HYSPLIT Tutorial Table of Contents

Last Revised 9 June 2011	**Index**	Next

Follow the HYSPLIT tutorial sections in the sequence shown below, working through each example. GUI menu screen images will be shown as needed. However, not all of the GUI options will be exercised with each example. Additional menu options will be introduced as needed. Some menus have a zoom button to show the required data entry values in a larger type. The tutorial is focused toward running HYSPLIT on a Windows PC. Although the operation of the GUI is similar on Linux and Mac platforms, not all of the GUI functions are available on all systems. If you are going through this tutorial from the CD, some of the examples will go faster if the contents of the CD are first copied to your hard drive (c:\Tutorial).

6. The Basic Air Concentration Simulation

7. Air Concentration Parameter Sensitivity

8. Air Concentration Uncertainty

9. Pollutant transformations and deposition

10. Source attribution methods

11. Alternate display options

1. [Enhanced labels](#)
2. [Google Earth](#)
3. [Shapefiles and ArcExplorer](#)
4. [Dynamic sampling](#)

12. Customized concentration simulations

1. [Dust storms](#)
2. [Volcanic Eruptions](#)
3. [Restarting the model from PARDUMP](#)
4. [Adjusting predictions using satellite data](#)

Tutorial Topic Index

A

[Adjoint, dispersion](#)
[Advection, Predictor-corrector](#)
[Aircraft sampling, CAPTEX](#)
[Air density conversions](#)
[AirNow PM10 measurments](#)
[Animation, example](#)
[Animation, CAPTEX](#)
[Aniosotropy, factor for TKE](#)
[ArcExplorer, example](#)
[ArcExplorer, install](#)
[Archived meteorology](#)

B

[Backward or upwind dispersion](#)
[Backward integration to find source](#)
[Backward trajectory reversibility](#)
[Batch file for concplot](#)
[Batch file scripting for trajectories](#)
[Beljaars-Holtslag](#)
[Box plot for ensembles](#)
[Bulk Richardson number](#)

C

[CAPTEX animation](#)
[CAPTEX configuration](#)
[CAPTEX overview](#)
[Climatology, trajectory](#)
[Cluster spatial variance](#)
[Clustering, trajectory](#)
[Concentration, binary to ASCII](#)
[Concentration, contouring](#)
[Concentration, convert to DATEM](#)
[Concentration, file listing](#)
[Concentration, grid display/a>](#)
[Concentration, set grid size](#)
[Conversion rates: chemrate.txt](#)

D

E

F

G

H

I

NARR - North American Regional Reanalysis
NetCDF format
NOMADS data server

P

PARDUMP, particle position file
PARINIT and PARDUMP files for model restarts
Particle (3D) calculation
Particle number release rate
Particle position adjustments
Particle position display
Particle size distribution
Physics ensemble
Plume arrival time graphic
PMCH tracer for CAPTEX
Pollutant menu, basic setting emissions
Pollutant transformation options
Postscript conversion to other formats
Profile, meteorology data
Puff growth, empirical
Puff growth, equations
Puff release mode, set puff or particle
Puff size, computing concentration
Puff splitting

Q

Quick start, concentration
Quick start, trajectory

R

Radioactive particles
Rainout for in-cloud wet deposition
Reanalysis data, download example
Reanalysis data, download menu
Receptor view, matrix
Release height variations
Residence time, trajectory
Restarting from a PARDUMP file
Reversible plume calculation

S

Satellite aerosol thickness
Scavenging ratio for below-cloud wet deposition
Sensible heat flux for stability
Shapefiles for GIS applications

Installing HYSPLIT on a Windows PC

HOME

The HYSPLIT installation file contains all the executables, documentation, and some test meteorological data. The graphical user interface requires Tcl/Tk, Ghostscript utilities, and ImageMagick. Optional programs such as Google Earth and ArcExplorer may be installed if needed.

1. Tcl/Tk Graphical User Interface

   The Tcl/Tk script interpreter is required to run the HYSPLIT GUI. Further, various computations can be automated through the use of Tcl scripts. Install the software to the suggested default directory.

   - Install Tcl/Tk 8.5.8
   - Tcl/Tk Home Page

2. Postscript Converter

   The HYSPLIT trajectory and concentration display programs create high resolution publication quality graphics files in Postscript format. These can be printed directly on any Postscript printer, viewed on the PC display monitor, or printed on any non-Postscript printer if Ghostscript has been installed. Install the software to the suggested default directories.

   - Install Ghostscript 8.63
   - Ghostscript Home Page

3. Postscript Viewer

   Ghostscript only provides for command line options. To more easily view and print Postscript files in a Windows environment, install Ghostview to the suggested default directories.

   - Install Ghostview 4.9
   - Ghostscript Home Page

4. ImageMagick File Converter

   The GUI has a built in link that permits the conversion of the Postscript graphics output file to most other graphical formats. This capability is enabled through the installation of ImageMagick, which requires the prior installation of Ghostscript to be able to read the Postscript files. Install the software to the suggested default directory.

   - Install ImageMagick 6.6.1
   - ImageMagick Home Page

5. Windows HYSPLIT Installation

The HYSPLIT PC installation simply requires running the self-installing executable. You will be prompted for a default installation directory, the suggested default is c:\hysplit4. If installation to another directory name is required, avoid directories with embedded spaces because many programs in the HYSPLIT system use the space as a file name delimiter. A desktop icon and quick-start drop down menu will be installed. If you do not want to install on top of an existing version, it is best to rename the old \hysplit4 directory before proceeding. Note that the registered version is identical to the trial version in all respects except that the dispersion model (for concentration predictions) cannot be run using forecast data with the trial version. Install the 64-bit version if you are expecting to read and write files larger than 2 GB.

- [CD-ROM 32-bit registered version](#)
- [CD-ROM 64-bit registered version](#)
- [WEB download trial version](#)
- [WEB download registered version](#)

6. *Optional* ArcExplorer GIS Viewer

The GUI includes an option to convert various graphical products to the ESRI shapefile format. These shapefiles can then be imported and viewed in ArcExplorer. It is then possible to overlay trajectories, meteorological data, and concentration contours, all on the same map background using ESRI GIS software. Note that administrator access is usually required to install this program. HYSPLIT also permits the use of shapefiles (.shp only) in defining the map background layers in the existing trajectory and concentration plotting programs.

- [ArcExplorer Home Page](#)

7. *Optional* Google Earth Viewer

HYSPLIT trajectory and concentration output files can be converted to a format that is compatible for display with Google Earth. The conversion results in zip file (.kmz) that contains all the files required by Google Earth. A double-click on the "kmz" file will open Google Earth and it will automatically zoom to the display. Google Earth gives the best results for computers connected to the Internet, permitting access to its on-line geographic database.

- [Google Earth Download Page](#)

8. *Optional* Tutorial Tips

There are two things that you can do to configure Windows to make it a little easier to follow along with some of the tutorial examples. One is to put a short-cut link to Notepad on the desktop so that files without text extensions can easily be opened and viewed. Open the Windows *Start Menu*, open *All Programs, Accessories*, and find and right-click on Notepad, and select *Send to, Desktop (create shortcut)*.

The second, if *File Explorer* is not already configured to view all file extensions, open the

[File Menu](#) in the Control Panel, and uncheck the box for *Hide extensions for known file types*.

Installing HYSPLIT on a Mac

[HOME](#)

The HYSPLIT Mac installation is similar to the PC except that the Mac OS supports the native display of Postscript files, therefore Ghostscript is not required. This version will only install under OSX 10.6.

1. Tcl/Tk Graphical User Interface

   Go to the Tcl/Tk web site to download the most recent Mac version.

   - [Tcl/Tk Home Page](#)

2. Postscript Converter

   On Mac systems Ghostscript is not required and therefore when using Preview, export the file to any non-Adobe format, which then can be converted to any other format using ImageMagick.

3. Postscript Viewer

   Not required. Use *Preview*, however, if there are too many Postscript frames in a file, *Preview* may have trouble converting the output to a viewable PDF. In this case you need to reduce the number of output frames in one file.

4. ImageMagick File Converter

   Go to the ImageMagick web site to download the most recent Mac version.

   - [ImageMagick Home Page](#)

5. Mac OSX 10.6 HYSPLIT Installation

   Download and open the installation package and HYSPLIT will be automatically installed in its own directory (Hysplit4) in your $HOME directory (user install) or in a system directory (root install). The Mac version was compiled under OSX 10.6 using the INTEL compiler. This version only installs and works under OSX 10.6.

   - [User directory install (CD-ROM only)](#)
   - [Root directory install (CD-ROM only)](#)
   - [WEB download registered version](#)
   - WEB download trial version not available

6. *Optional* ArcExplorer GIS Viewer

   Go to the ESRI web site to download the most recent Mac version.

- ○ [ESRI Home Page](#)
- ○ [ArcExplorer for MAC](#)

7. *Optional* Google Earth Viewer

   Go to the Google Earth web site to download the most recent Mac version.

   - ○ [Google Earth Download Page](#)

---

8. Starting the first time

   Once installed, open a terminal window or X-window and change directory to hysplit4/working. Then just execute the softlink *hysplit4.tcl* and the GUI should open if Tcl/Tk has been installed. The model should run in either terminal window. However, certain applications will only work from the X-terminal window. Once installed, insure that the X-directory location (usually /usr/X11/bin) in file *default_exec* points to the location of *xterm*, which can be determined from the command **which xterm**.

Graphical User Interface (GUI) Operation

The HYSPLIT package for computing trajectories and plume dispersion consists of a series of command line based executable programs that are integrated through a number of different scripts, all invoked through a Graphical User Interface (GUI). An overview of the GUI follows:

1. Once the installation is complete, that is the HYSPLIT code and all the auxiliary software are installed, then click the desktop icon **Run Hysplit** and a startup window will be shown. Select the **menu** button to proceed.

2. The main menu consists of four main tabs: *meteorology, trajectory, concentration,* and *advanced*. There are multiple sub-tabs under each main tab which are all shown in the open position in this document for illustration. Individual sub-menus will be discussed as needed.

3. The *meteorology* tab provides for different ways to access meteorological data files and load them into the local computer to perform trajectory or dispersion calculations. For the purposes of this tutorial, all required meteorological data files are provided with the HYSPLIT installation or in the directories of the tutorial CD-ROM.

4. The *trajectory* tab opens access to sub-menus to setup the trajectory simulation, run the calculation, and then display the results. A trajectory is just the integration of the position vector through a wind field that varies in space and time. The point is assumed to be passively transported by the wind.

5. The *concentration* tab has similar sub-menus to the trajectory calculation. The primary difference between the two is that the trajectory calculation only follows one point transported by the mean wind, while the concentration calculation may follow thousands of trajectories at the same time, the motion of each being composed of a mean (trajectory) and turbulent (dispersive) component. In addition, each "particle" trajectory associated with the concentration calculation has some mass assigned to it which means that the trajectory density can be used to compute an air concentration.

6. The *advanced* tab is used to set additional model parameters that can be used to provide further control or customization to either the trajectory or concentration calculation. The information is written to a namelist file, always called *SETUP.CFG*. A namelist file contains the value of various program variables defined by their internal code name. Some other miscellaneous features can also be found under this tab.

7. The following installed sub-directories will be found under **\hysplit4** ...

   - cluster - The default location for clustering trajectories.

- data2arl - The source code for programs not already available through the GUI that can be used to convert meteorological data files from models such as MM5 and WRF-ARW to the HYSPLIT compatible format.

- datem - Contains sample HYSPLIT input files for various experiments available from the DATEM repository and experimental data for CAPTEX

- document - Contains the technical manual, user's guide (pdf), and various README files.

- exec - Contains all the HYSPLIT executables, which may be for either 32-bit or 64-bit operating systems depending upon which file was downloaded.

- graphics - This directory contains the default ASCII map background file (*arlmap*) that is used by all the HYSPLIT graphical display programs. Other more detailed ASCII and binary shapefile map background files are also available in this directory.

- guicode - This directory contains all the TCL scripts required for the GUI. The root script is **hysplit4.tcl** which is also the target of the desktop icon.

- html - This directory contains all the context sensitive help files that are individually invoked from the GUI menus from the *Help* button. The **index.htm** and all other help pages can be opened in any browser.

- testing - This directory contains the **xrun.bat** batch file which can be used to test various model simulations. The script can be used as a template to develop other customized scripts.

- working - The working directory is the root directory for running HYSPLIT. By default the model looks for input files here and writes all the output files to this directory unless other paths are set in the simulation setup.

8. The basic model operation involves three steps. First *Setup Run* configures the simulation details and saves the information to a file called *default_traj* or *default_conc*. Second, when *Model Run* is invoked, the *default_????* file is copied to a file named *CONTROL* which is then read by the model executable. Third, the *Display* menu will call a program to read the model output file and will create a Postscript graphics file. These are all written to the working directory.

In subsequent tutorial pages these menus will be explored in considerably more detail.

Test Trajectory Calculation

From the top bar of the main menu select the *Trajectory / Quick Start / Run Example* menu tabs. The *Run Example* tab initiates a windows only program that displays a source selection menu. On non-windows system, the calculation just proceeds without any prompts. A left-click resets the source location, while a right-click closes the selection window. For the purposes of this test, just **right-click** to accept the default location, which then results in window termination message. Select **Yes** and then ...

1. A control file is created in the *working* directory with the starting time, location, meteorological data file name, and trajectory endpoints output file name.

2. The trajectory model is then run which creates an ASCII output file with the endpoint locations.

3. A trajectory plotting program is run which reads the endpoints file and creates the Postscript graphics file.

4. The Postscript graphic is displayed using Ghostview.

The display of the three-trajectory graphic means that all the HYSPLIT components have been correctly installed. In subsequent simulations through the GUI, the *Quick Start* menu would normally not be used because it automatically combines three individual steps: configuring the model simulation, running the simulation, and converting the output to a graphical format. These components will be explored in more detail individually. Many of the features available through the GUI apply to trajectory as well as air concentration calculations. After testing the air concentration simulation in the next section, the trajectory calculations will be explored in more detail.

Test Air Concentration Calculation

From the top bar of the main menu select the *Concentration / Quick Start / Run Example* menu tabs. The *Run Example* tab initiates a windows only program that displays a source selection menu. A left-click resets the source location, while a right-click closes the selection window. For the purposes of this test, just **right-click** to accept the default location, which then results in window termination message. Select **Yes** and then ...

1. A control file is created which contains the starting time, location, name of the meteorological data file, details of the pollutant emission, concentration grid, and output file name.

2. The concentration model is then run which creates a binary gridded concentration output file.

3. A concentration plotting program is run which reads the binary air concentration file to create the Postscript graphics file.

4. The final plume Postscript graphic is displayed using Ghostview.

The display of the air concentration plume graphic means that all the HYSPLIT components have been correctly installed. In the unlikely event that the installation failed and the graphic was not displayed, please contact the HYSPLIT help desk for further information.

Because a plume simulation may consist of thousands of individual trajectories but with an additional turbulent component to the motion to account for atmospheric dispersion, the trajectory calculation will be explored next in more detail.

Using CAPTEX data in this tutorial

HOME

In most of the following sections the trajectory and air concentration examples will be based on a real event where the pollutant emission rate is known and air concentrations have been measured at numerous locations. The tutorial focus will be on the second release of the Cross Appalachian Tracer Experiment. CAPTEX (Ferber et al., 1986) consisted of six 3 h perflurocarbon (C7F14) tracer releases (September 18th to October 29th, 1983), four from Dayton, Ohio and two from Sudbury, Ontario, Canada. Samples were collected at 84 sites, 300 to 800 km from the source, over 3 h and 6 h averaging periods, for about a 48 hour duration after each release.

The primary meteorological data used in most calculations will be the North American Regional Reanalysis (NARR) available at 32 km horizontal resolution every three hours. The meteorological data for this experiment are provided as part of the HYSPLIT distribution. The Gridded Binary (GRIB) files for the NARR for other time periods can be downloaded from the NOMADS web page. When selecting data to download, all variables and cycles should be obtained. Converting meteorological data from GRIB to a format HYSPLIT can process will be discussed in later sections.

To aid in the interpretation of the various modeling techniques that will be introduced in the tutorial, you can view the HYSPLIT simulation for CAPTEX release number 2. The animation shows the sequence of model calculated three hour average concentration patterns (in units of pg/m3 - pico grams per cubic meter) superimposed over the measured air concentrations averaged over the three day duration of the experimental sampling for release #2. In other examples the individual 3- or 6- hourly average concentrations will be used for the analysis.

Meteorological Data for the Tutorial

Most of the example calculations in the following tutorial sections use one or more of the five meteorological data files provided in the **\Tutorial\captex** directory on the CD (or your internal disk). These files contain meteorological data (u,v component wind speeds, temperature, and several other variables) on a regular grid at multiple levels and time periods. These files are already in a format that can be read by HYSPLIT directly. Converting data in other formats for use by HYSPLIT will be discussed in the next section. There are several programs available through the GUI that can be used to examine the contents of the meteorological data files.

1. To start, select the *Meteorology / Display Data / Grid Domain* menu tab to open the grid domain menu and set the file name to each of the meteorological files to see the spatial domain covered:

   - North American Regional Reanalysis captex2_narr.bin
   - Weather Research Forecast Model captex2_wrf27.bin
   - NCAR Global Reanalysis Extract-1 captex2_gblr.bin
   - NCAR Global Reanalysis Extract-2 RP198309.gbl
   - ECMWF ERA-40 Reanalysis captex2_era40.bin

   Note that the menu settings default to show latitude-longitude lines at 5-degree intervals and only every other data grid point. The NARR file seems tilted because the native data grid is on a Lambert Conformal projection where the Northeast U.S. extract shown is toward the edge of the projection. The data on the two global files are on a regular latitude-longitude grid.

2. To get more detailed information about the contents of any HYSPLIT meteorological data file, select the *Meteorology / Display Data / Check File* menu tab and select the data file in the check file menu which will then open a scroll box with more detailed information which is summarized below for each of the files. Do not try to open the link to the binary data files with the browser or any editor.

   - **captex2_narr.bin**
   - Time period: 25th 15Z -> 28th 15Z
   - Number of grid points: 50 x 52
   - 18 levels: 1000 to 500 hPa
   - Resolution: *32 km, 3 hr (180 min)*

   - **captex2_wrf27.bin**
   - Time period: 25th 12Z -> 28th 06Z
   - Number of grid points: 48 x 43
   - 25 levels: 0.998 to 0.310 sigma
   - Resolution: *27 km, 1 hr (60 min)*

   - **captex2_era40.bin**

- Time period: 25th 12Z -> 28th 12Z
- Number of grid points: 100 x 100
- 14 levels: 1000 to 100 hPa
- Resolution: *100 km (interpolated from 2.5 deg), 6 hr (360 min)*

- **captex2_gblr.bin**
- Time period: 25th 12Z -> 29th 00Z
- Number of grid points: 39 x 25
- 15 levels: 1000 to 50 hPa
- Resolution: *2.5 deg, 6 hr (360 min)*

- **RP198309.gbl**
- Time period: *1st 00Z -> 30th 18Z*
- Number of grid points: 39 x 25
- 15 levels: 1000 -> 50 hPa
- Resolution: 2.5 deg, 6 hr (360 min)

In summary, the WRF-ARW simulation (boundary conditions derived from NARR) provides the finest spatial and temporal resolution. The three global reanalysis files are just extracts for North America, two covering just the period of the experiment, while the third one covers the entire month. The NARR will be used for most of the examples.

Obtaining Meteorological Data using FTP

Although not needed for this tutorial, meteorological data files already formatted (ARL format) for use by HYSPLIT are available from several different FTP servers. These archives can be accessed directly using any FTP client or through the GUI from the *Meteorology / ARL Data FTP tab*. This menu provides access to **Forecast** data, a 24- or 48-h series of **Appended** forecasts (quasi-archive), an **Archive** of a variety of different regional and global data files, a special archive of the NCAR/NCEP global **Reanalysis**, and an option to **set the server** for FTP.

1. As an example of how this process works we can download one of the files that will be used later in the tutorial: the global reanalysis data for September 1983. Open the Reanalysis menu and set the year and month. The file name is automatically generated. *Get Data File* starts the transfer process which opens a progress bar in downloading the 119 Mb file. The downloaded file is much larger than the same named file in the *\Tutoria\captex* because it is global rather than a regional extract. If you are using a slower wireless network you may not want to download this file or if you are doing this example in a room with 50 other people, do not all click on download at the same time!

2. In the event of connectivity issues, you can change the FTP server location through the GUI from the Set Server menu selecting from one of three preset options: *primary, alternate, or backup.* The backup server can only access forecast or appended data files. The servers may have different directory structures.

3. As noted earlier, data files can also be obtained through other FTP clients or even the web browser. For instance, open the browser to the URL ftp://arlftp.arlhq.noaa.gov/pub/archives/reanalysis to view the files in the directory containing RP198309.gbl. In contrast, the directory structure at ftp://ftpprd.ncep.noaa.gov/pub/data/nccf/com/hysplit/prod is linked with the current date and only forecast data for today and yesterday are available for downloading.

One important consideration when downloading meteorological data files is that they are a composite of ASCII and binary fields, which means that you should not let the FTP client automatically determine the transfer mode, but always insure that it is set to **binary**.

Converting Meteorological Data for HYSPLIT

Meteorological data files are available from a variety of sources. However, most will need to be reformatted for use by HYSPLIT. The *Meteorology / Convert to ARL* menu tab provides several options that will be discussed only briefly below. These data can be in Gridded Binary Format (only GRIB-1 is supported), or Network Common Data Form (NetCDF), CMAQ-IOAPI, or custom binary formats, such as from NCAR's MM5. The HYSPLIT data conversion is necessary because each meteorological model may contain different variable names, data organization, horizontal grid projection, or vertical coordinate systems. Keeping the meteorological pre-processing external to HYSPLIT provides more stability to the base code structure. Note that some of the data conversion programs are only available for UNIX systems.

1. The *Convert to ARL* tab contains the following sub-menus:

    - WRF-ARW: The Advanced Weather Research model output files are in NetCDF (UNIX only).

    - NARR archive: The North America Regional Reanalysis is available in GRIB-1 format (PC and UNIX).

    - Global lat-lon: Regular latitude-longitude GRIB-1 files from NOAA and ECMWF global models can be processed from this menu (PC and UNIX).

    - ERA-40: GRIB-1 files from the ECMWF 40 year global or Interim reanalysis projects can be processed through this menu (PC and UNIX).

    - MM5V3: Version 5 of NCAR's mesoscale model can be converted from their binary format (PC and UNIX).

    - MCIP IOAPI: Meteorological files for the CMAQ model are available in this format, which is a variation of NetCDF (UNIX only).

    - User entered: This menu permits the user to manually enter one observation point but for several time periods to create a spatially homogeneous custom meteorological file (PC and UNIX).

2. Except for the *User Entered* option, the various data conversion options will not be discussed in any more detail because most require either the download of large data files or running your own meteorological model. Both of which are beyond the scope of this tutorial. However, the user data entry option will create a 3-dimensional gridded file with a uniform wind field (in height and space) that can be used to run HYSPLIT, or combined with another meteorological file to complete a simulation.

3. First select the [user entered](#) menu tab to open the menu to [set the grid center](#) which should be **40.7N 83.5W**. The grid center is set slightly northeast of the release location because of the wind direction. If the *stndata.txt* file does not already exist (it doesn't), then select **Create File**.

4. The meteorology [enter data](#) menu provides one line for each time period. Enter the information as shown at 6 hour intervals (25 12Z; 25 18Z; 26 00Z; 26 06Z), changing only the time. Set the wind direction and speed to **225** at **6.0** m/s and stability category **3** for all times. Then **Save Data to File** and **Run Convert** which will then create the binary meteorological file *stndata.bin* in the *\working* directory for use by HYSPLIT.

5. Open the [profile menu](#) and select the *stndata.bin* file. No other changes are necessary to see the [sounding](#) at the first time period. The other time periods will all be the same. The wind direction and speed have been converted to vector components at all levels and velocity variances correspond to values that will give plume growth similar to stability category 3 (C) at all levels below the mixed layer depth.

HYSPLIT requires meteorological data on an evenly spaced grid (latitude-longitude or conformal projection) at multiple heights and time periods over the duration of the simulation. These data can be obtained from various sources or converted to the proper format. The manually created data file from this section will be used for a more complex simulation later in the tutorial.

The Basic Trajectory Calculation

In the previous trajectory calculation to test the model installation, after selecting the source location, the sequence of simulation configuration, model execution, and trajectory display, was entirely automatic, with each step hidden within the GUI script. In all subsequent menus, each step will be addressed in sequence.

1. To start a new trajectory calculation, from the top bar of the main menu select *Trajectory / Setup Run* which will open a menu with multiple entry options.

2. The Trajectory setup menu is used to enter information, such as the starting time on the first line. Enter **83 09 25 17** to correspond with the time of the start of the tracer release (1700 UTC 25 September 1983).

3. On the second line change the number of starting locations to **1** and then press the *Setup starting locations* button to open a new window where you should now enter **39.90 -84.22 10.0**, which corresponds to the latitude and longitude of the tracer release location at 39.9N, 84.22W, at a starting height of 10 meters above ground level.

4. The other options on the setup menu will be discussed in more detail later, but for now enter total run time of **68** hours (the trajectory duration). The vertical motion method should be using the **data** field from the meteorological input file, the name of the output file with the trajectory end point latitude-longitudes should be called **tdump**, and after pressing the **clear** button add the meteorological data file **captex2_narr.bin** in the captex tutorial directory.

5. After all the changes have been made to the setup menu, press the **Save** button which copies all the information to a special file called *default_traj* and then closes the menu. Now the model simulation can be started from the *Trajectory / Run model* menu tab. This button causes two actions. First, the trajectory setup information is copied from *default_traj* to a file called *CONTROL*, which is the input name required by the HYSPLIT trajectory model executable (*hyts_std.exe*). Second, the GUI then launches the model.

6. As the model is running a progress message percent complete is displayed. Do not try to *Exit* this window until the calculation is complete or a beep is heard indicating a premature stop.

7. By default all calculations take place within the *\hysplit4\working* directory. The calculation created the trajectory endpoints file *tdump*. To turn this ASCII file into a graphic, open the *Trajectory / Display / Trajectory* menu.

8. This multi-entry *Trajectory Display* menu provides for several options, which will be discussed in more detail later as needed. For now, no changes are required and the **tdump** input file will be converted to a Postscript output file called **trajplot.ps** using the default map background file.

9. Pressing the **Execute Display** menu button will run the *trajplot* program and then open the Ghostscript viewer to display the [trajectory graphic](#).

10. If your simulation result matched the previous picture, then you should save the information contained in the [Trajectory setup](#) menu by selecting the **Save as** button from the trajectory setup menu and entering a file name such as [traj_base_control.txt](#). The default directory for these *Save as* actions is in the working directory. In the future, this information can be loaded using the **Retrieve** menu to reload the simulation information into the GUI. An example of this file can also be found in the tutorial [files](#) directory.

In summary, the basic trajectory calculation consists of three steps: setup, run, and display. Note how the low-level trajectory (started at 10 m AGL) follows the southern shoreline of Lake Ontario and Lake Erie. From the sampling data we already know the tracer from this short 3 hour release was spread all over New York and Pennsylvania, and even into southern Canada, suggesting that a single trajectory is insufficient to represent this pollutant dispersion episode. In subsequent sections, we will explore the different applications of the trajectory calculation as well has how multiple particle trajectories can be used to more accurately simulate pollutant dispersion.

The Trajectory Equation

The advection of a particle or puff is computed from the average of the three-dimensional velocity vectors at the initial-position P(t) and the first-guess position P'(t+Δt). The velocity vectors are linearly interpolated in both space and time. The first guess position is

- P'(t+Δt) = P(t) + V(P,t) Δt

and the final position is

- P(t+Δt) = P(t) + 0.5 [V(P,t) + V(P',t+Δt)] Δt.

The integration time step (Δt) can vary during the simulation. It is computed from the requirement that the advection distance per time-step should be less than the grid spacing. The maximum transport velocity is determined from the maximum transport speed during the previous hour. Time steps can vary from 1 minute to 1 hour and are computed from the relation,

- U_{max}(grid-units min^{-1}) Δt (min) < 0.75 (grid-units).

The integration method is very common (e.g. Kreyszig, 1968) and has been used for trajectory analysis (Petterssen, 1940) for quite some time. Higher order integration methods will not yield greater precision because the data observations are linearly interpolated from the grid to the integration point. Trajectories are terminated if they exit the meteorological data grid, but advection continues along the surface if trajectories intersect the ground.

Trajectories in the Mixed Layer

From the basic trajectory calculation shown in the previous section, it was clear that although the trajectory starting height was similar to the tracer release height, the low-level trajectory did not correspond to the tracer footprint or was representative of the levels that the tracer was transported. We can use several tools through the GUI to evaluate the best transport level.

1. The first step is to determine the mixing depth at the time and location of the tracer release. Go to the main menu and select the *Meteorology / Display Data / Text Profile* menu tab. This will call a program to read the values from the meteorological data file at that point and time and write the information to a text file.

2. The *Text profile* tab opens a menu where you need to select the appropriate meteorological data file **captex2_narr.bin** and set latitude and longitude of the release point: **39.90 -84.22**. Setting the correct time can be a little confusing using the two radio-buttons: **offset** and **increment**. This particular meteorology file contains data every 3 hours, so we could just select an increment of 3 hours and the contents of the entire file at that location will be extracted. However, we already know that the file starts at 15 UTC and the tracer release started at 17 UTC. Therefore by setting the **offset=3** hours and the **increment=0**, only one time period, 18 UTC will be extracted from the file.

3. The profile results will be shown in its own window and also written to the file *profile.txt*. In addition to the data contents at the selected grid point, the file also contains information about the first and last time periods. At this point all we need to know is the Height of the Planetary Boundary Layer (**HPBL**) which is shown to be **1756** meters. Information about each of the variables will be discussed later as needed. More information about these variables can be found in the *Users Guide* (see hysplit documents directory).

4. With a mixed layer depth of 1756 m AGL, it would be reasonable to bracket the transport layer with trajectories starting at 10, 750, and 1500 m AGL. Open the *Trajectory / Setup menu* and enter **3** for the *Number of Starting Locations* prior to pressing the **Setup Starting Locations** button. Then replace the 10 meter height in the 2nd and 3rd lines with **750** and **1500**. If the 2nd and 3rd lines do not have the same starting latitude and longitude, these also need to be changed to match the 1st entry line. Select **OK** and then **Save** to close the *Trajectory Setup* menu.

5. As before, in the previous trajectory example, run the model, then open the trajectory display menu which will create a graphic showing the three trajectories, which provide a much better representation of surface concentration distribution. However, the more southern measured concentrations still cannot be explained through these trajectories.

6. Before proceeding further with the case analysis, there is another way to let the model automatically select a height within the boundary layer. Open the *Advanced / Configuration Setup / Trajectory* menu. This menu creates a *namelist* file called *SETUP.CFG* which contains a list of internal HYSPLIT variable names and their default values. This menu

permits changes to those defaults.

7. Select submenu (2) to define MSL/AGL units and then select the fraction of the mixed layer radio-button. This option changes the interpretation of the starting heights defined in the trajectory setup menu from heights above ground level (the default), heights above mean-sea-level, or in this case to a fraction of the boundary layer height. In this situation, the absolute height is computed internally and may change day-to-day.

8. After saving each of the open configuration menus go back to the trajectory setup menu, replace the **3** locations with **1** and then open the starting locations menu and replace the height field with **0.5**. This will cause the trajectory to start at a height of one half the mixed layer depth.

9. After saving, proceed to the *Trajectory / Run Model* menu, where this time a new menu will appear to confirm that the model should be run using the *SETUP.CFG* namelist file. Select the Run using SETUP file button to continue with the calculation. The other button options exist in case the SETUP file was left over from a previous simulation and may not be needed. After the run completes, open the trajectory display menu where this 0.5Z simulation result is very similar to the previous 750 m trajectory.

10. As an end-note, go back to the *Advanced / Configuration / Trajectory* menu and save the configuration using the name traj_mixd_setup.txt.

Most of the samplers that detected tracer were to the right of the low-level trajectory. Because wind directions generally veer with height, this result is consistent with the idea that the bulk of the tracer was transported at higher levels above ground but still within the boundary layer.

Sources of Trajectory Error

In this section we will explore the possible causes of trajectory error. In the first calculation a forward trajectory will be compared to a backward trajectory started at the termination point of the forward trajectory. In the second part, the same calculation will be made using two different meteorological data files.

1. Start by retrieving the information into the trajectory setup menu from the previously save control file **traj_base_control.txt**, but change the starting height from 10 m to **750 m**, also rename the output file from tdump to **tdump_fwrd**, then save the changes and run the model. Select the **Delete file then Run** if the existing *SETUP.CFG* file prompt appears. If your trajectory matches the trajectory shown, save the control file as traj_fwrd_control.txt.

2. Now we need to setup a new trajectory calculation to start from the last point of the previous trajectory. To do this you need to open the output file tdump_fwrd and note the information on the last record in the file that indicates the time **83 9 28 13** and location **37.479 -75.202 343.4** of the last point. Then open the trajectory setup menu and enter that information as the start time and location. Two additional changes are required: select the **back** radio-button, which changes the run duration to a **negative** 68 hours. Also change the output file from tdump_fwrd to **tdump_back**.

3. If your result matches the trajectory trajectory shown, save the control file as traj_back_control.txt. Note the title label differences between the two calculations, the location of the source points, and the direction of time along the abcissa of the vertical trajectory projection.

4. The two trajectories look very similar. To compare them directly, we can use the trajectory display program to superimpose the forward and backward trajectories. Open the trajectory display menu and in the first entry line of *input endpoints* enter the two file names using a plus symbol (without spaces) between the two file names: **tdump_back+tdump_fwrd**. Select **Meters-agl** as the vertical coordinate in the display menu to see the results in height rather than pressure units.

5. The superimposed trajectories are so close that they almost appear to be identical. We can also examine the end of the backward trajectory output file to determine exact ending position **39.893 -84.209 743.9** and comparing it with the original starting location **39.90 -84.22 750.0** suggesting that the computational integration error is about 1 km horizontally and 6 m vertically after a 136 hour integration time.

6. Computational error is not a significant source of trajectory error. However, data resolution may be important. We can examine the effect of meteorological data resolution by re-running the forward calculation from 750 m but using the global reanalysis (2.5 deg every 6 h) instead of the NARR (32 km every 3 h).

7. Open the trajectory setup menu and retrieve **traj_fwrd_control.txt**. To change the meteorology file, first press the **clear** button and then **Add meteorology files** and select **captex2_gblr.bin**, rename the output file from tdump_fwrd to **tdump**, save, and then run the model. The trajectory should then be displayed and [superimposed](#) over the original trajectory (tdump_fwrd). Note how the differences between the two trajectories expand dramatically after 24 hours.

A trajectory represents the integration of the position vector in space and time through the time- and space-varying wind field. In the atmosphere, the wind direction and speed is a continuous field, but the numerical representation used in these calculations is discreet in space and time. How well this data represents the real atmospheric conditions can vary from day-to-day and is probably the most important source of trajectory error.

Absolute Trajectory Error

Up to this point the discussion of trajectory error has been a little abstract and perhaps unsatisfying. Considering the spatial extent of the ground-level concentrations, almost any combination of starting heights or meteorological data would result in a trajectory that passes over some non-zero concentrations. However in addition to the ground-level sampling, several aircraft were equipped with samplers and collected relatively short time-duration samples (6 or 10 min) making passes through the horizontal extent of the tracer plume at several different altitudes and downwind distances. This sampling information can be used to identify the plume center-line and if we compute a backward trajectory from that point, it should pass over or near the tracer release location. That nearest approach distance is one measure of the absolute trajectory error.

1. The sampling data for each of the five different flight levels are contained in files named according to the flight altitude in meters above mean-sea-level (MSL). For instance, the lowest sampling altitude was 914 m MSL and can be found the file named flight0914.txt where the highest concentration of 29,936 pg/m3 was measured over a 6 minute sample starting at **09 26 03 06** UTC with the sample centered over location **41.09N 82.52W**.

2. The information about that sample should be transferred to the trajectory setup menu. A little mental calculation is required to determine the run duration. We know that the tracer release started at 17 UTC on the 25th while the sample collection was at 03 UTC on the 26th (rounding to the nearest hour), therefore the run duration should be -10 hours (negative because it is a backward trajectory). Also rename the trajectory endpoints output file from tdump to **tdump_0914**. Change the meteorology file back to **captex2_narr.bin**. Upon completing the trajectory setup, it should be saved as traj_0914_control.txt. Note rounding to the nearest hour is suggested for these examples rather than using the minutes field. Otherwise you would need to insure the integration time step is consistent with the start time.

3. One last change is required. The starting height is specified as MSL rather an AGL (the default). MSL designations are typical of aircraft data. You should open *Advanced / Configuration / Trajectory* menu #2 vertical coordinates and select the MSL radio-button. **Save** this change and then from the *Create Optional Trajectory Namelist File: SETUP.CFG* configuration menu **save as** traj_abse_setup.txt prior to saving and closing the advanced menu.

4. After all the changes have been made go ahead and run the trajectory and then open the trajectory display menu. You can go ahead and create the graphic as we did in previous examples. Clearly the trajectory goes back to near the source location, but we can be more exact by superimposing the previously calculated 750 m AGL forward trajectory on this plot, which would then show the tracer release location. However, rather than using the + symbol between each output file, we will use a different method this time by specifying only one file that contains the file names of all the files we want to superimpose.

5. In this special case the special file name is preceded by the + symbol, which would be the

first character in the *Input Endpoints* field which should contain the file name of traj_files.txt. You then need to use *Notepad* to create **traj_files.txt** in the *\hysplit4\working* directory. At this point the file should only contain two entry lines: **tdump_fwrd** and **tdump_0914**. One file per line. The first line was our original 750 m forward trajectory calculation. Now when you run the trajectory display you will get the two trajectories superimposed and this particular aircraft sample based trajectory goes right back to the release location. Select the AGL radio-button in the display menu to show the trajectory in height units rather than pressure units.

6. This first calculation was reviewed in detail. To continue the exercise, go to each of the four remaining aircraft sampling files:

   - flight1219.txt
   - flight1524.txt
   - flight1829.txt
   - flight2134.txt

   and run a backward trajectory from the peak concentration in each file, saving the output files with unique names and then adding each of those to **traj_files.txt** and the create the final graphic with all the backward trajectories superimposed upon the initial forward trajectory.

In some respects it makes sense that one mid-boundary layer trajectory can be representative of so many different aircraft samples (all collected in the mid-boundary layer). However, the northern most sample had a completely different trajectory and naturally the complex and quite diffuse ground-level concentration pattern cannot be explained with a one-trajectory model. These issues will be explored further in subsequent sections.

Trajectory Vertical Motion

In most circumstances the input meteorological data will contain a vertical motion field, usually in pressure units. The trajectory and dispersion model calculations can use these data fields directly. If the vertical motion field is missing, or perhaps some special conditions are required for a simulation, the model has an option to replace these fields with an internally calculated vertical velocity based upon an assumption that the pollutant parcel is transported on some other surface. This is accomplished by computing the velocity (W_η) required to maintain a parcel on the selected η surface:

- $W_\eta = (-\partial\eta/\partial t - u\,\partial\eta/\partial x - v\,\partial\eta/\partial y) / (\partial\eta/\partial z)$

given the slope of the surface and its local rate of change and where the surfaces (η) can be either isobaric (p), isosigma (σ), isopycnic (ρ), or isentropic (θ). Note the equation is only an approximation because the velocity fields are not remapped to a new surface and therefore it is possible for a calculation to move off the surface.

1. The effect of changing the vertical motion method can be evaluated by recalculating the backward trajectory from the trajectory error discussion section. Retrieve the CONTROL file traj_back_control.txt which should show the trajectory setup after changing the output file from tdump_back to **tdump_data**. Save the change, delete the *SETUP.CFG* if it exists, run the model, and display the results. It should match the previous calculation.

2. Now repeat the process but configuring the simulation using the isobaric option. Make sure to change the output file name to **tdump_isob**, save and run the model. Repeat this process for each of the vertical motion options, naming the output file suffix with the name of the vertical motion method.

   - data - uses the vertical velocity field in the meteorological data file
   - isob - isobaric maintains the trajectory on a constant pressure surface
   - isen - isentropic maintains the trajectory on surfaces of constant potential temperature
   - dens - trajectories stay on constant density surfaces
   - sigma - vertical motion is zero and the trajectory stays on the same internal sigma
   - divg - the vertical motion is computed by vertical integration of the velocity divergence

3. When the calculations are finished, all trajectories can be superimposed on the same plot by using the + symbol between endpoint file names, or by creating the file traj_files.txt of file names which should be entered into the display menu. Remember to add the forward trajectory **tdump_fwrd** as the reference trajectory and the trajectory results will show only one other vertical motion method (besides data which should be identical) that is similar to the forward and backward data method.

4. Either examine each endpoints file, or go back and run the display by entering the endpoints file names, such as tdump_isen. This will show that the isentropic trajectory was closest to the one using the meteorological data field. For this display, the **theta** radio-button was

selected to show potential temperature as the vertical plot coordinate, where the temperature varied by only +/- one degree during most of the trajectory. This two degree range still translates into a variation of around 700 m, which can be determined by examining the meteorological profile near the tracer release point.

5. At this point it is not possible to determine a correct answer with absolute certainty because there are no tracer measurements at the off-shore starting location for all these back trajectories. However, the mid-boundary layer data and isentropic trajectories did pass through the middle of the tracer plume.

6. Another way to analyze the situation is to look at a something similar to a weather map. Open the *Meteorology / Display Data / Contour Map* menu tab and make the following changes to the contour map menu: select the global reanalysis file **captex2_gblr.bin** because the regional reanalysis covers too small a domain, select the geopotential height **HGTS** field, for level number **4** which will be the 850 mb surface, set the time offset radio-button to **48** to draw the map at the end of the sampling period near the start time of the back trajectory, set the map center to **40N 80W**, and increase the map radius to **25** degrees.

7. The resulting 850 mb heights map shows a high pressure system centered over the eastern U.S. with a divergent region just off the coast. Here the back trajectories easily got caught in different flow regimes, depending upon small differences in height between each method, resulting in very different horizontal trajectories primarily due to large variations of wind direction with height. The flow region to the north of the high pressure system contained most of the tracer.

In general, trajectory calculations should use the meteorological data's vertical velocity fields when available. Each of the computational approaches has its own limitations, isentropic in diabatic conditions (through clouds), isobaric over large terrain variations, the divergence is sensitive to small differences in velocity gradients, and even the data method becomes unreliable when meteorological grid sizes decrease but the data time interval remains unchanged resulting in under-sampling a field that may change direction multiple times between output intervals.

Trajectories and Terrain

The interaction of trajectories with the underlying terrain can be examined in more detail by forcing the trajectory to intersect the ground. The easiest way to approach this is by computing an isobaric trajectory starting just upwind of some large terrain feature. Although this is a rather artificial configuration, it is not unrealistic that a trajectory, using any of the vertical motion options discussed in the previous section, might intersect the ground under certain meteorological conditions.

1. Start by opening the trajectory setup menu and configuring a forward **isobaric** calculation to start on **83 09 01 00** for a duration of **72** hours from **45N 125W 500 m-AGL**, a location just off the west coast of the U.S. Name the output file **fdump** and find the global reanalysis file **RP198309.gbl**. For reuse later, save the configuration to a file named traj_isob_control.txt.

2. To see the terrain below the trajectory, open the *Advanced / Configuration Setup / Trajectory* tab and open menu #6, set the *Terrain Height* checkbox and *Save* to close each menu and then go ahead and run the model.

3. Now open the *Trajectory / Display* and select the Meters-AGL radio-button. Press *Execute Display* and you will see the trajectory intersect the mountains about 24 hours downwind. Subsequently, the trajectory continues to rise with the terrain and then proceed at its new pressure level.

4. Open the *Trajectory / Utilities / Simple Listing* menu to show the contents of the **fdump** endpoints file and copy the last endpoint position **49.573 -93.315 967.8** to the *Trajectory Setup* menu. You can also use *Notepad* to view the endpoints file. Note the time, **83 09 04 00** and enter it into the starting time field. Set the **backward** radio-button, rename the output file to **bdump**, save, and then run the trajectory model.

5. Display the backward trajectory graphic where you can see the back trajectory intersect the terrain and continue at that level rather than descending. This can be more clearly seen by combining the trajectory endpoints files **fdump+bdump** in the display menu to show both trajectories on the same image. In this particular case the backward trajectory is not reversible because there is no way for the backward model calculation to know which point along the forward calculation first intersected the terrain.

Although under most circumstances trajectories are fully reversible, the results shown here suggest that when trajectories intersect the ground information is lost. This may be a more common problem than is commonly recognized, such as when computing backward trajectories associated with ground-level sampling. This may be of particular concern in areas where typical upwind sectors are also associated with elevated terrain (the U.S. East coast).

Multiple Trajectories in Space and Time

The original trajectory calculation started at the beginning of the tracer release, but conditions can change with time and space. We can investigate both of these options to see if it improves the simulation with respect to the ground-level concentration pattern.

1. Start by configuring the simulation for the mid-boundary layer (750 m AGL) trajectory by retrieving traj_fwrd_control.txt into the *trajectory / setup* run menu.

2. Then go to the *advanced / trajectory / configuration* tab, press the *Reset* button, and then open menu #3 multiple trajectories in time. Set the *restart interval* to **1** hour, which will cause the model to start a new trajectory every hour from the starting point and time. The second entry, *trajectory duration*, should be set to **4** hours, which will cause the model to only start new trajectories for four hours regardless of the duration of the run.

3. Save all the changes and then run the model, open the trajectory display menu to view the result. The four trajectories, one hour apart, span the tracer release period from 17 to 20 UTC. Each successive trajectory is further south and west, indicating that changes to the flow field during this short 4 hour period could account for at least some of the tracer observed over Pennslyvania.

4. Because we already know that a single trajectory level and time is insufficient to capture the plume structure, we can combine the multiple starting heights with starting trajectories in-time. Start with the same trajectory setup used for the three mixed layer trajectories (10, 750, 1500 m AGL), and then save the changes.

5. Now open the configuration menu #3 again and change the interval to **6**, the duration to **24**, and the number of levels to **3**, consistent with the three starting heights. What happens in this variation is not intuitive. The input parameters have the same meaning as before, but instead of starting 3 new trajectories every 6 hours at the initial starting location, new trajectories are started at the end of each of all the previous trajectories. The calculation result illustrates how changing wind direction with height within the mixed layer can account for much of the observed tracer dispersion.

6. Another way of analyzing the flow field important for the tracer transport is to compute simultaneous trajectories over the whole domain. Open the trajectory setup menu and enter three starting locations, all at 750 m AGL: **38N 84W, 44N 74W, and 39N 83W**. The first two points represent the lower left and upper right corner of the domain over which trajectories will be started. The difference between the first point and the third point represents the spacing of a virtual grid from which trajectories will be started. Also reduce the *total run time* to **6** hours. Save the changes and run the trajectory. If the message pops up that the *SETUP.CFG namelist file found!*, select **Delete file then Run**. The namelist file was leftover from the previous calculations and is not needed for this illustration.

7. Only three trajectories are shown when the standard model run menu tab is selected. To create a matrix grid of trajectories go to the Trajectory / Special Runs / Matrix tab and you will get a prompt asking if the input was properly setup with three sources defining the grid domain. When the model run is finished, open the trajectory display, and you should see an illustration of the flow field over the domain.

8. One element to remember from this section is that when the setup menu was configured for three locations the resulting control file only showed those three points. However, when the model was run through the special runs tab, it invoked a pre-processor step, that converted the three starting locations into a control file with 77 starting locations. Complex control files can also be created manually with any text editor.

The primary result shown in this section was that the surface tracer concentration distribution could be explained in large part by the changing wind directions with height and time within the mixed layer.

Trajectory Frequency Analysis

In this section we will review different ways to analyze multiple trajectory output files. In contrast to the previous section, where multiple trajectories were written to a single output file, in this analysis approach, each output file contains a single trajectory resulting from a single execution of the trajectory model. This method would be used rather than the multiple trajectories in-one-file approach if additional meteorological information is required with each trajectory or to more easily sort trajectories associated with selected air samples. In this example, we will investigate the probability of conducting a successful CAPTEX tracer release during the month of September 1983.

1. Although a regional extract of meteorological data for September of 1983 is already provided on the CD-ROM, the complete global file can also be downloaded from the ARL server through the GUI meteorology menu tab. Enter the year and month into the download menu and the file name will be constructed automatically. A progress bar will be shown until the download completes. Remember all files are directed to the \working directory unless another location is specified.

2. Now go to the trajectory setup menu and configure the run for the same single mid-boundary layer trajectory as before (traj_fwrd_control.txt), but first change the starting time to the beginning of the month **83 09 01 00**, reduce the run time to **48** hours, rename the output file to **fdump** to avoid later confusion with previous simulations, and lastly change the meteorology file (first **clear**) to the global file, either in the CD-ROM CAPTEX directory or the working directory, if you just downloaded the file **RP198309.gbl**. Save the changes as *traj_freq_control.txt* in case we need to rerun this case and then save to exit the menu.

3. The run model tab will only create a single trajectory but the *Trajectory / Special Runs / Daily* tab will run a script based upon the start and end dates entered into the run daily menu. Change the end day from 31 to **28** because September only has 30 days. To complete a 48 h trajectory you can't start trajectories on the 29th or 30th without adding October to the meteorology input file list. The script execution creates a *CONTROL* for each trajectory starting time, runs the model, and creates a unique trajectory output file for each run: *fdump{yymmddhh}*.

4. After the script completes there should be 112 files starting with fdump in the *\working* directory. Rather than trying to display them individually, open the Display / Frequency menu tab. This opens the frequency menu. There are two steps involved in this process. First, enter the base name of the output files: **fdump**, this will be used as a wildcard to create a file of filenames (named *INFILE*) when the yellow button is pressed.

5. Check the working directory to insure that no **fdump** files exist without the number suffix. These would have been created by the run model tab. This file should be deleted and a new *INFILE* created, or you can just edit *INFILE* to delete the line that shows the unwanted file name.

6. The next step is to just **Execute Display** which runs two processes. The first is to count the number of trajectories that fall within each grid cell that covers the area. The grid resolution defaults to 1.0 degree. Other resolutions can be set through the menu. The trajectory frequency (F) is just the sum of the number of trajectories (T) that passed through each (i,j) grid cell divided by the total number (k) of trajectories analyzed:

   - $F_{i,j} = 100 \; \Sigma \; T_{i,j,k} \; / \; k$

   Note that all trajectories are counted once in the source location grid cell and each trajectory is counted once per intersecting grid cell if the residence time radio-button is set to **No**. The other option is to count multiple intersections if they occur. A height range can also be selected. Normally all trajectories are counted that pass over a grid cell. The trajectory summation results are written to a file and a normal completion will result in a simple termination message.

7. The second part of **Execute Display** automatically opens the display of the trajectory frequency output which shows flow in all directions during the month with one preferential direction to the northeast skirting along the edge of the CAPTEX sampling network. If the computation is repeated, but with the residence flag set to **Yes**, then the results show more transport to the east.

The results shown here present a simple approach to analyzing multiple trajectories. There are other methods which will be explored in more detail in other sections. For instance, counting a trajectory more than once in a grid cell because multiple points along the trajectory may stay within the same grid cell is a residence time weighted frequency. This type of particle trajectory analysis is the basis of the concentration calculation.

Trajectory Cluster Analysis

In the previous section the trajectories from multiple simulations were counted as they passed over an arbitrary grid. Although very simple and computationally efficient, this method tended to obscure the individual flow patterns that may have dominated during the computational period. Another approach is to merge trajectories that are near each other and represent those groups, called clusters, by their mean trajectory. Differences between trajectories within a cluster are minimized while differences between clusters are maximized. Computationally, trajectories are combined until the total variance of the individual trajectories about their cluster mean starts to increase. This occurs when disparate clusters are combined. The clustering computation is described in more detail in the next section.

1. Clustering requires a large number of single trajectory files which should have been created in the previous section. If these files are not already available, go back and complete that step. With the trajectory files completed for September 1983, open the Trajectory / Special Runs / Clustering Standard menu tab, which will open the main clustering menu.

2. Several changes need to be made to the default settings. First change the hours to cluster from 36 to **48** which permits all or part of the trajectories to be compared to each other. Second, change the endpoints folder, using the *browse* button, from ../cluster/endpts to **../working**, the endpoints location from the previous section. Third, change the base file name from tdump to **fdump** to be consistent with previous calculation. The time interval and skip options are used to select a subset of endpoints or trajectories for analysis to speed up the clustering of a large number of trajectories.

3. Just like with the frequency analysis, a file of file names for analysis must be created first by pressing the **Make INFILE** button. The INFILE contents can be manually edited to remove unwanted files prior to pressing the Run Cluster Analysis button which then shows the progress of the clustering.

4. When the clustering is complete, press the **Display Total Spatial Variance** button to display a graphic showing the change in the Total Spatial Variance (TSV) as the trajectories are merged into one cluster. In this particular case there is a large jump in TSV when going from 3 to 2 clusters, suggesting that perhaps 3, 4, or 5 clusters would be an appropriate solution. Another possibility is to use an objective percentage change criterion of either 20% or 30%.

5. The third and last step of this process is to decide the final cluster number and enter that number, for this example **4** into the *Number of Clusters* text field. Then press the **Run** button to Assign Trajectories to Clusters. The final step would be to Display Means graphic. The individual trajectories in each cluster can also be displayed. As an exercise rerun this step, but using three clusters to illustrate which two clusters get merged into one cluster, clearly illustrating why three clusters is not the correct answer.

6. All the intermediate clustering files and graphical results are saved in the *\cluster\working*

directory. For instance, the step that assigns the cluster number to individual trajectories is written to a file called CLUSLIST_{x}, where x is the final cluster number. This [file](#) can be used as input for other post-processing trajectory applications.

In summary the clustering results shown here for September 1983 present a more nuanced view of the probability of conducting a successful experiment: a 38% chance of simple west to east transport (Cluster #3) through the center of the sampling network.

Trajectory Clustering Equations

In the clustering process the spatial variance (SV) is computed between each endpoint (k) along trajectory (j) within its cluster (i):

- $SV_{i,j} = \Sigma_k (\mathbf{P}_{j,k} - \mathbf{M}_{i,k})^2$

where the sum is taken over then number of endpoints along the trajectory and $\mathbf{P}$ and $\mathbf{M}$ are the position vectors for the individual trajectory and its cluster mean trajectory, respectively. The cluster spatial variance (CSV) is then just the sum of the spatial variance of all trajectories within its cluster:

- $CSV_i = \Sigma_j SV_{i,j}$

and the total spatial variance (TSV) is the sum of the CSV over all clusters:

- $TSV = \Sigma_i CSV_{j,k}$

Clustering starts by assigning each trajectory to its own cluster, so that there are i clusters with j=1 trajectories in each cluster. In each iteration the cluster number is reduced by one as two clusters are merged together. So that after the 2nd iteration there will be i-1 clusters consisting of one cluster with two trajectories and the remainder with one trajectory. This process continues until only one cluster remains.

With each iteration, the TSV is computed for each cluster merge combination, that is the trajectories in cluster 1 are added to those in cluster 2, cluster 3, and so on, until the TSV is computed for all remaining cluster combinations, resulting in $(i^2-i)/2$ computations per iteration. The combination with the minimum TSV is passed on the the next iteration. This process continues until there is only one cluster. Large groups of trajectories could take quite some time to complete the clustering process.

Initially the TSV rises dramatically, then levels off for the remaining iterations until near the end of the computation, at which point disparate clusters start to be merged the TSV goes up again. The ideal final number of clusters would be prior to the point of rise.

Source Geolocation using Trajectories

One aspect of running multiple backward trajectories from various locations is if those trajectory locations and times correspond with high measured values then by superimposing these trajectories it may be possible to determine the source location of the measured pollutant. The GUI has an option to execute a script to run multiple iterations of the backward trajectory calculation which can then be summarized using the frequency plot menu option.

1. Before getting started it is necessay to define a forward trajectory using the trajectory setup menu that encompasses the time period of the sampling. We have already used this trajectory configuration for several previous examples: the 750 m trajectory saved to file name traj_fwrd_control.txt, which should be retrieved into the menu. Then just save. It is not necessary to run the trajectory again. Retrieving and saving just loads the run information into the GUI variables.

2. Now click the *Trajectory / Special Runs / Geolocation* menu tab which will open a relatively simple menu composed of just three steps. Step 1 defines the measured data input file used in this series of calculations. The trajectory model will be run backward, from each of the sampling locations. The sampling data for CAPTEX in the DATEM format and can be found the file captex2_meas.txt.

3. Step 2 creates three CONTROL.{xxx} files at the beginning, middle, and end of the sampling period for each sample with a non-zero measurement. 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. **Execute Step 2** and a completion message is shown after all 597 CONTROL files have been created in the working directory.

4. As an example of this process, examine the first non-zero sample in captex2_meas.txt which shows **1983 09 25 1800 0300 41.30 -82.22 15.6 316**. Three CONTROL files were created in the working directory for this sample: CONTROL.001, CONTROL.002, and CONTROL.003. In file 001, the trajectory starts at the end of the sample **83 09 25 21** and has a duration of -4 hour to take it back to the start of the release at 17 UTC. In contrast, file 003 corresponds to the start of the 3-h sampling period at **83 09 25 18** and has a duration of only -1 hours back to the release start time. The trajectory output file name consists of the sampling station number (316) and the trajectory start time. CONTROL files are created for all samples with some of the later ones having trajectory durations of as much as -64 hours.

5. Next **Execute Step 3** which invokes a Tcl script to sequentially run all 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.

6. Once all calculations have completed, go to the *Trajectory / Display / Frequency* menu to

grid and display the results. Make sure no unwanted (without the number suffix) *tdump_fwrd* files are listed in *INFILE*. Using a 0.5 degree grid (no residence time) shows a [pattern](#) with the maximum probabilities centered over Lake Erie rather than the actual location in western Ohio. This calculation was done assuming trajectories started at 750 m AGL for air samples actually taken near ground level (about 2 m AGL). As an exercise, reconfigure the simulation for a starting trajectory height of 10 m AGL, recreate the CONTROL files with the new starting height, run the trajectories, and the display the [frequency plot graphics](#). With this calculation, the results are even more ambiguous, with a maximum probability region in eastern Pennsylvania. This result is consistent with previous sections that showed the low-level trajectoriues to be not very representative of boundary-layer flow.

The trajectory geo-location results shown here only present a summary of the methodology rather than a definitive analysis for this particular event. Part of the issue is that the geography of the orientation of the tracer release location with the sampling network always required the same flow conditions for a successful experiment. For a more accurate geo-location calculation using only trajectories, it is necessary to sample a variety of different flow orientations. For instance, a geometric triangulation using trajectory analysis would be easier if the tracer release had been located within the center of the sampling network. The problem presented here with this single event analysis will be studied further in relation to the concentration calculation, where we can also account for the effects of sample timing and zero measured values.

Batch File Scripting

← Previous	**HOME**	→ Next

In the previous section hundreds of CONTROL files were created through the GUI and then the trajectory model was run for each file and the results analyzed; all under the cover of the GUI hidden from the user. In this section we will examine how these calculations can be run directly outside of the GUI using a Windows batch file script. Comparable scripting procedures exist under other operating systems.

1. To start, go back to the previous section and recreate the CONTROL files for the 750 m trajectory as outlined in sections 1, 2, and 3 (through Step 2).

2. From the *Tutorial**files* directory, copy the two batch files *batch_main.bat, batch_exec.bat* into the *hysplit4**working* directory. Although not required to run a batch file, open the *Command Prompt* by going to the Windows *Start Menu, All Programs, Accessories*, and the open the *Command Prompt*. From the command prompt change directory to the working directory: **chdir \hysplit4\working**.

3. Open the main script batch_main.bat in notepad where you can see that it is composed of seven sections, each preceded by a **REM**arks line. The first line runs the trajectory model script, passing as an argument, the name of the CONTROL file, the second step creates the file of file names, the next step accumulates the trajectories on a grid to compute the frequency, the next step creates the custom labels for the plot, then the postscript plot is created, displayed, and finally unneeded files are deleted.

4. Each of these commands could be typed line-by-line on the command line, or you could just simply type the name of the upper level batch file, **batch_main.bat** and windows knows to execute the commands in the file. Run this script and at its conclusion the final graphic will be similar but not identical to the one in the previous section because in this case the contours were customized to illustrate one of the advantages of scripting: providing for program options not always available through the GUI.

Other scripting examples can be found in *hysplit4**testing**xrun.bat*, which runs through a series of different calculations. Example scripts for Windows, TCL, and UNIX, can be found in *hysplit4**examples**scripts*. Command line options for various HYSPLIT programs can be found in the User's Guide and by typing the program name from the command prompt. All HYSPLIT programs are in the *exec* directory so for example to see the options associated with concplot, type: **..\exec\concplot** without any arguments. Batch file commands can also be displayed from the command prompt by typing **help**.

Meteorological Trajectory Ensemble

Another multiple trajectory approach, an extension of a previous section on sources of trajectory error, is a variation of an old manual technique, where trajectories are started about the point of interest, and the divergence of those trajectories would provide a more quantitative estimate of the uncertainty associated with the center point trajectory. In HYSPLIT, this method has been incorporated directly into the code so that trajectories are automatically computed about a 3-dimensional cube centered about the starting point. However, the initial positions are not offset, just the meteorological data point associated with each particular trajectory.

1. The first step would be to setup the trajectory simulation for the 750 m AGL mid-boundary layer forward trajectory by retrieving the traj_fwrd_control.txt file. Then save and exit the setup menu.

2. Instead of using the simple run model tab, go to the *Trajectory / Special Runs / Ensemble menu tab* to run the calculation. This tab calls a special trajectory executable (*..\exec\hyts_ens*). If the *SETUP.CFG* message appears, select to delete the file and then run.

3. A single endpoints output file is created which shows the forward trajectory results for the 27 trajectories that make up the points of the data cube about the starting location.

4. The same calculation can be performed for the backward trajectory point that was done in an earlier section by retrieving the traj_back_control.txt file into the trajectory setup menu and rerunning the ensemble which should show the equivalent 27 backward trajectory results. Only one of these would be identical to one of the forward trajectories, the others get caught in totally different flow regimes.

5. The computational details of the meteorological ensemble can be configured in the *Advanced / Configuration / Trajectory* meteorological ensemble configuration menu #11, which shows the default grid offset of 1 grid point in the horizontal and 0.01 sigma units in the vertical. The 27 members are created from 3 planes of 9 trajectories, each plane at +/- 0.1 sigma (about 250 m). The 9 trajectories on each plane represent all combinations of +/- horizontal combinations in x and y.

The difference between the forward and backward results show a dramatic difference in the "trajectory dispersion", the forward trajectory results are quite constrained while the backward pattern is quite disperse. This is consistent with the weather pattern associated with release #2, where the tracer flowed along the northern side of a high pressure system. The backward equivalent starts in a divergent region where small changes in position resulted in very different trajectories.

The Basic Concentration Calculation

The first step in understanding the nature of the air concentration dispersion calculation will be to modify the test example and reduce the simulation down to its most basic component, a single particle trajectory, which we will then enhance step-by-step until the calculation is optimized to represent a realistic concentration simulation.

1. First from the main menu press the **Reset** button to set the menu variables for the test calculation and then press the *Concentration / Setup Run* menu tab to open the concentration setup menu to set all the concentration run parameters. Change the starting time to **83 09 25 17**, the run duration to **12** hours, and the starting location to the tracer release point **39.90 -84.22 10.0**. Clear the meteorology files and then add **captex2_narr.bin** from the *Tutorial/captex* directory. When finished with the changes, **Save** to close the menu window.

2. Then go ahead and press the Run Model tab under the *Concentration* tab. If the SETUP.CFG namelist file found! message appears, select **Delete file and then Run** because we have not yet created a namelist file for this example and it is probably left over from a previous calculation. When complete, **Exit** and continue to the next step.

3. To create the concentration graphic, press the *Concentration / Display / Concentration / Contours* menu tab to open the display menu, where you should just accept the defaults, press *Execute Display* to open the plume graphic which shows color filled contours of 12-hour average air concentrations at factor of 10 intervals ranging from 10^{-12} to 10^{-15} mass units per cubic meter. This calculation is identical to the original test case except we moved the location and time to be consistent with CAPTEX release number two.

4. The test calculation release was one unit for a duration of one hour. To change this value, press the large bar labeled **Pollutant, Deposition, and Grids setup** under the meteorology files section of the *Concentration Setup* menu. Then under the left most column labeled Pollutant, press the **Specie 1** radio-button (there is only one pollutant). This then opens the emission menu where you will change the emission rate from 1.0 to **100.0** and the emission duration from 1.0 to **0.01**. Notice that although we have changed the mass release rate, the total mass released is still one unit, because the rate is 100 units per hour but only for 0.01 hours. Effectively this means all the mass is released in one time step. Save to close out the *Pollutant* menu.

5. Now open the middle menu, labeled **Grids** where we can configure the concentration grid which accumulates the mass of each particle as its trajectory takes it through the computational domain. At this point we will change only one line. Change the height of the level (averaging layer) from 100 to **5000** meters. Because we will be following only one particle trajectory, we need to make sure the sampling layer is deep enough not to miss the particle as the particle moves through different levels in the boundary layer due to vertical mixing. Then *Save* to close the menus

6. Before running the model, one more modification is required: we need to insure that only one particle is released over the emission period. The default is to release 2500 particles over the emission period. That is we would follow 2500 trajectories, each with a 1/2500 of pollutant mass. These changes are made through the namelist file: *SETUP.CFG*. Press the Advanced / Configuration Setup / Concentration menu tab and select menu #4 to change the release number limits from 2500 to **1**. Then *Save* to close out all menus.

7. Now from the main concentration tab, *Run Model*. You will be prompted again that the SETUP.CFG namelist file found!, which we created in the previous step, so this time select **Run using Setup File**. When the run has completed, again select the contour display menu. Note no changes are required, as the new layer height of 5000 m has been passed to the menu. Then **Execute Display** which will show a very narrow plume, essentially one concentration grid cell wide and very similar to the trajectories calculated in the first few sections of the tutorial.

8. To examine the details of the calculation we need to eliminate the temporal averaging. Open the *Concentration / Setup* menu and the open the grids menu and change the last line from 00 12 00 to **01 01 00**. This changes the particle mass accumulation from a 12 hour average to a snapshot value once an hour. The term "now" equals a one-time-step accumulation.

9. Save the change, run the model, and open the display menu. There will now be 12 frames in the graphic, one for each hour, the first frame shows the concentration pattern after one hour. Note the concentration grid cell size is represented by the red square and although it looks like the pattern covers several grid cells, a single particle calculation can only be contributing to one cell during a time step. The bleeding of the concentration contours into adjacent cells is just an artifact of the smoothing and contouring process.

10. To see all the frames in a single animated graphic, similar to a trajectory, press the *Concentration / Utilities / Convert Postscript* menu tab to open the ImageMagick conversion menu. Select the **Animate** and **crop** radio-buttons, and move the slider bar to a higher resolution (**140**) for a better quality image. After executing the conversion, the window closes with no message, but you will find the animated GIF, *concplot.gif* in the working directory. The animation is a little jumpy due to the atmospheric turbulence affecting this single particle trajectory.

The results shown here illustrate how a particle trajectory is used to compute air concentrations. This particular example, using one particle, is insufficient for a realistic simulation. These issues will be explored in more detail in the following sections.

Multiple Particle Concentration Calculation

To further expand upon the single-particle calculation discussed in the previous section, we will increase the particle number release rate until the simulation looks more realistic. If you have not completed the previous section, please go back and review that section before proceeding.

1. We ended the last section viewing the hourly concentration contribution of one particle as it was transported and dispersed along its path. Lets start by reducing the number of output frames to every three hours rather than hourly. Open the *Concentration / Setup Run / Grids* menu and change the last line from 01 01 00 to **01 03 00**. Save to close all the setup menus. Then open the *Advanced / Configuration Setup / Concentration / Release Number* limits (Menu #4) and change the *Particles Released per Cycle* from 1 to **100**. Save to close and exit all menus.

2. Now *Run Model*, open the contour display menu and when complete, view each of the four frames (at 20Z, 23Z, 02Z, and 05Z). Note at the inital time, all the particles are close together and the pattern is continuous, but as the particles spread out due to turbulence and vertical wind shear, the results quickly degrade and by the last frame it almost appears that each of the 100 particles are individually visible.

3. Run this exercise again for 1000 particles and 10000 particles: only the 10,000 particle simulation shows a continuous concentration pattern. Remember in the original example calculation we only released 2500 particles over one hour, a considerably smaller particle release rate, but the concentration pattern was very smooth. This is because we computed a 12 hour average concentration, rather than instantaneous concentrations. The model needs to sample a sufficient number of particles over the averaging interval and concentration grid size to insure robust results. The appropriate number can be determined by trial-and-error as the rate when the air concentration results are no longer sensitive to the particle release rate.

4. To illustrate the nature of the particle-trajectory calculation, we can output the individual particle positions in addition to the air concentrations by opening the *Advanced / Configuration Setup / Concentration / Input and Output of Particle Files* menu #9 and change the *First Output and Repeat Interval* from 0 to **3**. This will create a special output file called *PARDUMP* which will contain all the particle information every three hours. This is a more complex file than the ASCII trajectory endpoints file. It is binary and in addition to the particle position, it contains all the information needed to restart the model. Save to exit and close all menus, and then run the model.

5. A different program is used to display the contents of the particle endpoints file. Press the *Concentration / Display / Particle* menu tab to open the particle display menu. Accept the defaults (perhaps increasing the zoom if desired) and **Execute Display** to open the graphic. In addition to the horizontal plane view, the vertical cross-section is shown in the

lower panel, which shows very clearly why a single particle trajectory is insufficient to simulate the pollutant distribution. Particles that mixed to the upper-levels of the boundary layer travel at faster speeds. Winds aloft also tend to be more clockwise than those at the surface.

6. Previously we found that the simulation results for a given particle release rate were sensitive to averaging time. A similar sensitivity exists with regard to the concentration grid size. To run a simulation with a finer resolution grid, open the *Concentration / Setup Run / Grids* menu to change the spacing of the grid from 0.05 to **0.005** in both latitude and longitude. One degree spacing is approximately 100 km, so 0.005 degree spacing is about half a kilometer. Note that a grid center specification of zero means that the concentration is centered over the release point. Save to close the menu and then run the model.

7. When the run completes, open the display contour menu. With all those nearby particles, the visual look of the plot can be improved by removing the closed contour about each fill color by changing the *contour drawing options* to **none**. The final graphic shows much more detail than the previous simulation, but again individual particles are visible.

The simulations with various particle number release rates suggested that more particles are required for more detailed simulations, but at a cost of increased computational time. This may become especially significant for continuous releases. There are other simulation options to reduce the particle number requirements which will be explored in the next section. For future reference, the control (cpart_control.txt) and namelist (cpart_setup.txt) files should be saved.

Particle Growth using Puffs

In the previous section we needed to follow many thousands of particle trajectories to get a reasonably realistic simulation. Another option is, instead of following each individual particle that makes up the pollutant cloud, we follow the mean trajectory of the cloud and model the growth of horizontal (and optionally the vertical too) particle distribution; a single number to represent the particle distribution about the centroid point. There are two distribution options, the *Top-Hat* where the concentration is zero outside and a constant average value inside and the *Gaussian* option, which follows a normal distribution over a range of 3 σ.

1. To configure the two-dimensional Top-Hat puff simulation, open the *Advanced / Configuration Setup / Concentration / Particle-Puff Release Mode* (menu #3), and select the **Top-Hat-Horizontal Particle-vertical** radio-button, then save. Also open menu #4, and change the particle release number back to **1**, and save, run the model, and then display the concentration contours. The output should still be configured for snapshots every 3 hours which shows a growing circular puff. Note that after 12 hours the puff does not cover as much domain as the 3D particle simulation.

2. Go back to menu #3 and this time select the **Gaussian-horizontal particle-vertical** puff option. Save the change, rerun the model, and display the new result. Although the puff radius is about twice as large (3.0 versus 1.5 σ) as the top-hat calculation puff, it is still covers much less area than the 3D particle calculation. If the center point of either type of puff passes over a sampling location, the integrated concentration at that point will be the same.

3. You've probably noticed that these calculations have been taking quite some time considering that we are only following a single particle trajectory. The reason is that as the puff grows, at each integration time step, all the grid points covered by the puff radius accumulate mass. At hour +12, the Gaussian puff had a diameter of about 100 km and with a grid resolution of 0.005 (0.5 km), there would be about 15,000 grid points within the puff. Go to the *Concentration / Setup Run / Grids* menu and change the concentration grid resolution from 0.005 back to its original value of 0.05. Save, rerun the model, and display the result. Although with a slightly more ragged outer perimeter, the puff at the last time period (+12 h) still shows the same circular pattern. However, this time the calculation was much faster because 100 times fewer concentration grid cells were involved in the integration.

4. The remaining issue is why the single puff calculation was still insufficient to describe the more complex 3D particle calculation. In the previous section, the particle display showed particles transported at different levels, the higher levels having faster transport speeds. One puff can only describe the horizontal particle distribution at that level. Each level must have its own puff. Go the the *Advanced / Configuration Setup / Concentration / Release Number Limits (#4)* and change the *Particles Released per Cycle* from 1 to **100**. Save, rerun the model, and display the new result. After 12 hours the concentration pattern is much more complex and very similar to the previous 10,000 3D particle calculation.

Although these 100 Gaussian puffs were released the same time at a height of 10 m they quickly mixed to different levels. This is the advantage of one of the unique features of HYSPLIT, a hybrid calculation, where the horizontal dispersion is modeled through the puff approach, while vertical mixing is treated in the particle mode. Growing vertical puffs would have to be split up very frequently to properly simulate the boundary layer wind shear.

5. The puff splitting process also occurs in the horizontal when the puff grows larger that the meteorological grid size. To more clearly see this effect, go back to the 1 particle release calculation (configuration menu #4), but in the main setup menu, run the calculation for a duration of **48** hours instead of 12 hours. The simulation at 48 hours shows the effect of the horizontal splitting, particularly evident by the circular puffs near the edge of the main pollutant cloud.

6. The exact splitting times can be determined from the diagnostic message file. Press the *Advanced / View MESSAGES* menu tab to open the listing MESSAGE file. The lines starting with NOTICE main: give the simulation hour, the time in minutes, the number of particles/puffs, and the total mass of all the particles on the computational domain. The first split occurs between hours 14 to 15, when the calculation goes from 1 to 5 puffs. Note the total mass stays the same, at 1.0 unit, now distributed over 5 puffs. At the end of the calculation, we are following 161 puffs. Note that puff merging also occurs when previously split puffs are in the same location. So there is no simple formula to compute the puff number growth rate.

7. The results after 48 hours look somewhat discontinuous, puff calculations suffer the same limitations as the 3D particle calculation, there still needs to be a sufficient number to describe the complexity of the pattern, just fewer puffs are required for the same calculation. The use of snapshot concentrations is also not very realistic. For instance, if the 48 calculation is rerun, but computing 12 h averaged concentrations, the resulting pattern is much smoother.

The modeling of the change in the particle distribution with time rather than modeling individual turbulent particle trajectories can be a satisfactory alternative in computing air concentration patterns. The default HYSPLIT option is to compute 3D particle transport and dispersion. It is up to the user to recognize the limitations and if more particles or a different modeling approach are required. In the next section, we will explore the equations that are the basis for the particle and puff calculations.

Air Concentration Calculation Equations

| **HOME** |

This section provides a quick review of the dispersion equations for particles and puffs and how the air concentration is computed using each approach. The equations shown here are used to illustrate the calculation and the HYSPLIT Technical Memorandum (ARL-224) should be referenced for a more complete description.

1. The 3D particle calculation is composed of two steps. The first consists of the advection step, essentially the trajectory calculation component using the mean wind field from the input meteorological data file. In the second step, the mean position is adjusted by the turbulent wind.

   - $\mathbf{P}_{final}(t+\Delta t) = \mathbf{P}_{mean}(t+\Delta t) + \mathbf{U'}(t+\Delta t)\ \Delta t$

2. The horizontal turbulent velocity components at the current time $\mathbf{U'}(t+\Delta t)$ are computed from the turbulent velocity components at the previous time $\mathbf{U'}(t)$, an auto-correlation coefficient (R) that depends upon the time step, the Lagrangian time scale (T_{Li}), and a computer generated random component (U"). An exponential velocity auto-correlation is assumed.

   - $\mathbf{U'}(t+\Delta t) = R(\Delta t)\ \mathbf{U'}(t) + \mathbf{U"}\ (\ 1-R(\Delta t)^2)^{0.5}$
   - $R(\Delta t) = \exp(\ -\Delta t\ /\ T_{Li})$

3. The Gaussian random component $\mathbf{U"}$ comes from the computer generated random number (λ) and the standard deviation of the velocity σ_u, a statistical value that is estimated from the meteorological data fields (e.g. wind speed and stability).

   - $\mathbf{U"} = \sigma_u\ \lambda$
   - $\tan \sigma_\theta = \sigma_u\ /\ U$

4. The same standard deviation of the velocity component (σ_u) used to compute particle dispersion is also used to compute the horizontal puff growth rate.

   - $d\sigma_h/dt = \sigma_u$

5. Air concentrations are computed by summing the contribution of each 3D particle's mass (m) each time step that the particle resides in the grid cell and dividing the sum by the cell's volume, where x, y, and z define the grid cell's dimensions.

   - $\Delta c = m\ (\Delta x\ \Delta y\ \Delta z)^{-1}$

6. The incremental concentration contribution for a Top-Hat and Gaussian puff is computed at each grid cell center point when that point lies within the puff radius. Puffs must intersect the point to contribute to the concentration summation while a 3D particle can be anywhere within the grid cell. This means that puffs may pass between grid cell center points when the plume radius is small or the concentration grid resolution is too coarse. In this situation the volume is a combination of the puff radius and cell height.

   - {Top-Hat} $\Delta c = m (\pi r^2 \Delta z)^{-1}$
   - {Gaussian} $\Delta c = m (2 \pi \sigma_h^2 \Delta z)^{-1} \exp(-0.5 x^2/\sigma_h^2)$

Only a simplified version of the air concentration computational details are shown here. Symbols in bold are vectors and a form of these equations are applied in each velocity component direction. Furthermore, the vertical particle dispersion equation has an additional term (not shown here) to compensate for the accumulation of particles in low-wind and low-turbulence regions near the ground surface.

Configuring the CAPTEX #2 Release			
⬅️ Previous	**HOME**	**Zoom**	➡️ Next

Most of the essential HYSPLIT model parameters have been discussed in the previous sections. Now we will review in detail all the changes required to configure the model to simulate CAPTEX release number 2 and produce the **animation** shown in the introductory section.

1. First press the center **Reset** button on the main GUI to clear all previous changes and then press *Concentration / Setup Run* to open the **concentration setup** menu. Make all the changes shown:

   - change the starting time to **83 09 25 17**,
   - change the starting location to **39.90 -84.22 10.0**,
   - and make the total run time **68** hours, which coincides to about when the last air sample is collected.

2. Now press the large center button labeled **Pollutant, Deposition, and Grids Setup** to open the main **selection** menu. Start with the top left radio-button for species #1 to open the **pollutant** menu.

   - Enter the 4-character identification field, **PMCH**, for the material released (perfluromonomethylcyclohexane),
   - the hourly release rate, **67000** grams,
   - and the emission duration of **3.0** hours, which will result in a total release of 201 kg. The emission units are totally arbitrary as HYSPLIT only computes the dilution factor of any mass that is released. So if the emission units are grams then the air concentrations will be grams per cubic meter.
   - Leave the emission starting times as all zeros. When this field is zero, the emissions start at the beginning of the simulation. Save to close the menu.

3. Now press the center column radio-button for grid #1 to open the menu to define the characteristics of concentration **grid #1**.

   - Start by defining the center of the concentration grid approximately centered over the sampling domain **42.0 -78.0**. A zero in this field forces the grid center to be the release location.
   - Change the grid spacing to **0.25** in both directions. This should be sufficient for the large source to receptor distances of this experiment.
   - Change the grid span to **15.0** degrees latitude and **25.0** degrees longitude.
   - The output file will be written to the startup working directory (**./**) and give the binary concentration output file a unique name such as **hysplit2.bin**.
   - The concentration grid only needs one **100** m layer. When vertical particle dispersion is enabled, the heights represent layer tops, in this case from ground-level (0) to 100 m.
   - Now explicitly set the start (**83 09 25 18 00**) and stop (**83 09 28 15 00**)times for

the integration time on the concentration grid. Leaving the field as zeros starts the summation at the start of the run. But in this case we want the concentration grid times to match the actual times air samples were collected, which started at 18Z rather than the start of the release at 17Z.

- Air concentration samples were collected over 3 or 6 hours, therefore a **3** hour average covers all the possibilities (two 3h periods can be averaged together).

4. Now press the right column radio-button for species #1 deposition options. The PMCH tracer released does not deposit and therefore all these fields will remain zero. The menu has some [pre-set values](#) which will be discussed in more detail in a later section.

5. Now press the *Advanced / Concentration Setup / Concentration* [menu tab](#) to open the [namelist selection](#) menu. Only two menus need to be changed.

- Open menu #4, the particle/puff release [number limits](#) and change the default particle release number from 2500 to **50000** and the maximum particle number from 10000 to **100000**. Because the default mode is 3D particle, we know from the previous sections that the default is insufficient for a 3 day duration simulation.
- Open menu #9, the input and output of [particle files](#) and change the first output time from 0 to **1** hour and repeat interval from 0 to **3** so that the particle output time will be at the same time as the concentration grid output times. The *PARDUMP* output file will be used for display purposes in the next section.
- Save each menu and the selection menu to close out the *Concentration Setup* section.

6. Now from the main menu select *[Concentration / Run Model](#)* and when the simulation completes continue on to the next section to review all the concentration display options.

After the simulation run has completed, open the *MESSAGE* file to confirm that indeed 201 kg have been released and that concentrations (condsk) and particle positions (parout) were output every three hours. If satisfied, go back and save all the changes to the control and namelist file menus through *Save As* to [captex_control.txt](#) and [captex_setup.txt](#) for future examples.

Air Concentration Display Options

Do not proceed with this section unless the previous section has been completed and you have created two different output files in the working directory for CAPTEX release #2: *hysplit2.bin* with 3-hour average air concentrations and *PARDUMP* with all the particle positions every 3 hours.

1. Press the *Display / Concentration / Contour* menu tab to open the concentration display menu. Only a few changes are required from the defaults. Because we defined the release rate in grams and we know that the measured concentration data are reported in pico-grams per cubic meter, we need to define a concentration multiplier of **1.0E+12**, the number of pg in each gram. The air concentration label field should also be changed from blank to **pg**. If desired, increase the zoom to reduce the whitespace around the plot.

2. The Postscript viewer opens automatically and then you can scroll though the images frame-by-frame. The plot after 12 hours shows a very similar pattern to the test plots done in previous sections. The plot is not identical to the one shown in the introductory section where the contour values were fixed rather than letting the contouring program automatically select the interval. To animate the multi-frame Postscript file, press the *Utilities / Convert Postscript* menu tab to open the conversion menu. Set the **Animate** and **Crop** radio-buttons and increase the slider bar for better resolution if desired. When the menu disappears, the animated GIF graphic will be found in the */working* directory. Although different graphic conversions can be specified by changing the output file suffix, only GIFs can be animated.

3. To follow the individual particle trajectories, press the *Concentration / Display / Particle* menu tab to open the particle display menu. There are three radio-button options: 1) a horizontal plane view, 2) a vertical West->East and South->North projection, and 3) the default combination plane-view with a cross-section. Perhaps increase the zoom, but otherwise select the default options, and the viewer will open the multi-frame file *partplot.ps* (depending upon the speed of your computer, this may take several minutes), which like all other output files, unless otherwise directed, is located in the */working* directory. Skip to the frame representing the particle positions after about 12 hours and the image will show all the particle positions that contributed the 3-hr average air concentration map. Try the other particle display options to see the differences and perhaps create a particle animation.

4. To examine the temporal evolution of the released tracer, press the *Concentration / Display / Arrival* menu button to open the plume arrival time menu which will create a color-filled graphic representing the time after sampling has started that a grid cell shows a non-zero concentration. The menu permits setting a threshold concentration other than zero, as well as setting the number of contours and the time difference between contours. For this example, change the time difference from -1 (auto select) to **6** hours. The resulting output file *chron.ps* shows arrival times to the east coast of 42 hours. Only files with multiple time period output can be analyzed for arrival times.

5. Another display option is to see the concentration values in each grid cell without the

interpolation and smoothing introduced by the contouring program. Press the *Display / Concentration / Grid Values* [menu tab](#) to open grid cell display [menu](#). The default values are set to display the full range of potential concentrations. Change the contour base (the minimum) to **1.0E-10** and the contour delta to **2.0**. With the log scale box checked, the 2.0 is interpreted such that each color interval will be a factor of two larger than the previous one starting with the base value. The multi-frame postscript file shows the concentration value in each [grid cell](#) for all time periods.

The concentration display options reviewed in this section all create Postscript files that can be directly printed or converted to other formats. Some of the display menus also contained other options that would create GIS compatible output files such as ESRI Shapefiles and Google Earth KML. These options will be explored in more detail in later sections.

Air Concentration Utility Programs

In this section we will review how the HYSPLIT binary air concentration file can be converted to other formats or interpolated to a sampling location. Statistical analysis programs are provided to compare the measured and calculated values. The previous section should have been completed before proceeding with this section.

1. A quick listing of output file contents is obtained by pressing the *Concentration / Utilities / Simple Listing* menu tab. Use the *Set File Name* button to browse for the concentration file name **hysplit2.bin** and then press *Show File Contents* to open the file listing window, the GUI viewer of the output file conread.txt, which can be found in the */working* directory. The listing shows the maximum and minimum concentrations each time period.

2. A more complete listing is available through the *Utilities / Convert to ASCII* menu tab. The options menu provides several different format options to provide more spreadsheet import flexibility. For this example, set the **Single File** checkbox so that all time periods are in the same file rather than individual files. Also set the concentration units conversion to **1.0E+12** so that we get pg m^{-3} and then *Execute Conversion*. By default, the output file will always have the same name as the input file but with a .txt suffix: hysplit2.bin.txt. Concentration values for all non-zero grid points are listed. Try some other options to see the differences in the output format.

3. The ASCII conversion can also be performed at a single location by interpolating a value to a location. Select the *Utilities / Grid to Station* menu tab to open the options menu. For this example we will select a location near the center of the CAPTEX sampling domain, station number 510, Little Valley, NY, south of Buffalo, near the Pennsylvania border. Enter the station ID **C510** (C for calculated), and the location **42.25 -78.80**. Set the *Display Time Series* radio-button to **Yes**. The units conversion should be set to **1.0E+12**. Press *Extract Data* and the output file con2stn.txt will be created, but not opened in the GUI viewer. However, with the radio-button set, the time series plot will be displayed (*timeplot.ps*).

4. A variation of the interpolation to a location is the *Utilities / Convert to DATEM* tab which opens a similar options menu which converts the HYSPLIT output to the DATEM (Data Archive of Tracer Experiments and Meteorology) format by matching each value in the measurement file with a calculated value. First browse to find the measurement file: **/Tutorial/captex/captex2_meas.txt**. Then press **Create DATEM file** and the calculated data file hysplit.txt is created in the working directory. Pressing **Compute Statistics** analyzes the data and opens the GUI viewer to the results file: statA.txt. The scatter plot button opens a graphic showing the measured and calculated values identified by station number. The paired measured and calculated values are also written to the file: dataA.txt.

There are several options that can be used to convert the HYSPLIT binary air concentration file to a text formatted file, each with several different formatting options, one of which is linked with some statistical analysis programs. The binary data manipulation programs available through the

utilities menu tab will be discussed in other tutorial sections. Some supplemental exercises for this section are also [available](#).

Case Study Base Configuration

⬅️ **Previous**	**HOME**	**Zoom**	➡️ **Next**

Now that we have successfully configured an air concentration calculation and compared the results with the ground-level sampling data from CAPTEX release #2, we will experiment with different dispersion parameters and turbulence settings to determine their effect upon the calculation results. You should have saved the previous *CONTROL* and *SETUP.CFG* settings. Retrieve captex_control.txt into the *Setup Run* menu and captex_setup.txt into the *Concentration Configuration* menu. This will be the starting point for all the case study customizations.

1. To run through many model combinations as quickly as possible and limit the complexity of the analysis, we will only compare the model predictions to the first complete aircraft sampling pass about 200 km downwind from the tracer release point. See the CAPTEX report for a complete description of all the data. This first pass occurred around 0300 UTC on September 26th. Open the *Concentration / Setup Run menu* and change the run duration from 68 hours to **13** hours, enough time to take the calculation through 0600 on the 26th.

2. To reduce the number of graphical output frames, open the *Concentration Grid #1* menu and change the sampling start time from 83 09 25 18 00 to **83 09 26 03 00**. This insures that the binary concentration output file will only contain one 3-hour average air concentration period, covering the last three hours of the simulation. Press *Save* to close all menus and then press the **Run Model** tab.

3. When the run has completed, press the *Display / Concentration / Contours* menu tab to open the graphics menu. Make the same changes as in previous examples, that is the concentration multiplier should be **1.0E+12** and the output units will be **pg**. Three additional changes are required.

   ○ First, force the map center further to the northeast, rather than over the tracer release point, by selecting the map center **Set** checkbox and entering a new position of **41.0 -82.5**. In this way the map is centered over the plume.

   ○ Second, because we have a sense of the range of potential concentrations, we will set the contours by checking the **UserSet** radiobutton and entering the following seven contours using a plus symbol as a delimiter:
   50000+20000+10000+5000+2000+1000+500. The field window is too small to show all values at the same time, but you can use the cursor to view the whole string.

   ○ Third, increase the zoom slider bar to **80**.

   ○ Then *Execute Display* to open the graphic

4. In the trajectory section, we started a backward trajectory from the maximum concentration point defined in the 914 m MSL aircraft sampling flight. This file is in the DATEM format.

This aircraft pass managed to cover the entire horizontal extent of the plume. The concentration plotting program we have been using, *concplot*, has a command line option (-q) to plot the values from simple data files (ID LAT LON VALUE), but the data points must be reformatted. The measured concentrations from this flight have been copied to data_case.txt which you should either create manually or copy it from the tutorial directory to the HYSPLIT */working* directory.

5. Unfortunately, there is no GUI option to set the data plot command line option, but when *Execute Display* is pressed, the GUI script automatically creates a concplot batch file (or .sh in unix) with all the command line options set in the GUI. Open concplot.bat in notepad and replace one of the non-set switches (-:) with the string **-qdata_case.txt** and save to a unique name such as *conc_case_plot.bat*. Now from *Windows Explorer* or from the command line, run the concplot plot batch file and then open the output file, *concplot.ps*, to see the model predictions and measurements.

6. The large red square in the center of the plot shows the grid cell (to scale) with the maximum concentration. The 25 km resolution of the concentration grid may be appropriate for the full 68 hour simulation, but it is too coarse to examine the model prediction just 200 km downwind. Open the *Setup Run / Grids* menu and change the resolution from 0.25 to **0.05** degrees. Save to exit, then **Run Model**, but when it completes, instead of opening the *Display / Concentration* GUI, just run the previously saved *conc_case_plot.bat* file and open *concplot.ps* to see the new model prediction.

7. To examine the effect of using the puff parameterization instead of the default 3D particle, open the *Advanced / Configuration Setup / Concentration* menu #3 to switch from 3D particle to **Top-Hat-Horizontal Particle-Vertical** mode and also menu #4 to change the particle release number from 50000 to **5000**. Fewer puffs than particles are required for the same simulation. Save to exit, run the model and the *conc_case_plot.bat* file and open *concplot.ps* to see the top-hat puff prediction.

8. Follow the same process to configure the **Gaussian-horizontal particle-vertical** puff simulation. Now the graphic will show a slightly wider tracer plume because of the larger scan radius used in the Gaussian puff calculation compared with the previous top-hat puff computation. The particle/puff positions are the same in both calculations. Now save the control file settings to conc_case_control.txt and the namelist file parameters to conc_case_setup.txt.

We've found that for this particular case, the model's plume simulation 200 km downwind matched the position and width of the aircraft measured plume. Although there were differences in the model layer depths as well as averaging times, the magnitude of the concentration predictions were very similar to the observations. Matching the sampling times and layer depths more closely with the measurements is left as an exercise for the reader. Note the batch file short-cut introduced here can be used to add the surface measurement data to the 68 hour CAPTEX animation. This is another exercise left to the reader.

Vertical and Horizontal Turbulence

The [last calculation](#) in the previous section used all the turbulence computation defaults. These equations determine the way the meteorological data are processed to compute the horizontal and vertical turbulence. The method can be changed from the *Configuration Setup / Concentration / Turbulence Method* Menu #7. Some of these options will be explored in more detail in this section.

1. The default calculation uses the Kanthar-Clayson equations to compute the turbulence values from stability parameters estimated from the meteorological data. Within the boundary layer these equations have the following form:

   - $w'^2 = 3.0 \, u_*^2 (1 - z/Z_i)^{3/2}$
   - $u'^2 = 4.0 \, u_*^2 (1 - z/Z_i)^{3/2}$
   - $v'^2 = 4.5 \, u_*^2 (1 - z/Z_i)^{3/2}$

   where the turbulence is a function of the friction velocity, height, and boundary layer depth. The horizontal and vertical components are explicitly predicted when using this method.

2. The other turbulence computation is an older approach that follows the Beljaars-Holtslag equations parameterized in terms of the vertical diffusivity for heat:

   - $K_h = k \, w_h \, z \, (1 - z/Z_i)^2$

   where the stability parameter w_h is a function of the friction velocity, Monin-Obukhov length, and convective velocity scale:

   - $w_h = f(u_*, 1/L, w_*)$

   The vertical diffusivity profile is converted to a turbulence value:

   - $\sigma_w = (K_h / T_L)^{0.5}$

   assuming a constant value for the Lagrangian time scale. The horizontal turbulence components are computed by assuming that they are equal to the vertical components:

   $$w'^2 = u'^2 + v'^2$$

   To configure this calculation, open [Menu #7](#) and select the **Beljaars-Holtslag** radio-button for vertical turbulence. Save all menus to exit, run the model, and then run the previously saved display batch file and open the [resulting](#) graphic which shows a much narrower plume than the default calculation. The primary reason for this is that the turbulence is partitioned equally between the vertical and horizontal, while in the default calculation more turbulence goes into the horizontal component [3.0/(4.0+4.5)].

3. Another alternative is to use the meteorological model's Turbulent Kinetic Energy (TKE) field if that variable is available. In this case the turbulence components are derived from the definition of the TKE

   - $E = 0.5 \, (u'^2 + v'^2 + w'^2)$

   and the relationship between the components is either defined by the Kanthar-Clayson

equations or the turbulence aniosotropy factor: w' / (u' + v').

To configure this calculation, open Menu #7 and select the **Met model TKE field** radio-button for vertical turbulence. Save all menus to exit, run the model, and then run the previously saved display batch file and open the resulting graphic which shows a tracer cloud with dimensions more similar to the default Kanthar-Clayson approach than the Beljaars-Holtslag.

4. The TKE field only provides information about the total turbulence and the turbulence partition between the vertical and horizontal components must be defined (the anisotropy ratio). The default is to assume a value of 0.18. To test the sensitivity of the calculation to this parameter, open Menu #7 and change the anisotropy factors from 0.18 to **0.05**, an extreme change to illustrate its effect upon the calculation. Save all menus to exit, run the model, and then run the previously saved display batch file and open the resulting graphic which shows a slightly more circular plume but still very similar to the original calculation. The reason for this is that horizontal dispersion is not just a result of horizontal turbulence, but also of particles mixing to different levels with winds at different speeds and direction. An examination of the vertical mass profile shown in the MESSAGE file reveals that the 0.18 factor results in a plume that reaches 4 km rather than 2 km when the factor was 0.05.

5. Another way to approach the anisotropy issue is to use a different method to compute the horizontal turbulence. The default approach is to compute the horizontal turbulence as defined in the above approaches. However, the horizontal turbulence values can be replaced by a value computed from the deformation of the velocity field:

   ○ $K_{hor} = 2^{-0.5} (c\ X)^2 [(\partial v/\partial x + \partial u/\partial y)^2 + (\partial u/\partial x - \partial v/\partial y)^2]^{0.5}$

   To configure this calculation from the original default calculation, open Menu #7, press the **Reset** to set previous changes back to their defaults, and then select the **velocity deformation** radio-button for horizontal turbulence. Save all menus to exit, run the model, and then run the previously saved display batch file and open the resulting graphic which shows a narrower plume using the Kanthar-Clayson, more similar to the Beljaars-Holtslag calculation. In general the deformation approach should not be used for simulations where the grid spacing of the meteorological data under-samples the variations in the flow field (grid too coarse) because then the deformation provides no information about sub-grid scale turbulence.

The results shown here provide some rationale for the the default vertical and horizontal turbulence settings used in the model calculation, which has been shown to provide an excellent representation of the initial tracer cloud mixing. The turbulence options are intended to provide some flexibility when using different input meteorological data.

Stability Computation Method

The base calculation from the previous sections used the turbulence computation defaults. One of these defaults was to compute the atmospheric stability using the model predicted fluxes of heat (H) and momentum (M). The stability estimate, expressed as a Monin-Obukhov length, determines the magnitude of the turbulence associated with that stability. Most of the meteorological data files contain estimates of the fluxes, however if these fields are missing there is an option to use the vertical profile of wind and temperature to estimate the stability.

1. The default computation uses the momentum flux to the surface (M) to compute the friction velocity, the sensible heat flux (H) to compute the friction temperature, and the mixed layer depth to compute the convective velocity scale. Using these three values, the height normalized Monin-Obukhov (z/L) stability parameter is computed.
   - $u_* = (\ M\ /\rho)^{0.5}$
   - $t_* = -H\ (\rho\ C_p\ u_*)^{-1}$
   - $w_* = \ g\ u_*\ t_*\ Z_i\ T^{-1}\ ^{1/3}$
   - $z/L = Z_2 k\ g\ t_*(u_*^2 T_2)^{-1}$

2. When no fluxes are provided by the meteorological model, z/L can be estimated from the wind and temperature profiles by first computing the bulk Richardson Number from the two lowest data levels and the z/L can be computed using several different functional forms that depend upon the stability.
   - $R_b = g\ \Delta\theta\ \Delta Z\ \{\theta_{12}\ [(\Delta u)^2 + (\Delta v)^2]\}^{-1}$
   - $z/L = f(R_b)$

The plume prediction should be recalculated using the wind and temperature profile by opening *Configuration Setup / Concentration / Turbulence Method* Menu #7, press **Reset** to set previous changes back to their defaults, and then select the **Computed from U/T profile** radio-button for the boundary layer stability section. This calculation will take considerably longer than the default calculation because there is greater puff splitting in this calculation. When the run has completed, execute the display batch file and open the resulting graphic which shows a much longer and slightly wider plume with correspondingly lower concentrations. Examination of the *MESSAGE* shows the tracer to have mixed much higher into regions of faster winds causing the puff splitting without the opportunity for puffs to merge.

In this case using the wind and temperature profiles to compute stability caused a significantly different calculation result. Stability from profiles are instantaneous values valid at the model time step, while flux derived stabilities are based upon time-averaged heat and momentum fluxes. There is no single right answer that applies to all data files but it depends upon the frequency of the meteorological data and the time duration of the flux integral.

3. There is one other option in this section. Normally the vertical turbulence profile varies with

height, approaching zero near the ground, increasing to a peak in the mid-boundary layer, then decreasing again to the top of the mixed layer. This is the default approach. However, the height varying profile can be replaced by a single boundary layer average value. This approach would only be used when trying to configure the model to match the Gaussian analytic solution, where the vertical diffusivity is constant with height. The effect of this change can be compared with the default (press **Reset** first) by selecting the [Menu #7](#) radio-button **Replaced by PBL average**, save, run the model, display script, and then the resulting [graphic](#) shows a very similar result to the default calculation.

The results shown in this section suggest that there may be considerable sensitivity to the selection of how the stability is computed from the meteorological data. They key is understanding the sources of the data and their limitations. For instance, hourly fields generated by a mesoscale meteorological model may show more similarity between the flux and profile calculation that computations performed using regional or global model output that may only be available at 3- or 6-h intervals.

Mixed Layer Depth Calculation

From the previous sections, we found that both the computation of the stability and the estimate of the resulting turbulence was a function of the mixed layer or boundary layer depth (used interchangeably in these discussions). The default approach is to use the mixed layer depth that is output from the meteorological model. This field is not always available and if missing, the depth is computed from the temperature profile as the height at which the potential temperature exceeds the surface temperature by two degrees. The mixed layer depth can also be estimated from the TKE profile as the height when the TKE value first becomes less than 0.20.

1. To compute the plume using a different mixed layer depth method, open menu #7 and check the radio-button (press **Reset** first) marked From Temperature Profile, save the change, run the model, the display batch file, and then compare the resulting plume with the base calculation. It is narrower and the air concentrations are much higher.

2. Repeat the above sequence again, but this time select Compute from TKE Profile radio-button from Menu #7 and the resulting plume shows a concentration pattern very similar to the previous calculation.

3. During the earlier trajectory analysis discussion, we determined that the mixed layer depth for this case was 1756 m. We can force the calculation to use a constant mixed layer depth by setting the Set as Constant radio-button and entering the value **1750**. The button highlight will disappear when the value is changed from its default, but the calculation will use this value and not unexpectedly the resulting plume looks very much like the base calculation.

4. To contrast the previous calculation, reduce the mixed layer depth to half its previous value. Change the Set as Constant field to **875**, rerun the model, and now the resulting plume is a little smaller, but nowhere near a factor of two smaller in area. However at any one location, air concentrations may be a factor of two higher only if the original plume growth was restricted by the mixed layer. The mixed layer depth directly affects air concentrations but the effect on the plume size is more indirect, related more to other factors such as the wind shear through the depth of the plume.

In summary, the results show that the magnitude of the air concentration prediction is directly proportional to the mixed layer depth. However, this conclusion only applies in situations of strong vertical mixing, when the particles interact with this mixing boundary. The effect on plume size depends upon how much the wind direction and speed change with height. If there is little wind shear with height, then plume size will be much less sensitive to vertical mixing.

Puff Growth Simulation

HOME

There are a few namelist file options left in menu #7 that are more appropriate for certain customized applications. One of these would be when dealing with user defined data files, an example of which should have already been created in the working directory: *stndata.bin*. This file contains only the minimum number of meteorological fields required to run HYSPLIT.

1. Recall from the previous sections that the puff growth is computed from the velocity variances,

   ○ $d\sigma_h/dt = \sigma_u$

   a field which is not available in most meteorological model output files and must therefore be computed from the atmospheric stability and various turbulence parameterizations. However, a stability value was defined when the *User Defined* data file was created. This stability was immediately converted to a velocity variance using an empirical relationship that matched each stability category with a wind fluctuation. Therefore, to use this data file, open the *Concentration / Setup Run* menu and clear the meteorology file and *Add Meteorology File* and select stndata.bin. Save and then open the *Configuration Setup* menu #7 and select (press **Reset** first) the measured variances radio-button. Save, exit, run model and the display batch file, to see the graphical result. In this simulation, the wind speed and direction were constant with height throughout the boundary layer, and the resulting narrow plume illustrates the importance of wind variation to plume growth.

2. These constant wind simulations would not normally be applied over such long distances, but at much shorter ranges where the stability as well as the winds would not be expected to change. In these circumstances, it might be desirable for the plume growth to more closely match the empirical estimates that are found in published plume growth graphs. Most of these indicate a growth with time to a power of slightly less than one. This relation can be expressed in differential form and applied in the model calculation.

   ○ $\sigma_h = \sigma_u T^{0.9}$

   ○ $d\sigma_h/dt = 0.9\ \sigma_u\ dt\ /\ T^{0.1}$

   Open menu #7 and select the empirical puff growth, leave the other settings as before, save, run, and display the graphical result. The plume width appears to be about 50 km, which suggests a "σ_y" of about 10-15 km ($4\sigma \sim$ 95th percentile), consistent with published values, but much smaller than the reality indicated by the aircraft sampling.

The various parameter sensitivity tests reviewed in the last few sections probably leave a residual sense of uncertainty as to the best approach to use in a particular situation. However, these simple test results were only compared to a few samples at one downwind distance. The best approach is to at least run each test through the entire experiment and then the results should be compared to the measurement data as was discussed in the utility program tutorial.

Working Directory Cleanup

With all the simulations completed up to this point, the *working* directory may have become very cluttered, perhaps making it difficult to find specific files. If you have not already been managing your data files, then there is already a simple procedure built into the GUI to help with this process.

1. Press the *Advanced [Cleanup Working](#)* menu tab, which then opens a [system message](#) asking if the working directory can be renamed with a randomly generated suffix, in this case to *working.357*. If the number is acceptable, then *Continue*, which will rename the directory and close the GUI.

2. Now re-open the GUI from the desktop icon and a new *working* directory will be created with the minimum number of required files and the install directory *c:\hysplit4* will contain the new directory and all the previous [renamed directories.](#) On UNIX/MAC systems, change to the new directory and manually create the softlink (*ln -s ../guicode/hysplit4.tcl hysplit4.tcl*) before restarting HYSPLIT.

This process can be used as each tutorial section is completed and the directory renamed from its random assigned value to one more representative of its contents. Exercise caution in deleting renamed directories because the original installed working directory also contains two sample meteorological data files that are part of the standard installation.

Meteorological Grid Ensemble

The uncertainty of the concentration calculation can be addressed in similar way in which we earlier addressed trajectory uncertainty, by slightly offsetting the meteorological data to test the sensitivity of the advection calculation to the gradients in the meteorological data fields. Start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu. Note that these files may now be in your archived working directory as well as the \Tutorial\files directory.

1. Recall from the trajectory discussion that the internal grid offset is in the horizontal and vertical. Therefore, to take full advantage of the ensemble, the release height should be changed to **200** m from the *Setup Run / Starting Locations* menu. Also to reduce the number of output frames, open the grid menu and change the averaging time from 03 to **06** hours and the sampling start time from 18 to **21** to line up the model output times with the majority of the measurement data.

2. Open the *Advanced / Configuration Setup / Menu #4*. Because the GUI script will cycle through 27 simulations, we can speed up the calculation by reducing the particle release number from 50000 to **25000**. Then save to close all menus.

3. To start the model simulation (this calculation may take some time: ~1 hr), press the Special Runs / Ensemble / Meteorology menu tab and accept the prompts to continue and when finished, close the ensemble complete menu. The calculation results are saved to the *\working* directory and the base output file name, *hysplit2.bin* is appended with a simulation sequence number from **.001** to **.027**.

4. To analyze the simulation results, a special pre-processing program needs to be run. Press the *Display / Ensemble / View map* menu tab. This opens up the ensemble display menu. The upper part of the menu is used to change how the input data files are processed. In the middle section, change the output selection option *Concentration at Percentile* from its default 95% to **50%**. This means that the output maps will show the median concentration of all the ensemble members. There is one graphic for each time period. If you set the aggregation period from 1 to **10**, then all the time periods are included in the statistic and you only get one plot covering all times. If no plot is produced, your binary output files may not contain all 10 output time periods. Otherwise, reset the aggregation period back to **1** when finished.

5. The *View Map* processing of the ensemble output files leaves a variety of different files (prob??, cmax??, cmean) in the *working* directory. These files were previously displayed as maps (using concplot) or they can be displayed as box plots. Start from the *Display / Ensemble / box plot* tab. This opens a simple menu where you can set the location of the data extraction point. Use the same location, sampler 510 (Little Valley, NY), that we examined in the concentration utility tutorial by entering **42.25 -78.80**, then *Execute Display*.

6. The resulting box plot shows the ensemble concentration predictions at Little Valley for each 6-hr averaging period during the simulation. The box bottom and top shows the 25th and 75th percentile concentrations, the single lines the 10th and 90th percentiles, and the circles the 5th and 95th percentile concentrations. The plus symbol and middle line show the mean and median concentrations. Note there are no unit conversion options for any of these programs so the results are all shown as g m^{-3}. An additional graphic with the same axis labels is also created that shows the individual member concentrations indicated by member number.

7. To relate the box plot with the original graphic of median concentrations, the median box plot concentration on the 26th between 15 and 21 is perhaps 7x10^{-10}. Examining the graphic at *42.25 -78.80* shows the location to be in the blue (10^{-10}) region very close to the yellow (10^{-9}) contour.

8. To view how the measured data fall within the ensemble estimates, we can overlay the data points on the boxplot. In the concentration utility tutorial we created a file with just the measurements from station 510 for display purposes. Unfortunately, the box plot program has no overlay capability, but we can manually (using paint after converting the image to BMP) add the measurements to the box plot graphic after converting the numbers from pg back to g. Two of the three highest measured concentrations correspond with the smallest uncertainty range. Note that 10^{-11} is approximately the detection threshold for the measured concentrations. Values lower than this are effectively zero. The ensemble also provides an estimate of the potential maximum concentration.

There are many causes of concentration uncertainty, such as how the well the meteorological data represent the true flow field, errors in the parameterization of physical processes in the model, and even the effects of atmospheric turbulence not accounted for by the model. In this case we looked at the data issue. In the subsequent sections we will explore the other factors.

Turbulence Ensemble - Random Variations

Another component of the uncertainty in the concentration calculation is the contribution of random motions by atmospheric turbulence. The model already computes this turbulence when computing particle dispersal. However, normally we would try to release a sufficiently large number of particles to insure that each simulation gives similar results. In the turbulence ensemble approach, we reduce the particle release number and run multiple simulations, each with a different random number seed, and then examine the variations between simulations. Start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu.

1. After the *Setup Run* and the *Advanced Configuration* menus have been retrieved, open the *Advanced / Menu #4* and change the particle release per cycle from 50000 to **2500**. Although the turbulence ensemble can be composed of any number of members, to parallel the meteorological grid ensemble, 27 variations are also run in this case. The 2500 is determined by dividing 50000 by the number of members to maintain about the same total particle number when computing the mean concentration.

2. After saving the change, press the *Special Runs / Ensemble / Turbulence* menu tab. There are no data entry options, just a prompt menu to ask if you really want to continue with the ensemble turbulence calculation. The calculation will start and as each member calculation is completed, a message is added to the simulation log and finally a completion message when member 27 finishes.

3. Following the same procedure as previously with the meteorological ensemble, select the *Display / Ensemble / View Map* menu tab. This step is required to display probability maps or box plots because it invokes the pre-processor step that creates the probability files from the individual concentration simulations. Display any map and then open the box plot menu and enter the same position **42.25 -78.80**, sampler 510 (Little Valley, NY), used in the previous section.

4. The resulting box plot with values every 3-h rather than every 6-h as in the previous example, shows that for two periods with the highest concentrations, the 90th percentile concentration uncertainty range (5th to 95th) is about a factor of four.

The approach shown here, using the model's random number generator, provides some guidance as to how much variability might be introduced by atmospheric turbulence. On your own, try two additional simulations, one with a greater particle release rate and another with an even smaller release rate, and view the effect on the concentration uncertainty at sampler 510.

Physics Ensemble

Another component of the uncertainty in the concentration calculation is the variation that can be introduced by using different physical parameterizations, or model options. Most of these were already reviewed in the concentration modeling introductory sections. The model normally runs with its default options, unless a *SETUP.CFG* namelist file is created in the *Advanced / Configuration* menu section. Although various physical parameterization options were exercised in the introductory sections, the actual namelist parameters or their values were not addressed. These details are usually available through the context sensitive *HELP* menu button in each GUI. In the model physics ensemble section, a script is run that automatically sequences through the most common parameter variations. This automated process will be reviewed in this section. Start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu.

1. *The Special Runs / Ensemble / Physics* menu will sequence through 20 different calculations stating with the 3D-particle option, Gaussian puffs, Top-Hat puffs with linear growth, Top-Hat puffs with the empirical growth rate, variations in how the mixed layer depth is calculated, setting fixed mixed layer depths: 500, 1000, 1500 m, various turbulence and stability equations, varying the ratio of vertical to horizontal turbulence, and varying the Lagrangian time scale.

2. The physics ensemble menu will stay open as long as the model is running. WARNING - it may take 2 hours or more to finish all 20 simulations. Press **Execute Script** to start the process. As each simulation completes, the name and value of the namelist variable will be shown in the text box. The following variations are programmed in the script:

   - {file}.001 : initd = 0 initial distribution is particle (default=0)
   - {file}.002 : initd = 3 distribution gaussian horizontal-puff vertical-particle
   - {file}.003 : initd = 4 distribution top-hat horizontal-puff vertical-particle
   - {file}.004 : kpuff = 1 empirical puff growth rate (default=0 linear)
   - {file}.005 : kmixd = 1 mixed layer from temperature profile (default=0 input data)
   - {file}.006 : kmixd = 2 mixed layer from TKE
   - {file}.007 : kmixd = 500 use a constant 500 m for mixed layer
   - {file}.008 : kmixd = 1000
   - {file}.009 : kmixd = 1500
   - {file}.010 : kmix0 = 125 mimimum mixing depth (default=250)
   - {file}.011 : kzmix = 1 vertical mixing PBL average (default=0 use profile)
   - {file}.012 : kdef = 1 horizontal turbulence from deformation (0 = scale to vertical)
   - {file}.013 : kbls = 2 stability derived wind/temperature profile (default=1 fluxes)
   - {file}.014 : kblt = 1 use Beljaars turbulence parameterizations (default=2 Kanthar)
   - {file}.015 : kblt = 3 use TKE field for turbulence (default TKER=0.18)
   - {file}.016 : tker = 0.36 double vertical turbulence TKER = w'2/(u'2+v'2)
   - {file}.017 : vscale = 100.0 vertical Lagrangian time scale (default = 200 sec)
   - {file}.018 : hscale = 5400.0 horizontal Lagrangian time scale (default = 10800 sec)
   - {file}.019 : vscale = 400.0

- {file}.020 : hscale = 21600.0

3. When the last simulation has finished, the [calculations complete](#) message will be shown. Then go to the *Display / Ensemble / View Map* menu and select the 90th percentile map and page forward to the 27th from [0000-0300](#) which shows a value greater than 10^{-9} near sampling station 510, Little Valley, NY.

4. Now open the *Box Plots* menu and set the location for station 510 to **42.25 -78.80** which will show the [box plots](#) time series. The plot for the 27 03 (27th 00-03) shows the 90th percentile concentration (upper horizontal line) to be about 3×10^{-9}, within the range shown on the map for that location. What the 90th percentile value means is that only 10% of the ensemble members (about 3) have concentrations greater than that value at that location.

5. To determine which members produced the highest concentrations, look closely at the second graphic, the ensemble [member plot](#), which shows that members 5, 6, and 7 produced the highest concentrations at that time period. (HINT - right click on Postscript files to zoom). These were the simulations where the mixing depth computation was manipulated. As the script is running, the namelist variations for each member are written to the file [ensemble.txt](#).

The results shown here represent a wide range of model options. The physics ensemble script (*\hysplit4\guicode\conc_phys.tcl*) could easily be customized for different model options depending upon the problem under consideration. As should be more obvious by now, there is never going to be just one right answer due to limitations in how well the meteorological data represent the true flow, variability from atmospheric turbulence, and how well the model parameterizations capture these processes.

Ensemble Multiple Meteorological Data

The last ensemble that can be created is to run the dispersion simulation with different meteorological data files. There is no one-click option through the GUI. Each simulation must be configured manually, but the GUI can be used to analyze the products. As in all the previous ensemble sections, start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu.

1. Before running a simulation, we should delete all the ensemble files left over from the previous sections. There is a *Special Runs / Ensemble / cleanup* tab that opens the menu. There are no options, just press **Execute Script** and all ensemble related files will be deleted from the working directory. Only the model output concentration files with the root name set in the *Grid* menu with the *.000* suffix will be deleted.

2. Before starting the base simulation using NARR, open the *Setup Run / Grid Menu* and change the output file name from hysplit2.bin to **hysplit2.001**. The suffix will be manually incremented with each new simulation, following the same procedure used in the automated ensemble scripts. Save the changes and run the model. Once the simulation has completed, open the *Concentration / Utilities / Convert to DATEM* menu and as before select the measured data file, create the DATEM file, and finally **Compute Statistics**. Then rename the statistical results file, statA.txt, to a unique file name.

3. Now repeat the same process with each of the other three meteorological data file, giving the output file and resulting statistical file a unique names:

   - hysplit2.001 :: captex2_narr.bin ... statA_narr.txt
   - hysplit2.002 :: captex2_era40.bin . statA_era40.txt
   - hysplit2.003 :: captex2_gblr.bin .... statA_gblr.txt
   - hysplit2.004 :: captex2_wrf27.bin .. statA_wrf27.txt

4. When all the simulations have been completed, open the *Setup Run / Grid Menu* and rename the output file from hysplit2.00? to just **hysplit2**. The base name will then be passed through the GUI to the ensemble scripts, where the programs automatically search for the 3-digit suffix. Save the changes, run the *Display / Ensemble / View Map* to generate the probability files, then create the boxplot at Little Valley, NY (42.2N 78.8W). With only four members, it is not surprising that except for one time period, the concentration variations are larger than in the previous ensemble examples for this location. A view of the member plot shows that simulation 002 (the ERA40) gave the highest concentrations.

5. Although there are a variety of possible metrics, the correlation coefficients for each of the simulations

   - 0.51 NARR
   - 0.79 ERA
   - 0.62 GBL

- 0.68 WRF

suggests that the best performance is when using ECMWF meteorological data fields. Now in most modeling situations, we usually don't know the correct answer. One approach is to use the ensemble mean concentration for the simulation. This field has already been computed in the *View Map* step.

6. Then open the *Utilities / Setup Run / Grid* menu and change the base name from hysplit2 to **cmean**. The open the *Utility / Convert to DATEM* menu and run the statistical analysis for the ensemble mean, which shows a correlation of **0.81**, a better performance than any of the other ensemble members. A similar, but more qualitative comparison, can be made for the scatter plots, with the ensemble mean plot also showing excellent results.

The results shown here suggest that a practical application for ensemble products may be simply to compute the ensemble mean and use that as one would a single deterministic simulation. It might be an interesting exercise to go back to some of the previous ensemble examples and perform a similar analysis.

Linear Transformation of Pollutants

Normally when multiple pollutants are defined, each pollutant is released on its own particle and different pollutants cannot interact with each other because they follow different transport pathways. However, there is an option for a simple linear transformation from one pollutant to another by defining multiple pollutants on the same particle. The multiple pollutant single particle option should only be invoked when the pollutants have comparable transport characteristics.

1. Start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu and re-run the simulation if the results have not already been saved from one of the previous exercises. Create the concentration contour plots as before and save the graphical results to a unique file name as a reference to compare with the transformation simulations. This and all subsequent sections under pollutant transformations are just a theoretical exercise because the PMCH tracer used in CAPTEX is inert and does not deposit.

2. The pollutant transformation computation only requires defining an hourly conversion rate. The pollutant mass fraction converted each time step (β) is computed directly from the conversion rate (R) which has a default value of 0.10 hr^{-1}:
   - $\beta = R \, \Delta t$

   The mass (M_r) removed from pollutant M_1 when $\beta < 0.01$
   - $M_r = \beta \, M_1$

   but when $\beta > 0.01$
   - $M_r = (1 - \exp^{-\beta}) \, M_1$

   In each case, the mass on pollutant M_2 is increased by
   - $M_r \, W_2/W_1$

   where W_2/W_1 is the ratio between the molecular weights of the two pollutants. 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 as SO_2 and and #2 as SO_4, then the molecular weight adjustment factor should be set to 1.5 as SO_2 transforms to SO_4 (the conversion picks up two additional oxygen molecules).

3. To demonstrate the conversion calculation, open the *Setup Run* menu and then open the pollutant menu from the *Pollutant, Deposition, Grid* tab. At the top of the *Pollutant* column, change the num=1 to **2**, which then populates the Specie 2 sub-menu with the values from Specie 1 (PMCH). Click on *Specie 2* to open the emission rate menu and change the pollutant name from PMCH to **POL2**, and change both the emission rate and duration to **0.0**. We could emit both pollutants and transform them at the same time, but for this example, POL2 mass will only come by conversion from Specie 1.

4. Now open the *Advanced / Configuration / menu #10* conversion modules and select the 10% per hour radio-button. It is only necessary to define two different pollutants in the concentration setup menu and select the 10% /hr option. This combination automatically sets *MAXDIM=2* in the model code and calls the transformation routine every time step to convert pollutant #1 to #2 at a rate of 10% per hour. If more than two species are defined, then the single particle mass dimension needs to be explicitly set in the menu (last data entry line). Now save the changes and run the model.

5. After the simulation has completed, open the *Display / Concentration / Contour* menu. The menu now shows the two pollutants as display possibilities. First change the default Postscript output file name from its default concplot to a unique name, such as **pmch**. The .ps suffix is added automatically. Then select the **PMCH** radio-button as the pollutant to display. As in previous examples, set the **pg** units conversion to **1.0E+12** and increase the zoom to **80%**, then *Execute the Display*. You could also un-select the *View On* check-box because right now we only want to create all the Postscript files. The viewer is not yet required. Once the PMCH Postscript file has been created, change the options, and create another file for **POL2**.

6. Rather than going through a frame-by-frame comparison of the 3-hour PMCH and POL2 concentration averages (the plumes must cover identical regions because both pollutants are on the same particle), just find the maximum concentration on each graphic (printed toward the bottom of the contour labels text box), and note the value for each time period for the first 24 hours, for the base simulation with no transformation, the PMCH, and POL2 calculation. These values are also shown below and may differ slightly from your values due to differences introduced from the hardware/software dependent random number generator driving the 3D particle dispersion.

Day/Time	Base	PMCH	POL2
25/18-21	440000	350000	83000
25/21-00	130000	81000	52000
26/00-03	56000	27000	29000
26/03-06	50000	18000	34000
26/06-09	42000	11000	30000
26/09-12	32000	5900	25000
26/12-15	33000	4800	29000
26/15-18	25000	2600	23000

    The results show how much more rapidly the PMCH concentrations decrease above the base simulation due to the additional conversion and correspondingly the POL2 concentrations show only a small decline as decreasing concentration due to dispersion is compensated by increasing mass due to the conversion from PMCH. After 24-h into the simulation, the POL2 concentrations are comparable to the base calculation because most of the pollutant has been converted. As an independent exercise, rerun the display, but this time select pollutant **All**, which will add together all the pollutants prior to display, which will result in concentrations similar (but not identical due to rounding and interpolation errors) to the base calculation. Another exercise can be to select the fixed contour (**Fix-Exp**) rather than the dynamic contour radio-button. With this option the contours are not rescaled with each plot and stay the same between time periods, which will more dramatically illustrate the decrease of PMCH concentrations compared with POL2.

7. Normally other conversion rates or a greater number of pollutants are required for more realistic simulations. In these situations it is necessary to create a *CHEMRATE.TXT* file in the local directory. This file consists of one or more records, where each record defines a pollutant conversion. The data are free-format and consist of four fields, the integer "from" and "to" pollutant index (specie) numbers, the real hourly conversion rate, and molecular weight adjustment factor. For instance, a file representing the default conversion would consist of the following single line:

    o **1 2 0.10 1.0**

    Try creating the CHEMRATE.TXT file and running the conversion with a different conversion rate.

The HYSPLIT pollutant transformation option is not intended to replace the need for more complex chemical models that account for the non-linear simultaneous interaction of multiple pollutants, but to provide some first-order guidance as to the potential effect of transformations that can be represented by just a few pollutants. There are some advanced chemical modules available for HYSPLIT that have been developed for specific applications. However, all of these are beyond the scope of this tutorial.

Pollutant Dry Deposition

The term dry deposition in the context of how it is implemented within HYSPLIT refers to the depletion of pollutant mass from gases and particles when they interact with the ground surface in the absence of rainfall. Gases or particles within the surface layer will loose mass at a rate proportional to the deposition velocity. Also particles (but not gases) will gravitationally settle downward toward the surface where they can then be subject to dry deposition.

1. Naturally all the calculations in this section are just examples because the PMCH tracer does not deposit. Start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu. We will only focus on the first day's results, so set the run duration to 25 h and and re-run the base case simulation. Follow the same process as in the previous section and note the maximum concentration for each of the first eight time periods. Save the MESSAGE file to a unique name. From the MESSAGE file, note that at the end of the 25-h simulation the system mass is still 200968 grams with the profile showing about 18% of the mass within 200 m of the ground.

2. The dry deposition velocity is defined as the ratio of the deposition flux (mass/area/time) to the air concentration (mass/volume):
   - $V_d = D_{dry} / C$

   Dry removal is computed when the bottom of the puff or the particle center position is within the surface layer (Z_{sfc}), defined in the model as the top of the second meteorological data level. The deposition velocity can be expressed as a time constant:
   - $\beta_{dry} = V_d \, \Delta Z_{sfc}^{-1}$

   The total deposition from all removal processes can be expressed in terms of the time constants. The time constants can be added and hence the total deposition for particle mass m over a time step becomes:
   - $D_{dry} = m \, \{1 - \exp[-\Delta t \, (\beta_{dry} + \beta_{...})]\}$

3. To compute gaseous dry deposition, open the *Setup Run / Pollutant-Deposition-Grids / Deposition* menu and change the deposition velocity, the first number in the second line, from 0.0 to **0.01** (1 cm/s a relatively high removal rate). The other entries on this line will not be discussed here but are required if the resistance method is going to be used to compute the deposition velocity instead of explicitly setting a value. One other change is required. To be able to view the deposition amounts, rather than just its effect on air concentration, a deposition level needs to be added to the concentration grid.

4. Open the *Setup Run / concentration grid* menu and change the number of vertical levels from 1 to **2** and add the level height of **0** preceeding the 100 on the height of levels line. The deposited mass will be accumulated on level zero. Save the changes and run the model. When it completes, open the display menu and insure that the bottom level radio-button for height **0** and top-level height **100** is selected. On the deposition multiplier line check the

Total radio-button. This will show the deposition accumulate between sampling time periods rather that just showing the deposition for each time period. As in all previous examples, set the concentration multiplier and units label.

5. Execute the display and sequence through each frame and note the maximum concentration each time period. The last time period shows a maximum concentration of 5900. The total deposition frame is at the end and shows the deposition footprint as the plume passed over the region. Check the MESSAGE file which shows a mass of 109328 grams and only 9% of the mass within the three lowest model levels. The non-depositing run showed a maximum concentration of 25,000 at the end of the run. With half the mass lost to deposition and the lowest layers showing the greater mass losses (9% versus 18%), deposition accounts for the factor of 4 decrease in the maximum concentration.

6. To configure the simulation for particle deposition, it is necessary to define the particle's characteristics. The particle settling velocity (V_g) is calculated for a spherical particle from the particle diameter (d_p), air density (ρ), and particle density (ρ_g):

   - $Vg = d_p{}^2 \, g \, (\rho_g - \rho) \, (18 \, \mu)^{-1}$

   Open the *Setup Run / Deposition* menu and set the particle diameter, density, and shape all to **1.0**. Setting these to non-zero values defines the pollutant as a particle rather than a gas. Getting the density and diameter correct is essential in computing the correct settling velocity. However, for this exercise we will take a shortcut and force the model to use a fixed value, regardless of the particle settings. This means that the previously entered value of **0.01** (1 cm/s) will be used to compute the deposition, but more important this value will be added to the vertical velocity in the particle trajectory advection computation. Save the changes and run the model.

7. When the run completes, display the concentrations and note the maximum value each time period. At the end of the run the maximum concentration is now 11000 rather 5900 at the end of the gaseous deposition simulation. Open the MESSAGE file and the end mass is now 70381 grams, considerably less that the gas run but the concentrations are higher. The answer lies in the profile, which shows 23% of the mass in the lowest three layers. Although the deposition rate is the same between the gas and particle run, the additional gravitational settling of the particles moves more mass into the lower layers, providing more mass to be removed, and counter-intuitively, higher concentrations near the surface, at least during the earlier time periods.

8. All the previous simulations ended with the same number of particles as were released. However, instead of 4 grams per particle, each may only end up with considerably less mass by the end of the simulation. There is alternative approach, where instead of removing a fraction of the particle's mass, we can compute the probability that a particle will deposit all of its mass and then only a fraction of the particles in the deposition layer will be deposited each time step. In this situation, if R is a random number from 0 to 1, then a particle will deposit if

   - $R < \beta_{dry} \, \Delta t$

   In this situation, the particle number goes down as the particles stick to the surface. To set this option, open the *Advanced / Configuration / Conversion Modules Menu #10* and set the **Deposit Particles …** radio-button. Save the changes and run the model. The simulation log will indicate that the *dry deposition probability* option has been selected. When the run

has completed, again note the maximum concentrations each time period. Note they are identical to the previous simulation. Open the MESSAGE file which shows a mass of 70572 grams but this time distributed over 18,000 particles (4 g/particle) rather than 50,000.

The maximum concentration simulation results are summarized in the table shown below.

Day/Time	Base	GAS	PART	PROB
25/18-21	440000	280000	360000	370000
25/21-00	130000	78000	87000	84000
26/00-03	56000	34000	34000	33000
26/03-06	50000	27000	32000	33000
26/06-09	42000	19000	24000	24000
26/09-12	32000	13000	17000	17000
26/12-15	33000	10000	17000	17000
26/15-18	25000	5900	11000	11000

Pollutant Wet Deposition

The term wet deposition refers to the removal of pollutants, both gases and particles, by condensation, or rainfall, either within a cloud or below the cloud. Naturally all the calculations in this section are just examples because the PMCH tracer does not deposit. As in the previous sections, start by retrieving the previously saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu. We will only focus on the first day's results, so set the run duration to **25** h and as was done previously for dry deposition, open the *Setup Run / concentration grid* menu and change the number of vertical levels from 1 to **2** and add the level height of **0** preceeding the 100 on the height of levels line. Then re-run the base case simulation without any deposition, wet or dry.

1. The wet deposition of gases depends upon their solubility and for inert non-reactive gases it is a function of the Henry's Law constant (H), the ratio of the pollutant's equilibrium concentration in water to that in air. A gaseous wet deposition velocity can be defined as
   - $V_{gas} = H\,R\,T\,P$

   where R is the universal gas constant, T is temperature, and P is the precipitation. Then the gaseous wet removal time constant can be defined:
   - $\beta_{gas} = V_{gas}\,\Delta Z^{-1}$

   Note that the wet removal of gases is applied at all levels from the ground to the top of the cloud-layer. The wet removal time constant is added to the other removal constants to compute the particle mass loss each time step.

2. Open the *Setup Run / Deposition* menu and set the wet deposition radio-button to **Yes** to populate the wet deposition removal parameters with their default values. For gases, the default value of 1.0E+5 is the Henry's constant for hydrogen peroxide (H2O2). The other two values on that line are ignored for gases. Save the changes, run the model, and after it completes, open the display menu and advance to the last frame showing the total deposition pattern. It shows two distinct rainfall areas near 41.5N 81.5W and 41.5N 79.5W. Looking at the individual time-period deposition patterns shows that wet removal ocurred on the 26th between 00-03 and 06-12. The MESSAGE file shows a total mass of 173006 grams at the end of the run.

3. Wet deposition of particles is divided into two processes, those in which the polluted air is continuously ingested into a cloud from a polluted boundary layer and those in which rain falls through a polluted layer. A scavenging ratio is assumed for pollutants located within a cloud layer and the scavenging coefficient is used for pollutant removal in rain below a cloud layer. At the grid points where it is raining, the cloud bottom is defined at the level when the RH first reaches 80% and the cloud top is reached when the RH drops below 60%. All removal amounts are adjusted by the fraction of the pollutant mass that is within the cloud layer.

4. For the wet removal of particles by within-cloud processes a scavenging ratio (S), which is the ratio of the pollutant's concentration in water to its concentration in air, is expressed as a wet deposition velocity,
   - $V_{inc} = S\ P$

   where the precipitation rate is given by P. The time constant for within-cloud removal,
   - $\beta_{inc} = V_{inc}\ \Delta Z^{-1}$

   where the average scavenging ratio is $S = 3.2 \times 10^5$ by volume, and as before, ΔZ is the depth of the pollutant layer. Different scavenging ratios can be defined for different pollutants. Below-cloud removal is defined directly as a rate constant, independent of the precipitation rate. The below-cloud removal constant (s^{-1}) is given by,
   - $\beta_{bel} = 5 \times 10^{-5}$

5. Open the *Setup Run / Deposition* menu and reconfigure the emissions for particles by setting the three values on the first line all to one. However, to avoid computing dry deposition, force the dry deposition to a very small value (1E-10) so that we can see the only the effects of wet deposition. Save the changes, run the model, and display the results. The final particle deposition pattern looks very similar to the gaseous pattern but with slightly less deposition. The MESSAGE file shows a total mass of 193846 grams at the end of the run.

6. Wet removal can be very effective when the pollutant is concentrated in one area as it would be near the source. As an example of this, move the starting location to the first precipitation area. Open the *Setup Run / new location* menu and enter the position **41.5 - 81.5** and change the starting time to **83 09 26 00**. Save the changes and run the model. There is no need to display the results, but open the MESSAGE file, which shows a mass of 151163 grams after just 3-hours and 123382 grams at the end of the simulation. Essentially 25% of the mass released was deposited by the end of the release!

Dry deposition rates may be small but they occur everywhere at all times resulting in large losses over longer time periods, while large losses by wet deposition are limited to areas with rainfall and over much shorter time periods. However, model derived rainfall predictions may be very uncertain and access to observed precipitation such as from NASA TRMM may be useful in the interpretation of modeling results.

Radioactive Decay and Dose

In this section we're going to pretend the release consisted of radioactive particles which decay and deposit. The air concentration and deposition amounts will be converted to dose. Although we will try to make some reasonable assumptions, this is still a simplistic example of what can be a complex modeling problem. The details presented here should just be used as an example in configuring the model and not as a template for simulating a nuclear accident.

1. The decay of radioactive pollutants is treated the same way as transformation and deposition. The mass on a particle is reduced using the time constant approach:
   - $m_2 = m_1 \exp(-\beta_{rad} \Delta t)$

   In addition to the particle mass, deposited radioactive pollutants also decay, and hence deposition amounts are also reduced each time step. The decay constant for radioactive processes is defined by the half-life ($T_{\frac{1}{2}}$):
   - $\beta_{rad} = \ln 2 / T_{\frac{1}{2}}$

2. For the purposes of this example, we will assume a release from a hypothetical nuclear reactor located at the CAPTEX release point, essentially the same configuration we have been using for all the previous examples. Start by retrieving the saved *captex_control.txt* and *captex_setup.txt* settings into the GUI menu. We will assume that a 3000 MW (thermal) reactor that has been running for one year creates about 1.0E+17 Bq of Cesium-137 (and many other fission products). We also assume that 10% of the Cesium is released in the accident over a one-hour period.

3. To configure this release, set the run duration to **25** h, open the *Setup Run / Pollutant* menu and enter the **C137** label, release amount **1.0E+16**, and the **1.0** hour duration. Save the changes and open the *Setup Run / Grid* menu and change the name of the output file to **c137.bin**, and add the second level **0** for deposition. Then open the *Setup Run / Deposition* menu and check the Cs-137 radio-button to set the deposition defaults for Cesium. Save the changes and then run the model.

4. To convert the air concentration and ground deposition values into a number that can be more easily be related to health effects, we need to find the dose conversion factors for Cesium-137. For the airborne plume assume 3.4E-11 (REM/hr) / (Bq/m3) and 1.1E-12 (REM/hr) / (Bq/m2) for the deposited material. Because the air concentrations are three-hour averages, the air concentration dose conversion factor will be **1.0E-10** and if we compute the total deposition over 24 hours, then the deposition dose conversion factor becomes **2.6E-11**. Open the *Display / Contours* menu and enter the dose conversion factors. Before executing the display, the plot labels should be modified to reflect the changes. Just changing the units field in the menu to REM is insufficient because it will incorrectly show as REM/m3.

5. To make more complex changes to the graphics label, open the *Configuration Setup /*

Border Labels menu and enter **Cesium 137** for a new plot title, **Dose Equivalent** for the map type, and **REM** for the mass units into their respective text entry fields. Leave the other fields blank. Then save the changes and go back and execute the *Contour Display* menu and advance the frames to the end to see the one-day accumulated ground-shine dose map.

6. Because Cesium has such a long-half life, the deposited material will continue to be a problem for quite some time. The decay after one year is so small that we can compute the one-year ground-shine by multiplying the dose conversion factor by 8760 rather than 24 (9.6E-09). The accumulated dose becomes 365 times larger. The conversion factor could also be adjusted for the actual Cesium decay.

The example presented here was intended show the model can be configured for a radiological simulation. The emission and dose conversion values are only intended as examples and a guideline for an actual accident scenario, which is composed of a complex mix of short- and long-lived radionuclides. Other radiological simulations could also be configured with the model, but their complexity is beyond the scope of this tutorial. Although there are many public sites with radiological monitoring data, frequently these sites only show background values, except when there has been some event.

Converting Output to Mixing Ratio

In all previous examples, the pollutant release was specified by a mass emission rate and the resulting air concentrations by mass over volume. Another frequently used air concentration unit is a volume mixing ratio. This is especially common for gaseous pollutants where concentrations may be specified in units such as ppm (parts per million) or ppb (parts per billion). There is an option in the *Advanced / Configuration* menu to facilitate these conversions. All the original CAPTEX measured tracer concentration data were reported in units of fL/L (f=femto=1.0E-15) and were converted to mass/volume concentrations for model comparison applications.

1. First, the mass to volume conversion is based upon the perfect gas law (PV = nRT):
   - V/n = RT/P = (0.0821 L atm / K mole) * 273 K / 1 atm = 22.40 L/mole (at 273 K), then
   - POL [g/m3] = POL [L/L] * [g/mole] * (1/22.4) [mole/L] * 1000 [L/m3]
   - POL [g/m3] = POL [L/L] * [g/mole] * 44.64 [mole/m3]

   where L is liters and the conversion factor between mass and volume units is just based upon the molecular weight of the pollutant (POL). To compute the conversion factor for PMCH, which has a molecular weight of 350, from fL/L to pg/m3, substitute the following values:
   - PMCH [pg/m3] 1.0E-12 [g/pg] = PMCH [fL/L] * 1.0E-15 [L/fL] * 350 g/mole * 44.64
   - PMCH [pg/m3] = PMCH [fL/L] * 15.624

   One of the model options divides the pollutant mass by the air density prior to summing the mass to the concentration grid. This in effect replaces the constant temperature perfect gas law conversion with a dynamically changing value based upon height as well as temperature. The units of air density within the model are kg/m3, therefore if the pollutant emission units are in kg, the effect of dividing the pollutant mass be air density is the same as dividing the final air concentration kg-pol/m3 by air density kg-air/m3, resulting in a mass mixing ratio of kg-pol/kg-air. To convert the mass mixing ratio to a volume mixing ratio:
   - (liter-pol/liter-air) = (kg-pol/kg-air) * (kg-air/mole) / (kg-pol/mole) * (liter-pol/mole) / (liter-air/mole)

   Because the liters per mole is the same for all ideal gases, the conversion from a mass mixing ratio to a volume mixing ratio is simply proportional to the ratio of the molecular weight of air (29) to that of the pollutant. For the case of the PMCH tracer, the conversion factor to get the model simulation output in fL/L would be:
   - [fL/L] = 29/350 [L/L] * 1.0E+15 [fL/L] = 8.3E+13
   - or 8.3E+10 if the emissions are in grams rather than kg

2. To demonstrate the use of the model to generate mixing ratio output, go back and follow the instructions of the first two steps in the Case Study Base Configuration tutorial, where the results were compared to aircraft sampling data. Following those instructions, set the run duration to **13** hours and start the sampling at **83 09 26 03 00** so that only one output frame is created. Save the changes and open the *Advanced / Configuration / Conversion Modules Menu #10* and check the **Divide output by air density** radio-button. Save the

changes, and then run the model.

3. Before opening the display menu, we already know that the default label options are insufficient to describe this case. Open the borders label menu and set the mass units to **fL** and the volume to **/L**. The other descriptive fields are optional. Now open the *Display / Contour* menu and set the concentration multiplier to **8.3E+10**. Because we already know that the volume contours will be more than a factor of 10 less than the mass contours (15.6 to be precise), we can force a more realistic contour interval than the order-of-magnitude default. Check the **User Set** radio-button and enter **2000+1000+500+200+100** in the contour text field, then Execute Display.

4. Although the results look reasonable, it would be better to do a more quantitative comparison by showing the aircraft measurements in fL/L on the same graphic. The CAPTEX data report contains a tabulation of all collected samples in fL/L. To save a little time, the relevant data were transcribed to the file data_orig.txt in the \Tutorial\captex directory. This is identical to the data file that was used in the case study tutorial, except sampling units are in fL/L. Copy this file to the \hysplit4\working directory and edit the concplot batch file that was created to include the option **-q***data_orig.txt*. Run the script and the resulting graphic shows an excellent correspondence between model and measurements in the native reporting units.

A model feature was demonstrated that facilitates the conversion of model output air concentration units from mass/volume to either mass or volume mixing ratios. On your own try a more realistic example, perhaps for SO2 with emissions in kg and output in ppm. For instance, the Kilauea volcano in Hawaii emits about 2000 tons of SO2 per day. Assuming no conversion to SO4, what concentrations might be expected?

Emissions from a Known Location

In this section we will use the measurement data to estimate the magnitude of the emissions assuming we know the location of the source. Start by retrieving the previously saved *captex_control.txt* and captex_setup.txt settings into the GUI menu.

1. To simplify the example and produce results more quickly, we will only use the sampling data from the 3-hour duration collections. These occurred from 18Z September 25th to 12Z September 26th. Therefore, in the *Concentration / Setup Run* menu, change the run duration to **19** hours. Save to close and exit all menus.

2. Run the model and when the simulation completes, open the *Convert to DATEM* utility menu and browse for the measured data input file of the 3-hour duration data. You could manually create a subset from the master file captex2_meas.txt, but for convenience, this file is already provided ..\captex\captex2_3hr.txt. Then as in previous sections: create DATEM file, compute statistics, and open the Scatter Plot. The ground-level sampling covers the same time period as the aircraft sampling data used in the some of the previous sections and the model results are also quite good for these data with an over prediction (C/M) of 24% and a correlation coefficient of 0.46.

3. To use the measurement data to estimate emissions from the release location we need to agree about what is known and not known. In this case we assume that we know nothing about the emission rate nor the duration of the emissions, but we do know the release location. Open the Setup Run menu and start the simulation at the beginning of the meteorological data file. Change the start time from 17 to **15**, and increase the run duration from 19 to **21** hours. Now open the Pollutant Emission menu and change the emission rate from 67000 to **1.0** and the hours of emission from 3.0 to **21.0**. By using a unit emission rate we can easily compute the actual emission rate by dividing the measured values by the model computed dispersion factor. Save the changes and run the model.

4. After the simulation completes open the Convert to DATEM menu, use the same 3-hr sampling data file, but because the unit emission rate was so much smaller than the previous rate, set the unit conversion factor to **1.0E+15**, 1000 times larger than the default value to maintain a sufficient number of significant digits in the fixed DATEM format file. Just remember to divide all model values by 1000 in any calculations. Then create the DATEM file and compute the statistics. The scatter plot is not needed.

5. Before continuing, consider that the measured concentration (M) represents the product of the atmospheric dilution (D) from the source to the receptor and the emission rate (Q):
   - M [g/m3] = D [hr/m3] Q [g/hr]

   Because the model computes the dilution factor (DATEM output times 1E+15), we can simply re-arrange the equation, but this time adjusting for units and accounting for the fact that the model output represents a 3-h time average rather than an exposure:
   - Q [g/hr] = M [pg/m3] 1E-12 [g/pg] / (D [1/m3] * 3 hr * 1E-15)

Looking at the [statistical results](#) output, the mean measured concentration is 2303.92 and the mean calculated is 81.86, which means that the estimated emission rate is 9381 g/hr. We know that the actual emission rate was 67,000 g/hr but for only a 3-hour period. Because the 3-hr dilution factors and measurements represent a 12 h period, all we can infer is that the 9381 g/h would be the average over the 12-sampling period for a total emission of 112578 g, or about half of the actual release total.

6. It may be possible to infer the emission time variation be examining the M/D ratios by time period. The DATEM statistical program also creates an output file of the measurements and calculations paired by time and sampling location. Examining the [dataA.txt](#) file for the locations with the highest concentrations and computing the M/D ratio shows considerable variability but no clear temporal trends. The zero predictions prior to 00Z on the 26th in combination with an estimate of the transport time could be used to estimate the emission start time.

Measurement data in combination with the dilution factors computed by the model were used to estimate the source term from a known source location. There is considerably more uncertainty in estimating emissions than concentrations because the precision of the result is limited by the averaging time of the measurement data collection. Small errors in model transport can result in large errors in the emission estimate because the dilution factor is in the denominator and transport errors can cause its value to approach zero.

Backward Calculation from a Sampler

In the previous section we computed the dilution factor from the source to various sampling locations and then used the measured concentration value to estimate the emission rate. In situations where the source location is not known, a frequently employed option is to compute the dilution factor from the sampler to all possible source locations. If there are multiple samplers it may be possible to combine the information from each sampler to estimate the source location as well as the release rate. Some of these issues will be explored in subsequent sections. Here we will determine if the "backward dispersion" calculation from the sampler gives the same dilution factor as the forward calculation from the source.

1. Start with the same configuration as in the previous section where we were comparing results to the 3-hr sampling data. Open the *Setup Run / Pollutant Emission* menu and simplify the emissions even further, set the rate to **1.0** unit for **1** hour. Then open the concentration grid menu and change the averaging time from 03 hours to **01** hour and the start of the sampling back to **83 09 25 17**. Save the changes and run the model.

2. When the run has completed, open the *Utility / Grid to Station* menu and pick a site, such as 316, which we already know is within the calculated and measured plume. Set the location to **41.30 -82.22**. Also to keep enough significant digits in the fixed format output, increase the multiplier from 1.0E+12 to **1.0E+15**. This last step is necesssary because we reduced the emission rate from its actual value 67000.0 to a unit value. The resulting hourly output file at station 316 shows a value of 275 near the center time (0500-0600) of the plume passage.

3. To configure the reverse calculation, open the setup run menu and set the start time to **26 06** and the run duration to 13 hours; set the back radio-button to change the sign to negative. Open the starting location menu and change the starting location to the position of sampler 316 (41.30 -82.22). Then open the concentration grid menu and reverse the sampling start and stop times. Set the start time of sampling to **26 06** and the stop time to **25 17**. Save the changes and run the simulation.

4. When the run completes, open the Grid to Station menu and set the sampling site to the original release location **39.90 -84.22**. The resulting time series at the source location shows a value of 240 between 1800-1700, the same transport time as the original calculation to 0500-0600. There is about a 12% difference in the calculated dilution factors between the two approaches.

The results shown here indicate that the dilution factors between the forward and backward calculations are similar, they are not identical. Some of these issues were explored in previous sections, for instance when a particle intersects the ground the transport calculation is no longer reversible. Also the particle dispersion calculation depends upon the turbulence the previous time step:

- $U'(t+\Delta t) = R(\Delta t)\ U'(t) + ...$

through the auto-correlation, which means that the current dispersion rate depends upon its previous history. If the turbulence was the same during the computational period, then the forward and backward integration would be the same. If for example, the calculation period went from day to night, then the forward and backward calculations would have a different history.

Attribution from Multiple Samplers

In this section we will use the measurement data and the adjoint dispersion calculation (backward integration from the measurement location) to estimate the source location and magnitude of the emissions. Start by retrieving the previously saved *captex_control.txt* and captex_setup.txt settings into the GUI menu.

1. As in previous examples in this section, we will only use the sampling data from 3-hour duration collections. These occurred from 18Z September 25th to 12Z September 26th. Therefore, in the *Concentration / Setup Run* menu, change the run duration to **19** hours. Because we will be running the model for only 19 hours, fewer particles are needed. Open the *Advanced / Configuration / Menu #4* and reduce the particle release number to **25000**. Save to close and exit all menus.

2. Now press the *Special Runs / Geolocation* menu tab to open another data input menu composed of four steps. In this step you need to define the measured data file (DATEM format) that will be used to create the individual backward CONTROL files. You could manually create a subset of only the 3-hour sampling data from the master file captex2_meas.txt, but for convenience, this file is already provided ..\captex\captex2_3hr.txt. Use the browse button to find and select this file.

3. In step 2 leave the defaults and press the *Execute* button. After the completion message appears, 48 CONTROL files will have been created in the *working* directory corresponding to each of the measurements. As an example, file *CONTROL.023* contains the information from station 318, where the sample was collected from 00Z-03Z on the 26th. Note this simulation, like all others, starts at 12Z on the 26th, running for -19 hours (negative = backward), with the particle emissions occurring from 03Z to 00Z. In this way all model simulation files contain the same number of output time periods. The emission mass equals the measurement. Zero measurements are assigned a nominally small emission rate (10^{-11}). Now **Execute Step 3** to run the dispersion simulations.

4. When the calculations have completed, **Execute Step 4** with the default menu values to see the six frames (one for each time period) of the weighted source sensitivity function, the mean of the 48 simulations. The last frame shows the pattern for the time period corresponding to the tracer release. These patterns are weighted by the measurements so that nearby samplers, with the highest measurements and smallest model dilution factors, provide the greatest weight to the pattern. As an exercise try this again, by eliminating all measurements except those collected during the last 3-hour time period (just delete the appropriate hysplit2.bin.000 files) and rerun Step 4. Essentially we are computing a weighted trajectory pattern. Also in situations where air samples are collected both before and after the release, there would be multiple zero measurement points to constrain the source location solution.

5. As noted in an earlier section, the model computes M = D Q, where M is concentration, Q is

-3

the emission value (mass) and D is the atmospheric dilution (m) factor. Although not precisely correct, we must assume that D forward, the dilution factor from the source to the receptor, is the same as D backward, the dilution factor from the receptor to the source. Then the source term can be estimated from measurements as the ratio of M/D. However, the model only computes D, not its inverse. If we set the source term as 1/M, where in this case M is the measurement, the model will compute D/M which is the same as 1/Q. To perform this calculation, it is necessary to repeat Steps 2 and 3, but this time selecting the **Output as Inverse** radio-button. This will set the emission rate as the inverse of the measured value, an example of which is shown in the control file for station 318. Only the 22 non-zero measurements are used in this approach. Rerun the calculations and display, and now the frame corresponding to the emission time shows a more complex pattern, with the smallest values corresponding to the larger emission rates. For instance, the grid location near the known source location (40N 84W) shows a value of 10^{-17}. The inverse would be 10^{17} pg or 10^5 g or about 100 kg.

6. The post-processing of the source attribution output files is the same program that was used in processing the meteorological ensemble, resulting in different files (prob??, cmax?? , cmean) in the *working* directory. In this application, all the graphics are created from *cmean*, the mean value at each grid point for all the output files with the .000 suffix.

The results shown here use measurement data in conjunction with the dilution factors computed by HYSPLIT to estimate source location and magnitude. For this particular example, the flow was relatively uniform so that all the samplers were in the same general downwind direction, resulting in estimates of source area that were larger than if we had sampled multiple releases that went in different directions. Multiple downwind directions would result in a better triangulation of the source region and a smaller area of uncertainty about the possible source location.

Source-Receptor Matrix

In the previous section, to determine the location or magnitude of an unknown source, the dispersion model was integrated backwards in time from a measurement location to determine the geographic area of potential sources. To quantify the emission rate in these calculations, we assumed that the dilution factors are about the same in the forward or backward integration of the model. An alternative approach is to compute a forward dispersion calculation from all potential source locations and then determine which location provides the best fit to the measurement data.

1. Open the *Setup Run* menu and configure the simulation the same way as in previous simulations in this section, a **19** hour run duration which limits the results to the 3-hr measurement data. Following the same approach as was used in the trajectory matrix, open the source location menu for three locations and enter the lower left (**38,-85**), upper right (**45,-78**), and first internal grid point (**38.5,-84.5**). This will create a regular grid of emission points at 0.5 degree resolution.

2. Then open the concentration grid menu and change the sample starting time to **83 09 26 09 00** which will result in only one output time with one **03** hour average output to simplify the subsquent analysis. Save the change and open the pollutant menu and change the emission rate from its actual value to a unit value, in this case **0.333333** so that one unit of mass is released after three hours. Save the change and close the *Setup Run* menu.

3. Now open the *Advanced / Concentration / Conversion Modules* menu #10 and check the radio-button to restructure the concentration grid to the source-receptor format. The effect of this switch is that instead of all sources contributing mass to a single concentration grid, each source has its own concentration grid, which can be treated as a matrix with each row representing a source location and the columns representing the receptors (the concentration grid points). Plotting the values on a row gives a concentration map for that source. Plotting the values in a column gives the contribution of each source to that receptor. Save the changes and then run the model from the ***Special Runs / Matrix*** menu tab.

4. When the run completes, press the *Display / Source-Receptor / View* menu tab, to open the display menu. This menu calls a special program to extract the source or receptor information from the matrix output file. It writes out a single binary file that can be displayed with the normal concentration plotting program or any other concentration utility. Rename the binary output file to give it a unique name, such as **SRM_fwrd.bin**. The extraction method radio-button should be set to **source**, which means we are going to extract the row computed from the tracer source location entry box values: **39.90 -84.22**. Then execute to view the plume dilution factors for the 26th from 0900-1200. The source location is rounded to the nearest half degree point.

5. Go back and check the receptor radio-button and enter the location of sampler 316 at **41.3 -82.22** and give the output file a unique name, such as **SRM_back.bin** The resulting

source display map shows the dilution factors of for sources contained within the contoured region. The dilution factors can then be divided into the measurement to estimate the emission rate from that source location.

6. Naturally the forward and backward dilution factors must be identical because they are all derived from the same forward calculation. This can be checked by using the *Grid to Station* analysis as was done forward-backward analysis tutorial.

The results shown here are another approach to source location from the source perspective, relying only on a forward calculation from all potential source locations. Simply selecting a receptor location will show the contributions of all sources contributing to that location. The computation can be very resource demanding, in terms of time and memory, because a unique concentration grid is required for each source. Do not delete the HYSPLIT output file, it will be used in the next section.

Solving the Coefficient Matrix

The source-receptor coefficient matrix that was created in the previous section can be solved directly to determine the source term and location. The solution is the source term vector given a measured data vector and the coefficient matrix, which is composed of the dilution factors for each source-receptor pair created in the previous step.

1. 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:
   - $D_{ij} S_i = R_j$,

   where the dilution factors are defined as the coefficient matrix. A plot of the product $S_i D_{ij}$ can be presented as a map of the concentrations contributed by source i to all the receptors. A plot of $S_i D_{ij}$ for receptor j would show a map of the concentration contributed by each source to that receptor. 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 inverse of the coefficient matrix:
   - $S_i = (D_{ij})^{-1} R_j$.

   An example of using this approach to determine the CAPTEX source term follows from the previous tutorial. If those results are not available, go back and complete the previous section before proceeding.

2. Press the *Display / Source-Receptor / Solve* menu tab to open the matrix solution menu. The measured data vector file needs to be defined. An extract of the 3-hour sampling data should be used that only contains the measured values from the 26th from 0900-1200. The unit conversion factor of **1.0E-15** is the number of kg per pg (the measured data unit). Execute the iteration button to generate a solution, and then display the solution results which after pass #2 shows that an emission of 274 kg from 39.5 -84.5 would account for the measured data values. We know the correct answer is 201 kg. The results are written to a file called *matrix.txt*. Setting the verbose check box provides more detailed information on the solution process.

The solution of the coefficient matrix to determine source location or amount is an attractive simple and objective method as presented in this example. However, in reality there is an underlying subjective component which may require editing the measured data to reduce singularities. It may be difficult at times to obtain a solution because there will usually be many more source locations than measured data values. This section should be considered more experimental rather than a mature operational approach to source estimation.

Enhanced Graphic Labels

In the next few sections some alternative display methods will be reviewed. Configure the simulation the same way as in the [case study base configuration](#) where the results were compared with aircraft measurements. The simulation should be set for a **13** hour run duration, a sampling start day/hour of **26 03**, and a concentration grid resolution of **0.05** degrees. Save the changes and rerun the model.

1. In a previous section we had already defined a file that changed the border labels on the concentration plot. In this section we will add an additional text box at the bottom of the display. Start by pressing the *Advanced / Configuration Setup / Panel Labels* menu tab to open the [text entry](#) data menu. This menu creates the file *MAPTEXT.CFG* in the working directory. The text prompts on each line are just initial suggestions and can be replaced by any text. Save the changes to exit.

2. Open the concentration contour display menu and create the plume [graphic](#). The new text is automatically added to the bottom of the display. This text box will appear for all subsequent graphics until the *MAPTEXT.CFG* file is manually deleted from the *\working* directory.

There are two enhanced labeling options, the *borders label* menu creates a file called *LABELS.CFG*, which is used to modify the title line and concentration units label. The other option, the *panel labels* creates the *MAPTEXT.CFG* file, which provides user supplied supplemental information in a text box below the main graphic. Do not delete the model simulation results, they will be used in the next few sections.

Creating KML/KMZ for Google Earth

Several of the HYSPLIT display programs have an option to create a file that can be opened in Google Earth. If you do not have it already installed, go to the **download page** and follow the installation instructions before proceeding with this section.

1. Start with the calculation that created the **graphic** in the previous section. Assuming the binary output file was not deleted, open the *Display / Contour* **menu** and check the **Google Earth** radio-button on the GIS output line (5th down). Then execute the display.

2. Once the output file has been created, a **message box** will indicate that the output file *HYSPLITconc.kmz* has been created in the working directory. The "KMZ" file suffix is just a zip file containing the contours in *HYSPLIT_ps.kml* and various logos and label information: *logocon.gif, noaa_google.gif, GELABEL_ **_ps.gif*.

3. The HYSPLIT GUI cannot open GE internally as an application. Go to the \working directory and open the "KMZ" file in **Google Earth**.

The KMZ file is created in the GUI. If the concentration plotting program is run outside of the GUI, such as in a script as shown in a previous example, then only the KML file will created. This can still be displayed by Google Earth, but without any of the label information. Creating a KMZ file may also be an issue on a MAC unless Ghostscript has been installed.

Creating Shapefiles for GIS

Before we continue with the example from the previous section, insure that ESRI's software ArcExplorer has been installed. Using ArcExplorer it is possible to overlay multiple products, such as trajectories, concentration plumes, meteorological data contours, and even point data, all on the same display.

1. In the previous section, we had already computed the 3-hr average concentration pattern from 03-06 UTC on the 26th. Open the *Concentration / Display / Contour* menu and set the **ESRI Generate** radio-button. Execute will open the display and also create two ASCII text files, GIS_00100_ps_00.txt (and .att), in generate format. The file name changes slightly according to the time period and output layer. The .txt file contains the contour polygon points and .att file contains optional attribute information.

2. The next step is to convert the Generate format files to the binary shapefile format. Press the *Utilities / GIS to Shapefile* menu tab to open the conversion menu. Use the browse button to find the GIS text file then select the **polygons** radio-button for the conversion method (polygons are closed lines). Because an attributes file is available, select the **concentration** radio-button. Press **Process Data** and four output files will be created (concplot.shp .shx .dbf .prj) in the working directory. A system message will be displayed when the conversion is complete.

3. Open Arc Explorer and select the Add Layer icon to browse and select the concplot polygon file in the working directory. To add a map background file go to the \Tutorial\maps directory and select the states polygon file. As each layer is added it will appear on the left panel. Click the checkbox to display each layer. The concentration contours are below the states, therefore select the concentration box and drag it to the top of the column to show the plume on top of the state maps.

4. To fix the colors and transparency, double-click the left panel states box and select the transparent fill option. Next double-click on the concplot box and change the *Draw Features* option to unique symbols. Double-click on the contour colors to customize, then after some panning and zooming the final display graphic will show something very similar to previous displays.

The ESRI ArcExplorer option provides a powerful display tool that can be used to overlay a variety of different products on the same map. On your own, try to add a trajectory or even a meteorological analysis using the ESRI option in the meteorology and trajectory menus. The sample shapefiles on the CD were all obtained from public sources. As an alternative, software is provided in the \hysplit4\examples directory to convert output for display in GrADS (Grid Analysis and Display System).

Dynamic or Lagrangian Sampling

Although the output is a simple text file, in terms of alternate display options, the dynamic or Lagrangian sampling is very different than any of the other display options. The model can be configured to move a sampler through the computational domain, either passively, moving with the wind as a balloon, or as an aircraft with a defined direction and speed. Start with the same configuration as in the last few examples. We will make a few modifications.

1. We are going to configure the model to match the time and locations of the same 914 m AGL aircraft sampling flight that was used in several previous examples. Note the end of the last sample was on the 26th 0348 to 0354, which means we only need to run the model from the 25th 17Z to the 26th 04Z, a run duration of 11 hours. Open the *Concentration / Setup Run* menu to make that change.

2. Next open the Concentration Grid menu. Several changes are required. The aircraft is always above the 0-100 concentration layer. We need to define a concentration at the heights the aircraft will be flying. Change the number of vertical levels from 1 to **5** and define 5 layers on the next line: **200 400 600 800 1000**. If the sampling start time was set to 26 03 change it to an earlier time, such as **83 09 26 00 00** so that the entire last aircraft pass will be captured. The last change required is that the sampling needs to be changed from averaging (00) to snapshot (01), resulting in the last line showing **01 01 00**. The middle 01 doesn't matter, because we will not be examining the conventional binary output file.

3. In a snapshot grid definition, the particle masses are summed to the concentration grid each time step. As the dynamic sampler passes through the snapshot grid, the concentration of the grid cell occupied by the sampler that time step is summed to the dynamic sampler. Then the concentration grid is set to zero before the next time step calculation. To configure the dynamic sampling option, select the *Advanced / Configuration / Dynamic Sampling* menu tab.

4. In the first menu, define the number of samplers that will be followed at the same time. In our situation, we only need to define one aircraft pass. A pass is a segment that can be defined by a single velocity vector. Pressing the *Configure Samplers* button opens another menu, where by selecting the radio-button opens the configuration menu for the selected sampler.

5. Review the data from the sampling aircraft again. We will start the dynamic sampling from the beginning of the pass defined by:
   - 1983 09 26 0248 0006 40.86 -81.81 468.0

   On the first line set the aircraft start position to **40.86 -81.81 500.0**. The aircraft flight level was at 914 m MSL. However the input value requires a height in AGL. The elevation at that location is about 400 m: 900 - 400 = **500**. From the latitude-longitude positions it is possible to determine the aircraft direction, **290** degrees, and speed **50** m/s. Enter those

on the second line. The third line is the start time of the flight leg and the second line defines the start time of the sampling, in this case they are both at the same time: **83 09 26 02 48**. The next two lines define the sampler averaging time and disk output interval in minutes, in this case both values are set to **06** minutes. The output will be written to a file called *LAGOUT.TXT*. Save each of the menus to close the menus. The dynamic sampling information is written to a file called *LAGSET.CFG*, when found in the working directory turns on the dynamic sampling option.

6. Now run the model and when the simulation completes, open the LAGOUT.TXT file to see how the model results compare with the measurements. Two issues to note. One there is no units conversion factor option, hence values are g/m3. Second, the output times are at the end of the sample, while the measurement file times are at the beginning of each sample. The maximum calculated concentration occurs at:
   - 83 9 26 3 12 41.078 -82.617 616.6 0.4371E-07

   which corresponds to a concentration of 43710 pg/m3. The maximum measurement value for that flight segment also occurred for a sample collected for the same time period and approximately the same position:
   - 1983 09 26 0306 0006 41.09 -82.52 29936.4

   As with many other previous examples, your results may differ slightly from the results shown here.

The results shown here permit model simulations to be configured in a way to match aircraft or balloon borne sampling platforms. There are limitations to this approach in terms of multiple pollutants and concentration grids. Currently only simple single pollutant simulations are permitted.

Dust Storm Simulations

HYSPLIT contains two different wind-blown dust emission algorithms. The [original procedure](#) is available through the GUI, while the newest procedure must be configured manually. For both versions, the dust emission algorithm is invoked by setting the namelist parameter ICHEM=3 in the file SETUP.CFG. In both procedures, potential dust emission points are defined in the input CONTROL file by the two additional fields of threshold friction velocity and area associated with each dust emission location.

1. The original dust emission algorithm (an option not currently not available) was based upon describing the vertical dust flux as a fraction of the horizontal transport:
   - $Q = K \rho \, g^{-1} \, U_* \, (U_*^2 - U_{*t}^2)$

   where the soil emission factor K and threshold friction velocity U_{*t} varied by soil type and land use. This detailed approach proved to be impractical in locations where these details are unknown, hence a simplified method was applied:
   - $Q = 0.01 \, U_*^4$

   when the threshold friction velocity field is set to -1.0 and the area field represents the dust emission area (m2) centered about that point. Dust emissions would occur at that location when the "hardwired" threshold friction velocity (28 cm/s) is exceeded. The use of the GUI option *Special Runs / Dust-storm* to set [three data points](#) (bottom left, upper right, resolution) for dust emissions, just invokes a pre-processor to create a CONTROL file for all the desert area land-use locations within that domain. The CONTROL file is configured for this fixed threshold dust emission algorithm. The GUI procedure cannot be used in the continental U.S. because there are no desert locations covering a full one-degree grid point.

2. To demonstrate the dust-storm computation, we will focus on an event that occurred in Utah from 30-31 March 2010. From a satellite derived data base of dust sources, we have already identified 21 locations (0.25 degree grid) in the Sevier Lake region of Utah that are frequent dust sources to the Salt Lake City region. Open the [Setup Run](#) and retrieve the pre-configured control file [CONTROL_dust1.txt](#) from the *Tutorial\\dust* directory. Note that the 21 potential dust locations contain two additional fields, the -1 indicating the use of the first algorithm and area value representing a 0.25 degree square emission area. All the other input values should already be set. Note that in the [Concentration Grid](#) menu the sampling start time is set for **00 00 00 06 00**, which means that sampling will start 6 hours after the start of the simulation, for a 24-hour duration sample. The model results wil be compared with the daily averaged (local midnight to midnight) AirNow measurements. Then save to exit.

3. Next open the *Advanced / Concentration / [menu #10](#)* and check the **Enable PM10 dust storm emission algorithm** radio-button. Save to exit and then open [menu #4](#) to increase the particle emission rate to **100000** with a maximum of **50000**. These changes can also be invoked by retrieving the [SETUP_dust.txt](#) file. Save the changes to exit.

4. Now go ahead and press the *Run Model* menu tab. The standard output message will indicate that the [PM10 dust emission](#) algorithm has been enabled. Note we are just doing a standard run and not through the *Special Runs / Dust-storm* menu which configures the control file. On your own try this option and you will see that it doesn't work because there are no desert-only land-use cells in the HYSPLIT data base. When the run completes, open the concentration [display](#) menu and set the units conversion to **1.0E+06** to convert grams/m3 to ug/3. Also set the contour interval to fixed values of **200 100 50 20 10**, then execute the display to show the [dust plume](#).

5. The calculation can be compared to the AirNow measurements in the Salt Lake City area for that day. Open the *Utilities / [Convert to DATEM](#)* menu and set the measured data input file to [AirNow_dust.txt](#) and with the conversion factor of **1.0E+06**. The statistical [results](#) show under-prediction by about a factor of 10 and a correlation coefficient of 0.30. A performance level confirmed by the [scatter diagram](#).

6. In the revised dust emission algorithm, the threshold friction velocity and dust emission area vary for each location and dust locations are predefined by month based upon a climatology of dust sources developed from satellite data. In this approach, the dust emissions are defined by:
   - $Q = K\ A\ (U_* - U_{*t})$

   where the positive value in the threshold friction velocity field (cm/s) triggers the use of the new algorithm. The second field is the product of the soil-dust density (K) and emission area (A).

7. To use the alternate emission algorithm, open the *Setup Run* and retrieve the pre-configured control file [CONTROL_dust2.txt](#) from the *\Tutorial\dust* directory. Note that the 21 potential dust locations are the same but the two additional fields now show a varying threshold friction velocity and the product of the dust density and emission area (KA). This approach provides more user control of the emission configuration. Save the changes and run the model. Once it completes go right to the *Convert to DATEM* step. The model [results](#) show a higher correlation (0.51), but the model under-prediction has increased to about a factor of 400!

8. There are a lot of uncertainties in these calculations, especially when more detailed soil and land-use information is required. In this case, the climatological values for U_* and KA may not be representative for 2010, perhaps because of flooding in previous years built up erodible sediment that was not present during the period of the climatological analysis of the dust emission sources. A simple test of the sensitivity would be to increase the emission factor. We don't need to rerun the model, but can simply change the conversion factor in the *Convert to DATEM* menu to **4.0E+08**, 400 times larger. The statistical results show a comparable [correlation](#) (0.45). The corresponding [scatter diagram](#) shows values for all the measurement stations in the Salt Lake City area over a wide range of air concentrations, suggesting that varying the emission factors by location can provide a method to improve model performance.

The dust storm emission calculations are very sensitive to the emission parameters and the module should not be treated as a black box. However, using the revised module with spatially varying characteristics, it may be possible to "calibrate" the model, refining the emission factors using measured data, and then using the calibrated model for predictions for a specific location.

Volcanic Eruptions

In the following example we will configure the model to simulate the Eyjafjallajokull eruption that started 14 April 2010 following a real-time scenario which means that the model is run in steps with every new forecast cycle, incorporating the ash emitted during previous simulations. Each new simulation may be specified with a different release height or emission rate.

1. To simplify the setup, start by retrieving the example control_volc.txt control file from the \Tutorial\volcano directory. We will review the key elements of the configuration.

2. Open the starting locations menu and note how the two locations are identical in horizontal position (63.63N 19.62W) but with different height. The model interprets this as a vertical line source and will distribute particles uniformly through the layer 100 to 6000 meters AGL.

3. Open the pollutant menu and note that four pollutants are defined. Lets assume a mass release rate of 10,000 kT/hr which means that if we set the emission rate to the equivalent 1.0E+16 µg/hr then the output units will be µg/m^3. Note there are four pollutants defined, each representing a different particle size:

LABEL	Diameter	Percent	Release Rate
P006	0.6µm	1%	0.008E+16
P020	2.0µm	7%	0.068E+16
P060	6.0µm	25%	0.250E+16
P200	20.0µm	67%	0.670E+16

   We will only run the model for 12 hours at a time and therefore emissions are all set to 12 hours. Check the other three pollutants to insure that the settings follow the table suggestions.

4. Open the grid definition menu where only one vertical level has been defined resulting in average concentrations in the layer from the ground to 10,000 meters. Six hour average air concentrations will be output because we will focus on the particle display output. However, if you want to create animations, a more frequent interval could be set.

5. The last menu in this section defines deposition for each of the four pollutants. For instance, in the pollutant #1 (P006) menu, the particle diameter is set to 0.6µm assuming a density of 2.5 g/cc for a spherical particle (1.0). Gravitational settling is computed based upon the previous values. The within cloud (3.2E+05 l/l) and below-cloud (5.0E-05 /s) wet removal coefficients will be applied to the local ash concentration and precipitation rate for each grid cell. Except for the particle diameter, these values are also applied to the other pollutants.

6. Save to close the setup run menu and open the *Concentration / Configuration* menu and retrieve the setup_volc.txt file. There were only two changes to the default values. First the

particle number release rate and maximum was raised to 5,000 and 50,000. Second, the input and output of the particle files was set to 12 hours.

7. Save the changes, run the model for 12 hours, and then open the particle display menu to view the ash plume valid at 1200 UTC 14 April 2010. Note how the particles are evenly distributed in the vertical layer. There are two ways in which non-uniform vertical mass distributions can be defined, either by defining multiple release height pairs or through the *EMITIMES* file. This exercise is left to the reader.

8. To complete the exercise, open the concentration display menu and check the **All** radio-button to sum the four particle sizes into the same graphic. Also fix the concentration contour intervals (**100+50+20+10**) and units of **ug** to get the final plume display.

The volcanic ash plume simulation is only an approximation of the actual event to illustrate the process for multiple particle sizes. In the next section, we will continue the calculation for another 24 hours.

Restarting from the PARDUMP File

In the last section, the simulation ended after 12 hours, at 1200 UTC 14 April 2010. Assume that now we have new information about the release, for instance that the eruption height maximum is now 12,000 m AGL. So we can restart the simulation at 12Z with this new information, keeping all the previous ash particles on the computational domain.

1. Open the setup run menu and change the start time from 10 04 14 00 to **10 04 14 12** and open the starting locations menu and change the top height from 6000 to **12000**. Save the changes and exit.

2. In the previous run we already set the input/output particle file options to output the endpoints every 12 hours. Note that one of the default options is to read the particle positions in a file called *PARINIT* when the model simulation starts. Therefore, go to the \hysplit4\working directory and rename the file *PARDUMP* created at the end of the last simulation to **PARINIT**. Then save the changes and run the model.

3. After the simulation completes, open the display menu to view the particle cross-section on the 15th at 00Z. The different release height periods are clearly evident in the display.

4. Go through this process one more time, change the start time to **10 04 15 00** and change the release height maximum back to 6000 m. Save the changes, and go back to the *working* directory and rename PARDUMP to **PARINIT**. You need to delete or rename the previous *PARINIT*. Then run the model. If uncertain, you can always confirm that the particle file is being opened by viewing the *MESSAGE* file. When the run completes, open the display to view the new particle cross-section on the 15th at 12Z. It should be evident that temporally varying release heights can result in quite complex plume structures.

In this section we illustrated how the standard model input procedure using the *CONTROL* file can be used to create a complex time-varying emission scenario. When the model is restarted, any of the model simulation parameters, either in the CONTROL file, the SETUP.CFG file, or even the meteorology file can be changed. Do not delete any files. In the next section, we will compare the model results with observational data.

Adjusting Predictions using Satellite Data

	[HOME](#)	**[Zoom](#)**	

In the previous section, the last valid time of the particle position file was 12 UTC on the 15th of April. We can compare the particle positions with the aerosol index from the [NASA OMI/TOMS](#) satellite archives available on-line. These are sun synchronous orbits which means that the pass over Iceland-England would occur around local solar noon or about 1200 UTC.

1. Start by pressing the *Advanced / Satellite Data / [FTP NASA TOMS](#)* menu tab to open the [download](#) menu. Set your **email address** for the anonymous FTP password field and enter the download date to **10 04 15** and press *Get Data File*. A pop-up message will appear indicating the name of the file accessed. All files get renamed to a standard convention. This particular file will be renamed to [ga100415.txt](#). In the event, the FTP fails, copy the file from *\Tutorial\volcano* to the *\Hysplit4\working* directory.

2. Before we open the satellite data viewer, go to the working directory and rename the concentration output file *cdump* to another name, such as **cdump_100415**. This is not necessary, but the viewer will display the satellite data, particle file, and concentration file. It is easier to view only two fields rather than three.

3. Open the [TOMS viewer](#). No changes are required from the default settings. It works in a similar manner to the *Quick Start* interface. Press and hold the left mouse button while dragging the pointer from the lower-left to upper-right corners of the desired map zoom area. Then right-click the mouse to redraw the display in the zoomed box. Subsequent left-clicks will advance the display to the next time period. The particle-satellite [display](#) should show the bulk of the particles on the northern edge of the higher Aerosol Index grid cells.

4. Actually the overlap between the model calculation and observations is quite good. The small difference for the first 1000 km may be just due to variations in release height. There is a procedure we can use to adjust the particle positions before continuing the calculation. Press the *Concentration / Utilities / [Particle Adjustment](#)* menu tab to open the [shift menu](#).

5. There are two adjustment options, defining a window and translating particles, or rotating them about a point. We will choose the latter option. Select the **rotation** radio-button. The rotation point defaults to the source location and enter a rotaton angle of **10** degrees (positive = clockwise) to a distance of **1000** km. All particles within this distance will be rotated. The menu already defaults to writing the adjusted particles to *PARINIT* which would then default to the input file for the next simulation cycle. **Process the points** and the script will automatically open the [particle display](#) where there is an obvious discontinuity at 1000 km. This could be eliminated by selecting the **blend** option.

6. Go back and run the particle-satellite viewer, but this time enter the **PARINIT** file in the particle file text entry field to see how the adjusted particle [positions](#) compare with the observations. It appears that perhaps 10 degrees was too much and 5 degrees would have

been a better choice.

On your own try a few of the other adjustment options and then restart the calculation. The fit with observations for this case is somewhat fortuitous as no particular effort was made to get detailed source amount or release height information. Although the GUI is linked to the TOMS data files, there are other public sites available with [OMI](#) and [MODIS](#) image data.