. However, to display the probabilities associated with the multiple simulations, it is necessary to pre-process the data through the Display Ensemble menu tab. Using the default configurations for the sample simulation, the illustration below represents the 90th percentile concentrations aggregating all four output time periods. For instance the blue contour in this 90th percentile plot represents the region in which only 10% of the ensemble members have air concentrations greater than 10^{-15}. If the meteorological ensemble is run through a script or batch file instead of the GUI, the executable, with a command line parameter of the member number, must be run once for each of the 27 members.



Ensemble-Turbulence

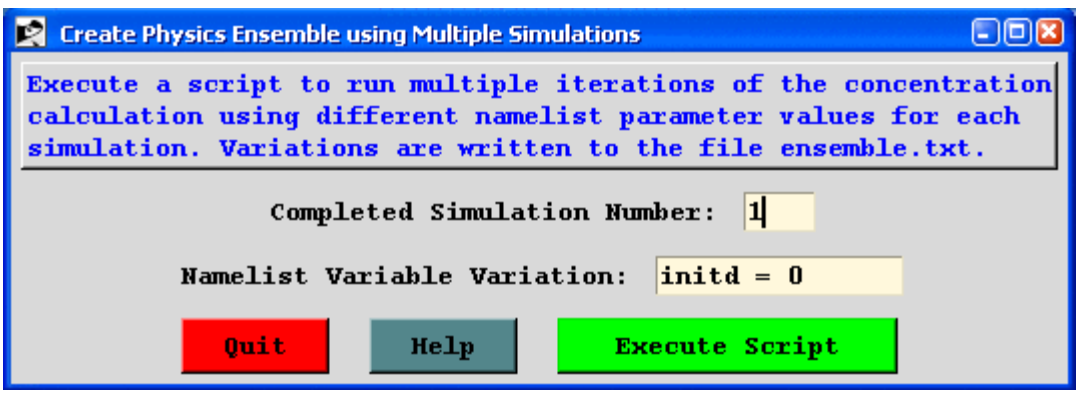
Another ensemble variation is the *turbulence* option, which also creates 27 ensemble members, but due to variations in turbulence rather than variations due to gradients in the gridded meteorological input data. The variance ensemble

should only be run in the 3D particle mode and with fewer particles, in proportion to the number of ensemble members to the number of particles required for a single simulation. For instance, if 27,000 particles are required to obtain a smooth plume representation, then each member should be run for 1000 particles. Normally the same random number seed is used when computing the turbulent component of the particle motion. However, in the variance ensemble, the seed is different for each member, resulting in each member representing one realization of the ensemble.

The variance ensemble can also be used to determine the number of particles required for a simulation, by progressively increasing the particle number until the variance decrease with increasing particle number is no longer significant. Because the number of particles required for a simulation increases with increasing distance from the source, a typical downwind receptor location needs to be selected and then by using the box plot display option, the concentration variability (max-min range) can be estimated and then determining when the decrease in range is no longer cost effective (in terms of computational time) with increasing particle number.

Ensemble-Physics

The physics ensemble is created by running a script that varies in turn the value of one namelist parameters from its default value. These are the parameters defined in the file *SETUP.CFG* and normally set in the Advanced Concentration Configuration menu tab. If the namelist parameters have not been defined through the menu, then the default values are assigned. In this first iteration, the GUI menu permits no deviation from the values assigned by the script. The entry box is for information purposes only to show the progress of the computation.



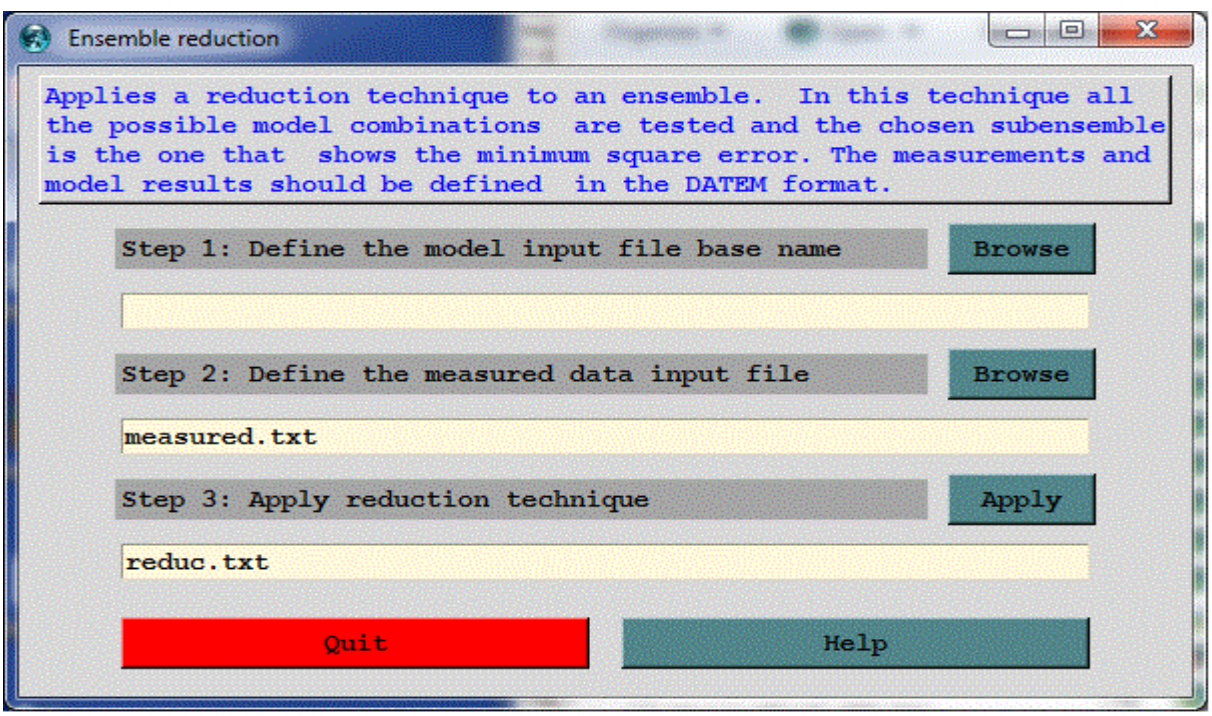
A summary of the current 20 ensemble variations is also written to the file *ensemble.txt* showing the name of the concentration output file and member variation. Check the advanced menu help files for more information on each variable.

cdump.001 : initd = 0
cdump.002 : initd = 3
cdump.003 : initd = 4
cdump.004 : kpuff = 1
cdump.005 : kmixd = 1
cdump.006 : kmixd = 2
cdump.007 : kmixd = 1500
cdump.008 : kmix0 = 50
cdump.009 : kzmix = 1
cdump.010 : kzmix = 2 ; tvmix =0.5
cdump.011 : kzmix = 2 ; tvmix =2.0
cdump.012 : kdef = 1
cdump.013 : kbls = 2
cdump.014 : kblt = 1
cdump.015 : kblt = 3
cdump.016 : tker = 0.10
cdump.017 : vscales = 5.0
cdump.018 : vscaleu = 1000.0

cdump.019 : hscale = 5400.0
cdump.020 : hscale = 21600.0

Ensemble reduction based on minimization of square error

Over the last few years, the use of dispersion model ensembles has been an increasingly attractive approach to study atmospheric transport in the lower troposphere. Ensembles are constructed either by combining multiple numerical weather prediction simulations, different dispersion models, introducing variations in a particular model's physics parameterizations or different combinations of these variations. The determination of the optimum number of multi-model members and/or individual model physical features to vary is the primary difficulty to overcome when constructing these dispersion simulation ensembles. In many studies the ensemble members just consisted of the available model outputs from different research groups regardless of the model characteristics or the result of performing an arbitrary number of runs with different configurations by individual researchers. Both approaches increase the possibility of redundancy which means that many of the ensemble members may not be much different from each other. In general, any ensemble might contain redundant information that overemphasizes certain transport and dispersion features that can be inaccurate. For example, perhaps a sub-group of members all use the same meteorological data, which might not be as accurate as another meteorological data set that is used by fewer members. Therefore, simply due to a dependency among many of the members to the same data, the ensemble including these members would be less accurate than one constructed from an ensemble based upon only the independent members. Conversely, independence among ensemble members does not necessarily imply that the reduced group of runs will be more accurate than the full ensemble because, by chance, the later could be also over emphasizing redundant members that happen to be more accurate. Consequently, we can apply reduction techniques with the intent to produce more accurate results than those obtained with the full ensemble and therefore requiring fewer computing resources. Solazzo and Galmarini (2014) demonstrated that an ensemble can be reduced by optimizing the skills of the mean taken among all the possible subsets of ensemble members. Following this methodology we calculate the average of all the possible model combinations composed by an increasing number of sub ensemble members up to the total number of members of the full ensemble and estimate their MSE. Furthermore, if M is the total number of ensemble members and n is the number of sub ensemble members, then the number of possible combinations is given by M!/(n!*(M-n)!). In other words, if our ensemble has, say, 24 members we will combine them in 276 pairs, 2024 trios, 10626 quartets, etc. and determine which combination provides the minimum MSE. The reduction technique is applied by running a postprocessing program that reads the different ensemble member outputs along with the measured data (all in DATEM format) and calculates the minimum square errors for each possible model output combination.



E. Solazzo, S. Galmarini, 2014. The Fukushima-137Cs deposition case study: properties of the multi-model ensemble,

Journal of Environmental Radioactivity, Available online 22 March 2014, ISSN 0265-931X, http://dx.doi.org/10.1016/j.jenvrad.2014.02.017

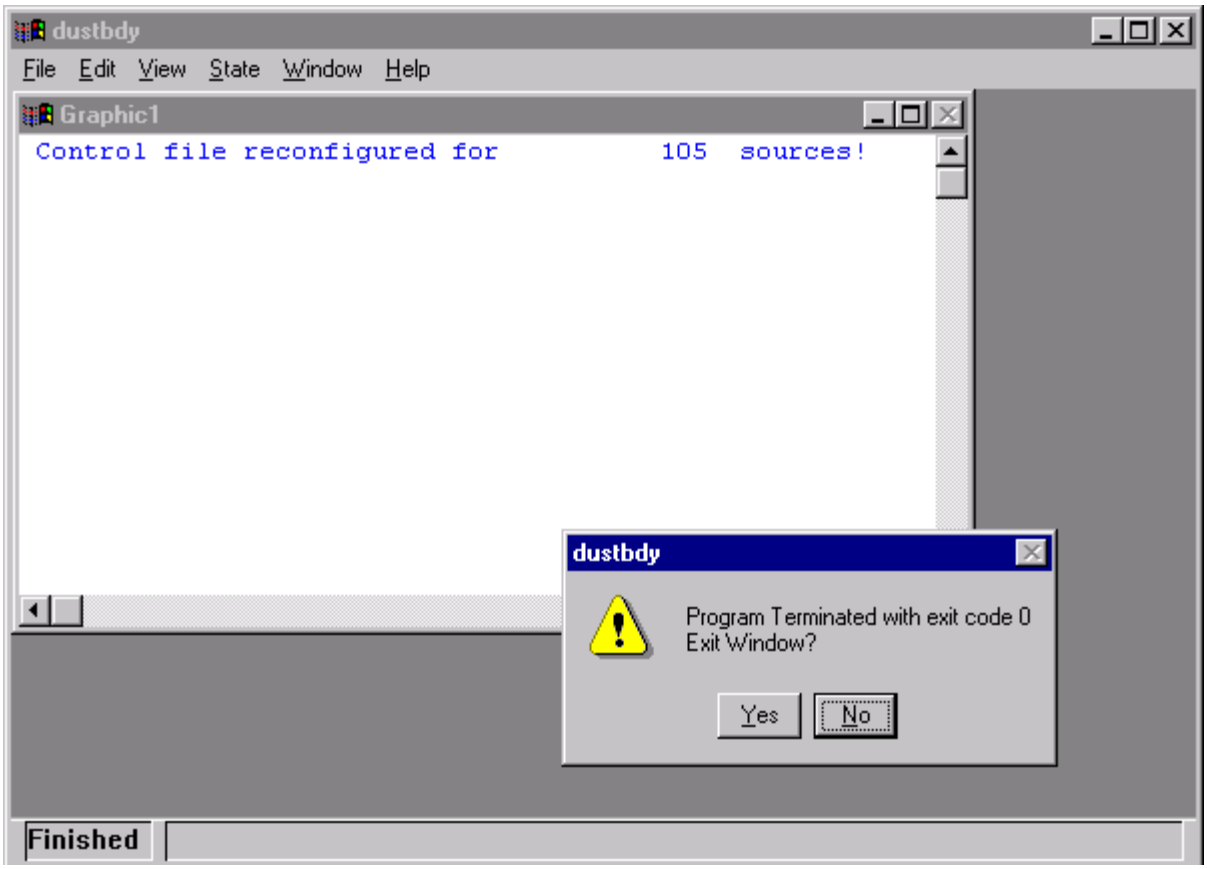
Global

The global simulation is a HYSPLIT "grid-in-plume" option, in which the Lagrangian particle mass can be transferred to a global Eulerian model after a designated number of hours. Lagrangian and Eulerian dispersion and transport can occur simultaneously. Each *model* has its own output grid. The advantange of this approach is that at times very long-range calculations may require too many particles to properly represent the pollutant distribution. In this way it is possible to take advantage of the the more precise Lagrangian approach near the source and the more computationally efficient Eulerian computation at the hemispheric and global scales. More information on how to configure this simulation can be found in the global model help menu.

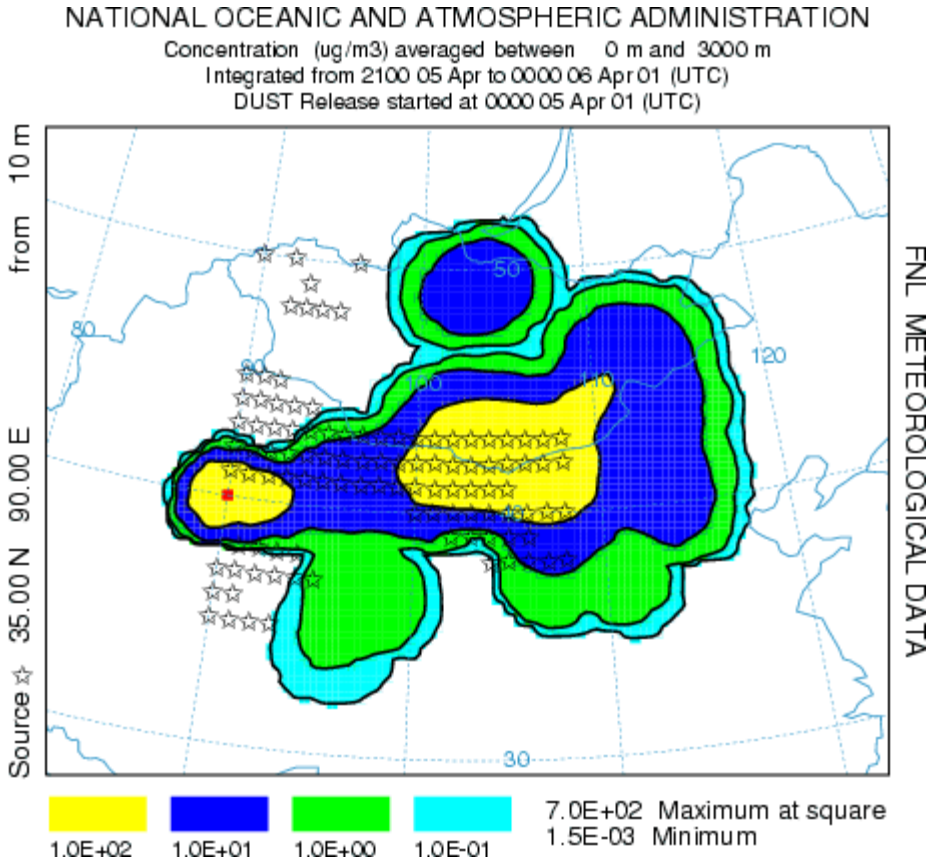
Dust Storms

A model for the emission of PM10 dust has been constructed (Draxler, R.R, Gillette, D.A., Kirkpatrick, J.S., Heller, J., 2001, Estimating PM10 Air Concentrations from Dust Storms in Iraq, Kuwait, and Saudi Arabia, Atmospheric Environment, Vol. 35, 4315-4330) using the concept of a threshold friction velocity which is dependent on surface roughness. Surface roughness was correlated with geomorphology or soil properties and a dust emission rate is computed where the local wind velocity exceeds the threshold velocity for the soil characteristics of that emission cell. A pre-processing program was developed that accesses the HYSPLIT land-use file over any selected domain and modify the input CONTROL file such that each emission point entry corresponds with a "desert" (active sand sheet) land-use grid cell. The original PM10 flux equation was replaced by a more generic relationship (Westphal, D.L., Toon, O.B., Carlson, T.N., 1987. A two-dimensional numerical investigation of the dynamics and microphysics of Saharan dust storms. J. Geophys. Res., 92, 3027-3029).

The dust storm simulation is configured in the same way as the matrix calculation in that it is necessary to define three source locations, the first two representing the limits of the domain, and the third defining the emission grid resolution. The pre-processor then finds all emission points within that domain that have a desert category and modify the *CONTROL* file accordingly. The dust box must be checked in the advanced configuration menu to compute the PM10 emission rate. As an example, we can configure the model to run the large Mongolian dust storm of April 2001. An animation of the calculation results can be downloaded. To run the same simulation it will be necessary to obtain the first two weeks of northern-hemisphere meteorological analysis data (FNL.NH.APR01.001). A pre-configured *CONTROL* file (*dust_conc*) should be retrieved from the working directory. The *CONTROL* file defines the emission domain by the three starting locations: 35N-90W to 50N-120W with the grid increment to 36N-91W. There is no point in defining an emission grid of less than one-degree resolution because the resolution of the land-use data file is one-degree and the meteorological data is closer to two-degrees. Once the model is setup for the simulation, including the dust check-box in the configuration menu, execute the model from the *Special Simulations / Run Dust Storm* menu tab. Not available through the GUI, but another option in the *SETUP.CFG* namelist file, is the emission threshold sensitivity factor, which normally defaults to one. For instance, adding the line *P10F=0.5* to the namelist file, would cause dust emissions to occur at half the normal threshold velocities. Starting the model will cause the window shown below will open to indicate the revision of the *CONTROL* file.



The message indicates that the initial 3-location *CONTROL* file was reconfigured by the *dustbdy* program for 105 source locations. That means in the domain specified, 105 one-degree latititude-longitude grid cells were found to have a desert land-use category. If none are found, then the *CONTROL* file is deleted to prevent model execution. Click on Yes or No to continue - yes just deletes the window. The model execution will then start. PM10 pollutant dust particles are only emitted from those 105 cells where the wind speed exceeds the emission threshold. Therefore it is possible to have simulations with no emissions. An example of the output after 24 hours simulation time is shown in the illustration below.



The concentrations represent a 3-hour average from 21 to 24 hours after the start of the simulations. It is not possible to say exactly from when or where particles are emitted except to note that the 105 potential source locations are shown. The emission algorithm emits in units of grams, but the in configuring the concentration display, the units were changed to ug by defining a conversion factor of 10^6. Maximum concentrations are on the-order-of 100, but the layer was defined with a depth of 3 km to facilitate comparison with satellite observations. The simulation could be rerun with a smaller layer to obtain concentrations more representative of near-ground-level exposures.

Daughter Products

A nuclide daughter product module has been incorporated into HYSPLIT. Given a chain of decay from a parent nuclide, the model can calculate the additional radiological activity due to in-growth of daughter products using the Bateman equations. Information about the available daughter products available in the model can be found in ../auxiliary/ICRP-07.NDX. More information on how to configure this simulation can be found in the daughter product help menu.

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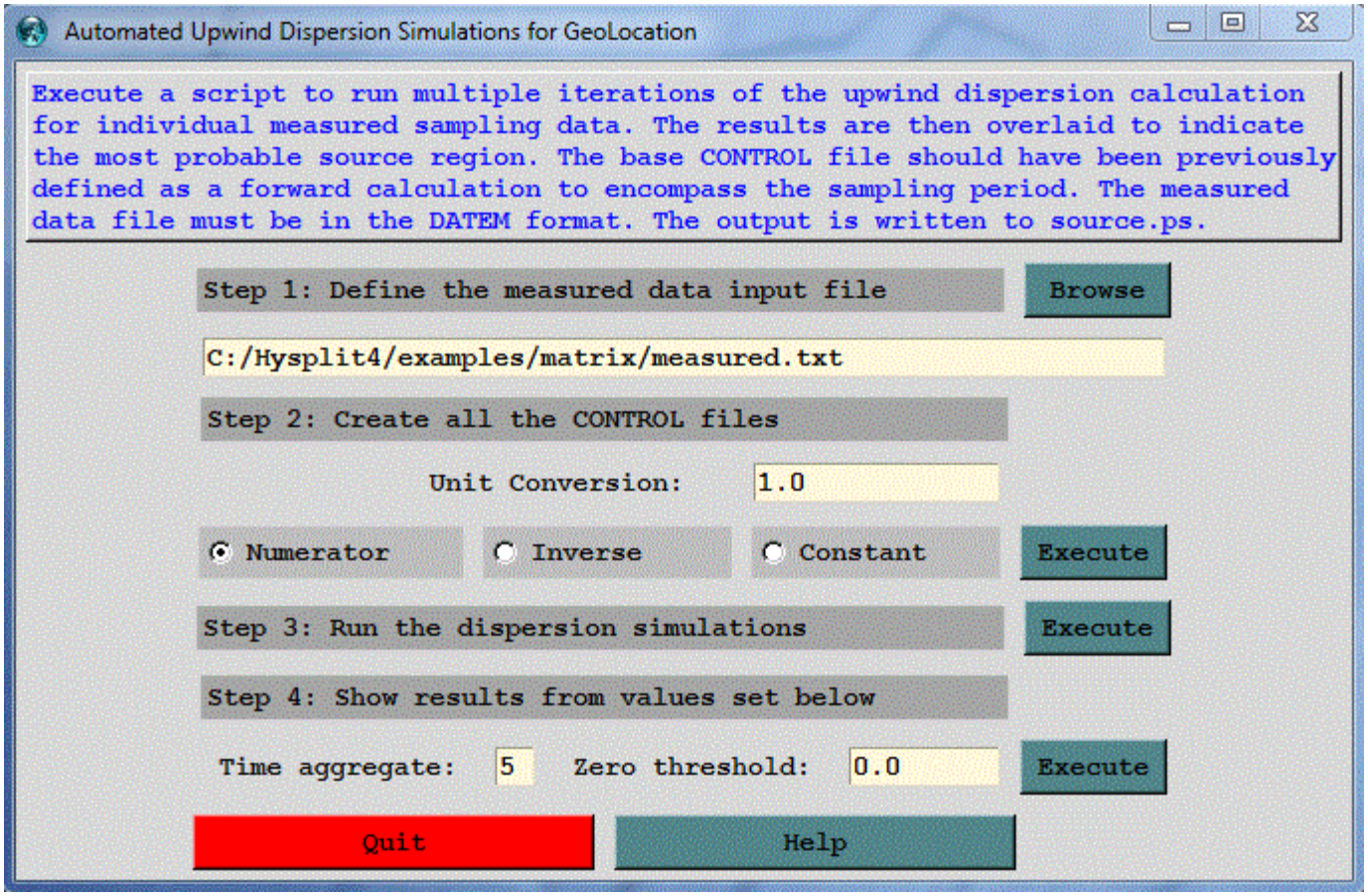
Concentration / Special Runs / GeoLocation

Summary: This menu is used to configure the model to execute a script to run multiple iterations of the upwind dispersion calculation for periods that correspond with individual measured sampling data. The model results are then overlaid to indicate the most probable source regions. The CONTROL file should have been previously defined for a forward calculation that corresponds to the sampling period of the measured data. The measured data file must be in the DATEM format. The output is written to the source.ps Postscript file in the working directory.



Step 1: defines the measured data input used in this series of calculations. The dispersion model is run in its backward mode, from each of the sampling locations, with a particle mass proportional to the measured concentration and with the particles released over a period corresponding to the sample collection period. Sampling data files are in the ASCII text DATEM format. The first record provides some general information, the second record identifies all the variables that then follow on all subsequent records. There is one data record for each sample collected. All times are given in UTC. The DATEM sampling data records have the following format:

- INTEGER - Four digit year for sample start
- INTEGER - Two digit month for sample start
- INTEGER - Two digit day for sample start
- INTEGER - Four digit hour-minutes for sample start
- INTEGER - Four digit hour-minutes for duration of the sample
- REAL - Latitude of the sampling point (Positive is north)
- REAL - Longitude of the sampling point (Positive is east)
- REAL - Air concentration in mass units per cubic meter
- INTEGER - Site identification

An sampling data file which is used in the following calculations can be found in examples\matrix\measured.txt. These

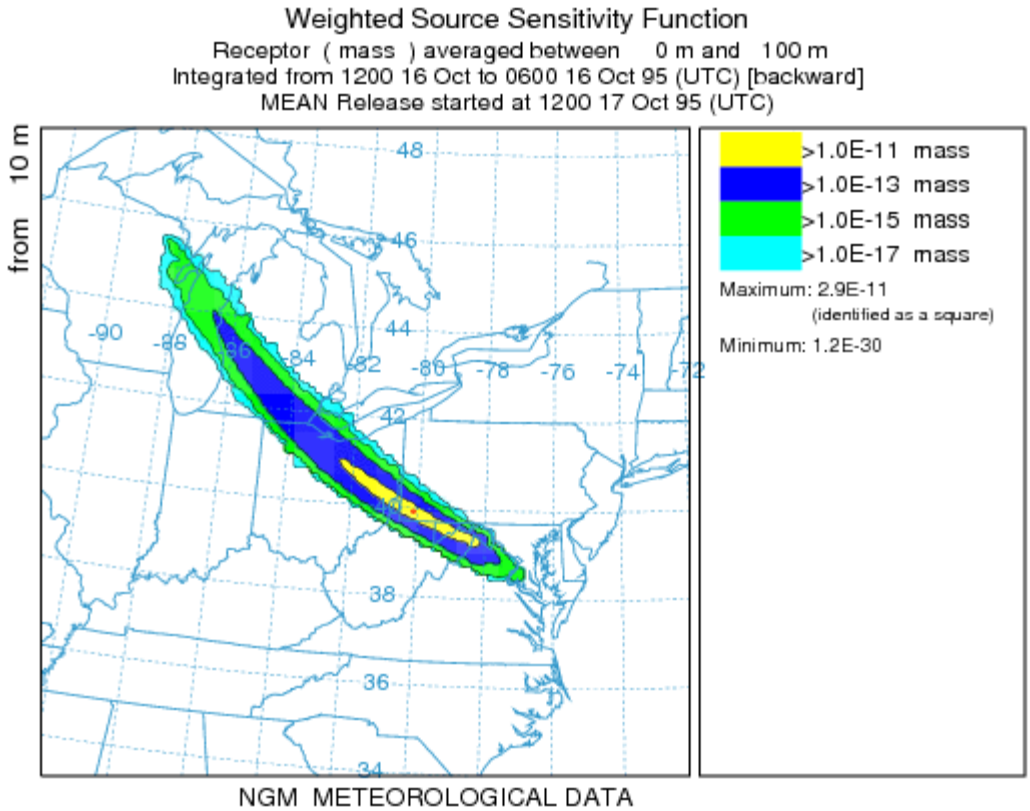
synthetic measurements (units = picograms per cubic meter) were created from a model simulation using the sample meteorological data in the working directory for a hypothetical 6-minute (0.1 hr) duration release of 10 kg of material from 40N 80W starting at 1200 UTC 16 Oct 1995.

Step 2: creates one CONTROL.{xxx} file for each sample (data record) in the previously defined measured data file. The CONTROL files are numbered sequentially from 001 to a maximum of 999, the current limitation of the program used to overlay the simulation results. The individual simulation control files are created from the current configuration shown in the concentration setup menu. The examples\matrix\control_geo file and the examples\matrix\setup_geo file templates should be retrieved into the setup and configuration menus. The template is a configuration for a forward simulation that encompasses the entire sampling period, with output intervals that correspond with the sampling intervals of the measured data. Essentially a configuration that could be used to predict the concentrations at the measurement locations if you knew the actual location and amount of the release. This step calls the pre-processor program (*dat2cntl*) which uses the configuration as a template to design each individual simulation CONTROL file. Each of these CONTROL files is configured as a backward simulation for the entire computational period, with the particle release occurring over the time of the sample collection. This insures that each simulation output file will contain an identical number of output periods, regardless of the time of the particle release. The template control file should have all key parameters specified such as the starting time and the center of the concentration grid. Do not use the zero default options in the CONTROL file, explicity set all variables. All simulations must be identical.

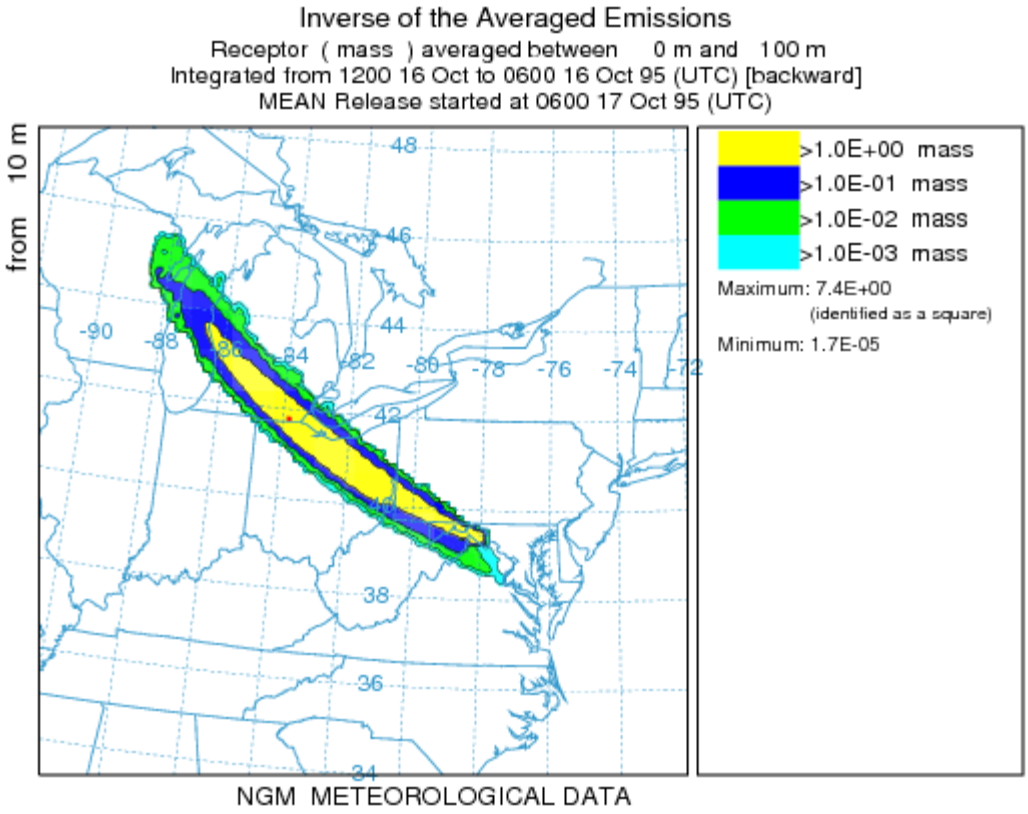
There are three solution options. The default option *Numerator*, discussed above, uses the measured concentration in the numerator as the emission rate, resulting in a source sensitivity map weighted by the measured data. Checking the *Inverse* box sets the source term as the inverse of the measured concentration. This modeling scenario is comparable to the S = R/D situation described in the matrix solution help file>. In this case the model is computing D/R, where D is the dilution factor computed by the model and R is the measured concentration. The source term for the calculation is set to 1/R and only measurements where R is greater than or equal to zero are considered. Therefore, the resulting output (D/R) is an estimate of the inverse of the source term (1/Q) required to match the measured value for that simulation. A unit conversion factor needs to be set to output the appropriate mass units. The last option is to set the *Constant* radiobutton which results in the emission rate equal to the value set in the constant conversion factor entry box. In this type of simulation, each sample gets equal weight and the model results may be used to determine the optimal emission rate required to match the measured data.

Step 3: sequentially runs the dispersion simulations starting with CONTROL.001 through the last available control file. Each simulation uses the same namelist configuration shown in the menu. Note that a simulation is run for each measurement, high values as well as zero measurements. Non-zero measurements result in an hourly emission rate equal to the measurement value, while zero measurements are set to a very small, but non-zero value. In the context of this particular calculation, the intent of the source-attribution is primarily to determine the source location and perhaps its timing rather than estimating the emission rate from the measurements. Determination of emission rates should be done through the matrix menu option. The measurement data are only used to weight the source-sensitivity results for each simulation. Depending upon the model setup and configuration, simulation wall-clock times may vary considerably. Each simulation output results in a binary concentration file and message file with the same run number suffix as the control file.

Step 4: shows the multiple simulation results by averaging the source sensitivity function at each grid point over all the simulations. The dispersion model result of the upwind (backward) calculation looks similar to the air concentration field of the downwind (forward) calculation, but represents not concentration, but the source regions that may contribute to the air concentration at the measurement location from which the upwind calculation was started. There are two optional parameters that influence the output graphic. The time aggregate default is one, meaning that each sampling period is represented by one graphic. In the example calculation shown below, the source sensitivity function is shown for the last time period of the simulation and represents the average of all the simulations (zero and non-zero) from different time periods valid for that 6-hour sampling period. A time aggregation value of 5 would average the results from all 5 time periods into one graphic. The zero threshold value can be used eliminate the very low level contours that result from the zero-emission simulations. For instance, selecting a value of 1.0E-15 (1/1000 of a pg/m3) would set to zero any grid points less than that value.



The comparable graphic for the inverse calculation is shown below for the mean emission values for 15 simulations that had non-zero measurements. Before creating control files for the inverse simulation, previous control files should be deleted to avoid mixing together the two types of simulations. For this example, the measured data file has 15 non-zero measurements and 30 zero measurements and the units conversion factor should be set to 1.0E-15 to go from pg to kg. The resulting interpretation of the graphic is that the central contour (value = 1) indicates an average emission of 1 kg in that region. The outermost contour (0.01) would require 100 kg to be released to match the measured data. Greater dilution (D is smaller) require greater corresponding emissions to match the measured data.



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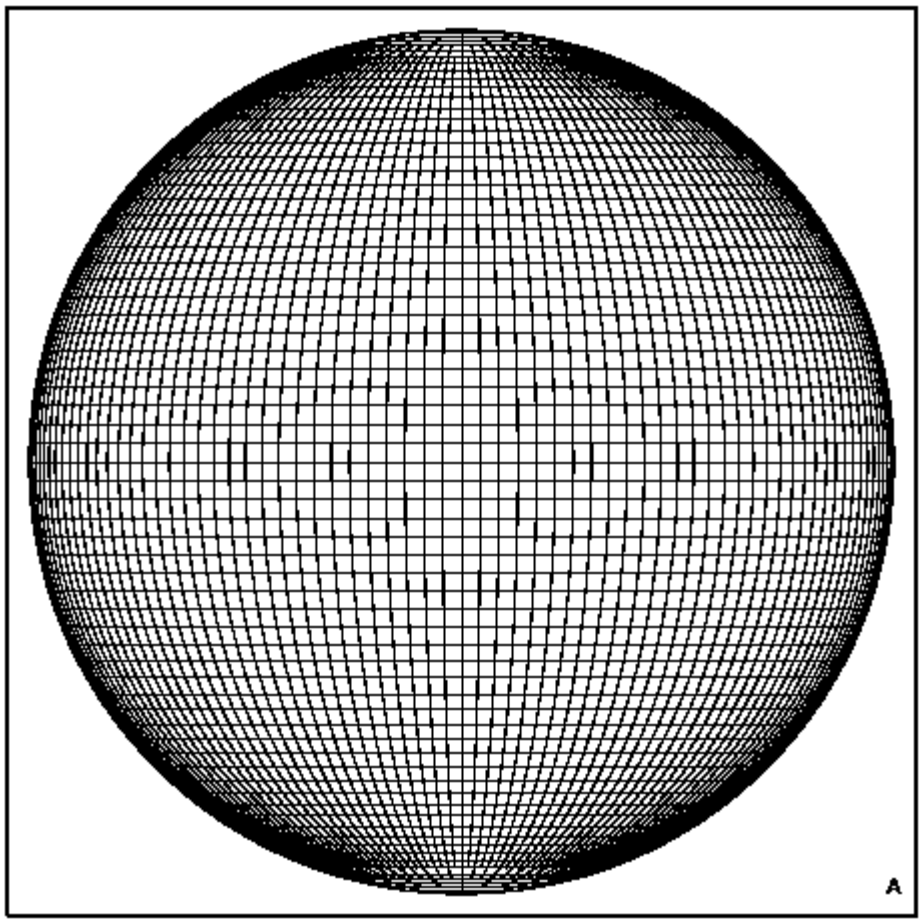
Concentration / Special Runs / Global

The Global Eulerian Model (GEM) is invoked as a series of subroutines within the main HYSPLIT transport and dispersion code. Particles or puffs are always first released in the Lagrangian framework and carried within HYSPLIT until they exceed a certain age at which point their mass is transferred to the GEM routines. Particles can be released and transferred for the entire duration of the simulation. The only requirement is that at one pressure-level global meteorological grid (2.5 degree reanalysis or 1 degree GFS) needs to be defined for the HYSPLIT calculation. Additional finer resolution regional meteorological grids can be defined for the Lagrangian portion of the transport calculation. Details of the global model have been previously published: Draxler, R.R., 2007, Demonstration of a global modeling methodology to determine the relative importance of local and long-distance sources, *Atmospheric Environment*, 41:776-789, doi:10.1016/j.atmosenv.2006.08.052.



General Instructions

Although the HYSPLIT-GEM version has its own executable, without the required namelist file *GEMPARM.CFG* the calculation will proceed as a standard Lagrangian HYSPLIT simulation. In this situation, the model will write the default file *gemparm.bak* as a reminder that a GEM configuration file is required to invoke the global subroutines. This file can then be edited and renamed if not using the GUI interface. GEM and HYSPLIT each create their own concentration output files and if the total concentration is required, the results from the two calculations must be added together. The program *concadd* is included in the distribution and can be accessed from the global display menu by selecting the plume add checkbox. Furthermore, the GEM concentration grid is always a snapshot concentration. There is no averaging option. In general, the model simulation is configured like any other HYSPLIT simulation, through the *CONTROL* and *SETUP.CFG* files. Additional GEM specific options are set in the *GEMPARM.CFG* file. Not all GEM options are available through the GUI and can only be modified by editing the file directly.

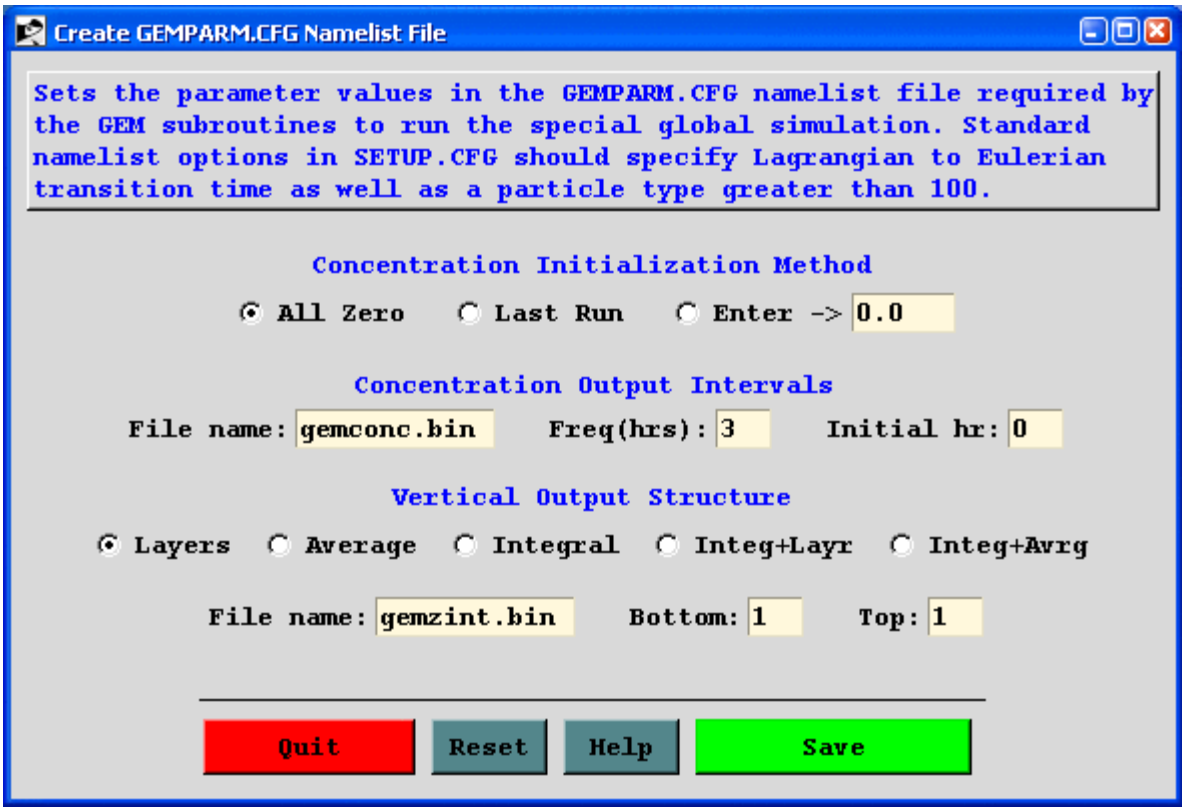
SETUP.CFG Namelist Configuration

There are several parameters in the HYSPLIT namelist that are important for the GEM subroutines. In particular, pay attention to the following:

1. Set INITD to one of the conversion variables, any value >100, for instance 109
2. Set CONAGE (default=48 hours) for particle conversion into the global model. Note that when CONAGE<0 the particles switch to the GEM grid when the particle meteorology grid switches to global meteorological grid or when the particle age=|conage|
3. When using an *EMITIMES* file, QCYCLE is not used for emission cycling. Also if the *EMITIMES* file has fewer sources than defined in the *CONTROL* file, the emissions specified in the *CONTROL* file need to be set correctly and match the first value in *EMITIMES*.

GEMPARM.CFG GUI Namelist Options

Only a subset of the namelist options are available to be set through the GUI. Note that concentration (mass/m3) output will always be written to *gemconc.bin* as individual or averaged layers, but the integrated output (mass/m2) will only be written to *gemzint.bin*. The bottom and top values are given as index numbers where 1 is the bottom layer. Layer thickness corresponds with the input meteorological data and cannot be modified. The GUI interface is shown below:



GEMPARM.CFG Namelist Description

HMIX=200000.0 - horizontal mixing (m2/s) at the equator
VMIX=50.0 - maximum vertical mixing (m2/s)
KMASS=2 - flag set to conserve mass (0:skip 1:show 2:yes)
KINIT=0 - concentration initialization (<0:no_run 0:zero 1:lat_bands 2:dew-point 3:last_dump 4:global_v37)
CKON=0.0 - value of initial concentration field if kinit>4
CMIN=0.0 - minimum value when using regression initialization (kinit=1|2)
CMAX=1.0E+25 - regression fit maximum value
WFACT=1.0 - sensitivity of advection to vertical velocity
KDIVG=0 - flag to compute vertical velocity from the divergence field (kdivg=1)
GEMDUMP='gemdump.bin' - daily 3-dimensional dump of concentration field (for initialization kinit=3)
GEMCONC='gemconc.bin' - HYSPLIT formatted concentration output file

GEMZINT='gemzint.bin' - HYSPLIT formatted vertically integrated concentration
CFACT=1.0 - internal (model) concentration to external (output) concentration units conversion factor
KZBOT=1 - grid cell index for the bottom output (or integration/averaging) level
KZTOP=1 - grid cell index for the top output (or integration/averaging) level
KZAVG=0 - flag for vertical averaging (0:none 1:average{bot-top} 2:integral{bot-top} 3:{2+0} 4:{2+1})
WFREQ=3 - output frequency in hours
IHOUR=0 - initial UTC output hour

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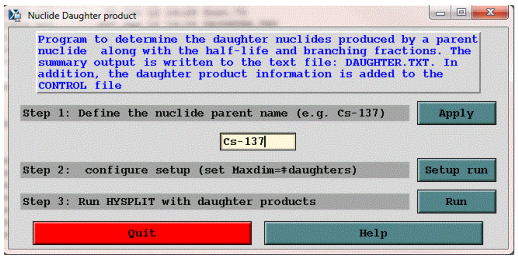
Concentration / Special Runs / Daughter products

Setting up this run consists in the following steps.

Step 1: Define the nuclide parent name (e.g. Cs-137) and run a preprocessor (nuctree) that creates a summary text file (DAUGHTER.TXT) that contains the daughter nuclides produced by a parent nuclide along with the half-life and branching fractions. This file is required to be in the working directory when running HYSPLIT for this application. In addition, the preprocessor will read the CONTROL file and create a new (CONTROL.DAUGHTER) file containing the daughter information. The names of the species will be given in numbers that correspond to the daughter products names written in the DAUGHTER.TXT file. Finaly, the GUI will copy the CONTROL.DAUGHTER back to CONTROL.

Step 2: configure setup (SETUP.CFG) indicating that the daughter products module will be used (ICHEM=11) and set Maxdim=#daughters obtained from DAUGHTER.TXT



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Concentration / Multi-processor

Special simulations may require a different executable file, modifications to the Control file that are not supported by the GUI, or interactions with other items under the Advanced Menu tab. More information is provided below for each special simulation that can be run under a multi-processor environment that supports MPI. These special simulations are available only for UNIX operating systems. All the MPI simulations execute the special script *run_mpi.sh* which can be found in the */exec* directory. This script executes the appropriate MPI executable variation of the concentration model and almost certainly will require some customization to match the local operating system environment.

Run MPI Model

The standard concentration model can be run on multi-processor systems. As pollutant particles are released during the simulation, they are parsed out in sequence to the available processors. The calculation proceeds independently until the end of a concentration averaging period. At this point, the concentrations from each processor are summed, and only one concentration output file is updated. The MPI version can be quite effective in speeding up simulations requiring the release of many particles. No special configuration or control file is required and output can be viewed using the standard concentration display menu.

Run Matrix Model

The multiprocessor version of the matrix calculation is configured the same way as for a single processor system. The MPI calculation proceeds as described above for the standard MPI model simulation.

Run Ensemble Model

The ensemble model automatically starts each member on a single processor in a multi-processor environment. The multiprocessor version of the ensemble calculation is configured the same way as for a single processor system. Note that if fewer than 27 processors are available, the ensemble configuration menu permits starting the calculation at any ensemble member number within the valid range of 001 to 027.

The Model Launch Menu

The model launch menu contains four entries: the number of processors requested for the simualation, the name of the executable, the Prep-Code, and the working directory. Each of these is assigned a default value depending upon the calling menu. Normally there should be no reason to change any of these values except the number of processors. If the working directory is changed and does not already exist, a new directory is created, and the script changes to that directory before starting the simulation.

The Prep-Code is just an internal flag to set any preprocessor options:

- M = matrix
- E = ensemble
- S = standard

If the Prep-Code field is left blank, the MPI script is not called, and the named executable will be run in background. In this way multiple jobs can be submitted on a multi-processor system in a non-MPI environment. However, in both MPI and non-MPI applications, when simultaneous calculations are desired, it is important that each simulation have its own working directory.

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Concentration / Display / File Format

Concentration packing has been implemented with HYSPLIT version 4.5. The updated format is downward compatible in that all display programs can read files produced from versions prior to 4.5, but older versions of the display programs cannot read the new packed output format. Note that HYSPLIT V4.5 can be configured to produced the older style unpacked concentration files. Concentration file packing does not write the same information in fewer bytes, but rather writes the same information using twice as many bytes. The packed files are generally smaller because only concentration values at the non-zero grid points are written to the output file by the model. However this requires the grid point location to be written with the concentration, hence the additional bytes. If most of the grid is expected to have non-zero concentrations, then the old style format will save space. The output format of the unformatted binary (big-endian) concentration file written by dispersion model (*hycs_std)* and read by all concentration display programs is as follows:

<u>Record #1</u>

- CHAR*4 Meteorological *MODEL* Identification
- INT*4 Meteorological file starting time (*YEAR, MONTH, DAY, HOUR, FORECAST-HOUR*)
- INT*4 *NUMBER* of starting locations
- INT*4 Concentration packing flag (0=no 1=yes)

<u>Record #2</u> Loop to record: <u>Number of starting locations</u>

- INT*4 Release starting time (*YEAR, MONTH, DAY, HOUR*)
- REAL*4 Starting location and height (*LATITUDE, LONGITUDE, METERS*)
- INT*4 Release starting time (*MINUTES*)

<u>Record #3</u>

- INT*4 Number of (*LATITUDE-POINTS, LONGITUDE-POINTS*)
- REAL*4 Grid spacing (*DELTA-LATITUDE,DELTA-LONGITUDE*)
- REAL*4 Grid lower left corner (*LATITUDE, LONGITUDE*)

<u>Record #4</u>

- INT*4 *NUMBER* of vertical levels in concentration grid
- INT*4 *HEIGHT* of each level (meters above ground)

<u>Record #5</u>

- INT*4 *NUMBER* of different pollutants in grid
- CHAR*4 Identification *STRING* for each pollutant

<u>Record #6</u> Loop to record: <u>Number of output times</u>

- INT*4 Sample start (*YEAR MONTH DAY HOUR MINUTE FORECAST*)

<u>Record #7</u> Loop to record: <u>Number of output times</u>

- INT*4 Sample stop (*YEAR MONTH DAY HOUR MINUTE FORECAST*)

<u>Record #8</u> Loop to record: <u>Number levels, Number of pollutant types</u>

- CHAR*4 Pollutant type identification *STRING*
- INT*4 Output *LEVEL* (meters) of this record

No Packing (all elements)

- REAL*4 Concentration output *ARRAY*

Packing (only non-zero elements)

INT*4 Loop non-zero elements

- INT*2 First (I) index value
- INT*2 - Second (J) index value
- REAL*4 - Concentration at (I,J)

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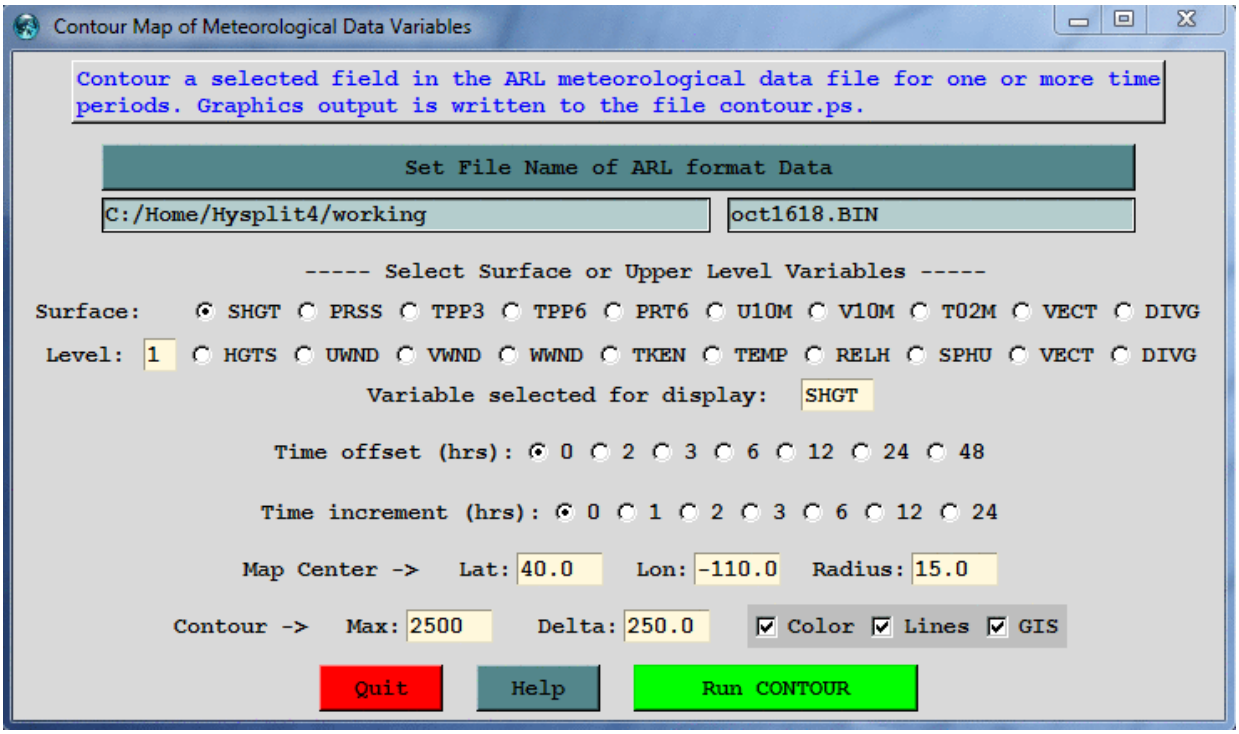
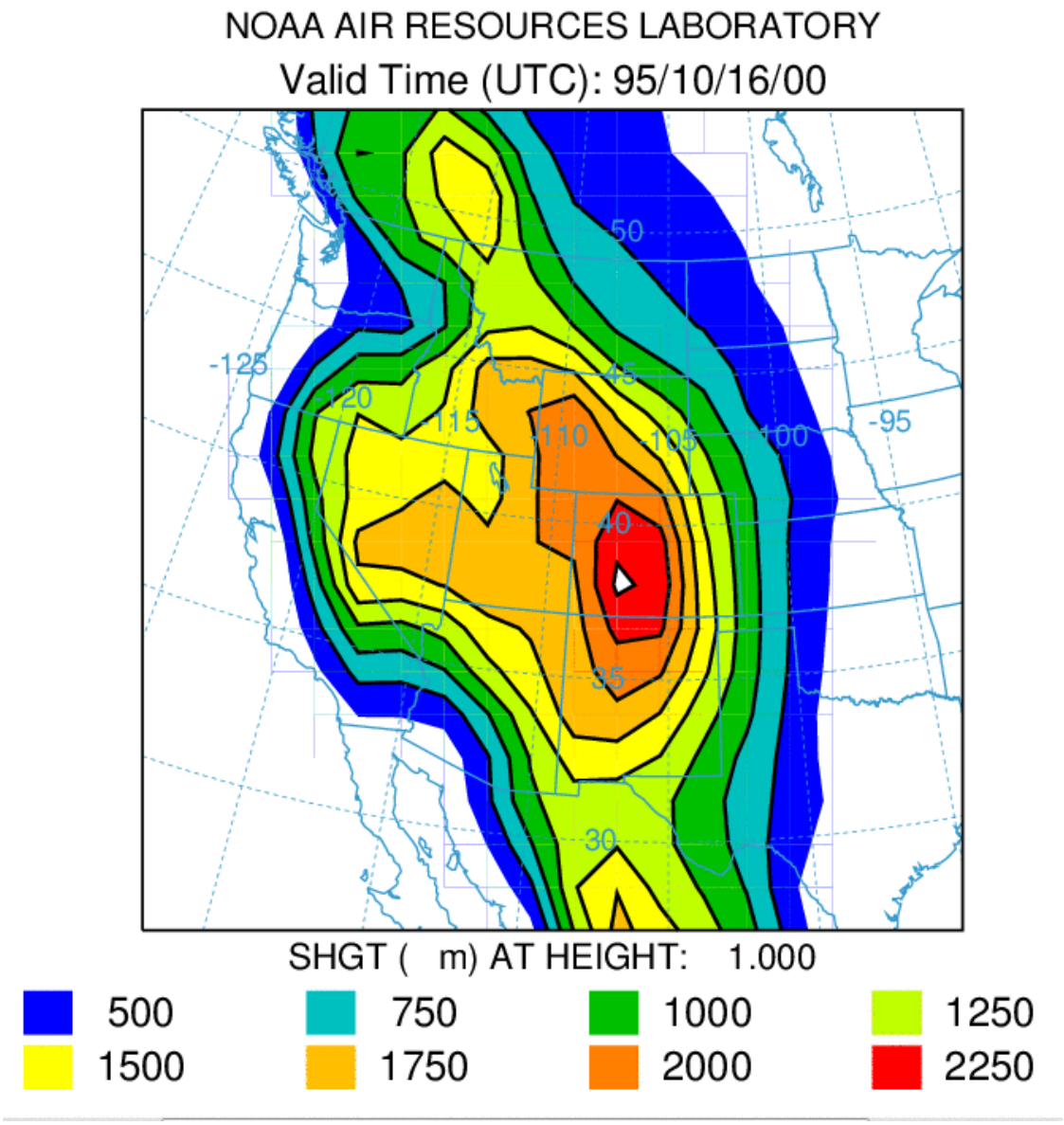
Concentration / Display Data / Terrain Overlay

The use of several menu features is demonstrated here that will permit the creation of a map of the concentration plume with political boundaries and contours of the terrain as defined by the meteorological data. The basic process is to create a shapefile of the terrain and add that file to a shapefile of the political boundaries. Although this demonstration is for terrain and concentration any line or contour based shapefile can be displayed through the concentration or trajectory plotting programs.

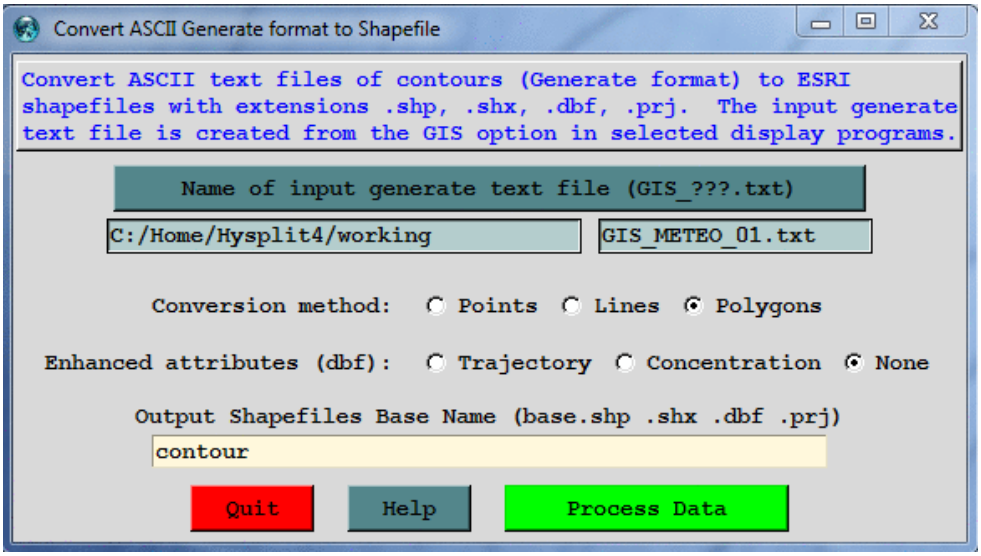
Open the Meteorology / Display Data / Contour Map menu and select the meteorological data file, the station height field (SHGT=terrain), and set the GIS checkbox, which will output the terrain field in generate format. It might be necessary to force the contours and the center of the map to get a nice looking display over the region of interest. In this case for the west coast of the U.S. the maximum terrain height was set to 2500 m with an interval of 250 meters between contours.



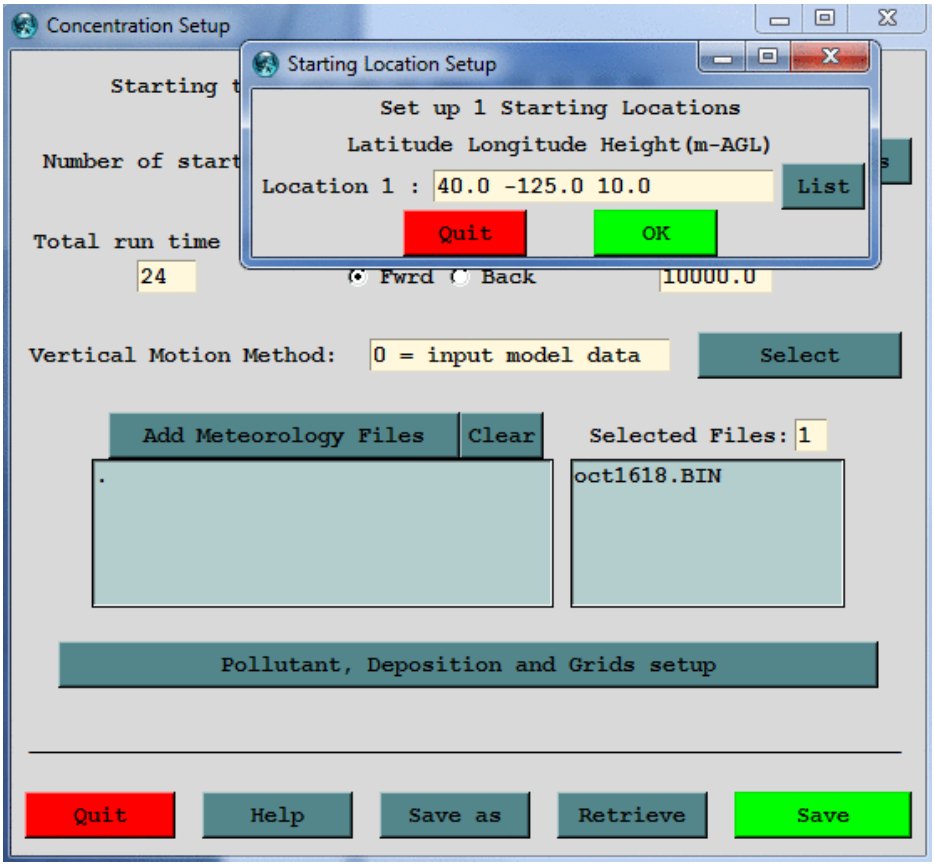
Run the contour program and the display shown below will be created. In the *working* there will be an additional file called *GIS_METEO_01.txt* which is the generate format text file of the terrain contours.



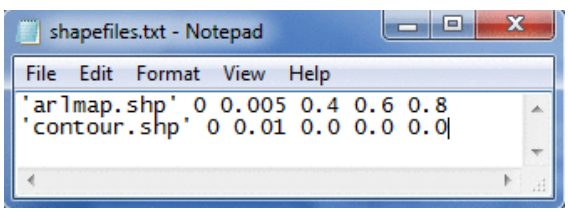
Now open the GIS to Shapefile utility menu and browse for the generate format file name. Select the "Polygons" radiobutton to insure that the terrain polygons are treated as closed connected lines. After processing the input file, four output files will be created with the base name of contour. The subsequent plotting programs only need the *contour.shp* file, but the other files may be needed for import into other GIS applications.



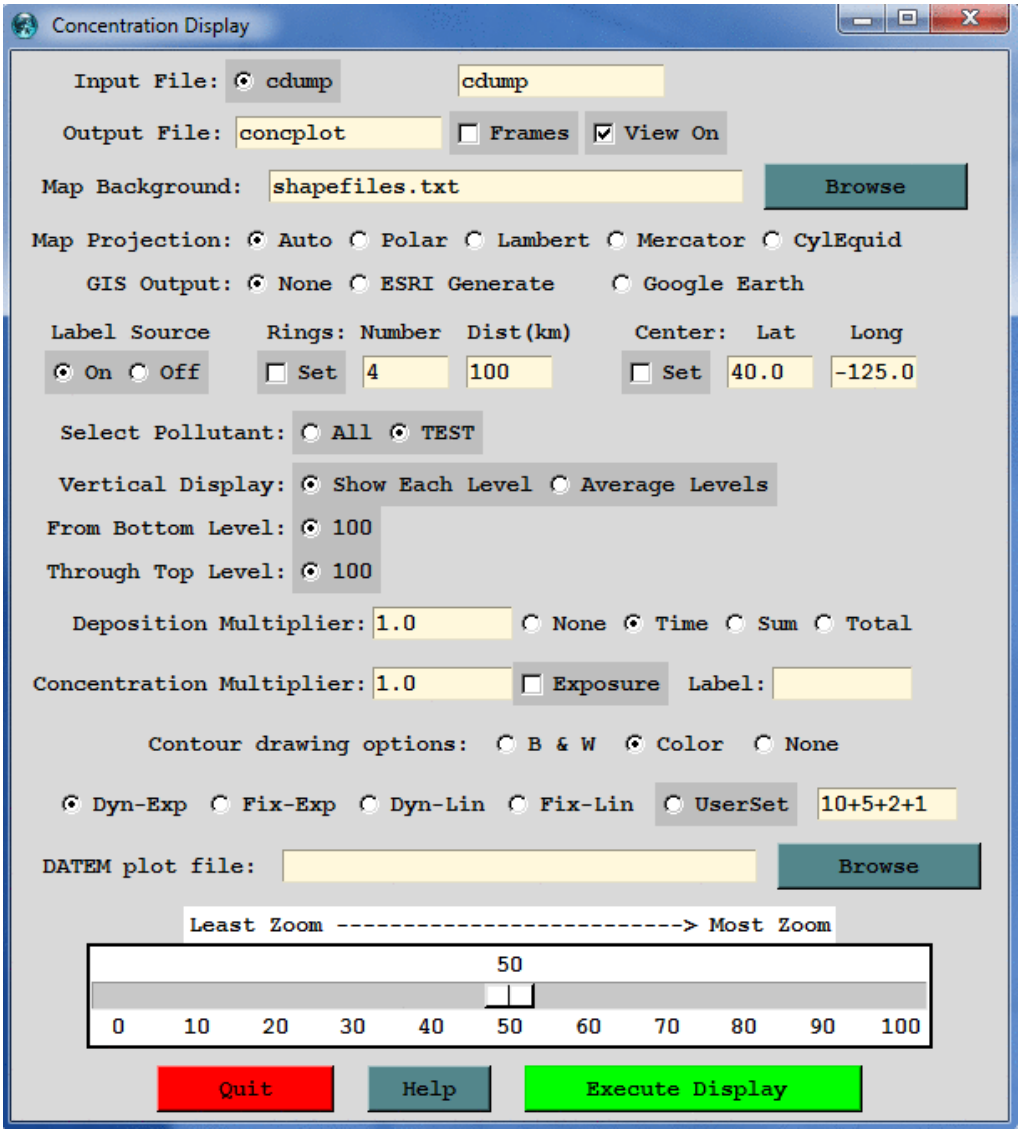
If you do not have a plume simulation already completed, open the concentration setup menu and run the default test case, but move the starting location to 40N 125W and run the model for 24 rather than 12 hours. To simplify the output, set the concentration grid averaging time to 24 h and reduce the grid resolution from 0.05 to 0.10. Then run the model.



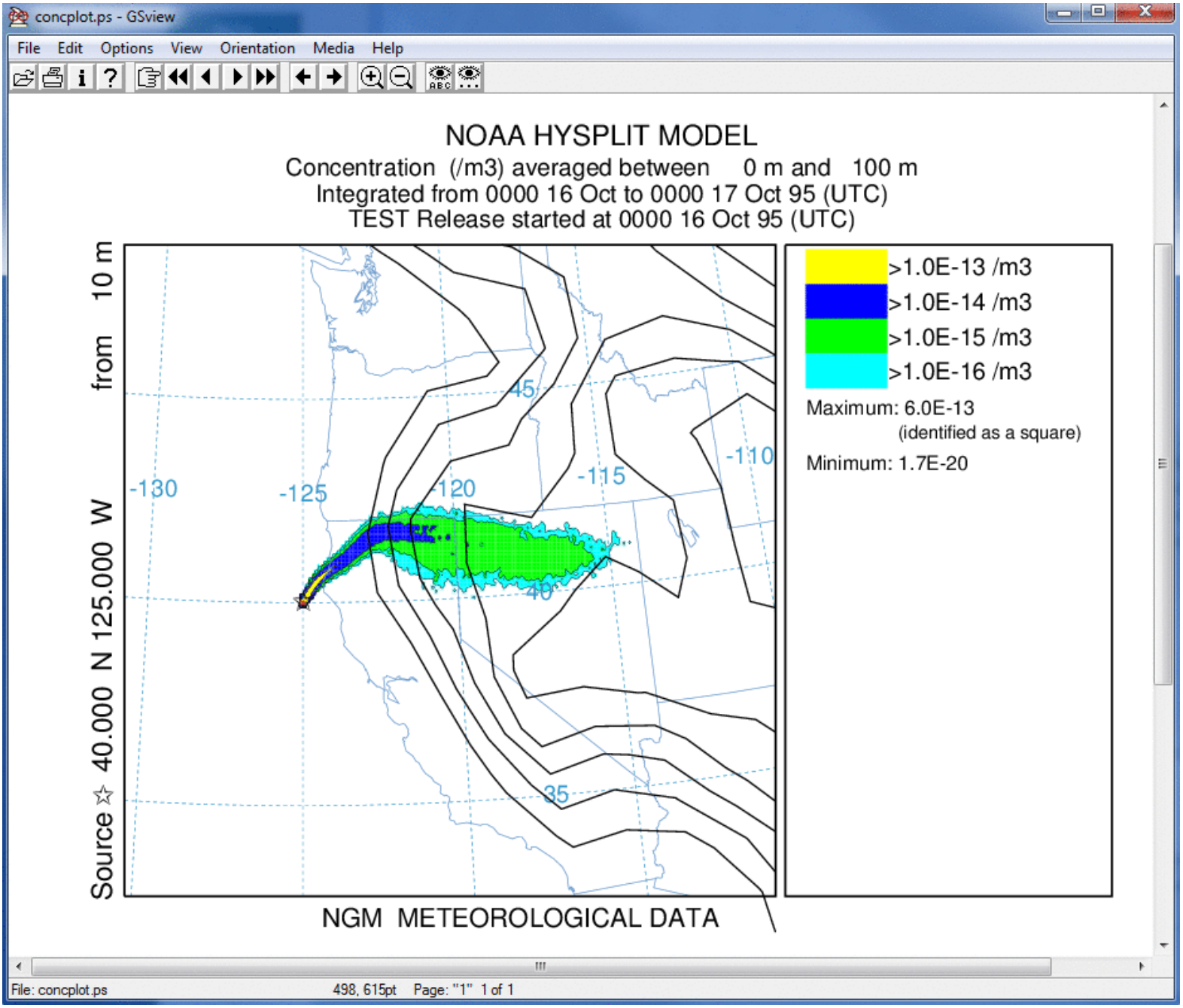
After the run completes, go to the *hysplit/graphics* directory and copy *arlmap.shp* and *shapefiles_arl.txt* to the working directory. Rename *shapefiles_arl.txt* to *shapefiles.txt*. Then open notepad in working to edit *shapefiles.txt* to add the additional file (line) defining the shapefile with the terrain. For this display, the line is twice as thick as the map background and the color is defined as black (0.0 0.0 0.0).



Now open the concentration / display / contours menu and define the *shapefiles.txt* in the field for the map background. This will cause the display program to use the files defined in this file rather than the default map background. Multiple shapefiles can be displayed at the same time.



Executing the display will result in the following image showing the intersection of the plume with the elevated terrain as it moves to the east.



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Advanced / Configuration Setup

This section provides some guidance in configuring the model input to perform certain specialized calculations. The default configuration supplied with the test meteorological data is confined to a simple trajectory and inert transport and dispersion calculation. More complex scenarios can be configured through the *Advanced / Configuration Setup* menu tabs. There are seven sub menus available.

1. The **Trajectory** tab opens a menu creation or modification of the *SETUP.CFG* namelist file. This can be accomplished through the GUI or by directly editing the namelist file. The file is required to be in the model startup directory, usually *./working* when running the model through the GUI. More information about the trajectory namelist variables can be found in the trajectories help file.

2. The **Concentration** tab opens a similar menu to the trajectory tab, but with many more options. The *trajectory* and *concentration* menus are confined to the variables relevant to the respective model calculation. More information about the concentration namelist variables can be found in the concentration help file.

3. The **Global** tab opens a menu to create or edit a special namelist file that configures the Global Eulerian Model (GEM), a series of subroutines within the main HYSPLIT transport and dispersion code. Particles or puffs are always first released in the Lagrangian framework and carried within HYSPLIT until they exceed a certain age at which point their mass is transferred to the GEM routines. Particles can be released and transferred for the entire duration of the simulation.

4. The **Dynamic Sampling** menu is used to configure a special virtual sampler that can move in space and time through the computational domain during the concentration simulation. Dynamic samplers can move passively with the wind or have a define pathway, similar to an airplane.

5. The **Emissions File** opens a menu to edit or create a point-source emission file that can define more complex release scenarios than could be created using just the CONTROL file. Simple scenarios like time-varying emissions to more complex moving line or point sources cab be configured.

6. The **Set Directories** menu is used to configure the GUI's directory structure as well as the location and name of certain executable programs used by the GUI. The structure is written to the *default_exec* file. If that file is not found in the startup directory, the GUI attempts to set all the values. Significant differences are found between Windows, Apple, and UNIX installations.

7. The **Extra Labeling** menu opens a simple editor menu to create a file of extra label information that is added to the bottom of all trajectory or concentration plots. Only these two display programs support the extra label function.

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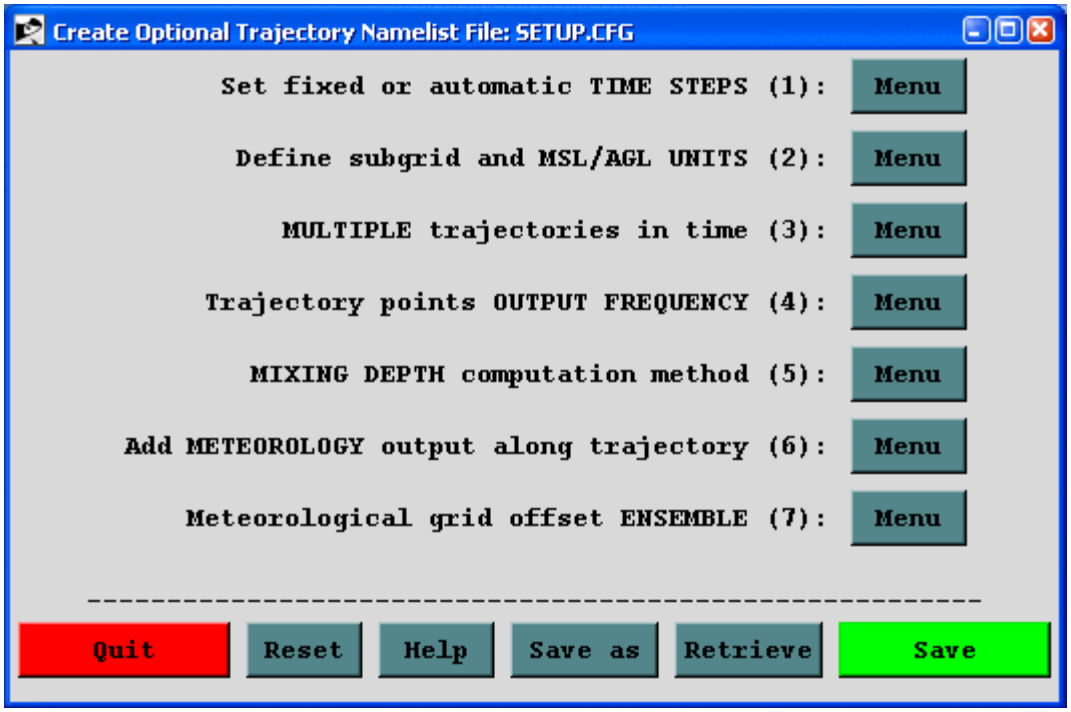
Advanced / Configuration Setup / Trajectory

This section provides some guidance in configuring the model input to perform certain specialized calculations. The default configuration supplied with the test meteorological data is confined to a simple trajectory calculation. More complex scenarios can be configured through the *Advanced*, *Configuration Setup*, *Trajectory* menu tab. The menu is used to modify the *SETUP.CFG* namelist file. This file is not required, and if not present in the root startup directory, default values are used. These parameters can all be changed without recompilation by modification of the contents of *SETUP.CFG* and in some cases their modification will substantially change the nature of the simulation. The configuration file should be present in the root directory. An illustration of the menu is shown below.



When using the GUI, the namelist file will be deleted and all variables are returned to their default value by selecting the "*Reset*" button. The following summarizes the namelist variables and their corresponding section in the GUI menu.

1. Set fixed or automatic TIME STEPS
2. Define subgrid and MSL/AGL UNITS
3. MULTIPLE trajectories in time
4. Trajectory points OUTPUT FREQUENCY
5. MIXING DEPTH computation method
6. Add METEOROLOGY output along trajectory
7. Meteorological grid offset ENSEMBLE
8. Summary of all NAMELIST variable defaults

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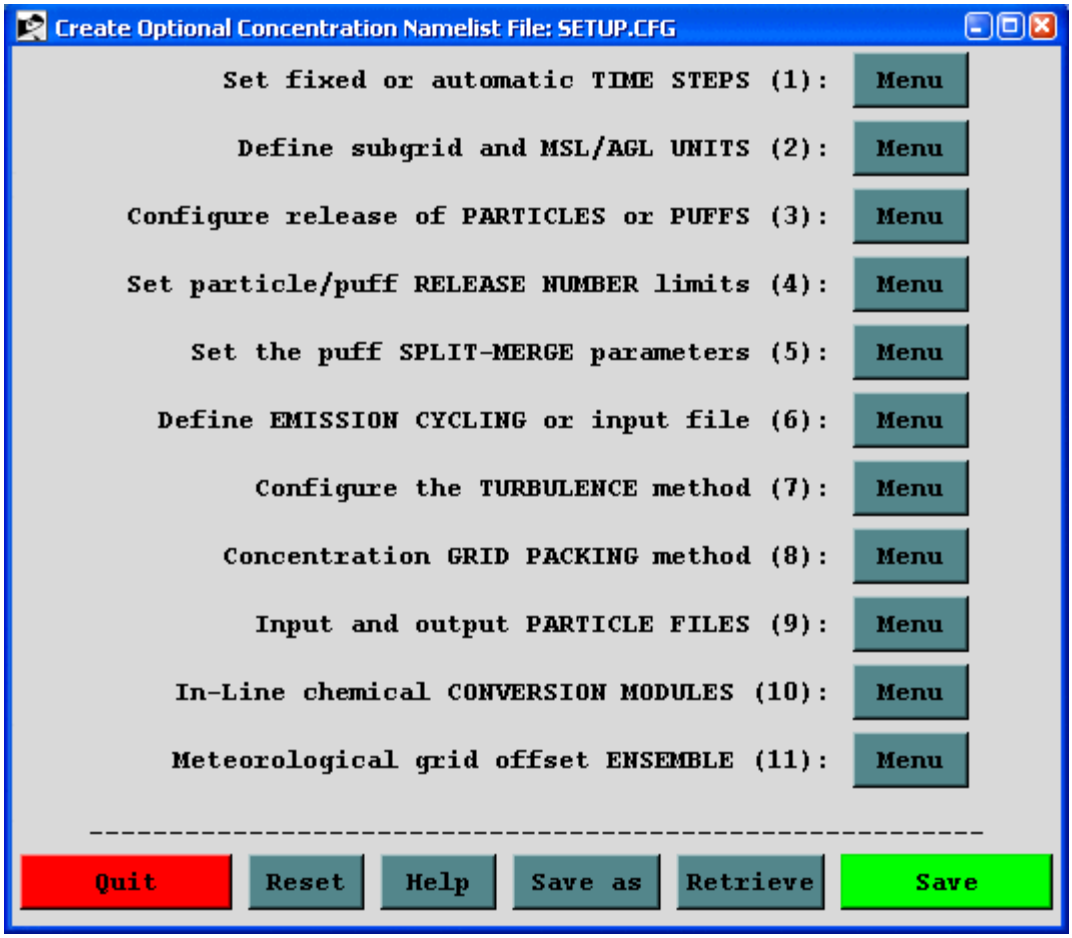
Advanced / Configuration Setup / Concentration

This section provides some guidance in configuring the model input to perform certain specialized calculations. The default configuration supplied with the test meteorological data is confined to a simple dispersion calculation. More complex scenarios can be configured through the *Advanced / Configuration / Concentration Setup* menu tab. The menu is used to modify the *SETUP.CFG* namelist file. This file is not required, and if not present in the root startup directory, default values are used. These parameters can all be changed without recompilation by modification of the contents of *SETUP.CFG* and in some cases their modification will substantially change the nature of the simulation. The configuration file should be present in the root directory. An illustration of the upper-level menu is shown below.



When using the GUI, the namelist file will be deleted and all variables are returned to their default value by selecting the "*Reset*" button. The following summarizes the namelist variables and their corresponding section in the GUI menu. Not all variables can be set through the menu system but may be modified by directly editing the namelist file.

1. Set fixed or automatic TIME STEPS
2. Define subgrid and MSL/AGL UNITS
3. Configure release of PARTICLES or PUFFS
4. Set the particle/puff RELEASE NUMBER limits
5. Set the puff SPLIT-MERGE parameters
6. Define EMISSION CYCLING or input file
7. Configure the TURBULENCE method
8. Concentration GRID PACKING method
9. Input and output PARTICLE FILES
10. In-line chemical CONVERSION MODULES
11. Meteorological grid offset ENSEMBLE
12. Summary of all NAMELIST variable defaults

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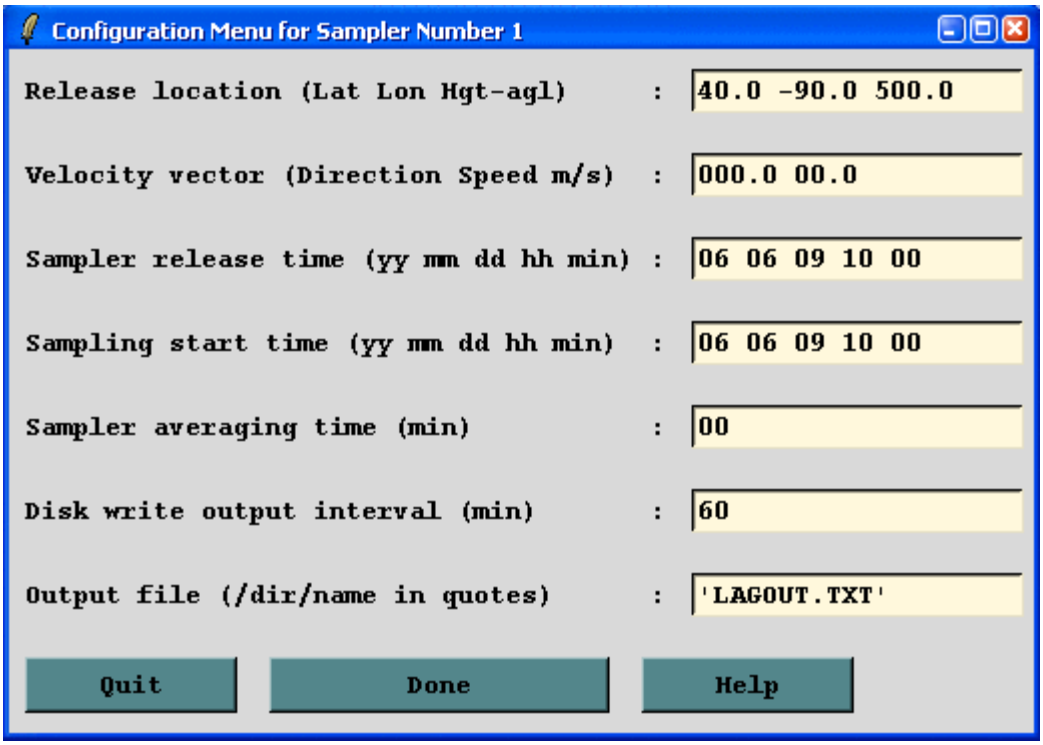
Advanced / File Edit / Dynamic Sampling

This menu creates the optional LAGSET.CFG file which is used to configure a dynamic sampler. A dynamic sampler is defined as a moving sampler that can pass through the model simulation domain, either passively with the wind (Lagrangian mode) or by using a pre-defined velocity vector (Forced mode). In the current version the dynamic sampler transport is always vertically isobaric regardless of the vertical motion method selected for the pollutant transport. The dynamic sampler samples model produced values that are generated internally on a snapshot concentration grid.

The first menu tab defaults to the configuration for one sampler. If multiple samplers are required, then enter the number in this menu. After pressing the *Configure Samplers* button, another menu comes up to select the sampler number to configure. Pressing the sampler number button brings up the menu shown below. Each defined sampler must be configured according to the following instructions.



The dynamic sampler configuration file must be located in the model's startup directory to be found and the name should always be in uppercase. The following is an example of the contents of LAGSET.CFG for one dynamic sampler. Multiple samplers would repeat the last seven line sequence.

1 : number of dynamic samplers

40.0 -90.0 500.0 : release location and height (agl)

0.0 0.0 : force vector - direction, speed (m/s)

95 10 16 00 00 : release start - year month day hour minute

95 10 16 00 00 : sampling start - year month day hour minute

00 : sample averaging (min)

60 : disk file output interval (min)

'LAGOUT.TXT' : sampler output file

Number of dynamic samplers: Due to file unit number restrictions, the current version only supports 9 simultaneous sampler definitions. The following seven lines need to be repeated for every defined sampler.

Release location and height: The location is the latitude-longitude point at which the trajectory of the sampler path is started. Although the subsequent vertical motion is isobaric, the initial starting height must be defined in meters above ground-level. Note that the isobaric sampler trajectory will not be identical to the HYSPLIT trajectory model isobaric trajectory because of differences in how the vertical motion is computed between the two models.

Force vector: If the direction (downwind) and speed (m/s) set to zero, then the model computes the sampler trajectory according to the meteorological input data wind velocity. If any of these values are not zero, then the sampler trajectory is computed using these values for its entire length. To simulate a more complex aircraft sampling path, each leg of the flight pattern requires its own sampler definition. For instance, an aircraft flying east with have a direction vector of 090.

Release start: The release time of the sampler gives the date and time that sampler starts from the previously defined release location. Note that in the current version, zero's for this field (relative start time) are not supported.

Sampling start: The sampler may proceed on its trajectory for quite some time before sampling is started. The sampler start time must be greater than or equal to the release start time.

Sample averaging (minutes): At every computational time step the model determines the sampler position in the concentration grid and accumulates the concentration value in memory. When the sampler accumulation time reaches the sample averaging time, all sums are reset to zero. A sample averaging time of zero means that the sample is only accumulated for one model integration time step.

Disk file output interval (minutes): At the disk output interval, the sampler concentration values are written to the output file defined on the next input line. The value written is the accumulated concentration divided by the accumulated minutes. The disk output interval is independent from the sample averaging time.

Sampler output file: The directory and file name should be enclosed in single quotes. If the file is defined without a directory it is written to the model startup directory.

Concentration Grid Configuration

Note that dynamic sampling will only work if the sampler trajectory passes through a concentration grid covering the region of interest. That means that a concentration grid of sufficient resolution, in both the horizontal and vertical is required for a sampler to capture the pollutant. However too much resolution (too fine a grid) may mean that there could be an insufficient number of pollutant particles to provide a uniform distribution and therefore the sampling could provide unrepresentative results. The concentration grid is required to be defined as a snapshot grid. In the current version, only one pollutant species per simulation is supported.

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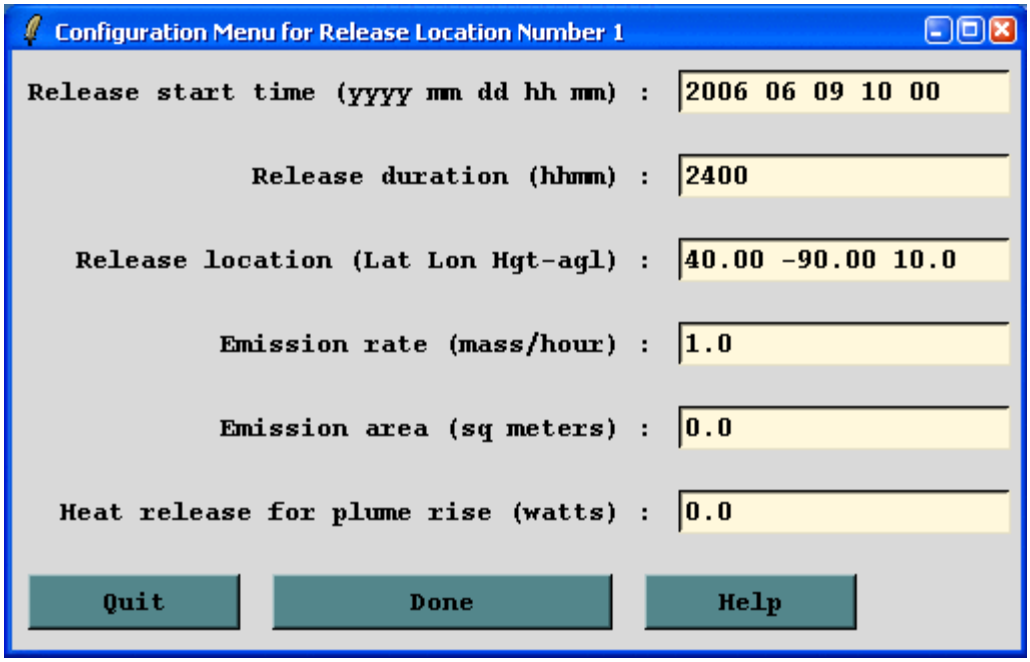
Advanced / File Edit / Emissions File

This menu creates the optional EMITIMES file which is used to configure more complex point source emissions scenarios. In the standard model simulation, the CONTROL file can only be used to define one pollutant release cycle which applies equally to all source locations. Although multiple release cycles can be defined, they must all be at the same interval. Using the EMITIMES file to define the point source emissions, multiple release locations can each have their own emission characteristics, each with different pollutants, if desired. Furthermore, multiple emission cycles, at non-regular intervals can also be defined. By appropriately locating multiple sources in space and time, line- source as well as other non-regular emissions configurations can be created. In version 4.8 the format of this file has changed from previous HYSPLIT versions to such an extent that they are incompatible with each other. In all versions the file name is defined by the *EFILE* variable in the namelist configuration file created thorough the *Advanced / Configuration* menu tab.



The first menu tab defaults to the configuration for one source. If multiple sources are required, then enter the number in this menu. After pressing the *Configure Locations* button, another menu comes up to select the location number to configure. Pressing the location number button brings up the menu shown below. The GUI menu only supports the creation of a file for one pollutant for one emission cycle. If multiple pollutants are defined, or multiple cycles are required, then the file must be edited manually by duplicating the emission record at each location for all pollutants in the order they are defined in the CONTROL file. Each defined release location must be configured according to the following instructions. The point source emissions file must be located in the startup directory the name should always be in uppercase. The following is an example of the contents of EMITIMES file for one location. Multiple locations would have one line per location. The number of data records should equal the number of sources defined in the CONTROL file times the number of pollutants released.

The EMITIMES file may also be configured to construct a vertical line source by having two consecutive emission points defined at the same spatial location but each with different heights. Unlike the vertical line source definition through the CONTROL file, where the same emission rate is defined for all sources, here the emission rate may be varied through the column. For instance, if the source record N is at the same location as record N-1, the the emission rate defined for record N-1 will be used for all particles released in the column from N-1 to N. This means that the emission value given for the last record, in a series of records at the same location will not be used.

- Record 1 - Identification record describing the emission cycle header record
- Record 2 - Identification record describing a location emission data record
- Record 3 - First emission cycle header record

- Record 4 - First emission data record in the first emission cycle

Emission Cycle Header Record: {YYYY} {MM} {DD} {HH} {hhhh} {#rec}

- {YYYY} {MM} {DD} {HH} - Starting time of the emission cycle, with each new emission cycle, all previous emission records are replaced with those in the new cycle.
- {hhhh} - Duration in hours that this emission cycle is valid.
- {#rec} - Number of emission records in this cycle (= # sources times # pollutants).

Emission Cycle Data Record: {YYYY} {MM} {DD} {HH} {mm} {HHmm} {Lat} {Lon} {Hgt} {Rate} {Area} {Heat}

- {YYYY} {MM} {DD} {HH} {mm} - Emission start time at this location
- {HHmm} - Release duration in hours and minutes (no space).
- {Lat} {Lon} {Hgt} - Position and height of the release.
- {Rate} - Emission rate in mass units per hour.
- {Area} - Emission area in square meters. Zero is treated as a point source and non-zero values only apply to one of the horizontal distribution models (top-hat or Gaussian).
- {Heat} - Heat released during the emission. Non-zero values result in a bouyancy plume rise calculation, replacing the previous height value.

The emisson cycle header record defines the valid time period for the subsequent data records. At the end of the header record time period {hhhh}, the model will attempt to read the next emission cycle header record. If no header record is found, then the EMITIMES emission processing is terminated and the model reverts to using the emission values defined in the CONTROL file. For instance, this means that if a short emission duration is defined in the data records, but the model simulation covers a longer period, the header record duration {hhhh} should be long enough to cover the entire simulation period. Unless it is indended to use both methods, the emission rate and duration in the CONTROL file should both be set to zero when using an EMITIMES file.

Special Case: Backward simulations

In the case of backward simulations, the cycle header record should point to the first (oldest) emission cycle and all subsequent emission cycles should be earlier in time. The emission start time within a cycle corresponds to a time such that the duration of emissions proceeds backward from that starting time. The internal backward flag has already been set from the negative run duration in the CONTROL file and therefore all time durations in the EMITIMES file should be expressed as positive numbers.

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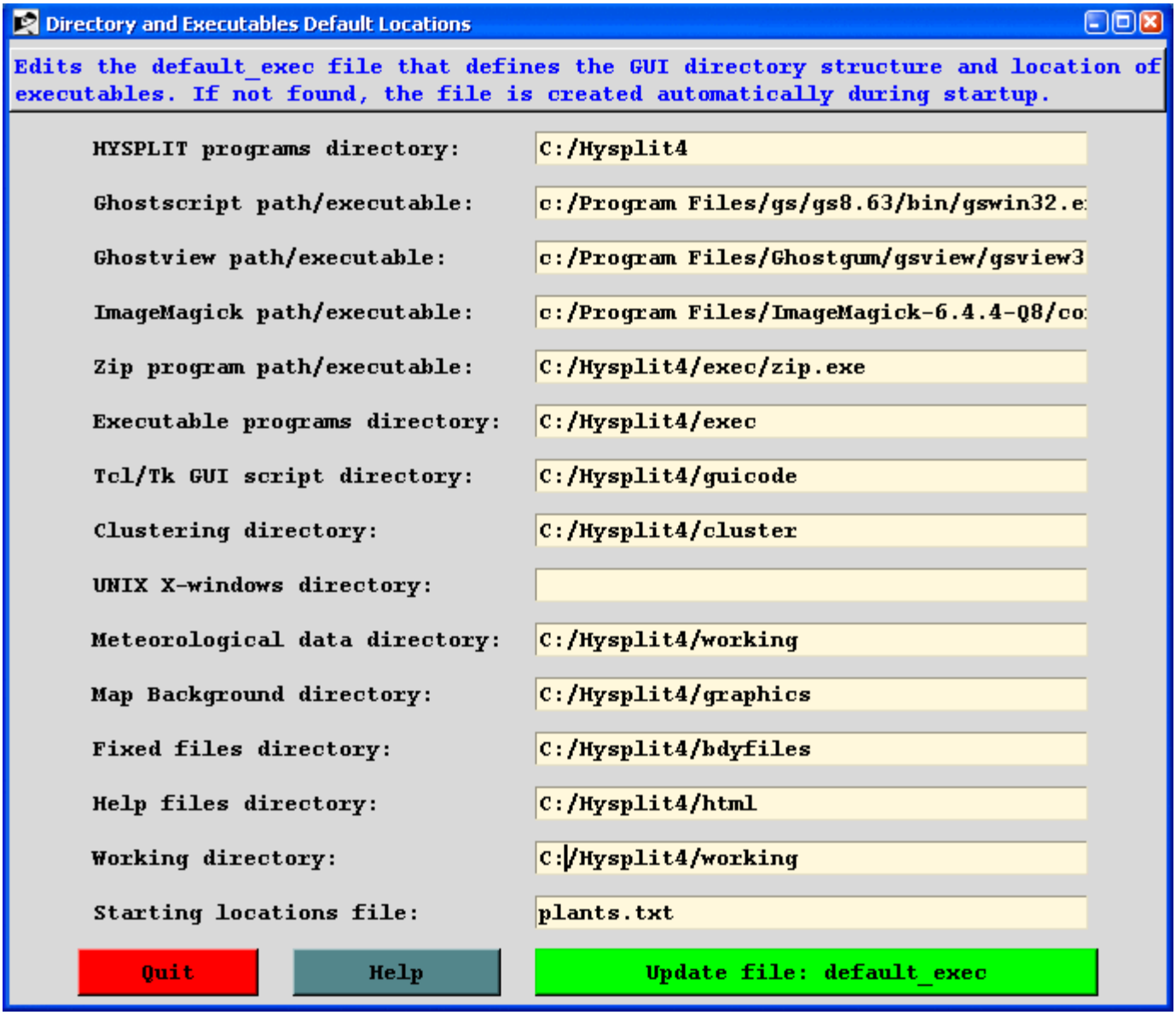
Advanced / Configuration Setup / Set Directories

The installation program installs all code and executables to your selected directory, and creates a shortcut on the Window's desktop to /guicode/hysplit4.tcl with the *Start In* directory as your selected default. On Unix systems the link would appear in the /working directory. When the GUI is first started, it looks for the supplemental programs such as Ghostscript, Ghostview, ImageMagick, and Tcl/tk in certain standard directories, and writes those paths to a file called *default_exec*. If this file already exists, those locations are used instead of the default search paths. The directories specified in this file may be edited through the *Set Directories* menu tab. Copying the *default_exec* file to another computer with a different directory structure may cause the GUI to fail to open. In these situations, either delete the file, or manually edit the file to reflect the correct directory strucuture.



The *default_exec* values either reflect a directory location, a file name, or a directory/executable name. The content is mostly self-explanatory. Under UNIX systems, the X-windows directory should point to the location of the *xterm* program. This is optional. If the directory is defined, then many of the programs called by the GUI will run in their own *xterm* window.

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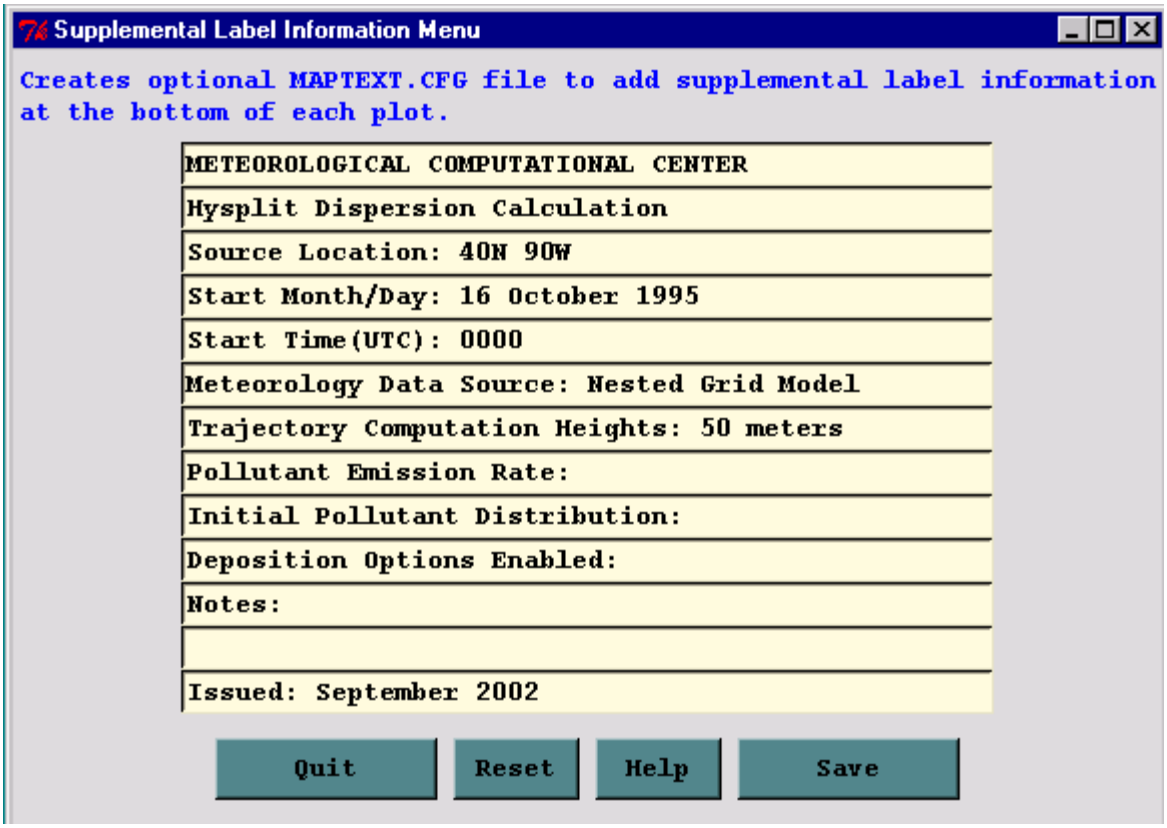
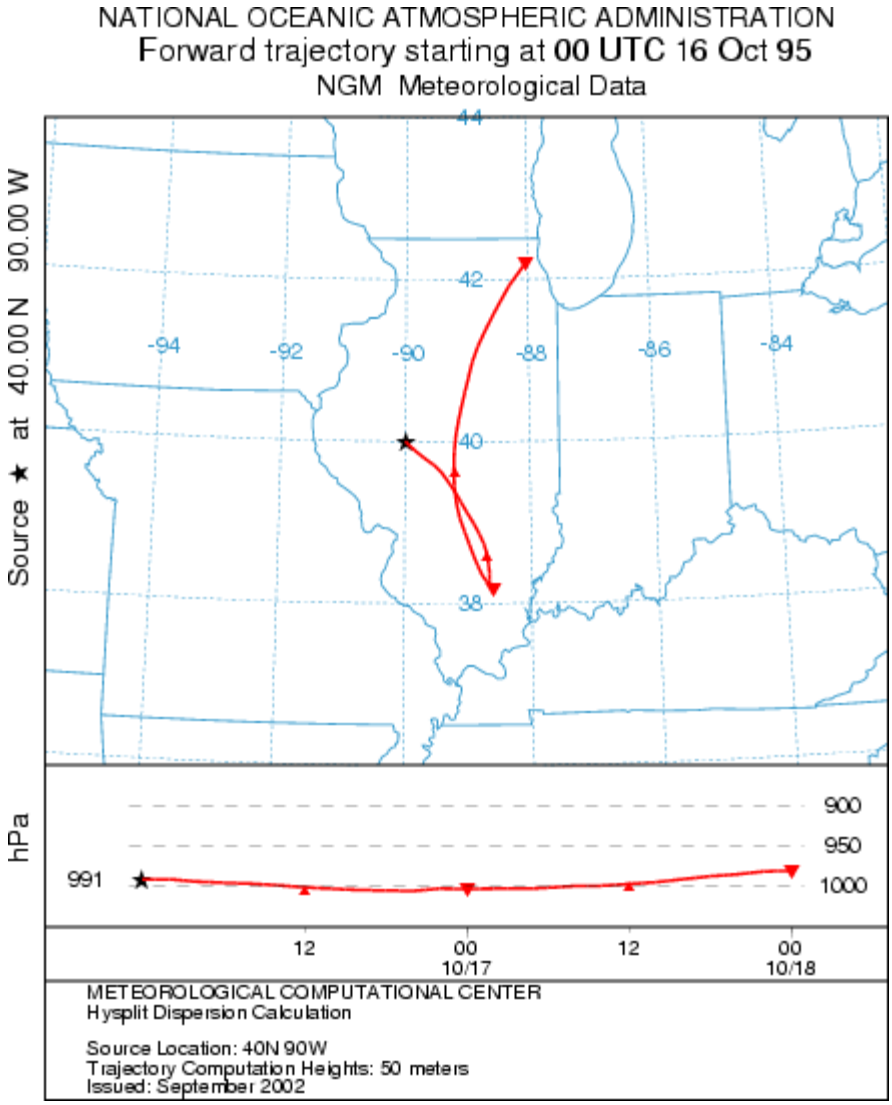
Advanced / File Edit / Panel Labels

If a file called *MAPTEXT.CFG* is found in the root or working directory during the execution of either the trajectory or concentration plotting program, additional label information is written at the bottom of each graphic. The *Extra Label* menu tab can be used to edit this information. An illustration of the menu is shown below, followed by the resulting trajectory graphic for the example simulation. Note that the menu entries are entirely text based and there are no restrictions regarding content. However, not all plotting programs display all lines. The example header text indicates the appropriate application.





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Advanced / File Edit / Border Labels

Many of the Postscript graphics programs have label information that can be customized to some extent. This is accomplished by placing a file called *LABELS.CFG* in the working directory which should contain one or more of the following valid entries (all in single quotes terminated by &). Replace the second text string with the new desired text. Not all label strings are valid with every plotting program. This file can be created and edited through the menu system. Quotes and string terminators are not required in the edit menu.

- 'TITLE&','NOAA AIR RESOURCES LABORATORY&'
- 'MAPID&','Air Concentration&'
- 'LAYER&','Layer Averaged&'
- 'UNITS&','Bq&'
- 'VOLUM&','/m3&'
- 'TZONE&','UTC+00&'
- 'RELEASE&','Release info&'
- 'ALLTD&','m&'

The time zone variable can be used to force a specific time zone for the air concentration contour plot. All calculations are performed in UTC, but prior to plotting, all times are converted by the time zone adjustment. The field should always be six characters in length. The first three represent the time zone label, such as UTC, the next character is the sign field (+ to the east or - to the west), and last two digits are the hours difference of the time zone from UTC.

Altitude units (ALTTD) may be set to feet for concentration output plots.

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Advanced / File Edit / FMDV Decay

Foot and Mouth Disease

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Foot and Mouth Disease is a contagious viral disease of cattle and sheep, causing ulceration of the hoofs and around the mouth. Evidence has shown[1] that the Foot and Mouth Disease Virus (FMDV) can be transported via airborne means making even a single outbreak highly infectious.

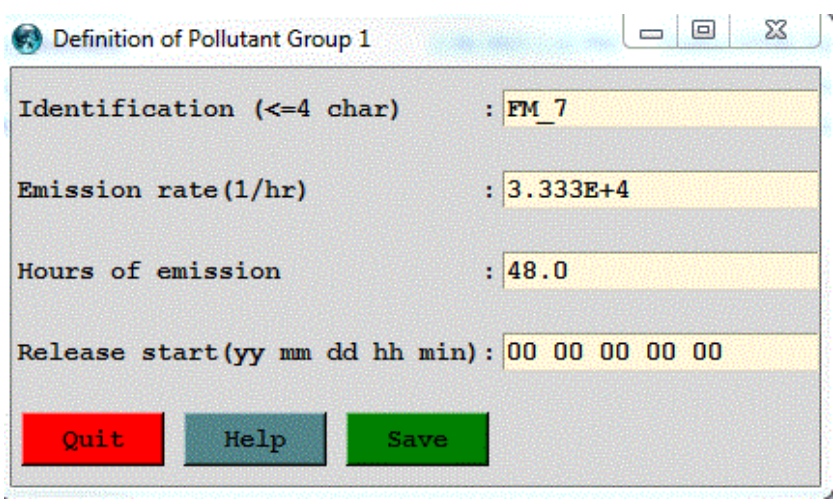
HYSPLIT is capable of modelling the dispersion of airborne FMDV. The survival of the FMDV particle is dependent on (a) the age of the particle, the virus has a natural lifespan which is simulated within the model with a half-life factor, (b) the air temperature, retrieved from the meteorological file and (c) the air humidity also retrieved from the meteorological file. In reality, wet and dry deposition also influence the distance travelled by the airborne FMDV.

To activate the Foot and Mouth Disease algorithm in HYSPLIT the species identification label must be set to either FM_0 or FM_1 or .... FM_7 where the integer behaves as a binary switch for including or excluding particle aging, temperature or humidity dependence as desired.

The Table below shows the dependences of Foot and Mouth virus survival to the species identification string. FM_7 is the most realistic option.

Identification	Particle Aging	Temperature	Humidity
FM_0	False	False	False
FM_1	False	False	True
FM_2	False	True	False
FM_3	False	True	True
FM_4	True	False	False
FM_5	True	False	True
FM_6	True	True	False
FM_7	True	True	True

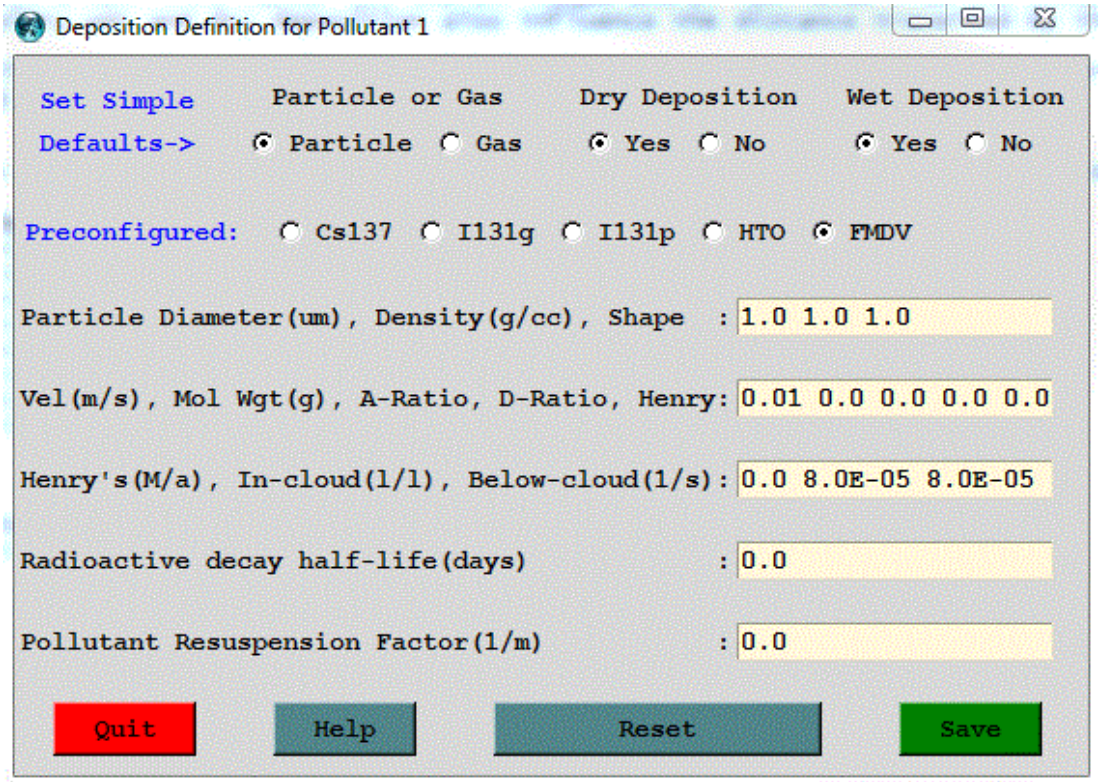
The species identification string can be set in the pollutant emission rate setup menu or automatically using the **FMDV** radiobutton in the deposition setup menu in the following section.



Default FMDV settings

- Deposition

The species identification string can also be set to a default value by selecting the **FMDV** radiobutton in the deposition menu. This button will also set default values for wet and dry deposition. For the Foot and Mouth virus a dry deposition velocity of 0.01m/s is assumed[1], but it can be changed by the user if required. FMDV wet deposition defaults are simply those for small particles using the removal time constant of $8x10^{-5}$ for both in-cloud and below-cloud removal which is similar to the value ($5x10^{-5}$) used by Garner[1].



- Particle age

Various publications use a virus decay constant to simulate particle ageing. For the Foot and Mouth virus estimates of an effective half-life range from 30 mins[1] to 2 hours[2]. This constant is also dependent on the strain of the virus. To be conservative the virus decay constant has been defined to be 2 hours by default but this can be easily redefined by the user in the advanced settings menu (see below). Particle ageing can be turned off altogether if desired by using the species identification label outlined above.

- Temperature

The survival of the virus depends on temperature. Taking the default temperature threshold of $24^{o}C$, all virus particles of $24^{o}C$ and under are unaffected. The concentration mass of virus particles linearly decreases between $24^{o}C$ and $30^{o}C$ so that none remain by the time they reach $30^{o}C$. This threshold of $24^{o}C$ can be user defined in advanced settings (preserving the $6^{o}C$ linear fall off) or the temperature dependence can be turned off altogether if required by selecting the appropriate species identification string outlined above.

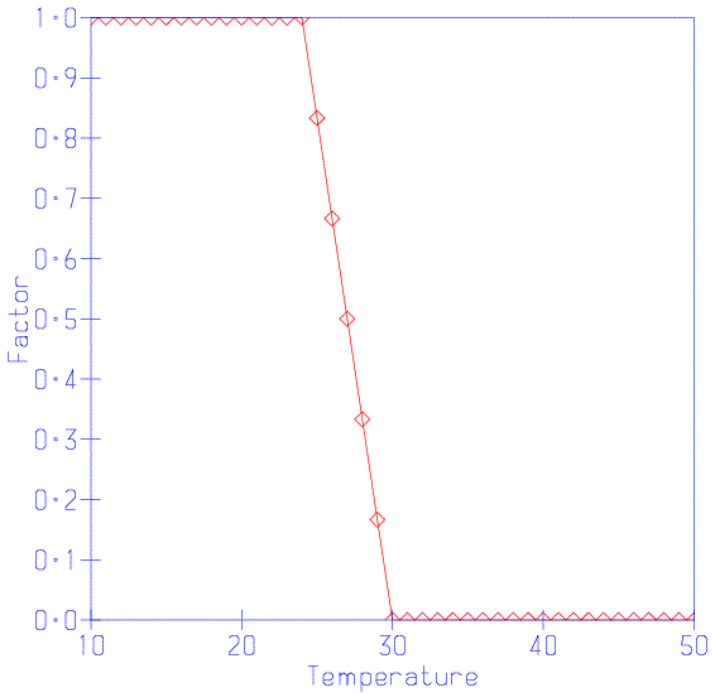
- Humidity

The survival of the virus also depends on humidity. The virus survives better in higher humidity. Virus concentrations with relative humidity higher than 60% are left unaffected. Concentrations decrease exponentially as the humidity falls from 60% to 1%. This threshold of 60% can be user defined in the advanced settings or the humidity dependence can be turned off

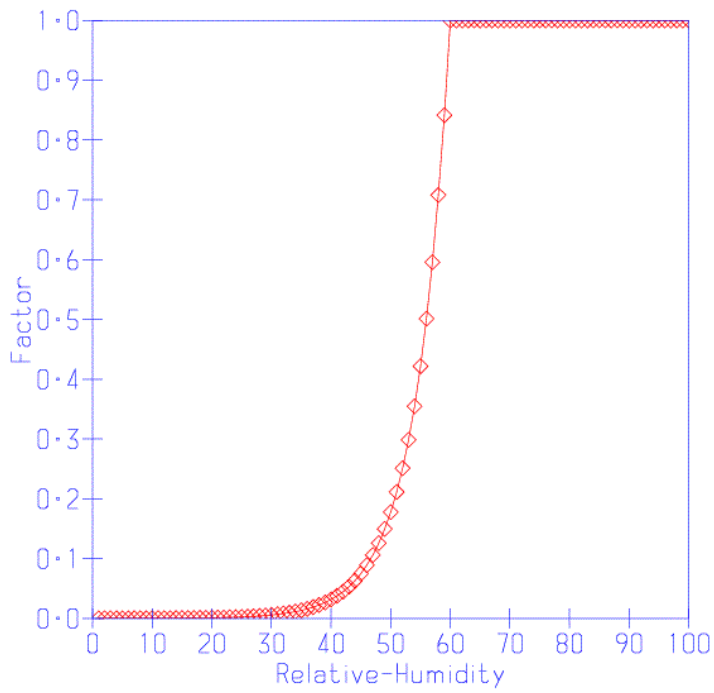
altogether if required by selecting the appropriate species identification string outlined above.

FMDV Survival Dependence

... upon Temperature

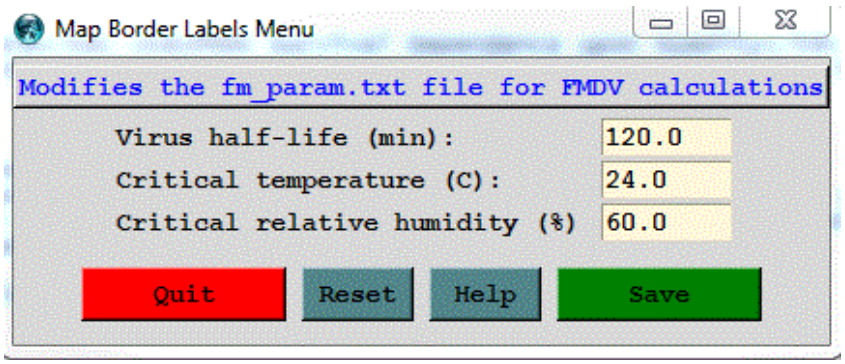


... upon Humdity



How to change default FMDV dependency thresholds

There are many different variants of FMDV each with their own characteristics. If a different set of threshold dependencies are know the default FMDV can be changed. To do this open the *Advanced / File Edit / FMDV Decay* menu to edit the decay, and critical temperature and humidity defaults. This information is written into the *fm_param.txt* file which is read when the HYSPLIT calculation starts.



References

[1] M.G. Garner, G.D. Hess and X. Yang, An integrated modelling approach to access the risk of wind-borne spread of foot-and-mouth disease virus from infected premises, Environmental Modelling & Assessment (2006) 11: 195-207.

[2] J.H. Sorensen, C.O. Jensen, T. Mikkelsen, D.K.J. Mackay and A.I. Donaldson, Modelling the Atmospheric Dispersion of Foot and Mouth Virus for Emergency Preparedness, Phys. Chem. Earth (B), Vol. 26, No. 2, pp. 93-97, 2001.

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Advanced / Configuration Setup / Namelist Variables

This section provides a summary of the *SETUP.CFG* namelist file parameters required in configuring the model to perform certain specialized calculations. The default value is shown in **bold** with each variable and a link to the User's Guide page with a more detailed discussion of the options. The namelist options that only affect *trajectories* are shown in italics.

- **CAPEMIN=-1** enhanced vertical mixing when CAPE exceeds this value (J/kg)
- **CMASS=0** compute grid concentrations (0) or grid mass (1)
- **CONAGE=48** particle to or from puff conversions at conage (hours)
- **CPACK=1** binary concentration packing 0:none 1:nonzero 2:points 3:polar
- **DELT=0.0** integration time step (0=autoset GT-0=constant LT-0=minimum)
- **DXF=1.0** horizontal X-grid adjustment factor for ensemble
- **DYF=1.0** horizontal Y-grid adjustment factor for ensemble
- **DZF=0.01** vertical (0.01 ~ 250m) factor for ensemble
- **EFILE=' '** temporal emission file name
- **FRHMAX=3.0** maximum value for the horizontal rounding parameter
- **FRHS=1.00** standard horizontal puff rounding fraction for merge
- **FRME=0.10** mass rounding fraction for enhanced merging
- **FRMR=0.0** mass removal fraction during enhanced merging
- **FRTS=0.10** temporal puff rounding fraction
- **FRVS=0.01** vertical puff rounding fraction
- **HSCALE=10800.0** horizontal Lagrangian time scale (sec)
- **ICHEM=0** chemistry conversion modules 0:none 1:matrix 2:convert 3:dust ...
- **INITD=0** initial distribution, particle, puff, or combination
- **KAGL=1** trajectory output heights are written as AGL (1) or as MSL (0)
- **KBLS=1** boundary layer stability derived from 1:fluxes 2:wind_temperature
- **KBLT=2** boundary layer turbulence parameterizations 1:Beljaars 2:Kanthar 3:TKE
- **KDEF=0** horizontal turbulence 0=vertical 1=deformation
- **KHINP=0** when non-zero sets the age (h) for particles read from *PINPF*
- **KHMAX=9999** maximum duration (h) for a particle or trajectory
- **KMIXD=0** mixed layer obtained from 0:input 1:temperature 2:TKE
- **KMIX0=250** minimum mixing depth
- **KMSL=0** starting heights default to AGL=0 or MSL=1
- **KPUFF=0** horizontal puff dispersion linear (0) or empirical (1) growth
- **KRAND=2** method to calculate random number 1=precalculated 2=calculated in pardsp 3=none
- **KRND=6** enhanced merge interval (hours)
- **KSPL=1** standard splitting interval (hours)
- **KWET=0** precipitation from an external file
- **KZMIX=0** vertical mixing adjustments: 0=none 1=PBL-average 2=scale_TVMIX
- **MAXDIM=1** maximum number of pollutants to carry on one particle
- **MAXPAR=10000** maximum number of particles carried in simulation
- **MESSG='MESSAGE'** diagnostic message file base name
- **MGMIN=10** minimum meteorological subgrid size
- **MHRS=9999** *trajectory* restart duration limit (hours)
- **NBPTYP=1** number of redistributed particle size bins per pollutant type
- **NINIT=1** particle initialization (0-none; 1-once; 2-add; 3-replace)
- **NCYCL=0** pardump output cycle time
- **NDUMP=0** dump particles to/from file 0-none or nhrs-output interval
- **NSTR=0** *trajectory* restart time interval in hours
- **NUMPAR=2500** number of puffs or particles to released per cycle
- **NVER=0** *trajectory* vertical split number
- **P10F=1.0** dust threshold velocity sensitivity factor

- **PINBC=' '** particle input file name for time-varying boundary conditions
- **PINPF=' '** particle input file name for initialization or boundary conditions
- **POUTF=' '** particle output file name
- **QCYCLE=0.0** optional cycling of emissions (hours)
- **RHB=80** is the RH defining the base of a cloud
- **RHT=60** is the RH defining the top of a cloud
- **SPLITF=1.0** automatic size adjustment (<0=disable) factor for horizontal splitting
- **TKERD=0.18** unstable turbulent kinetic energy ratio = w'2/(u'2+v'2)
- **TKERN=0.18** stable turbulent kinetic energy ratio
- **TM_PRES=0** *trajectory* diagnostic output pressure variable marker flag
- **TM_TPOT=0** *trajectory* diagnostic output potential temperature
- **TM_TAMB=0** *trajectory* diagnostic output ambient temperature
- **TM_RAIN=0** *trajectory* diagnostic output rainfall rate
- **TM_MIXD=0** *trajectory* diagnostic output mixed layer depth
- **TM_TERR=0** *trajectory* diagnostic output terrain height
- **TM_DSWF=0** *trajectory* diagnostic output downward short-wave flux
- **TM_RELH=0** *trajectory* diagnostic output relative humidity
- **TOUT=60** *trajectory* output interval in minutes
- **TRATIO=0.75** advection stability ratio
- **TVMIX=1.0** vertical mixing scale factor
- **VDIST='VMSDIST'** diagnostic file vertical mass distribution
- **VSCALE=200.0** vertical Lagrangian time scale (sec)
- **VSCALEU=200.0** vertical Lagrangian time scale (sec) for unstable PBL
- **VSCALES=200.0** vertical Lagrangian time scale (sec) for stable PBL

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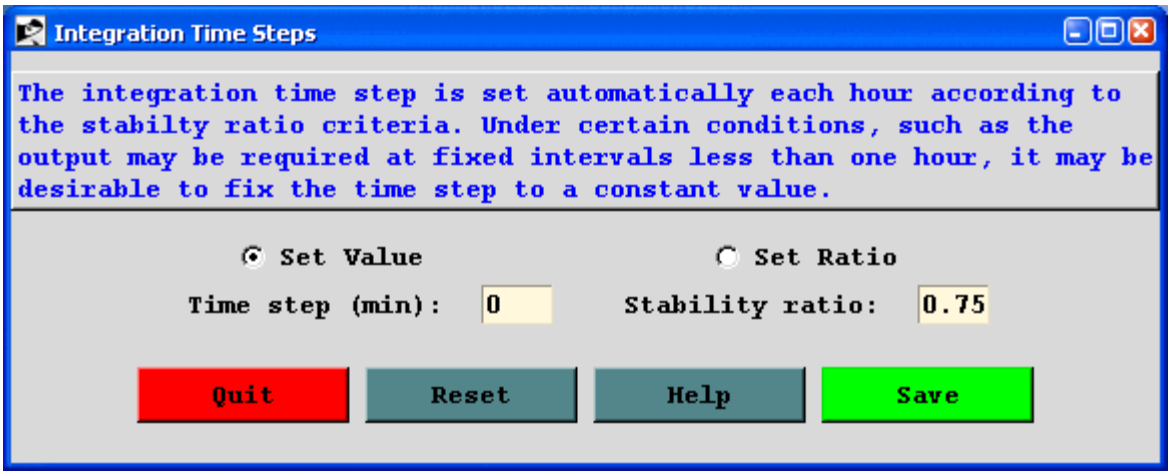
Advanced / Configuration Setup / Time Step Selection Criteria

Set Ratio - *TRATIO* (0.75) - defines the fraction of a grid cell that a particle or trajectory is permitted to transit in one advection time step. Reducing this value will reduce the time step and increase computational times. Smaller time steps result in less integration error. Integration errors can be estimated by computing a backward trajectory from the forward trajectory end position and computing the ratio of the distance between that endpoint and the original starting point divided by the total forward and backward trajectory distance.

Set Value - *DELT* (0.0) - is used to set the integration time step to a fixed value in minutes from 1 to 60. It should be evenly divisible into 60. The default value of zero causes the program to compute the time step each hour according to the maximum wind speed, meteorological and concentration grid spacing, and the *TRATIO* parameter. The fixed time step option should only be used when strong winds in regions not relevant to the dispersion simulation (perhaps the upper troposphere) are causing the model to run with small time steps. Improper specification of the time step could cause aliasing errors in advection and underestimation of air concentrations. An alternate approach is to set the a negative value which will result in that value (abs) being used as the minimum time step.



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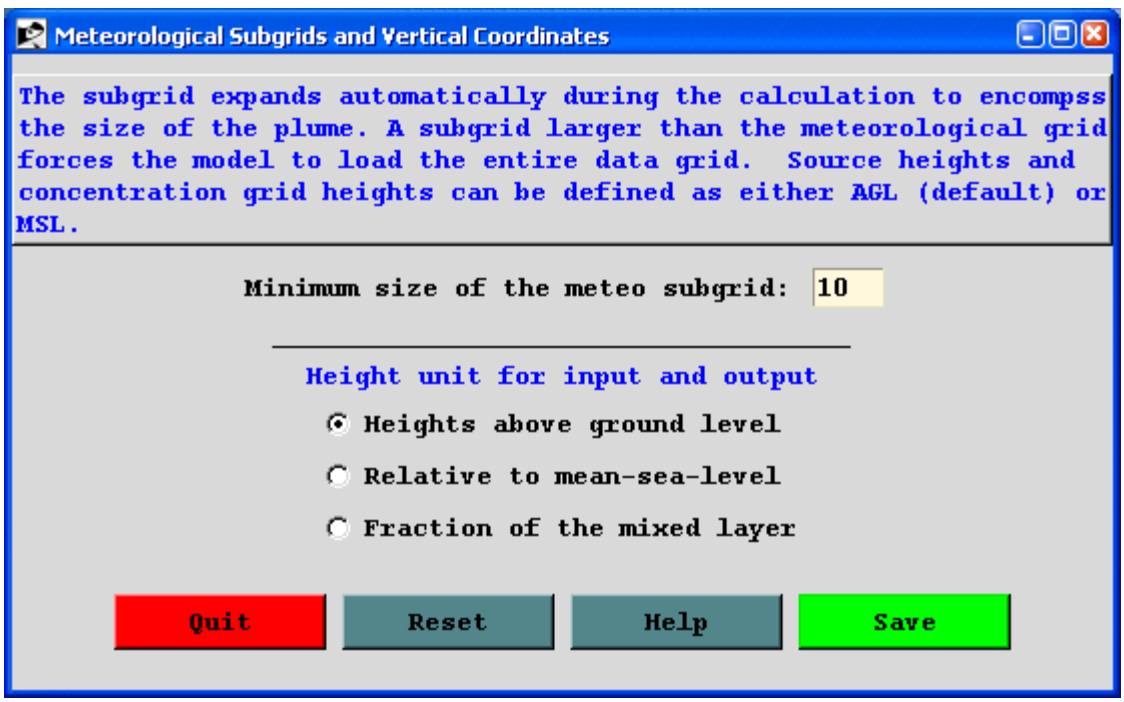
Advanced / Configuration Setup / Define subgrid and MSL/AGL units

Meteorological Sub-grid Size

MGMIN (10) - is the minimum size in grid units of the meteorological sub-grid. The sub-grid is set dynamically during the calculation and depends upon the horizontal distribution of end-points and the wind speed. Larger sub-grids than necessary will slow down the calculation by forcing the processing of meteorological data in regions where no transport or dispersion calculations are being performed. In some situations, such as when the computation is between meteorological data files that have no temporal overlap or insufficient spatial overlap, the model may try to reload meteorological data with a new sub-grid. This will result in a fatal error. One solution to this error would be to increase the minimum grid size larger than the meteorological grid to force a full-grid data load.

Height Unit for Input

KMSL (0) - sets the default for input heights to be relative to the terrain height of the meteorological model. Hence input heights are specified as AGL. Setting this parameter to "1" forces the model to subtract the local terrain height from source input heights before further processing. Hence input heights should be specified as relative to Mean Sea Level (MSL). In concentration simulations, the MSL option also forces the vertical concentration grid heights to be considered relative to mean sea level. The special option (xBL) sets KMSL to 2 and treats the input height as a fraction of the boundary layer (or mixed layer) depth at the trajectory starting location and time. This option is not valid with any multiple trajectory in time configurations or any of the concentration-dispersion calculations. Valid starting heights can be defined as any non-zero fraction less than 2.0.



Height Unit for Output

The namelist variable KAGL (=1) only applies to trajectories, not concentration simulations. For trajectory simulations, the default option is to write the heights as AGL (KAGL=1), setting KAGL=0 converts the trajectory output heights to MSL. The KMSL namelist parameter described above only applies to how heights are interpreted in the CONTROL file, while KAGL determines how the model heights are written to the output file. This variable is not available through the GUI.

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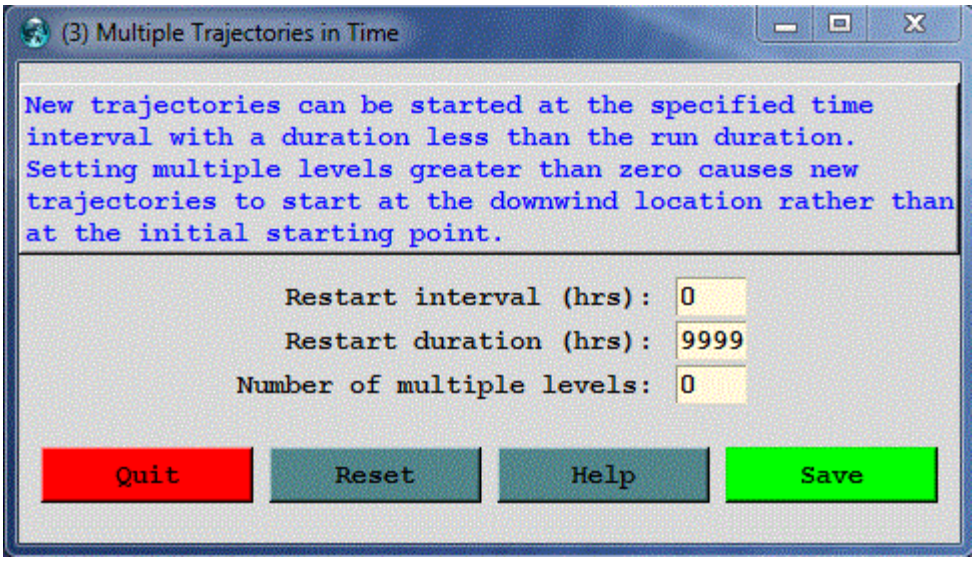
Advanced / Configuration Setup / Multiple Trajectories in Time

Restart Interval - *NSTR* (0) - Hours between trajectory starts for multiple trajectory-in-time simulations. When greater than zero, new trajectories will be started from the original starting location every NSTR hours from the initial trajectory starting time. See the special trajectory simulation section for more information.

Number of Multiple Levels - *NVER* (0) - Number of vertical levels that trajectories are restarted when trajectories for multiple trajectory-in-time-and-space simulations. When greater than zero, new trajectories will be started at this number of levels from the endpoint position at the NSTR interval. The level heights are set in the CONTROL file and must match the number of starting locations. See the special trajectory simulation section for more information.

Trajectory Duration - *MHRS* (9999) - Sets the maximum temporal trajectory restart period. For instance if you want to compute one month's worth of two-day trajectories, then the run duration would be 720 hours, *MHRS* would be set to 672 hours (720-48), and *KHMAX* (see below) would be set to 48 hours.



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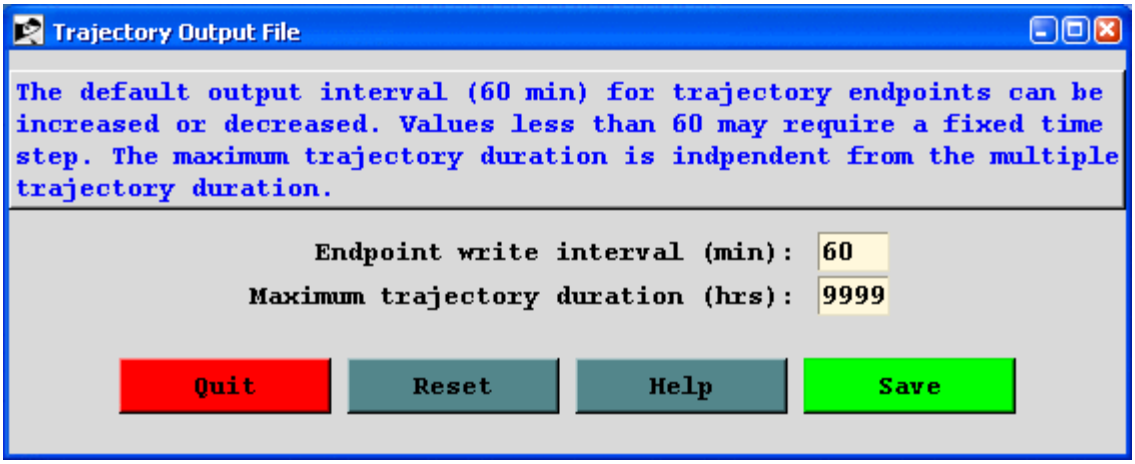
Advanced / Configuration Setup / Trajectory Points Output Frequency

The endpoint write interval *TOUT(60)* sets the time interval in minutes at which trajectory end-point positions will be written to the output file. Output intervals of less than 60 minutes can be selected. This will also force the internal time step to be an even multiple of the output interval.

The maximum trajectory duration *KHMAX* (9999) is the maximum duration of any one trajectory in hours.



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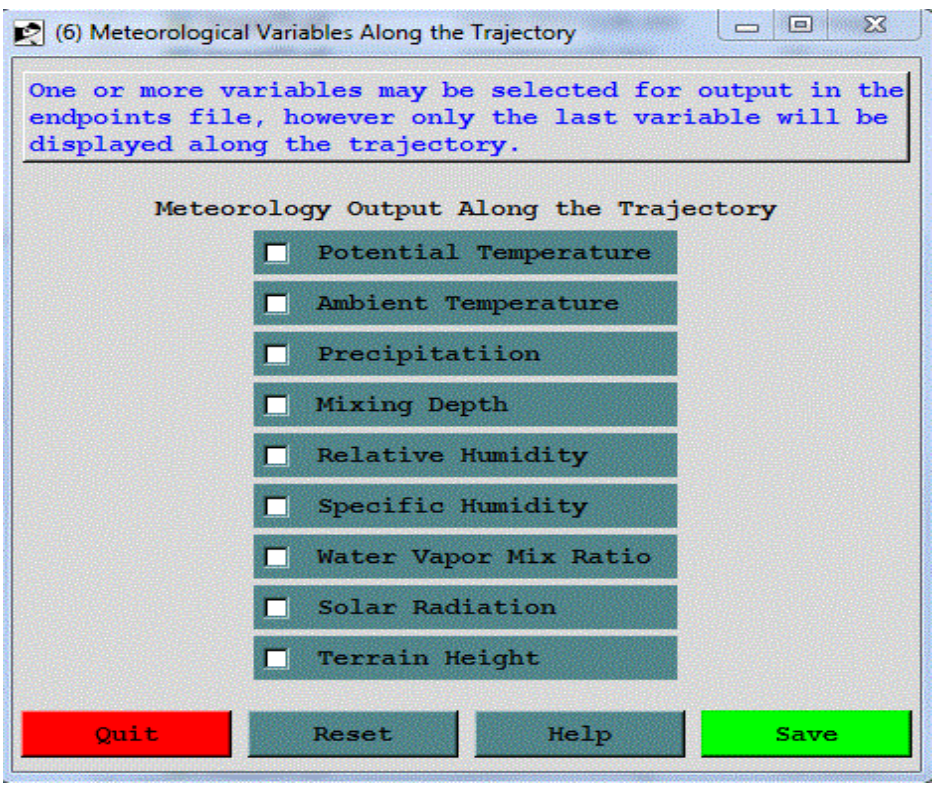
Advanced / Configuration Setup / Add Meteorology Output Along Trajectory

Sets the option to write the value of certain meteorological variables along the trajectory to the trajectory output file. The marker variables are set to (1) to turn on the option. Multiple variables may be selected for simultaneous output but only one variable may be plotted. If multiple variables are selected in conjunction with the trajectory display option, then only the last variable output will be shown in the graphic. The variable output order is fixed in the program and cannot be changed.

- **Potential Temperature** in degrees Kelvin *TM_TPOT (0|1)*
- **Ambient Temperature** in degrees Kelvin *TM_TAMB (0|1)*
- **Precipitation** rainfall in mm per hour *TM_RAIN (0|1)*
- **Mixing Depth** in meters *TM_MIXD (0|1)*
- **Relative Humidity** in percent *TM_RELH (0|1)*
- **Specific Humidity** in g/(kg air) *TM_SPHU (0|1)*
- **Water Vapor Mixing Ratio** in g/(kg dry-air) *TM_MIXR (0|1)*
- **Solar Radiation** downward solar radiation flux in watts per square meter *TM_DSWF (0|1)*
- **Terrain Height** in meters required for the trajectory plot to show underlying terrain *TM_TERR (0|1)*



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Advanced / Configuration Setup / Meteorological Grid Offset Ensemble

Sets the dimensions at which the meteorological grid will be offset for the ensemble calculation. Only one offset (+ or -) in either X, Y, or Z is applied per member.

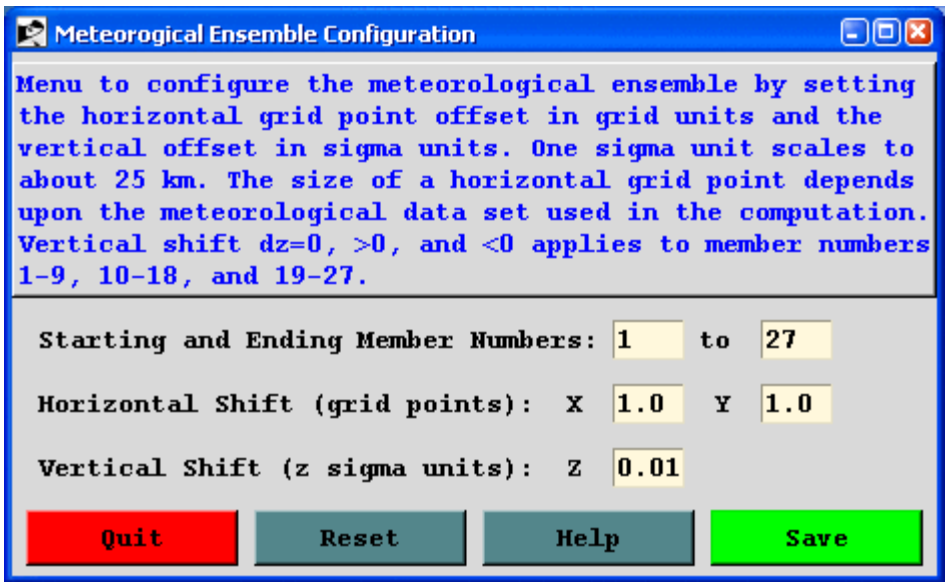
Horizontal Shift

Starting and ending member numbers can be selected where:

- the range 1-9 applies for no vertical shift,
- the range 10-18 applies for a positive vertical shift,
- the range 19-27 applies to a negative vertical shift,
- and DZF (0.01) is the vertical grid offset factor (0.01 ~ 250m).

Horizontal Shift

- DXF (1.0) is the west to east grid factor for offsetting the meteorological grid in the ensemble calculation.
- DYF (1.0) is the south to north grid factor for offsetting the meteorological grid in the ensemble calculation



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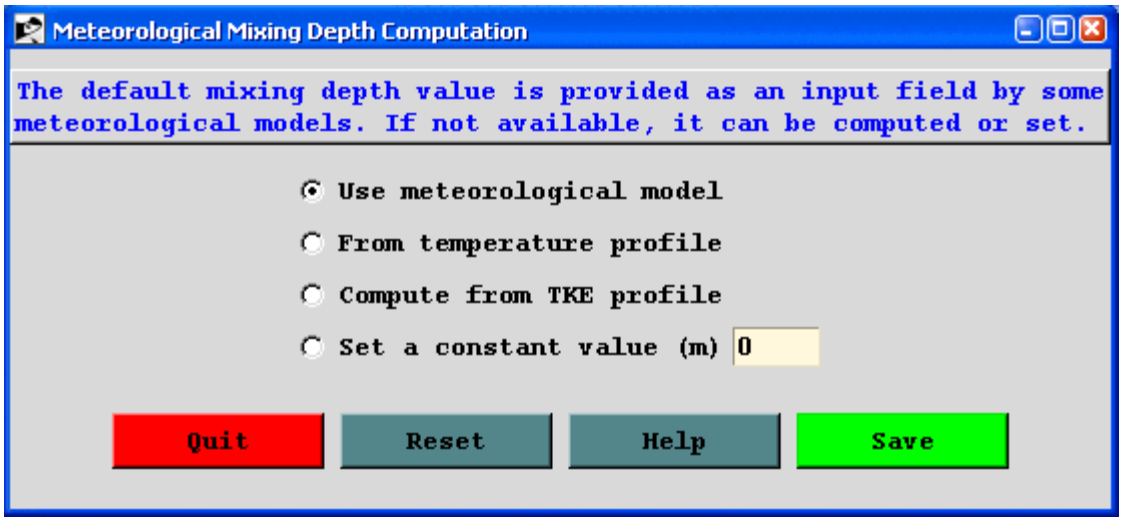
Advanced / Configuration Setup / Mixing Depth Computation Method

Permits the selection of the method used to compute the mixed layer depth. The mixed layer depth does not affect the trajectory computation, only the dispersion and resulting air concentrations by changing the rate of dispersion as well as providing a lid to vertical mixing of pollutants. Options include the following:

- Use meteorological model - uses the mixed layer depth value from the meteorological model. Not all model outputs provide mixed layer depths. Valid field IDs are MXHT, HPBL, and PBLH.
- From temperature profile - computes the height of the mixed layer as the height at which the potential temperature is at least two degrees greater than the minimum potential temperature. The computation is made from the top down.
- Compute from TKE profile - uses the meteorological model's TKE profile to estimate the mixing depth at the height at which the TKE either decreases by a factor of two or falls to a value of less than 0.21. Not all model outputs contain the TKE field.
- Set a constant value (m) - as a last resort the mixing depth can also be set to a constant value (meters). The *kmixd* namelist variable either contains the mixing depth value or the integers 0,1,2 indicating one of the other choices.



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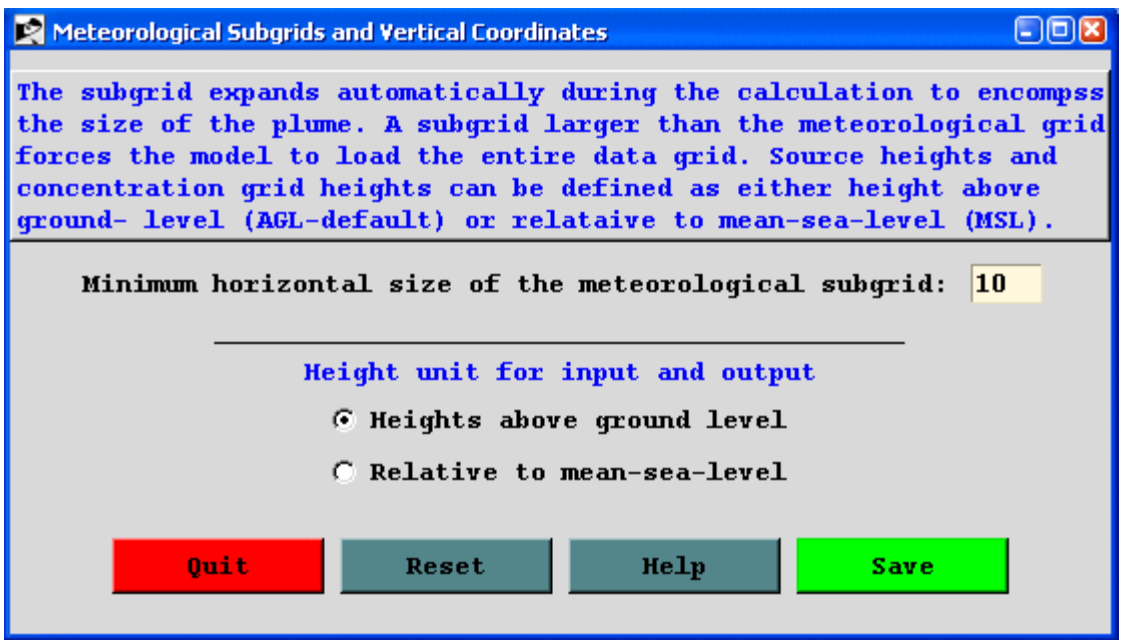
Advanced / Configuration Setup / Sub-grid Size and Vertical Coordinate

Meteorological Sub-grid Size

MGMIN (10) is the minimum size in grid units of the meteorological sub-grid. The sub-grid is set dynamically during the calculation and depends upon the horizontal distribution of end-points and the wind speed. Larger sub-grids than necessary will slow down the calculation by forcing the processing of meteorological data in regions where no transport or dispersion calculations are being performed. In some situations, such as when the computation is between meteorological data files that have no temporal overlap or insufficient spatial overlap, the model may try to reload meteorological data with a new sub-grid. This will result in a fatal error. One solution to this error would be to increase the minimum grid size larger than the meteorological grid to force a full-grid data load.

Vertical Grid Coordinate System

KMSL (0) sets the default for input heights to be relative to the terrain height of the meteorological model. Hence input heights are specified as AGL. Setting this parameter to "1" forces the model to subtract the local terrain height from source input heights before further processing. Hence input heights should be specified as relative to Mean Sea Level (MSL). In concentration simulations, the MSL option also forces the vertical concentration grid heights to be considered relative to mean sea level. The option to set the release height dynamically as a fraction of the mixed layer depth is not available for concentration-dispersion simulations.



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Advanced / Configuration Setup / Release Particles or Puffs

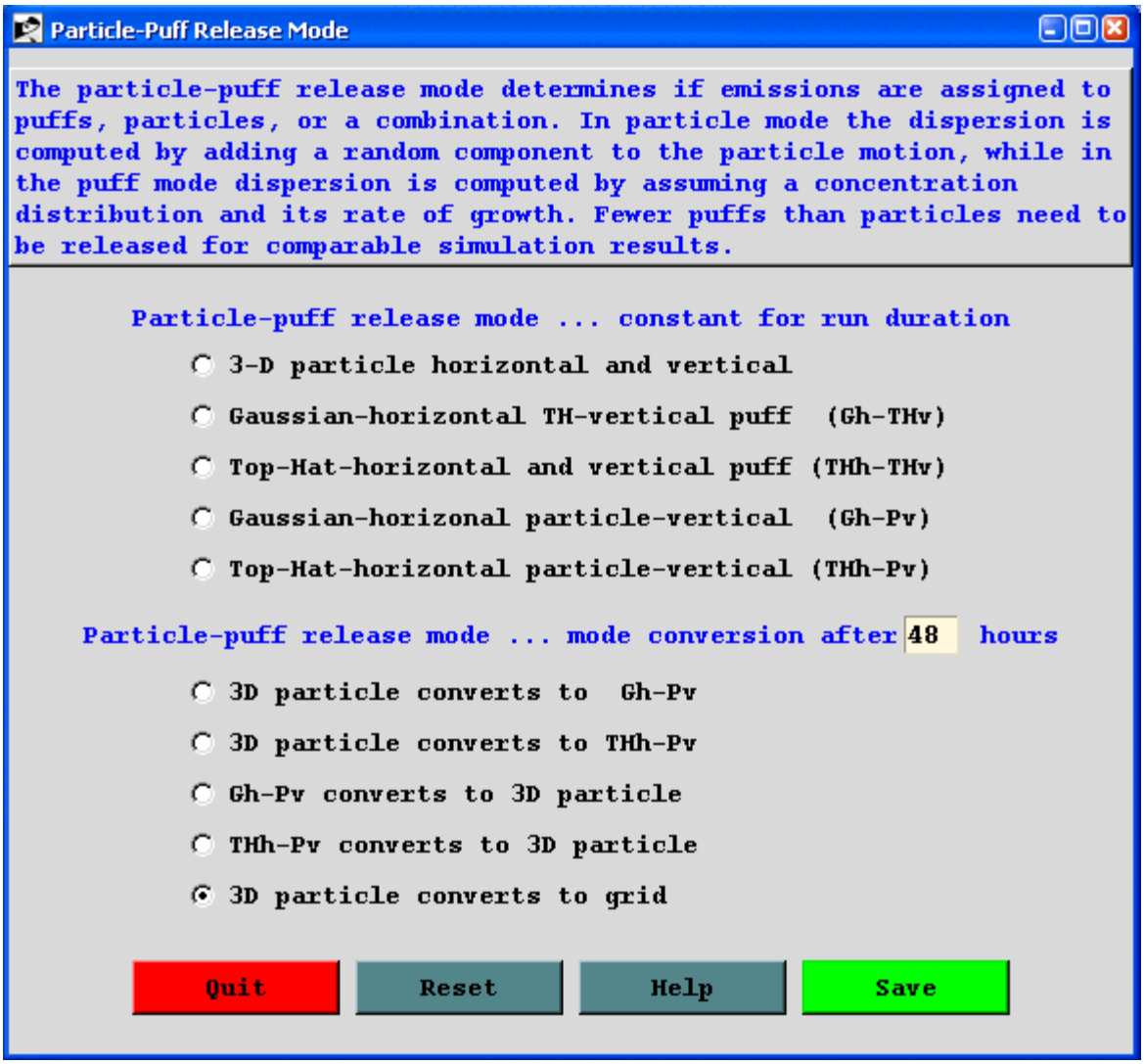
The menu is divided into two sections. In each case the value of the *INITD* namelist parameter is being set. In the upper portion of the menu, the model is configured as either a full 3D particle or puff model, or some hybrid combination of the two. The released particles or puffs maintain their mode for the entire duration of the simulation. Valid options are:

- 0 - 3D particle horizontal and vertical (**DEFAULT**)
- 1 - Gaussian-horizontal and Top-Hat vertical puff (Gh-THv)
- 2 - Top-Hat-horizontal and vertical puff (THh-THv)
- 3 - Gaussian-horizontal puff and vertical particle distribution (Gh-Pv)
- 4 - Top-Hat-horizontal puff and vertical particle distribution (THh-Pv)

Introduced with the September 2004 version are mixed mode model calculations, where the mode can change during transport depending upon the age (from release) of the particle. A mixed-mode may be selected to take advantage of the more accurate representation of the 3D particle approach near the source and the smoother horizontal distribution provided by one of the hybrid puff approaches at the longer transport distances. In a long-range or regional puff simulation, where the concentration grid may be rather coarse, puffs may pass between concentration sampling nodes during the initial stages of the transport, a stage when the plume is still narrow. Using mode #104 would start the simulation with particles (and concentration grid cells) and then switch to puff mode (and concentration sampling nodes) when the particles are distributed over multiple concentration grid cells. Valid options are:

- 103 - 3D particle (#0) converts to Gh-Pv (#3)
- 104 - 3D particle (#0) converts to THh-Pv (#4)
- 130 - Gh-Pv (#3) converts to 3D particle (#0)
- 140 - THh-Pv (#4) converts to 3D particle (#0)
- 109 - 3D particle converts to grid (global model)

A new option (109) introduced with the January 2009 version (4.9), converts 3D particles to the Global Eulerian Model grid. The particles are transferred to the global grid after the specified number of hours. This approach should only be used for very long-range (hemispheric) transport due to the artificial diffusion introduced when converting pollutant plumes to a gridded advection-diffusion computational approach. The method is ideal for estimating contributions to background concentrations. All mixed- mode particles/puffs (not just 3D) will convert to the global grid if the global option is selected from the special runs menu.



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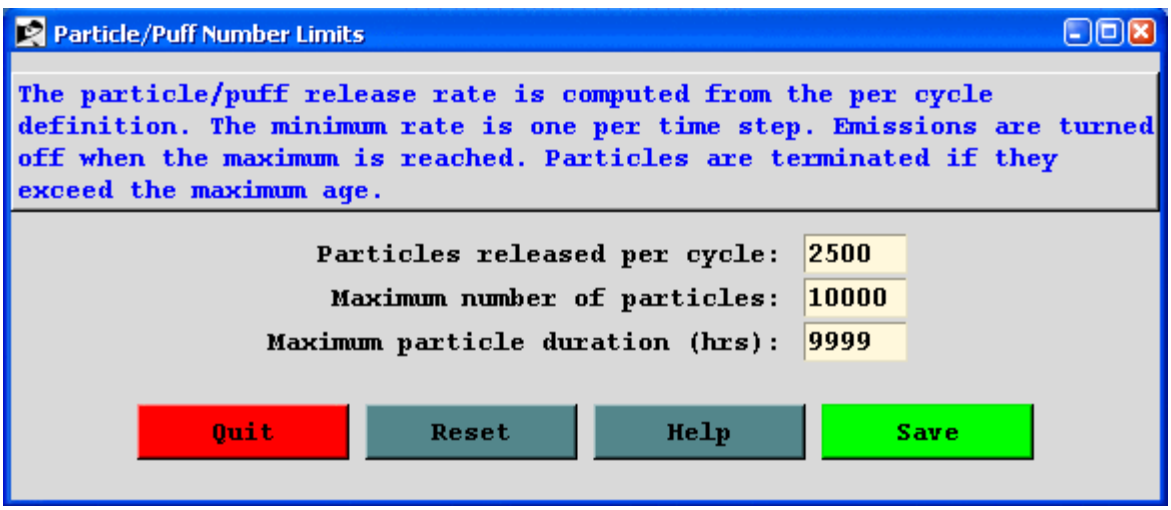
Advanced / Configuration Setup / Particle-Puff Release Number Limits

The number of particles released per cycle *NUMPAR (2500)* would be the maximum number of particles or puffs released over the duration of the emission. *NUMPAR* has a different meaning for puff and particle simulations. In a full puff simulation (*INITD* = 1 or 2), only one puff per time step is released, regardless of the value of *NUMPAR*. In a particle or mixed particle-puff simulation (*INITD* = 0, 3, 4), *NUMPAR* represents the total number of particles that are released during one release cycle. Multiple release cycles cannot produce more than *MAXPAR* number of particles. For a mixed simulation (particle-puff), *NUMPAR* should be greater than one but does not need to be anything close to what is required for a full 3D particle simulation.

To simplify certain simulations when a constant particle number release rate is required, specifying a negative value for *NUMPAR* will over-ride the particle number release rate calculations (in terms of the number of sources, hours emission, and pollutants) and force the particle release rate to be |*NUMPAR*| particles per hour for each source and pollutant.

The maximum number of particles *MAXPAR (10000)* is the maximum number permitted to be carried at any time during a simulation. In all simulation types, particle or puffs are only emitted if the particle count is less than *MAXPAR*. Note that there are situations where *NUMPAR* can (and should) exceed *MAXPAR* because the actual particle release rate is computed by dividing *NUMPAR* by the number of sources, pollutants, and release hours.

The maximum particle duration *KHMAX (9999)* is the number of hours after release that a particle is dropped from the simulation. For simulations using regional meteorological grids, particles are dropped when the reach the grid boundary. However, when using global meteorological data, it may be computationally prudent to drop particles after they are no longer over the region of interest.



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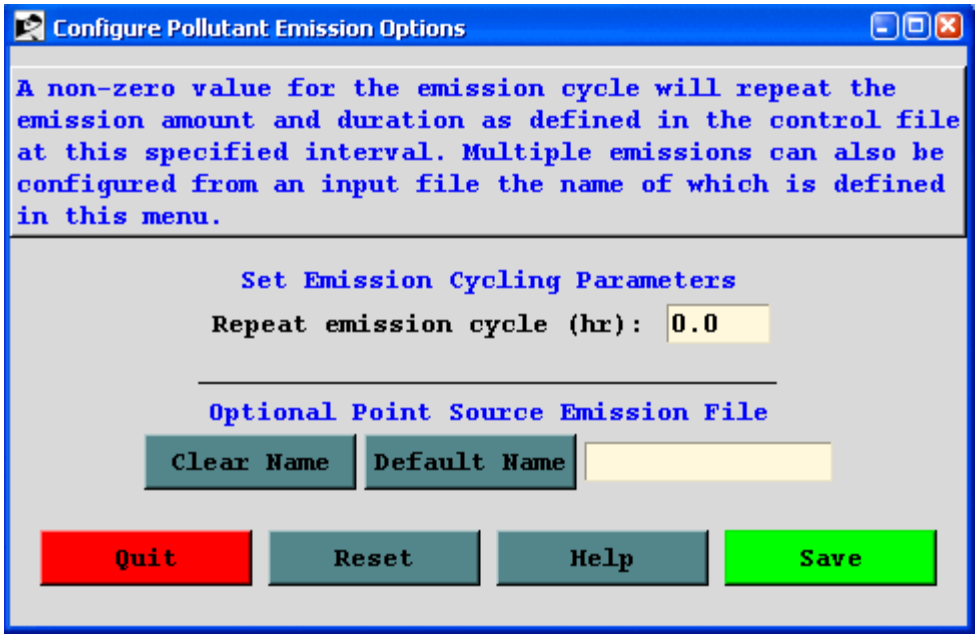
Advanced / Configuration Setup / Emission Cycling and Point Source File

Emission Cycling

QCYCLE (0.0) are the number of hours between emission start cycles. A zero value means that the emissions are not cycled. When non-zero, the number of emission hours is repeated again at *QCYCLE* hours after the starting emission time specified in the input *CONTROL* file. The *NUMPAR* parameter set in the release number limits menu is defined as the number of particles released over the emission duration per cycle unless its value is less than zero, in that case it defines the hourly particle number release rate directly as |*NUMPAR*|. The *QCYCLE* parameter is also used in conjunction with namelist option ICHEM=10 to that the concentrations from each release cycle are saved in their own concentration array.

Optional Point-Source Emission File

EFILE (undefined) is the file name that contains point-source temporal emission factors, where each record contains the {year month day hour duration latitude longitude emission-rate} for each emission period. Multiple emission periods can be defined. The values in this file replace the values set in the *CONTROL* file. The emission file can be created from the Advanced Menu tab. The format of this file is more complex than the one used to multiply time-varying unit-source dispersion factors created by the *ICHEM=10* option described above.



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Advanced / Configuration Setup / Configure Turbulence-Dispersion Computation

Vertical Turbulence

KBLT is a flag used to set the vertical turbulence computational method, that is how the turbulent velocity variances are computed from either the heat and momentum fluxes or the model profiles of wind and temperature. Two different computational approaches (Beljaars/Holtslag and Kanthar/Clayson - see the technical documentation for details) are defined. Another option is the use the TKE (Turbulent Kinetic Energy) output from the meteorological model provided in the input meteorological data file. Not all model data contain the TKE field. The last option is a special case where the input meteorological data are assumed to contain the 3-dimensional component velocity variance fields, usually a measured component.

- 1 - Beljaars/Holtslag and Betchov/Yaglom
- 2 - Kanthar/Clayson (**DEFAULT**)
- 3 - TKE field from the input meteorology data file
- 4 - Measured velocity variances from the input meteorology

Horizontal Turbulence

KDEF defines the way the horizontal turbulence is computed. The default approach is to compute the horizontal mixing in proportion to the vertical mixing using one of the methods defined above (see the technical documentation for details). The original computation was to compute the mixing from the deformation of the horizontal wind field. The limitation of this method is that for shorter-range dispersion simulations (<100 km) the deformation parameterization used in conjunction with larger scale meteorological fields will not reflect the diurnal variations in horizontal turbulence. Using diurnal sensitive methods will not effect longer-range calculations because the particles are distributed over many meteorological grid cells where variations in the transport vector dominate the horizontal dispersion process.

- 0 - In proportion to the vertical turbulence (**DEFAULT**)
- 1 - Computed from the velocity deformation

Boundary Layer Stability

KBLS defines how the stability is computed. Normally when turbulent fluxes (heat and momentum) are available from the meteorological data file, they are used to compute stability. Sometimes it may be desirable to force the stability to be computed from the wind and temperature profiles, especially if the fluxes represent long-time period averages rather than instantaneous values. If fluxes are not present, the profiles are used for the stability computation.

- 1 - Heat and momentum fluxes (**DEFAULT**)
- 2 - Wind and temperature profiles

Vertical Mixing Profile

KZMIX determines if any additional processing is to be performed on the vertical mixing profile. The current default is for no adjustments. In previous versions the boundary layer mixing profile was replaced with its average value. This compensated for some meteorological data sets with poor vertical data resolution that might result in particles being trapped near the surface due to insufficient mixing. The last two options are scale factors that can be applied to the mixing coefficients and currently are not available for modification through the GUI.

- 0 - NONE vertical diffusivity in PBL varies with height (**DEFAULT**)
- 1 - Vertical diffusivity in PBL single average value
- 2 - scale boundary-layer values multiplied by *TVMIX*

3 - scale free-troposphere values multiplied by *TVMIX*

Mixed Layer Depth Computation

KMIXD is used to control how the boundary layer depth is computed. In addition as acting as a vertical lid to particle dispersion (advection is not affected), the mixed layer depth is also used to scale the boundary layer mixing coefficients and computing turbulent fluxes from wind and temperature profiles. The default is to use the value provided by the meteorological model through the input data set. The profile can also be used if available. The computation defaults to use temperature profiles if the mixed layer field is not available. Another option to use for testing is to replace the index value (0,1,2) with a value greater than 10. In this situation, that value will be used as the mixed layer depth and will be constant for the duration of the simulation.

- 0 = Use meteorological model MIXD if available (**DEFAULT**)
- 1 = Compute from the temperature profile
- 2 = Compute from the TKE profile
- > = 10 use this value as a constant

KMIX0 is a related parameter that sets the minimum mixing depth. The default value is 250 meters and is related to the typical vertical resolution of the meteorological data. A resolution near the surface of 25 hPa is typical of pressure-level data files. This suggests that it is impossible to infer a mixed layer depth of less than 250 m (10 m per hPa) for most meteorological input data.

- 250 = The minimum mixing depth (**DEFAULT**)

Puff Growth Computation Method

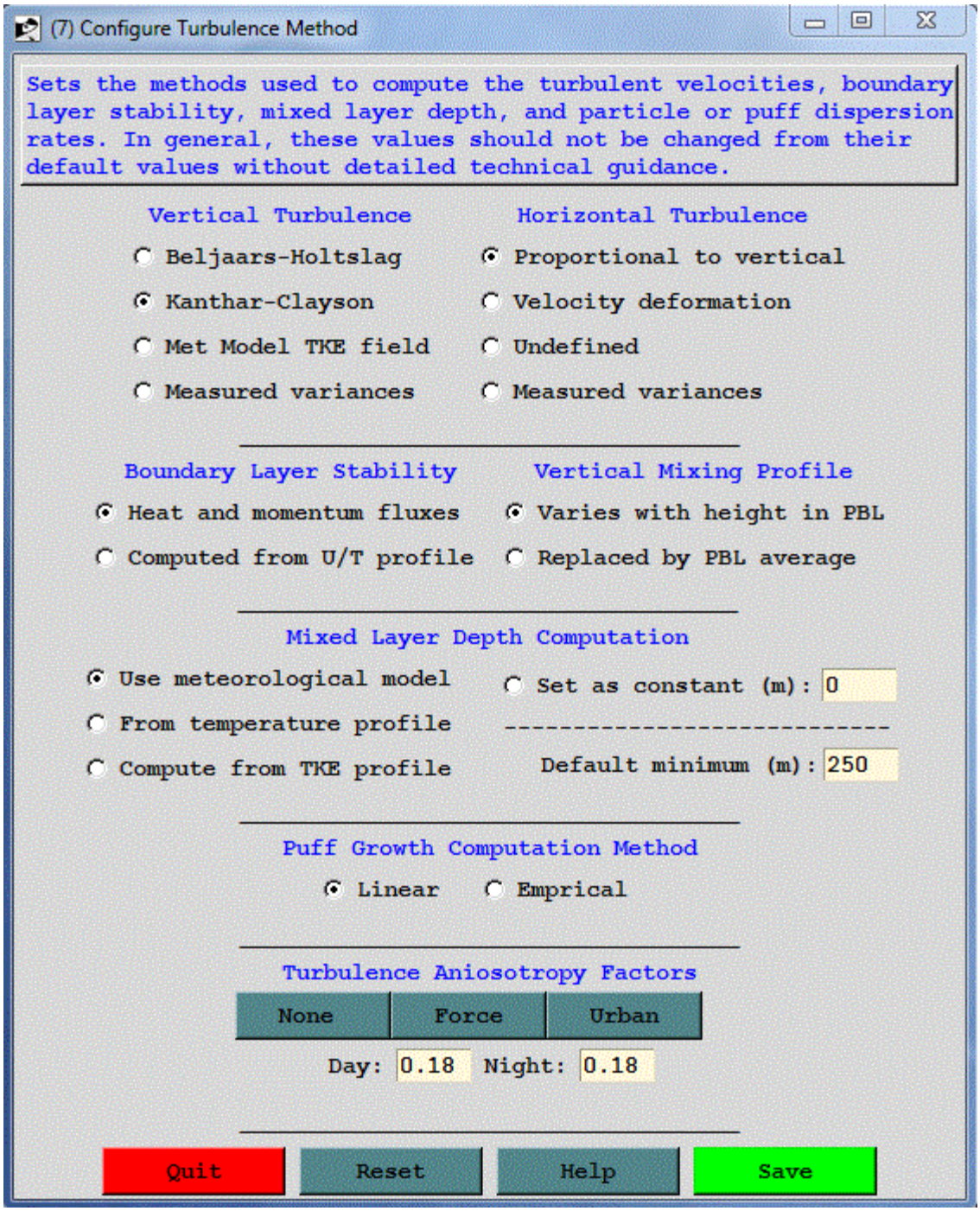
KPUFF is the flag to use either the linear with time or the empirical fit with time dispersion equations for the horizontal growth rate of puffs. This parameter does not affect particle dispersion. The linear with time approach suggests that not all turbulent scales have been sampled and puffs grow in proportion to increasing time. The empirical fit equation is similiar but the rate of puff growth decreases with time. Slower puff growth rate in the linear approach is represented by the separation of puffs after splitting due to variations in the flow. The empirical approach should only be used in those situations where puff splitting is constrained because of memory or computing time limitations.

- 0 = Linear with time puff growth (**DEFAULT**)
- 1 = Empirical fit to the puff growth

Turbulence Anisotropy Factors

TKERD and TKERN are the ratios of the vertical to the horizontal turbulence for daytime and nighttime, respectively. *TKER{D|N}* is defined as W'2/(U'2+V'2). A zero value forces the model to compute a TKE ratio consistent with its turbulence parameterization. A non-zero value forces the vertical and horizontal values derived from the TKE to match the specified ratio. This option is only valid with *KBLT=3*. The *Urban* button increases the internal TKE by 40% and slightly raises the nighttime ratio to account for enhanced turbulence in an urban setting. The landuse file supplied with the model is not of sufficient resolution to define urban areas and hence the urban setting applies to all points in the computational domain.

- 0.18 = *TKERD* day (unstable) turbulent kinetic energy ratio
- 0.18 = *TKERN* night (stable) turbulent kinetic energy ratio



Turbulence Parameters Not Defined in GUI

- 1.0 = *TVMIX* vertical mixing scale factor (in conjunction with *KZMIX*
- 200.0 = *VSCALE* vertical Lagrangian time scale (sec)
- 200.0 = *VSCALEU* vertical Lagrangian time scale (sec) for unstable PBL
- 200.0 = *VSCALES* vertical Lagrangian time scale (sec) for stable PBL
- 10800.0 = *HSCALE* horizontal Lagrangian time scale (sec)
- 1 = *KRAND* method to calculate random number (1=precompute 2=dynamic 3=none)

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Advanced / Configuration Setup / Concentration Packing and Output Units

Concentration Packing Method

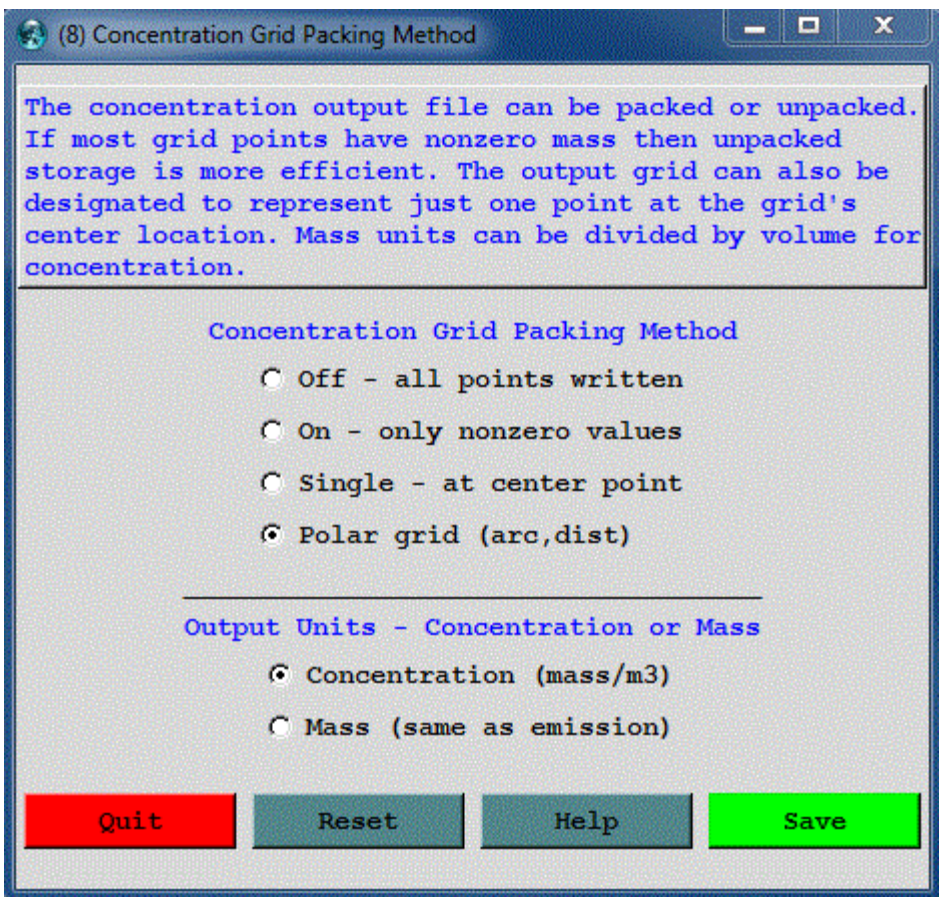
CPACK is the flag to turn off (set to 0) concentration output packing. The default is to write the binary concentration file at only those grid points that have a non-zero concentration value (set to 1). Setting the flag to zero results in the output of the entire concentration grid. Due to the nature of the packing method, if the plume covers more than 50% of the concentration grid, the default concentration packing will result in larger output file than an unpacked concentration file.

The *Point* option (*CPACK=2*) is a special feature that forces the concentration grid to have a size of one grid point over the location of the center point. It is a way to define a single sampling location.

In the case where *CPACK=3* defines a polar concentration grid defined by radial sectors centered about the origin latitude-longitude position. In this case the grid spacing and span defined in the CONTROL file define the arc sector size (latitude values) and the sector distances (longitude values). Polar concentration grids may be displayed using the program *poleplot*.

Concentration or Mass Output Units

The default option (*CMASS=0*) is to output units of mass/volume. However, if mass-only output is desired, then setting *CMASS=1* will cause the model not to divide the grid cell sum by its volume.



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Advanced / Configuration Setup / Input and Output of Particle Files

Particle File Initialization Options

NINIT sets the type of initialization performed. There are two types of initializations. One occurs at model startup, prior to the start of the calculations. This sets the initial conditions for the calculation, any particles on the computational grid at model startup are loaded. In the second situation, during the model simulation, particles are loaded each time step, if a matching time is found in the boundary condition file. These particles may represent emissions from a previous calculation and can be added to or replace the existing particles in the simulation. When *NINIT* is set to "0" no particle initialization occurs even if the input file is defined. A value of "1" reads the file only during the initialization process. No initialization will occur if the time of the particle dump does not match the time of the model initialization. A value of "2" will check the file each hour during the simulation, and if the times match, the particles will be added to those already contained in the simulation. A value of "3" is similar to the previous case, except the particles in the file replace all the particles in the simulation.

PINPF sets the default name *PARINIT* for the particle input file that can be used for initialization or boundary conditions. Note that particle files are just a dump of all the pollutants tracked by the model at a particular time and the file can consist of either puffs, particles, or a combination of both.

PINBC with a default name *PARINBC* is a special file that can be used for boundary conditions while *PINPF* can be used for initial conditions or boundary conditions. Setting the *PINBC* file name is not available through the GUI. For instance, *PINPF* can be used for both initial (NINIT=1) and boundary conditions (NINIT>1), but when *PINBC* is also defined, then it would replace *PINPF* after the initial input time.

Also not yet available through the GUI, the namelist variable *KHINP<>0* sets the particle age that will be read from the particle initialization file that may contain particles of many different ages each output time period. This option is intended to be used with continuous initialization (*NINIT=2*). An example of this application may be to create a particle file using high resolution regional meteorology, but only for the first few hours of transport. In the case of continuous emissions, this file would be read each time period during the coarser grid simulation, but only initializing with particles that are of age = *KHINP*. The final output requires that the concentration grids from the two simulations be added together.

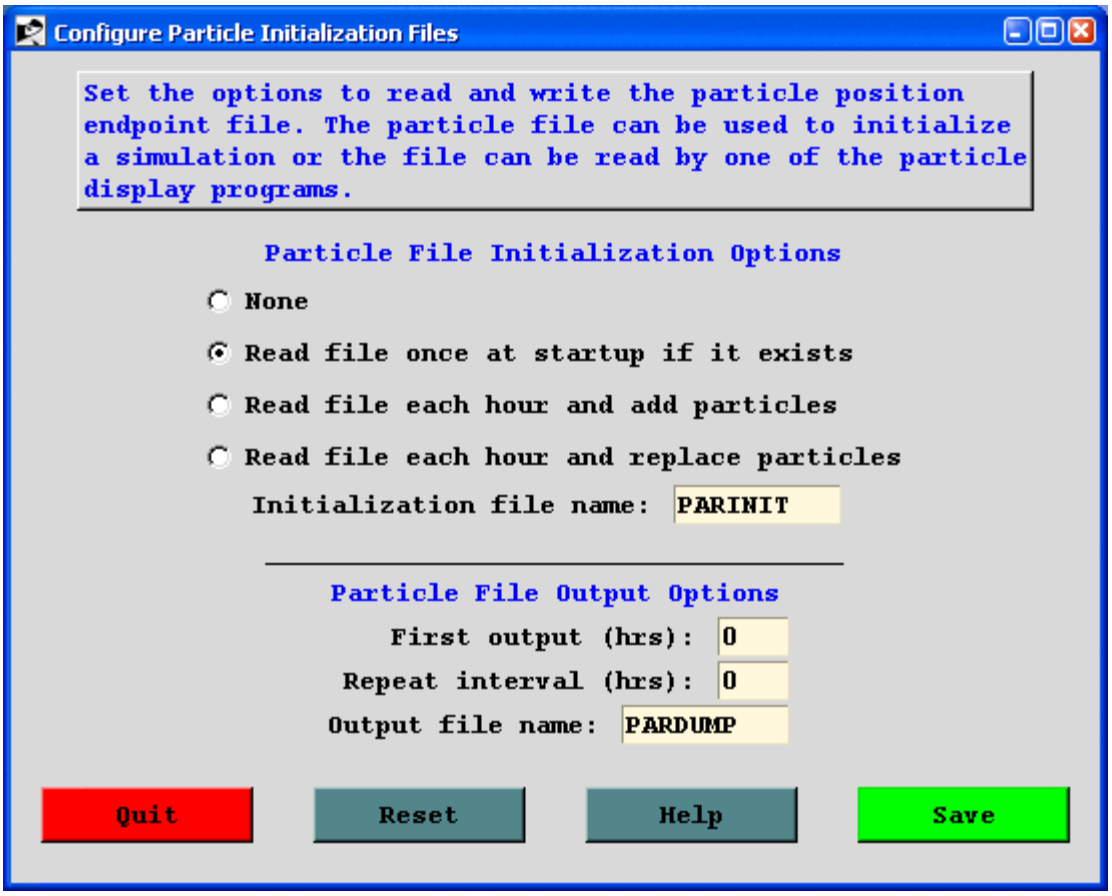
Also note that when a particle file is used for initialization of a simulation, the meteorological grid identification of a particle is retained from the previous simulation (except when *KHINP<>0*). This means that if different meteorological input files are defined in the two simulations, a particle on the second simulation may not be defined on the intended meteorological grid at the start of the calculation.

Particle File Output Options

NDUMP can be set to dump out all the particle/puff points at selected time intervals to a file called *PARDUMP*. This file can be read from the root directory at the start of a new simulation to continue the previous calculation. Valid *NDUMP* settings are [0] for no I/O or [hours] to set the number of hours from the start of the simulation at which all the endpoint positions will be written to the file. A negative value for *NDUMP* will dump out the particle/puff points at each model time step from the start of the simulation up to *NDUMP* hours. The file must exist in the root directory and *NDUMP*<>0 for the model to initialize pollutant particles from the file. *NDUMP* is used in conjunction with *NCYCL* (see below).

NCYCL sets the repeat interval at which the *PARDUMP* file is to be written after the first write at hours *NDUMP*. For instance, in a multi-day simulation, one application would be to set *NDUMP*=24 and *NCYCL*=24 to output all points at the end of every simulation day. If the model were to crash unexpectedly, the simulation could be restarted from the last *PARDUMP* output. If *NCYCL* is less than zero, then the *PARDUMP* file is over-written, rather than appended, at that interval. This means that the file will always contain one time period, a more compact file for initialization purposes. Also note that if *NDUMP* is negative, the *NCYCL* field is ignored.

POUTF is default name for the particle dump output file *PARDUMP*.



Although not yet available through the GUI, there is a command line program par2conc that can be used to convert the particle position file to a binary concentration file.

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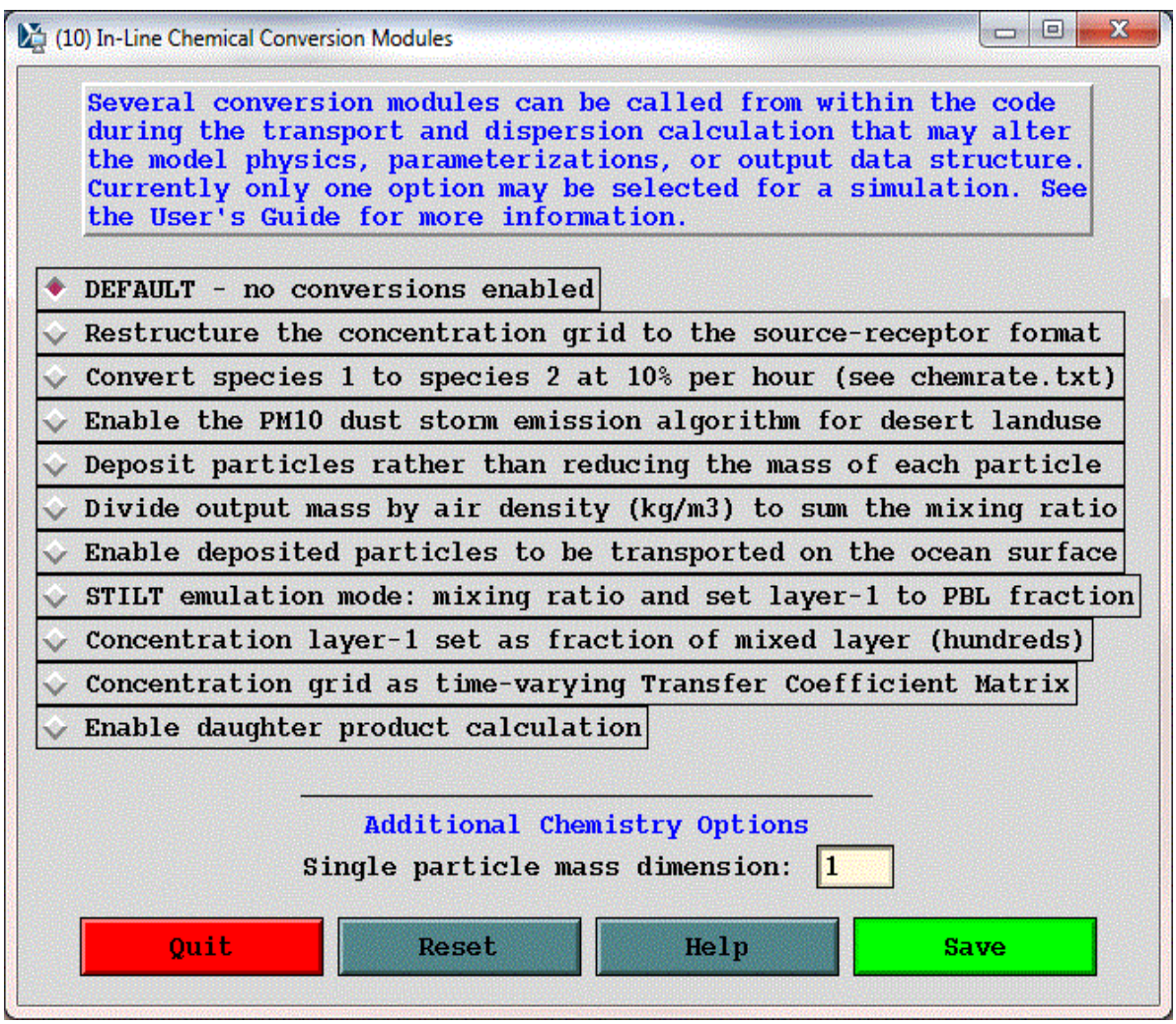
Advanced / Configuration Setup / In-Line Conversion Modules

Setting the *ICHEM* variable to a non-zero value changes the model's internal configuration in terms of how it treats the pollutants. Some conversion options require additional modules and specific requirements in setting up the *CONTROL* file. See the linked discussion under each option for more information.

***ICHEM* is chemistry module selection index:**

- 0=none (**DEFAULT**)
- 1=Restructure the concentration grid to a source-receptor format
- 2=Convert species #1 to species #2 at 10% per hour
- 3=Enable the PM10 dust storm emission algorithm
- 4=Force concentration grid to be identical to meteorology grid
- 5=Deposit particles rather than reducing their mass
- 6=Divide output mass by air density (kg/m3) to sum as mixing ratio
- 7=Transport deposited particles on the ocean surface
- 8=STILT emulation mode: mixing ratio (#6) and varying layer (#9)
- 9=Set concentration layer one to a fraction of the boundary layer
- 10=Restructure concentration grid into time-varying transfer matrix
- 11=Enable daughter product calculation



Additional Chemistry Options

MAXDIM is the maximum number of pollutants that can be attached to one particle. Otherwise, if multiple pollutants

are defined they are released as individual particles. This feature is usually required with chemical conversion modules, which are not part of the standard distribution. However, the species 1->2 conversion option will automatically set MAXDIM=2. Both the standard point source and emissions file input routines are enabled to release multiple species on the same particle. In addition, for the daughter product calculation MAXDIM needs to be set equal to the number of daughter nuclides. Setting MAXDIM greater than one forces all the species on the same particle, with the limitation that the number of defined pollutants must equal MAXDIM. No other combinations are permitted. The advantage of this approach is that not as many particles are required for the calculation as in the situation where every pollutant is on its own particle. The limitation is that each species on the particle should have comparable dynamic characteristics, such that they are all gases or have similar settling velocities; otherwise the transport and dispersion simulation would not be very realistic. In the case of multiple species defined on a single particle, the gravitational settling routine will use the characteristics of the last defined pollutant to compute settling for that particle. Deposition, decay, and other removal processes are still handled for independently for each pollutant on that particle.

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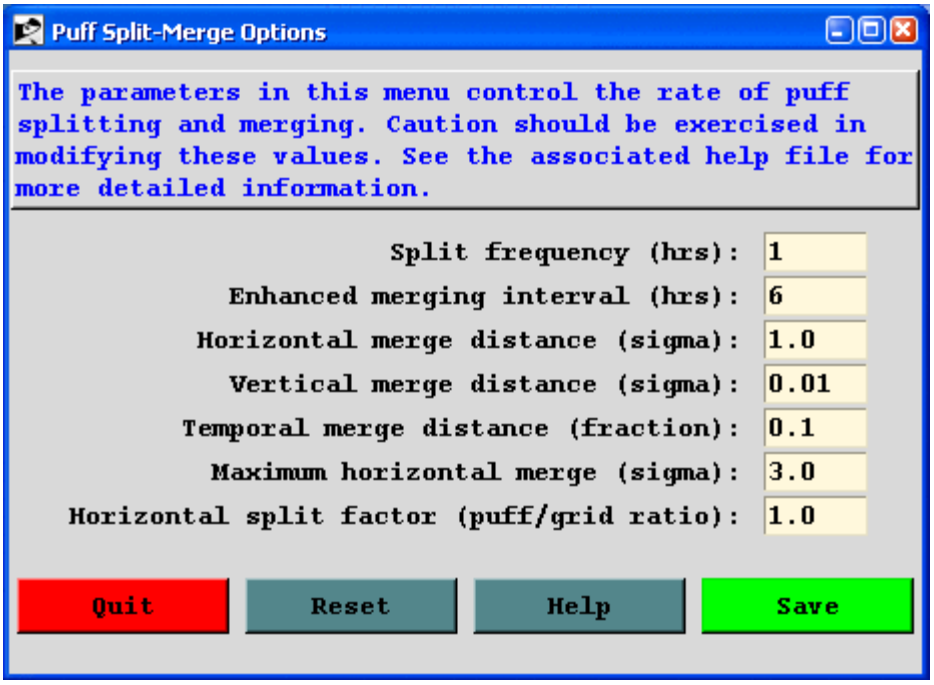
Advanced / Special Topics / Puff Split-Merge Issues

When the model is run in 3D particle mode a fixed number of particles are released and followed for the duration of the computational period. A sufficient number of particles need to be released so that at the end of the simulation, after particles have spread out, adjacent concentration grid cells, have enough particles to be able to properly represent the concentration gradients. For very long duration simulations, a large particle number may be required and the computational times may become prohibitive. One compromise is to use one of the hybrid particle-puff combinations. Fewer number of puffs need to be released because as they grow to the size of the meteorological grid, they will split into multiple particles. To avoid the particle-puff number quickly exceed the computational array limits, puffs occupying the same location may be merged. There are several different parameter settings that control the splitting and merging. These are discussed in more detail in this section.



Basic Namelist Parameters

The namelist parameters *KSPL, FRHS, FRVS, FRTS, KRND, FRMR, FRME* control the split-merge routines. Normally these should all be left at their default values. Split routines are called at *KSPL* intervals and merging is always called hourly. Merging is most sensitive to the horizontal parameter *FRHS*. When going from the default value of 1 to 4 almost all the puffs are merged once *FRHS=4*. Because merging is called after splitting, most puffs that are merged are already in the same vertical position; hence there is little sensitivity to the vertical parameter *FRVS*. The time parameter *FRTS* only matters when there are continuous emissions. *KRND* controls the interval at which the enhanced merging routines are invoked. Enhanced merging is similar to standard merging except the parameters are 50% larger and selectively applied to those puffs at the lower end of the mass range as defined by *FRME*. Its default value of 0.10 means that only puffs whose total mass only represents 0.10 of the mass of all puffs will be subjected to enhanced merging.

- **KSPL** (1) is the interval in hours at which the puff splitting routines are called.
- **FRHS** (1.0) is the horizontal distance between puffs in sigma units that puffs have to be within each other to be permitted to merge.
- **FRVS** (0.01) is the vertical distance between puffs in sigma units that puffs have to be within each other to be permitted to merge. This parameter only applies to 3d puff simulations.
- **FRTS** (0.10) is the fractional difference in the age that puffs have to be within each other to be permitted to merge.
- **KRND** (6) is the interval in hours at which enhanced puff merging takes place. Enhanced merging is less

restrictive (*FRHS*, *FRVS*, *FRTS* are 50% larger) and will degrade the accuracy of the simulation. Puffs can be further apart and still be merged into the same position. Enhanced merging only occurs when the puff number exceeds 25% of *MAXPAR*.

- **FRME** (0.10) is the fraction of the total mass that represents a puff mass at which all puffs with a mass less that puff value will only account for *FRME* of the total mass. These "Low Mass" puffs will be subject to enhanced merging.
- **FRMR** (0.0) is the fraction of the mass that is permitted to be removed at *KRND* intervals. The normal situation is to permit no mass loss. However for certain simulations, such as when a pollutant has a high ambient background relative to a typical plume signal, a small removal rate could significantly reduce the number of puffs on the grid with no loss in the accuracy of the simulation. This removal procedure can also be specified for 3D particle simulations.

Automated Split-Merge Procedures

When the puff-particle number approaches the array limits, further splitting is restricted until the merge procedures have freed up additional array space. Each time splitting shuts down, *FRHS* is automatically incremented by 0.5 to increase the effectiveness of puff merging, to a maximum value of 3 (*FRHMAX* in the namelist). Further, when splitting shuts down, those remaining puffs that are eligible to split but cannot due to the split restriction are prevented from increasing in size (both horizontal and vertical) until the split restriction has been removed. Also at the first occurrence of the split restriction, the size to which a puff is permitted to grow before splitting is increased in proportion to the namelist parameter *SPLITF*. Puff splitting occurs when the size of the puff reaches *SPLITF x METEOROLOGY_GRID_SIZE*, or concentration grid size, whichever is larger. A termination message to standard output has been added prior to HYSPLIT completion if puff splitting restrictions are in place at the end of the simulation. Such a message would suggest that it might be necessary to rerun the simulation with added array space or different merge parameters.

- **FRHMAX** (3.0) is the maximum permissible value for FRHS.
- **SPLITF** (1.0) at the default value of 1.0 is automatically recomputed to be the ratio of the number of concentration grid cells to the maximum number of particles permitted. For values less than one this feature is disabled and splitting occurs as before. For values greater than one, that value is used to determine when a puff splits. The distance adjustment is based upon how many particles are required to cover the concentration grid (assuming 20% in the PBL). If there are insufficient number of particles, then the puffs are allowed to grow larger before they split, providing for smoother patterns.

Theoretical Considerations

For example, if a global simulation is required using a 1-degree resolution concentration grid, that results in about 65,000 grid points at the surface. Clearly a very long duration simulation that is expected to spread over much of the domain will require a comparable number of puffs as grid cells to provide smooth concentration patterns. If we assume the lowest layer only represents about 10 percent of the volume over which the puffs have been transported and mixed, it is not unrealistic to expect such a simulation to require 10 times as many puffs. An alternate approach, would be to dump the puffs into a global grid model rather than splitting them as they grow to the size of the meteorological grid. Concentrations at any point would then be a sum from the two modeling approaches. This is a variation of a plume-in-grid model.

Parameter Considerations

Very long duration simulations or simulations using very fine resolution meteorological data, which have an insufficient initial allocation of the puff array space (*MAXPAR* in the namelist) can result in split shutdown messages or perhaps even emission shutdown messages. If any of these occur, the simulation results should be viewed with caution. The results may be noisy and inaccurate if the emissions (new puffs released) have also been restricted. A simulation with puff split restrictions may be improved by first increasing the array space to a value that still results in acceptable simulation times. If not effective, or the CPU times become too long, the second choice could be to increase the frequency of enhanced merging (perhaps decreasing *KRND* from 6, to 3, 2, or even 1), and perhaps in combination with

decreasing the split interval (increasing *KSPLT* from 1 to 3, 6, or 12). Although decreasing the split interval will not be effective once splitting has shutdown, it may extend the time at which splitting first shuts down. Enhanced merging has little effect if most of the puffs have the same mass, perhaps because they were released at the same time. It is most effective for continuous emission simulations, where there is a large range in puff mass due to the different number of splits each puff has been subjected. An effective removal method is setting *FRMR* to a non-zero value. This has the effect of purging the simulation of low-mass puffs and would be most appropriate for continuous emissions simulations, where the puffs at longer distances have less importance. Used incorrectly, setting this parameter to a non-zero value can seriously bias the model results. For long-duration continuous emission simulations, it may also be just as effective to stagger the emissions because it would not be necessary to emit puffs every time step for realistic (and accurate) results. This could be accomplished by emitting more mass over a shorter duration and then cycling the emissions. For instance instead of a continuous emission, one could emit 10 times the normal hourly amount over 0.1 hours (6 min) and the repeat the emission cycle (*QCYCLE* parameter) each hour. The emission cycle could even be staggered over longer times.

CPU Time Considerations

Long simulations may result in excessive CPU times because puffs will almost certainly be transported to the upper regions of the atmosphere where the winds are strongest which results in very small integration time steps. If computational accuracy in these upper regions is not required, perhaps because the only interest is boundary layer transport, the time step should be set to a fixed value. Given the same number of puffs, the enhanced merging version of the model should run substantially faster than the original version because when puff splitting shuts down and puffs continue to grow, they become quite large and cover many more concentration grid points which must all be sampled. Unrestricted puff splitting or restricting puff growth avoids this computational problem.

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Advanced / Configuration Setup / Variables Not Set in the GUI

- *CAPEMIN (-1)* - defines the threshold value of CAPE (convective available potential energy J/kg) to initiate enhanced vertical mixing. A value less than zero (default = -1) skips the CAPE computation such that if CAPE is not available in the input meteorological data file then it is NOT computed. When the value is greater than zero, CAPE enhanced mixing is turned on and if CAPE is not available in the input data file, it is computed for each grid point, which may substantially slow down the overall calculation. CAPE enhanced mixing results in particles in the cloud-layer being randomly redistributed within the cloud-layer if they reside in a grid cell where CAPE exceeds *CAPEMIN*. A initial value of 500 J/kg is suggested to test this computation.
- *DECAY (1)* - when (1=default) lets deposited material radioactively decay after accumulation on the deposition grid until it is written to the output file. When (0) then deposited material does not decay. In both situations, when the radioactive half-life is defined in the CONTROL file, the mass on the particles while airborne will decay in both cases. This flag only determines what happens after the material is deposited on the grid and before the information is written to the the output file.
- *HSCALE (10800.0)* - the horizontal Lagrangian time scale in seconds. The default value is about equal to 1/f, the Coriolis parameter.
- *K10M (1)* - when (1=default) the 10m/2m values for winds and temperatures are used as the lowest data level if available in the meteorological file. When set to zero, these data values will not be used in any computations.
- *KAGL (1)* - KAGL only applies to trajectories, not concentration simulations. For trajectory simulations, the default option is to write the heights as AGL (KAGL=1), setting KAGL=0 converts the trajectory output heights to MSL. The KMSL namelist parameter only applies to how heights are interpreted in the CONTROL file, while KAGL determines how the model heights are written to the output file.
- *KHINP (0)* - when non-zero sets the particle age in hours that will be read from the particle initialization file (*PARINIT*) that may contain particles of many different ages each output time period. This option is intended to be used with continuous initialization (*NINIT=2*) in which the calculation is continued from a previous simulation in which particles older than *KHINP* had been terminated by using the namelist variable *KHMAX=KHINP*. These continuous emission simulations require particles to be added each time step. This configuration works best when the integration time step is set to the same fixed value for all simulations.
- *KRAND (2)* - if not otherwise explicitly set, krand=1 when NUMPAR is greater than 5000, which precomputes all the random numbers required for the particle turbulence calculations. When NUMPAR is less than or equal to 5000 then krand=2 and the random numbers are computed at each dispersion time step. The dynamic method is slightly more acurate than the precomputed random numbers but it requires about twice as much CPU time. With large particle release rates both methods will provide comparable results. The special case of krand=3 will result in no turbulent mixing being added to the particle position; the particle track will follow the mean trajectory. This option is primarily intended for diagnostic testing.
- *KWET (1)* - when (1=default) the code uses the precipitation values in the defined meteorological input data file. When KWET=2, the code will try to open a file called *raindata.txt* which defines the directory, base, and suffix name of an external precipitation file that is in the ARL standard format. The text file also defines the 4-character name of the precipitation variable as well as the conversion factor from file units to model units (meters/min). The file name is automatically constructed from the prefix and suffix names using current calculation date following the convention: {prefix}{YYYYMMDD}{suffix}. If the *raindata.txt* file is not found in the startup directory, the model will create a template for manual editing and then stop.
- *MAXDIM (1)* - is the maximum number of pollutants that can be attached to one particle. Otherwise, if multiple pollutants are defined they are released as individual particles. This feature is only required with chemical conversion modules, which are not part of the standard distribution. However, the species 1->2 conversion option will automatically set MAXDIM=2, but the standard emissions routine will still put each species on a different particle in its appropriate array element. The only emissions routine that is enabled to release multiple species on the same particle is the emissions file option. Setting MAXDIM greater than one forces all the species on the same particle with the limitation that the number of defined pollutants must equal MAXDIM. No other combinations are permitted. The advantage of this approach is that not as many particles are required for the calculation as in the situation where every pollutant is on its own particle. The limitation is that each species on the particle should have comparable dynamic characteristics, such that they are all gases or have similar settling velocities, otherwise the transport and dispersion simulation would not be very realistic.

- *MESSG (MESSAGE)* - is the default base name of the diagnostic MESSAGE file. In normal simulations, the name defaults to the base name. In an ensemble multi-processor calculation, the message file name would be automatically set to correspond with the process number by appending the process number to the base name: {base}.{000}, where the process number can be any integer between 001 and 999.
- *NBPTYP (1)* - defines the number of bins assigned to each particle size as defined in the pollutant section of the CONTROL file. The default value of one uses the input parameters. A value larger than one will create that number of particle size bins centered about each value in the CONTROL file. The program creates the mass distribution for a range of particle sizes given just a few points within the distribution. We assume that dV/d(log R) is linear between the defined points for an increasing cumulative mass distribution with respect to particle diameter. The input points in the CONTROL file should be sorted by increasing particle size within the array. For instance, if the CONTROL file defines 3 particle sizes (5, 20, and 50), and NBPTYP=10, then for the 5 micron particle generates sizes from 2.3 to 8.1 microns while the 50 micron input particle generates sizes from 30.2 to 68.9 microns.
- *OUTDT (0)* - defines the output frequency in minutes of the endpoint positions in the *PARTICLE.DAT* file when the STILT emulation mode is configured. The default value of 0 results in output each time step while the positive value gives the output frequency in minutes. A negative value disables output. The output frequency should be an even multiple of the time step and be evenly divisible into 60. In STILT emulation mode, the time step is forced to one minute.
- *PINBC* - defines the input particle file name (default=PARINBC) that can be used for boundary conditions during the simulation.
- *RHB (80)* - defines the initial relative humidity required to define the base of a cloud.
- *RHT (60)* - the cloud continues upward until the relative humidity drops below this value. The values represent a compromise between the cases when the cloud (and precipitation) covers an entire grid cell and those situations where the cloud may only cover a fraction of the meteorological grid cell. For example, using the cloud fractions as defined in the EDAS (40 km resolution) data, 70% of the time 100% cloud cover occurs when the RH exceeds 80%.
- *TVMIX* - vertical mixing scale factor is applied to vertical mixing coefficents when *KZMIX* = 2 for boundary layer values and *KZMIX* = 3 for free-troposerhere values.
- *VDIST (VMSDIST)* - an output file that contains the hourly vertical mass distribution, similar to the values shown in the MESSAGE file every six hours. The output can be disabled by setting the default file name to blank or null length. Programs *vmsmerge and vmsread* are available in the exec directory to view and process these files.
- *VSCALE (200.0)* - the vertical Lagrangian time scale in seconds controls the transition of the dispersion rate from linear to square root growth as a function of time.
- *VSCALEU (200.0)* - the vertical Lagrangian time scale in seconds controls the transition of the dispersion rate from linear to square root growth as a function of time for unstable PBL conditions.
- *VSCALES (200.0)* - the vertical Lagrangian time scale in seconds controls the transition of the dispersion rate from linear to square root growth as a function of time for stable PBL conditions.

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Advanced / Satellite / FTP NASA TOMS

The FTP menu gets TOMS (Total Ozone Mapping Spectrometer) data from the following site and directories:

ftp://jwocky.gsfc.nasa.gov/pub/{eptoms|nimbus7}/data/aerosol/{year}/
file = L3_aersl_{ept|n7t}_{year}{month}{day}.txt

More current information is available from the README files on the NASA server.

TOMS Earthprobe datasets are located in the following directory paths:

data/ozYYYY/gaYYMMDD.ept (YYYY=1996 >>) (EarthProbe still reporting data)
Daily gridded (g), ASCII (a) files from year YY, month MM and day DD. The data in these ASCII files are in the format used for the Nimbus-7 and Meteor-3 CD-ROM. Details of this format are explained in the EarthProbe Data Products User's Guide, EARTHPROBE_USERGUIDE.PDF, available in the parent directory. A stub program, RDGRID.FOR may be used to read these datasets.

The values are in 3 digit groups 111222333444555
Sample ozone value: 234 = 234 du 0 = fill value

---

data/reflYYYY/gaYYMMDD.epr
Daily reflectivity data. Format similar to that of ozone data.
The vales are in 3 digit groups 111222333444555
Sample reflectivity value: _83 = 83% 999=fill value

---

data/a1YYYY/gaYYMMDD.epa
Daily aerosol data. Format similar to that of ozone data.

The data are an aerosol index formed directly from the measured radiances in two TOMS channels. Positive values generally represent absorbing aerosols (dust and smoke) while negative values represent nonabsorbing aerosols. The identification is not perfect because of geophysical reasons (e.g., aerosol too low to the ground). There will soon be a corresponding data set of optical depths and single scattering albedos.

The values are in 3 digit groups 111222333444555
The numbers have been multiplied by 10
--1=0.1 -11=1.1 111=11.1
999 = missing or bad data
-- stands for blanks

References:

- Herman, J.R., P.K. Bhartia, O.Torres, C. Hsu, C. Seftor, E. Celarier, Global Distribution of UV-Absorbing Aerosols From Nimbus-7/TOMS Data, J.Geophys. Res., 102, 16,911-16,922, 1997.
- Torres, O., P.K. Bhartia, J.R. Herman, Z. Ahmad, and J. Gleason, Derivation of aerosol properties from satellite measurements of backscattered ultraviolet radiation: Theoretical basis, J. Geophys. Res. 103, 17099-17110, 1998.

UV Erythemal Irradiance

data/uvYYYY/gaYYMMDD.epe
Daily uv data. RDGRID.FOR may be used to read these data but see 1README.UV and erynotes.pdf for

information about interpreting/decoding the uv data file format.

The values are in 3 digit groups 111222333444555

123 = 2.3x10^1 J/m2 -23 = 2.3 --3 = 0.3 999 = missing or bad data

---

data/monthly_averages/gmYYMM.ept .

This directory contains gridded monthly (gm) averages of ozone data from year YY and month MM. At least 20 days of data must be available for monthly averages to be considered valid.

Monthly averages of aerosol, UV and reflectivity are also provided in directories located in a path structure similar to that for ozone averages.

The Fortran statements that wrote the data records of these monthly files are:

```
      DO 570 IL=1,180
      DO 560 jj=1,288
560   OZONE(JJ)=ozav(JJ,IL)
      write(21,'(1X,25I3)') (OZONE(jj),jj=1,275)
      write(21,'(1X,13I3,1A17)') (OZONE(jj),jj=276,288), latlab(IL)
570   CONTINUE
```

---

data/overpass/OVPxxx.ept

A subset (seconds UT, latitude, longitude, total ozone, surface reflectivity, solar zenith angle,aerosol index, SOI index, etc) of EarthProbe data specific to a particular latitude-longitude location. xxx designates a numerical site location as listed in file "1Sitelist" in this directory.

Fortran statements that can be used to read the 1st header record and the data records in the OVPxxx files are the following:
For the header record:

```
      CHARACTER*28 site_name
      INTEGER*4    site_id, site_alt
      REAL*4       site_lat, site_lon
      Read(lun,2) site_name, site_id, site_lat,site_lon, site_alt
    2 Format(A30,4X,I3,7X,F7.2,7X,F7.2,7X,I4)
```

and for the data records:

```
Format(F7.1,1X,I4,1X,I3,1X,I5,2X,I2,1X,F6.2,1X,F7.2,1X,
I3,1X,I3,1X,F5.2,1X,F5.1,1X,F5.1,1X,F6.2,1X,I4)
```

1README, in this directory, provides more information about the OVPxxx files.

---

data/zonal_means/zm_month.ept and zmday_ YY.ept

Zonal means files. File "zm_month.ept" contains monthly averages of zonal mean column ozone over each 5 degrees of latitude for each year of EarthProbe operation to date. Additional files, named "zmday_YY.ept" (YY=96, 97...) provide zonal means on a daily basis. At least 2/3 of possible data must be present for a zonal mean to be considered valid.

The Fortran statements that wrote the header and data records of file zm_month are the following:

```
      CHARACTER*69 MONLAB
      Data MONLAB/'Jan   Feb   Mar   Apr   May   Jun   Jul   Aug   Sep
     & Oct   Nov   Dec'/
      do 20 j=1,37
      lat(j)=-95 + 5*j
   20 continue
      write(22,'(8x,A69)') MONLAB
```

```
      DO 300 IZ=1,36
      write(22,'(I3,I4,12f6.1)') lat(IZ),lat(IZ+1),(ozm(IM,IZ),IM=1,12)
300   CONTINUE
      write(22,'(I3,I4,12f6.1)') -65,0,(ozm(IM,37),IM=1,12)
      write(22,'(I3,I4,12f6.1)') 0,65,(ozm(IM,38),IM=1,12)
      write(22,'(I3,I4,12f6.1)') -65,65,(ozm(IM,39),IM=1,12)
```

The Fortran statement that wrote the data records of the zmday_YY files is:

```
write(21,'(A12,F9.3,1X,36F6.1,3X,3F6.1)') date,yd,zmd
```

If these EarthProbe/TOMS data are downloaded and used in publication, please give proper credit to the NASA/GSFC TOMS Ozone Processing Team (OPT).

For more information on the EarthProbe/TOMS data set, contact

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Advanced / Satellite / TOMS Viewer

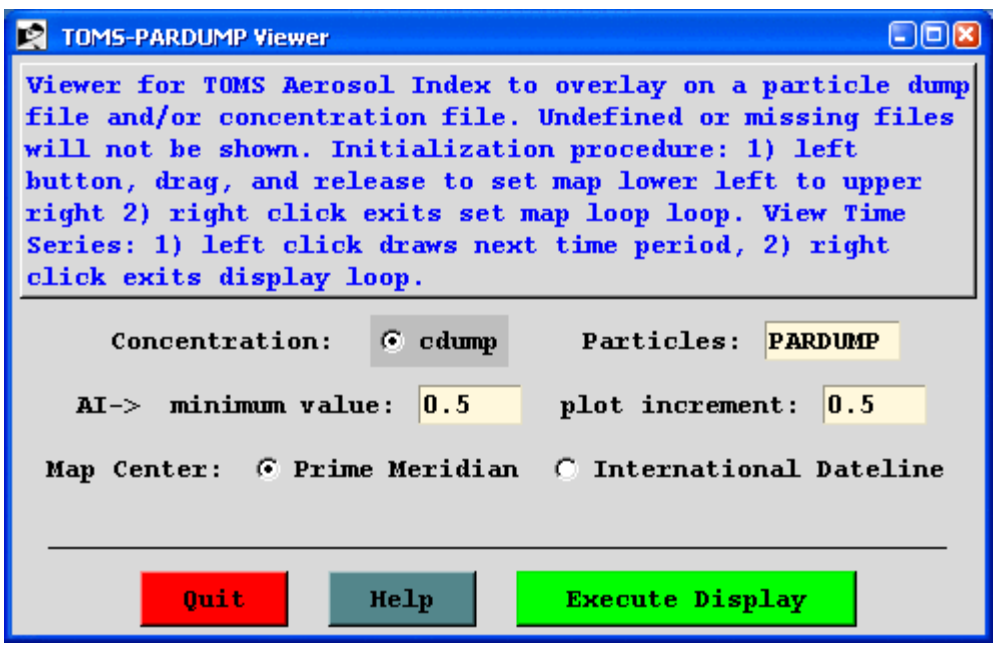
The viewer for the TOMS Aerosol Index provides a quick and qualitative way to evaluate the model calculation for dust storms, fires, and other events that may inject a significant number of particles into the atmosphere. This is accomplished by overlaying the AI values with the model particle positions from the particle dump file and/or the concentration field. The TOMS display provides a color coded representation of analysis of aerosols from the "Total Ozone Mapping Spectrometer". A range of warmer colors represents various positive values corresponding to absorbing aerosols.

The particle position dump file should have been created during the simulation by configuring the output of particle files (item 9) in the advanced configuration menu. Note that output is only required once-per-day because each TOMS data file represents all the overpasses for one day. For any given longitude, the satellite overpass occurs approximately near solar noon. Therefore the output time should be determined according to the predominant particle longitude. For instance, for the eastern United States, solar noon occurs around 1600 UTC.

The viewer has several input options that can all be selected through the GUI. The map center can be set for the dateline or prime meridians; the AI display has a minimum value below which nothing will be shown; and there is an AI color increment that represents the AI difference between the colors. Colors change from cold (blue) to warm (red) with increasing AI.

The times in the output files are not matched and they are just displayed in time sequence, with the TOMS file opened according to the date-time indicator written in the particle file. Therefore multiple particle or concentration files could be written for each day, but only one TOMS file will be opened for that day.

There are two steps involved in viewing these files. First the map domain needs to be initialization by first clicking and holding the left mouse button from the lower left corner and releasing the button at the upper right corner. The map will then be redrawn. Then each left button mouse click draws next data for the next time period. A right button click will exit the display loop.



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Advanced / Special Topics

This section provides some guidance in configuring the model input to for certain specialized calculations. The default configuration supplied with the test meteorological data is confined to a simple trajectory and inert transport and dispersion calculation. Some of these more complex scenarios are configured through the *Advanced* menu Configuration Setup tab which modifies the "*SETUP.CFG*" namelist file.

Particle or Puff Releases

The concentration model default simulation assumes 3D particle dispersion (horizontal and vertical). Other options are set with the INITD parameter of the *SETUP.CFG* namelist file defined in the advanced menu section. Normally changes to the dispersion distribution are straightforward. However, there are some considerations with regard to the initial number of particles released. The default release is set to be 2500 particles over the duration of the emission cycle (see NUMPAR). A 3-dimensional (3D) particle simulation requires many more particles to simulate the proper pollutant distribution, the number depending upon the maximum downwind distance of the simulation and the duration of the release, longer in each case require more particles. Too few particles result in noisy concentration fields. A 3D puff simulation starts with one puff as the puff-splitting process in conjunction with the vertical dispersion quickly generates a sufficient number of puffs to represent the complex dispersion process.

Continuous Emissions

As noted above the default release is 2500 particles over the duration of the emission cycle. If continuous emissions are specified (e.g. over the duration of the simulation), then those 2500 particles are spread out over that time period. This may easily result in the release of too few particles each hour to provide smooth temporal changes in the concentration field. Imagine a single particle passing in and out of the vertical concentration cell due to turbulent diffusion. One solution would be to increase the NUMPAR parameter until smoother results are obtained. Another possibility would be to cycle the emissions by emitting particles only for the first time step of each hour. Those particles would contain the total mass for a one-hour release (see how to set QCYCLE).

Time Variation of the Emission Rate

One way to incorporate a time varying emission rate into the existing model structure is to use the particle dump feature to restart the model each time with a new emission rate. Another option is to assign the name of a temporal emission input file to the "EFILE" variable in the setup.cfg namelist file. This ASCII file must consist of at least three records, the first two of which are used for identification purposes, and the third, and all subsequent records, define the temporal sequence of emissions. Each emission record contains the start time, duration, location, and emission rate. If the EFILE is present, the first emission record's values replace the emission values set in the control file. Once the model computation time has passed the emission period defined on the first emission record, the emission data from the second record are loaded and the calculation continues with the new emission data. The format of the emission file is given below:

Record #3 -> end

- I4 - Start year
- I3 - Start month
- I3 - Start day
- I3 - Start hour
- I2 - Start minute
- I3 - Duration hours
- I2 - Duration minutes
- F6.2 - Latitude
- F8.2 - Longitude
- F8.0 - Emission rate in units/hour

Time-Varying Unit Source Simuations

The previous approach defined a time-varying emissions file to use with a single simulation. An alternate approach is run the model with a unit source emission rate and in a post-processing step, apply a time-varying emissions factor. This can be accomplished by multiple simulations, one for each emission time period, and then the concentration output results can be added together or through a single simulation where individual release time periods are tagged as distinct pollutants. This is accomplished using the namelist parameters QCYCLE and ICHEM.

As an example, if hourly (the minuimum) resolution is desired over a 24 hour simulation period, then the emission rate needs to be set to emit one one unit for a duration of one hour. The namelist variable *QCYCLE* should also be set to 1.0 hour so that the emissions effectively become continuous at a rate of one unit per hour. This in combination with *ICHEM=10* will result in the creation of 24 concentration arrays with each particle being tagged according to its release hour and those particles will only contribute to concentrations on the grid with the same release-time tag. The pollutant identification field is used and its value corresponds to hours after the start of the simulation. The output concentration grid will appear to be like any other but with 24 pollutants, one for each release period as defined by the *QCYCLE* parameter. Make sure that a sufficient number of particles have been released to provide consistent results for all time perioids.

The output can be processed like any other concentration file by selecting the specific pollutant (= release time) or by two different post-processing applications that are configured to decode the output file. The apply source concentration utility menu multiplies each concentration field with its associated emission rate defined in an external file. Another option is to use the convert to station menu to extract the time series of concentrations contributed by each release time to each sampling period for a specific pre-selected location. The **TCM format** checkbox should be selected to enable the proper conversion option.

Area Source Emissions

Normally emissions are assumed to be point or vertical line sources. Virtual point sources (initial source area >0) can be defined two ways: 1) through the definition of an initial area on the source location input line of the CONTROL file or 2) by the definition of a gridded emissions file. If the model's root startup directory contains the file *Emission.txt*, then the pollutants are emitted from each grid cell according to the definitions previously set in the *Control* file. Two source points should be selected, which define the lower left (1st point) and upper right (2nd point) corner of the emissions grid that will be used in the simulation. This should be a subset of the grid defined in *emission.txt*. The release height represents the height from the ground through which pollutants will be initially distributed. Note that the structure of the "*emission.txt* " file has changed with the HYSPLIT 4.6 revision of October 2003.

The "emission.txt" file contains all the information that is required to interpret the data in the gridded emission inventory file. The file that contains the inventory is now independent of the emission.txt file. The file's first record contains information about the internal grid cell size that is used by the dispersion model to accumulate the file's emissions. The emission file defines the emissions at latitude-longitude points, which may represent the emissions from an area or from a point. The values at these points are accumulated in an internal grid, the size of which is defined on the first record. This value can be arbitrarily changed according to the desired resolution of the simulation. The pollutant puffs are released with an initial size comparable to the accumulation cell size. Because the emission file data are remapped to an internal grid, the file can consist of emissions data on a regular grid or just a collection of individual cells. The emission rate in the Control file is used as an additional multiplication factor for the data in the emission file. Also note that previously discussed particle number restrictions still apply. The particles are spread out over the duration of the emission and the number of grid cells that are defined in the emission domain. The format of the emission.txt file is given below:

Record #1

- I4 - Number (n) of pollutant species in file
- I4 - Number of emissions defined for each 24 hour period
- F10.4 - Conversion factor: file units to model units/hour

2F10.4 - Accumulation cell size (latitude & longitude)

Record #2

- nA4 - Four character pollutant identification string for each pollutant

Record #3

- A - The /directory/filename of the emission data file

The actual emission data file will contain one record identifying the grid location and then two records for each pollutant species. The first record defines emissions from GMT hours 0 to 12 and the second record from hours 12 to 24. This pair of records is repeated for each pollutant species:

Records Loop #1 to the number of i,j grid point

- 2I4 - I,J grid point of emission cell (arbitrary units for identification)
- 2F10.4 - Southwest corner Longitude and Latitude of this emission cell

Record Loop #2 to the number of pollutant species

- 12E10.3 - emissions for pollutant#1 hours 1-12
- 12E10.3 - emissions for pollutant#1 hours 13-24

Multiple Pollutants

The model can easily be configured to simulate more complex pollutant episodes with multiple pollutant types on different particles or multiple pollutant species on the same particle. The former is accomplished by defining additional pollutants in the *CONTROL* file. In this configuration, multiple species are emitted, have no interaction, and may track differently. This situation may represent a volcanic ash plume, where each pollutant, a different sized particle, settles at a different rate. An example configuration *control_volcano* can be retrieved in the SETUP menu.

Pollutant Transformations

In the latter situation, when multiple pollutants are defined on the same particle, an external chemistry routine is required that converts mass from one species to another, all tracking together (advecting and dispersing). In this situation, *MAXDIM* should be raised to the required value. Increasing the *MAXDIM* value always requires an external routine to adjust the mass between species. A simple species conversion program is included with the standard model distribution. In the default configuration it is only necessary to define two different pollutants in the concentration setup menu and select the 10% /hr checkbox in the advanced configuration menu's conversion section. This option combination sets *MAXDIM=2* and calls the transformation routine every time step to convert pollutant #1 to #2 at a rate of 10% per hour. Other conversion rates or a greater number of pollutants can be defined by creating the *CHEMRATE.TXT* file in the local directory. This file would consist of one or more records, each record defining a pollutant conversion. The data are free-format and consist of four fields, the integer "from" and "to" pollutant index numbers, and the real hourly conversion "rate", and molecular weight adjustment "factor". For instance, if the file were to be defined for the default case, the one data record would have the following values: (1 2 0.10 1.0). The molecular weight adjustment factor can be used to account for other reactions not considered in the simple conversion module. For instance, if one were to define pollutants #1 and #2 as SO2 and SO4, respectively, then the molecular weight adjustment factor should be 1.5 as SO2 transforms to SO4 (the conversion picks up two additional oxygen molecules).

Complex Chemistry

Although there are other more complex chemical conversion modules available for HYSPLIT, they are not incorporated into the standard compilation. More information on these special compilations may be found at http://www.ready.noaa.gov/HYSPLIT_pcchem.php

One feature, required for all these modules, is that there is a more complex interaction between the individual pollutant plumes, requiring a close link between the concentration grid and the meteorological data grid. This option is available in the standard model compilation. By setting the namelist file parameter ICHEM=4, the concentration grid is redefined to be equal to the meteorological data grid in terms of spatial resolution and extent. This simplifies the computation of the grid based chemical reactions that are dependent upon the meteorological conditions within each concentration grid cell.

Deposition and Decay

A simple particle deposition configuration (*control_nuclear*) for radioactive Cs-137 can be retrieved into the *SETUP* menu, which shows the default settings for radioactive decay and wet and dry deposition. In conjunction, a list of sites can be loaded into any *SETUP* menu, from the "Set Starting Locations" tab by pressing the LIST button. The site locations can be found in the file "*\working\plants.txt*" and could be replaced by any user generated location file listing.

The normal deposition mode is for particles to loose mass to deposition when those particles are within the deposition layer. An additional option was added to deposit the entire particle's mass at the surface (the particle is removed) when subjected to deposition. To insure the same mass removal rates between the two methods, a probability of deposition is computed, so that only a fraction of the particles within the deposition layer are deposited in any one time step. The probability of deposition is a function of the deposition velocity, time step, and depth of the layer. One limitation of this method is that only one mass species may be assigned to a particle. The probability deposition method can be invoked from the namelist file with ICHEM=5.

Compilation Limits

With HYSPLIT V4.5 most compilation array limits have been eliminated through the use of dynamic array allocation. However, one restriction remains with regard to the meteorological input data: meteorological data files are limited to a maximum of 12 per simulation, with no more than 75 levels or 35 variables in each file. This restriction does not limit any computation with data files available through the ARL web site, because all available data files meet the number of variable and levels restriction.

The use of dynamic memory allocation can result in unpredictable results if the computer's hardware memory limits are exceeded. Although there are several memory error allocation traps that will result in a message and execution termination, memory limits can be exceeded in a variety of different locations, such as when opening a file. Memory usage is a primarily a function of the meteorological sub-grid size, meteorological data grid size, concentration grid size, and the number of pollutants.

Script Automation and Configuration

Most of the discussion in various sections of the User's Guide are tailored to individually configured simulations. However there are several features to the model that can be used to automate the computational environment. For instance, a sample *Auto_traj.tcl* script is provided in the */examples/scripts/tcl* directory that can be used as a guide to automate many applications.

```
# Auto_traj.tcl
# the next line restarts using wish
# exec wish "$0" "$@"
set Start_hgt "10.0"
set Traj_path "../exec"
set Start_time "00 00 00 00"
set Run_hours "24"
set Vert_coord "0"
set Top_model "10000.0"
set Meteo_path "../metdata/"
set Meteo_file "oct1618.BIN"
```

```
set Output_path "./"
set Output_base "tdump"
set Output_numb 1
foreach {Start_lat Start_lon} {35.0 -90.0 40.0 -90.0 45.0 -90.0} {
set Start_loc "$Start_lat $Start_lon $Start_hgt"
set Output_file "$Output_base$Output_numb"
file delete Control
set f [open Control w]
puts $f "$Start_time"
puts $f "1"
puts $f "$Start_loc"
puts $f "$Run_hours"
puts $f "$Vert_coord"
puts $f "$Top_model"
puts $f "1"
puts $f "$Meteo_path"
puts $f "$Meteo_file"
puts $f "$Output_path"
puts $f "$Output_file"
close $f
exec "$Traj_path/hyts_std.exe"
incr Output_numb}
```

In this particular example the test trajectory case is run for three different starting locations, each simulation writing a new endpoints file with a unique file name. The *CONTROL* file is recreated for each simulation. It would be trivial to rewrite the script to set the latitude-longitude and loop through a different number of starting days and hours. With Tcl/Tk installed, this script can be run under Windows or Unix. For instance, to compute new forecast trajectories each day, the process can be automated by including a data FTP at the beginning of the script to get the most recent meteorological forecast file, setting the starting time as "00 00 00 00" so that the trajectories will start at the beginning of the file, and finally calling the script once-a-day though the Unix crontable or the Window's scheduler commands.

One problem with automated operations is that it is possible to generate simultaneous multiple jobs which may interfere with each other. The executables, hycs_std and hyts_std have a command line option of adding the process ID (PID): e.g. hyts_std [PID]. In this situation all standard named input and output files [those not defined in the Control file] have the PID added as a suffix to the file name: e.g. Control.[PID], Setup.[PID], Message.[PID].

An example of another type of operational configuration is the extended simulation of a pollutant emission using archive data to bring the simulation to the current time and then using forecast meteorological data to provide a daily projection. Each day the archive simulation must be updated with the new archive data and a new forecast product generated. This process can also be automated through a script, but for illustration purposes one can use the advanced features of the GUI to configure such a case. Assume a one-hour duration accidental pollutant release that occurred 48 hours prior to the current time. The following sequence applies:

1) From the "*Meteorology*" menu tab download the appropriate archive meteorological data and the most recent forecast meteorological data (assume it is available to +48h).

2) Setup the concentration simulation to run 96 hours using two meteorological files starting with the archive data and then switching to the forecast data.

3) Under the *Advanced* menu tab and *Configuration Setup* write the initialization file after 72 hours.

4) Run the model.

At the completion of the simulation you will have the plume projection from release (-48 h) through the current forecast (+48 h). The *PARDUMP* file will contain all the endpoint positions at +24 hours, corresponding to the initialization

time of when the next forecast will be available (assume there is one forecast per day).

The next day, when the new forecast data are available, reconfigure the model to run only with the forecast meteorological data for a duration of 48 hours. Then write the initialization file after 24 hours and run the model to obtain the new projection. In this second part, we assume that the first 24 hours of the forecast are not much different than the analysis. In practice, this procedure can be run at the same frequency that the new forecast data are available, typically 4 times per day. Data at the initial forecast hour are identical to the analysis data.

Source Attribution with Dispersion

A common application of atmospheric trajectory and dispersion models is to try to determine the source of a pollution measurement. If a high value has been collected at a particular receptor, from which pollutant source region did the air originate? One approach is to calculate the trajectory "backwards" from the receptor site. In the trajectory calculation this is accomplished by setting the integration time step to a negative value. However, the trajectory only represents the upwind path of a single point, while the pollutant measurement may require of hundreds or thousands of trajectories to represent the dispersion of the pollutant in time and space.

Another approach is the run the entire dispersion-trajectory model upstream (backwards), which is computationally attractive because in a 3D particle model the dispersion process is represented by a turbulent component added to the trajectory calculation and the advection process (the trajectory) is fully reversible. The trajectory equation can be correctly integrated in either direction. The interpretation of the output is a bit more complex because dispersion is an irreversible process. The upstream numerical calculation will yield a result because the integration of the dispersion equation is still in the downstream mode while the advection is integrated backward upstream. The meaning of the upwind dispersion result is not as easily interpreted as the downwind calculation. In any event, as noted in the earlier instructions, it is possible to run the dispersion model "backwards" by setting the run duration to its equivalent negative value. The stop time of the sampling should be set prior to the start time. All start and stop times should be set to their exact values - relative start-stop times are not supported in the backward mode.

Transport of Particles Deposited on Water Surfaces

The main code was modified (October 2003 Version 4.6) to permit particles deposited on water surfaces to continue to be transported on the water surface by the wind generated drift current. The transport output is treated as a deposition surface for display purposes. This new deposition method then creates particles that can be transported on water surfaces. Particles can be deposited on any surface. However, if the surface is defined as water, then the particle is assigned a unique identification code to distinguish it from atmospheric particles or puffs. These new particles may continue to be transported along the surface of the water contributing to deposition each time step but not air concentration. Dispersion is not computed for these particles. When they approach a land surface they are deleted. The water surface transport option is invoked from the namelist file with ICHEM=7. This option automatically forces the probability deposition computation (ICHEM=5) and should only be used only with the 3D particle mode (IN ITD=0). Surface water deposition can only be displayed if the deposition output level (0) is defined. Although particles may deposit over land, over-land deposition values are never shown.

The wind induced surface water drift current is assumed to equal the vector atmospheric friction velocity. The friction velocity represents the momentum transport to the surface and it is an approximation of the surface water movement. Currently only the GFS meteorological model output file contains the vector momentum flux components.

Mixing Ratio Output

Setting this option forces the concentration summation calls within the main program to integrate the mass divided by the air density (kg/m3) rather than just the mass, thereby permitting the output fields to be more easily converted from mass/volume to mixing ratio. This option would most likely be used in conjunction with the CMASS namelist variable that can be set to sum mass/volume or just mass.

STILT emulation mode

The STILT model is a variation of HYSPLIT developed by Lin et al. (2003 - JGR, VOL. 108, NO. D16, 4493, doi:10.1029/2002JD003161) that can be used to estimate upwind surface fluxes from atmospheric measurements. Although HYSPLIT does not contain the mass conservation adjustments and coupled vertical-mixing horizontal-transport features of STILT, setting this flag causes the HYSPLIT concentration output field units to be similar to the STILT configuration. Two changes are introduced; the mass summation is divided by air density resulting in a mixing ratio output field (ICHEM=6) and the lowest concentration summation layer (concentration layer top depth) is permitted to vary with the mixed layer depth (ICHEM=9), so that only particles below 50% of the mixed layer depth at each time step are summed to the lowest layer. The ICHEM=8 switch turns on both density and varying layer depth. A text file of particle position information (PARTICLE.DAT) at each time step will also be created unless the namelist parameter OUTDT defining the output interval (min) is changed.

Concentration layer varies with mixed layer depth

This option changes the height of the lowest concentration layer from a fixed value to a variable, which changes according to the mixed layer depth each time step. The depth, as a fraction of the mixed layer, is computed by the height value of the lowest level, where the height is interpreted in hundreds, such that the a fraction representing 0.5 of the mixed layer depth would be entered as 50. Note that in this mode it may be desired to change the default minimum mixing depth KMIX0 from its default value of 250 m, which would result in a minimum sampling layer of 125 m. Concentration levels above the first level are unaffected by this option.

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Advanced / Special Topics / Particle Dump File Format

The concentration configuration menu provides an option to write a model initialization file, which by default is always named "PARDUMP" (for particle dump). This file can be written at regular intervals during the simulation, a convenient way to restart a simulation in case of unexpected failure. To restart the model using the PARDUMP file it is only necessary for the file to be present in the root working directory. If the internal time stamp of the file matches the start time of the simulation, the model will initialize the particle count from the file before emitting new particles according to the emission scenario defined in the control file. The format of the PARDUMP file is given below:

Record #1

- INT*4 Number of particles
- INT*4 Number of pollutants
- INT*4 Time of particle dump (YEAR, MONTH, DAY, HOUR, MINUTES)

Record #2 - Loop to record: Number of particles

- REAL*4 Particle pollutant mass (times the number of pollutants)
- REAL*4 Particle LATITUDE, LONGITUDE, HEIGHT, SIGMA-U,SIGMA-V, SIGMA-X
- INT*4 Particle AGE, DISTRIBUTION, POLLUTANT, METEO-GRID,SORT-INDEX

The "Particle" tab of the "Special File Display" menu brings up a Windows based viewer that shows the particle positions over a map background. The display can be zoomed and otherwise adjusted using the left and right mouse buttons in conjunction with the shift and cntl keys. Help is provided on the screen with the left and right side comments corresponding to the respective mouse button. The particle viewer can also be used to overlay satellite images on the particle positions. More information on this is provided "FTP Satellite Data" help menu. The particle position file may be converted to a binary concentration file through the command line utility program par2conc.

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Advanced / Special Topics / Verification Statistics

See the DATEM (Data Archive of Tracer Experiments and Meteorology) web page for more detailed information on each of these tracer experiments. The model verification statistics are presented for the un-averaged data, where each measured and calculated concentration is paired in space and time. Zero-zero pairs are always excluded. Results are also presented after temporally averaging the measured and calculated values over the duration of each experiment. These latter results are paired in space but not time and hence represent the calculation's spatial performance. Statistics presented are the correlation coefficient (R), the fractional bias (FB), the figure-of-merit in space (FMS), the KS parameter representing the departure of the measured and calculated cumulative distributions from each other, and the normalized rank (0 to 4) which is computed from the normalized sum of the previous four parameters. The URL includes links to download the measurement data, meteorological data, statistical programs, and HYSPLIT configuration files.

Unless otherwise noted, all HYSPLIT calculations used the NCEP North American Regional Reanalysis (3 hr; 32 km) meteorological data for the dispersion calculations. The main characteristics of each experimental data set are summarized as follows:

ACURATE - consisted of measuring the Kr 85 air concentrations from emissions of the Savannah River Plant, SC. Twelve and 24 hour average air concentrations were collected for 19 months (March 1982 - September 1983) at 5 locations along the United States east coast from 300 to 1000 km from the plant (Fayetteville, NC to Murray Hill, NJ).

INEL74 - consisted of a little over two months of Kr-85 releases (February 27th to May 5th, 1974) from Idaho and continuous 12 h sampling (February 27th to May 4th, 1974) at 11 locations in a line about 1500 km downwind (Oklahoma City, OK to Minneapolis, MN).

ANATEX - consisted of 66 PerFluorocarbon Tracer (PFT) releases (33 each from two different locations - January 5th to March 26th, 1987) every two and one half days. Air samples were collected for 3 months (January 5th to March 29th, 1987) over 24 h periods at 75 sites covering most of the eastern US and southeastern Canada. PTCH (perfluro-trimethylcyclohexane) was released from Glasgow, Montana (GGW), and PDCH (perfluro-dimethylcyclohexane) and PMCH (perfluro-monomethylcyclohexane) from St. Cloud, Minnesota (STC).

CAPTEX - during September and October of 1983, consisted of six 3 h PFT releases (September 18th to October 29th, 1983), four from Dayton, Ohio and two from Sudbury, Ontario, Canada with samples collected at 84 sites, 300 to 800 km from the source, at 3 h and 6 h averages for about a 48 hour duration after each release (September 18th to October 30th, 1983).

OKC80 - consisted of single release of two different PFT tracers (July 8th, 1980) over a 3 hour duration with samples of 3 hour duration collected at 10 sites 100 km and 35 sites 600 km downwind from the Oklahoma City release point from July 8th to July 11th, 1980.

ETEX - although there were two releases, the primary evaluation data set is from the first release on October 23, 1994 from western France. Three hour duration sampling was conducted in western europe from October 23 through October 27th.

METREX - consisted of 6 hour emissions of perfluorocarbons simulaneously, from two different locations, every 36 hours. The tracer release locations were in suburban Washington, D.C, while 8 hour air samples were colleced at three locations within the urban area. The experiment ran for one full year. In addition monthly air concentration samples were collected at about 60 locations throughout the region.

SRP76 - consisted of continuous emissions of Krypton-85 from the Savannah River Plant near Aiken, SC. About 15 sampling locations were placed around the plant at varying distances (15 - 150 km) and directions. Weekly samples were collected between September 1975 and August 1977. Twice-daily samples were collected over four months (November 1976, February, April, July of 1977).

Verification Statistics Summary

The HYSPLIT model performance by rank for the time mean (spatial correlation) and individual sample paired concentrations for the most recent version of HYSPLIT is given. The rank is computed from the sum of the correlation, fractional bias, figure-of-merit in space, and the Kolmogorov-Smirnov parameter. In addition, all required data are provided with the HYSPLIT distribution to run CAPTEX release #2 and compute the resulting performance statistics through the GUI.

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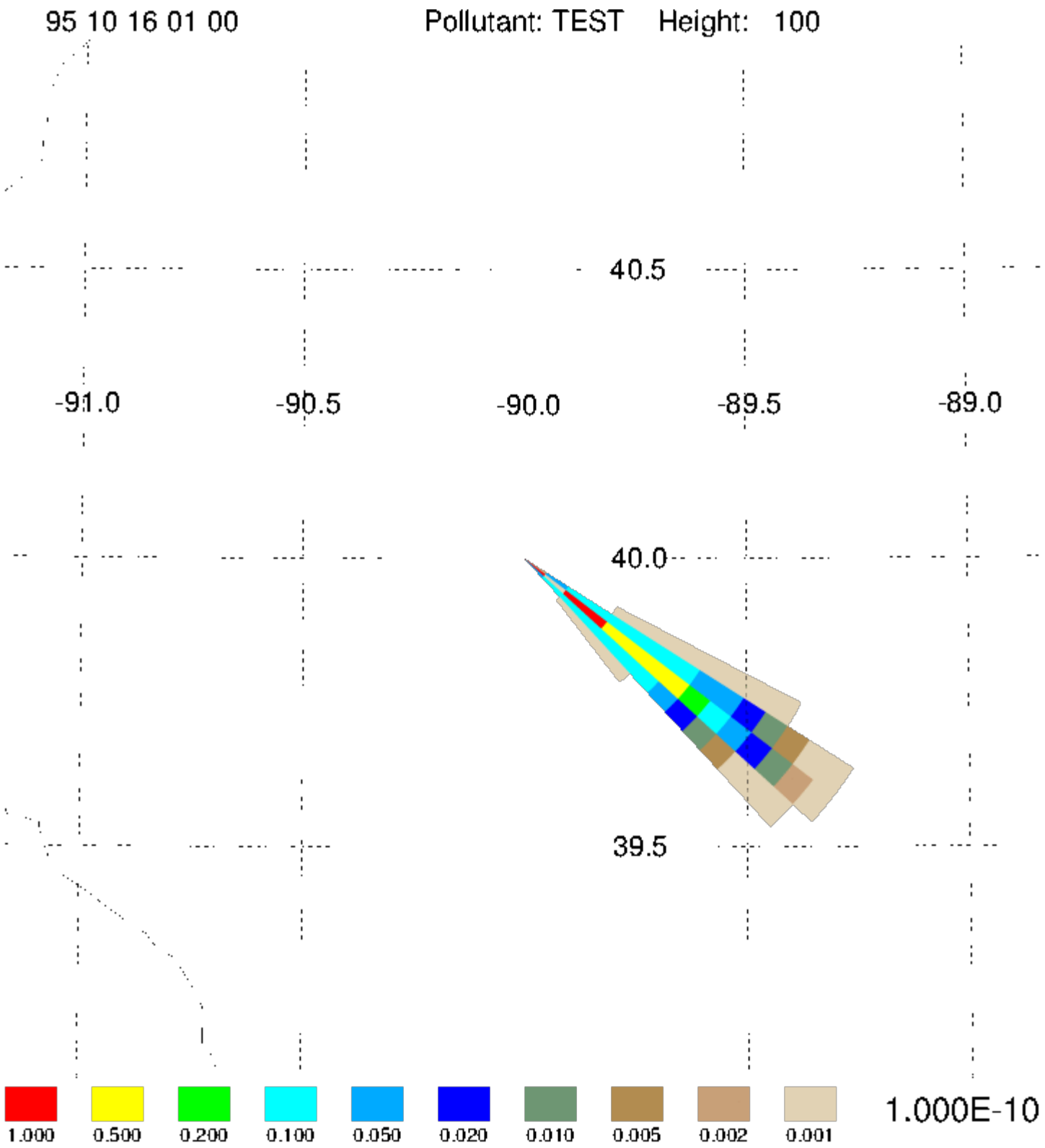
source 40N 80W; start 95101612; 10 kg over 0.1 hrs

year	mn	dy	shr	dur	lat	lon	pg/m3	stn
1995	10	16	0600	0600	39.15	-78.25	0.0	3978
1995	10	16	0600	0600	39.27	-78.07	0.0	4078
1995	10	16	0600	0600	39.38	-77.92	0.0	4077
1995	10	16	0600	0600	38.48	-76.85	0.0	3877
1995	10	16	0600	0600	38.68	-76.64	0.0	3977
1995	10	16	0600	0600	38.92	-76.43	0.0	3976
1995	10	16	0600	0600	37.86	-75.59	0.0	3876
1995	10	16	0600	0600	38.14	-75.40	0.0	3875
1995	10	16	0600	0600	38.40	-75.21	0.0	3975
1995	10	16	1200	0600	39.15	-78.25	308.8	3978
1995	10	16	1200	0600	39.27	-78.07	1605.3	4078
1995	10	16	1200	0600	39.38	-77.92	8.7	4077
1995	10	16	1200	0600	38.48	-76.85	0.0	3877
1995	10	16	1200	0600	38.68	-76.64	0.0	3977
1995	10	16	1200	0600	38.92	-76.43	0.0	3976
1995	10	16	1200	0600	37.86	-75.59	0.0	3876
1995	10	16	1200	0600	38.14	-75.40	0.0	3875
1995	10	16	1200	0600	38.40	-75.21	0.0	3975
1995	10	16	1800	0600	39.15	-78.25	5.8	3978
1995	10	16	1800	0600	39.27	-78.07	121.9	4078
1995	10	16	1800	0600	39.38	-77.92	37.8	4077
1995	10	16	1800	0600	38.48	-76.85	445.0	3877
1995	10	16	1800	0600	38.68	-76.64	614.5	3977
1995	10	16	1800	0600	38.92	-76.43	2.9	3976
1995	10	16	1800	0600	37.86	-75.59	106.8	3876
1995	10	16	1800	0600	38.14	-75.40	411.1	3875
1995	10	16	1800	0600	38.40	-75.21	0.0	3975
1995	10	17	0000	0600	39.15	-78.25	0.0	3978
1995	10	17	0000	0600	39.27	-78.07	0.0	4078
1995	10	17	0000	0600	39.38	-77.92	0.0	4077
1995	10	17	0000	0600	38.48	-76.85	0.0	3877
1995	10	17	0000	0600	38.68	-76.64	2.9	3977
1995	10	17	0000	0600	38.92	-76.43	0.0	3976
1995	10	17	0000	0600	37.86	-75.59	21.9	3876
1995	10	17	0000	0600	38.14	-75.40	224.4	3875
1995	10	17	0000	0600	38.40	-75.21	10.9	3975
1995	10	17	0600	0600	39.15	-78.25	0.0	3978
1995	10	17	0600	0600	39.27	-78.07	0.0	4078
1995	10	17	0600	0600	39.38	-77.92	0.0	4077
1995	10	17	0600	0600	38.48	-76.85	0.0	3877
1995	10	17	0600	0600	38.68	-76.64	0.0	3977
1995	10	17	0600	0600	38.92	-76.43	0.0	3976
1995	10	17	0600	0600	37.86	-75.59	0.0	3876
1995	10	17	0600	0600	38.14	-75.40	0.0	3875
1995	10	17	0600	0600	38.40	-75.21	0.0	3975

95 10 16 06
1
40.0 -80.0 10.0
30
0
10000.0
1
./
oct1618.BIN
1
TEST
100.0
0.1
00 00 00 06 00
1
38.0 -76.0
0.10 0.10
15.0 25.0
./
cdump
1
100
00 00 00 00 00
00 00 00 00 00
00 06 00
1
0.0 0.0 0.0
0.0 0.0 0.0 0.0 0.0
0.0 0.0 0.0
0.0
0.0

```
&SETUP
tratio = 0.75,
initd = 0,
kpuff = 0,
khmax = 9999,
numpar = 5000,
qcycle = 0.0,
efile = '',
tkerd = 0.18,
tkern = 0.18,
ninit = 1,
ndump = 0,
ncycl = 0,
pinpf = 'PARINIT',
poutf = 'PARDUMP',
mgmin = 10,
kmsl = 0,
maxpar = 5000,
cpack = 1,
cmass = 0,
dxf = 1.0,
dyf = 1.0,
dzf = 0.01,
ichem = 0,
/
```


95 10 16 01 00
Pollutant: TEST Height: 100
40.5
-91.0
-90.5
-90.0
-89.5
-89.0
40.0
39.5
1.000
0.500
0.200
0.100
0.050
0.020
0.010
0.005
0.002
0.001
1.000E-10