

Instructions and Sample Problems for Using the MACCS/HYSPLIT Capability

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Table of Contents

Table of Figures	3
Table of Tables	3
Abbreviations and Acronyms	4
Introduction.....	5
Installing HYSPLIT and Other Software.....	6
Python.....	6
MPI.....	8
HYSPLIT	9
HYSPLIT Sample Problem, Five Days of Data	11
Download Meteorological Files on Linux	11
Download Meteorological Files on Windows.....	11
Run MacMetGen	12
Run GenHysplit.....	13
HYSPLIT Sample Problem, One Year of Data	17
Download Meteorological Files on Linux	17
Download Meteorological Files on Windows.....	18
Run MacMetGen	19
Run GenHysplit.....	20
Using the HYSPLIT Model from WinMACCS.....	24
Overview	24
Create MACCS-HYSPLIT Files	24
Define WinMACCS Parameters	26
Running WinMACCS Using the MACCS-HYSPLIT Model.....	32
MACCS-HYSPLIT Model Results	35
WinMACCS Sample Problem – HYSPLIT Fixed Start Time.....	37
Locate HYSPLIT Data	37
Create Project	37
Select the HYSPLIT Model	37
Define the MACCS-HYSPLIT Variables	37
Run the MACCS-HYSPLIT Model	42
WinMACCS Sample Problem – HYSPLIT Weather Sampling.....	44
Locate HYSPLIT Data	44
Create Project	44
Select the HYSPLIT Model	44
Define the MACCS-HYSPLIT Variables	44
Run the MACCS-HYSPLIT Model	49

Table of Figures

Figure 1. Convert HYSPLIT files to MACCS Grid Form.....	25
Figure 2. Selecting the HYSPLIT model.....	27
Figure 3. Results after successful MACCS-HYSPLIT file validation	33
Figure 4. Form to define location of MACCS-HYSPLIT files	38
Figure 5. Fixed Start Time Sample Problem File Extensions and Lower Bounds	39
Figure 6. Fixed Start Time Sample Problem HYSPLIT Fixed Start Time Data	40
Figure 7. Fixed Start Time Sample Problem Extended Time.....	41
Figure 8. Fixed Start Time Sample Problem Spatial Intervals	42
Figure 9. Run Models form.....	43
Figure 10. Weather Sampling Sample Problem File Extensions and Lower Bounds	46
Figure 11. Weather Sampling Sample Problem HYSPLIT Transport Dates.....	47
Figure 12. Weather Sampling Sample Problem Extended Time	48
Figure 13. Weather Sampling Sample Problem Spatial Intervals.....	49

Table of Tables

Table 1. MACCS-HYSPLIT files variable definition	28
Table 2. File extensions and lower bounds variable definitions.....	29
Table 3. Fixed start time data variable definitions.....	30
Table 4. Transport dates variable definitions.....	31
Table 5. Extended time variable definitions	31
Table 6. Specify model results variable definitions.....	32
Table 7. MACCS-HYSPLIT data file validation tests.....	34
Table 8. MACCS-HYSPLIT data files required by weather sampling method	35
Table 9. Type 0 outputs when using the HYSPLIT transport model.....	36

Abbreviations and Acronyms

Op5	0.5-degree latitude and longitude increments
12	12-km increments
GDAS	Global Data Assimilation System
HYSPLIT	HYbrid Single-Particle Lagrangian Integrated Trajectory
MACCS	MELCOR Accident Consequence Code System
MPI	Message Passage Interface
MPI4PY	MPI for Python
NAM	North American Mesoscale
NOAA	National Oceanic and Atmospheric Administration

Introduction

The capability to use HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) atmospheric transport and dispersion results has been integrated with MELCOR Accident Consequence Code System (MACCS) and serves as an alternative to the original Gaussian plume segment model. The process of using this model starts with downloading meteorological files from the Air Resources Laboratory (or other source that provides compatible files), which is under the National Oceanographic and Atmospheric Administration, (NOAA). These files are processed for the HYSPLIT modeling software and are available from NOAA. They can be obtained manually or through the Python scripts designed for this MACCS application discussed below. The output files created by running the HYSPLIT application can then be linked to WinMACCS, a graphical interface to MACCS. Additionally, the MacMetGen application is available to create a MACCS formatted meteorological file from the files downloaded from NOAA or another source of meteorological data.

HyGridConvert can be run from WinMACCS or independently of WinMACCS to create air and ground concentration files that are compatible with MACCS. The MACCS-formatted files created by HyGridConvert can be linked to the WinMACCS project or used directly by MACCS as a batch application.

The explanations and examples following this file are based on WinMACCS 4.1.0 and the HYSPLIT/MACCS tools suite. These codes and tools are available from Sandia National Laboratories via the MACCS download site.

Installing HYSPLIT and Other Software

Python

Install Python version 3.3 or later. This is a command language interpreter that is used to generate HYSPLIT files using a Sandia-provided Python3 script, GenHysplit. Python downloads can be found at the following site:

<https://www.python.org/downloads/>

The process described in this document was tested using Python 3.7. Newer versions are not guaranteed to be fully compatible with the software supplied with this version of WinMACCS.

Linux:

The following can be added to a bash script or can be run from the command line:

```
# Make sure proxy is set up when using a proxy, e.g.,
export HTTPS_PROXY=http://server.org.name:PP
export HTTP_PROXY=${HTTPS_PROXY}
export http_proxy=${HTTPS_PROXY}
export https_proxy=${HTTPS_PROXY}
```

where server.org.name is the proxy server, and PP is the prescribed port number

Important Note: Versions ≥ 3.7 must have libffi installed on system for ctypes

```
curl http://mirror.centos.org/centos/6/os/x86_64/Packages/libffi-devel-3.0.5-3.2.el6.x86_64.rpm >
libffi-devel-3.0.5-3.2.el6.x86_64.rpm
sudo rpm -ivv libffi-devel-3.0.5-3.2.el6.x86_64.rpm
rm libffi-devel-3.0.5-3.2.el6.x86_64.rpm
```

Change as needed

```
PYTHON_VERSION=3.7.0
PYTHON_SHORT_VERSION=3.7
```

Change dir when needed (This is an example location)

```
PYTHON_INSTALL_DIR=/projects/python${PYTHON_SHORT_VERSION}
```

Make directory for new Python

```
rm -rf ${PYTHON_INSTALL_DIR}
mkdir ${PYTHON_INSTALL_DIR}
```

Important Note: Versions ≥ 3.7 need to make sure newer openssl installed

```
OPENSSL_VERSION=1.1.0h
```

Download OpenSSL and install to Python dir

```
curl -k https://www.openssl.org/source/openssl- $\{OPENSSL\_VERSION\}$ .tar.gz > openssl- $\{OPENSSL\_VERSION\}$ .tar.gz
tar xvf openssl- $\{OPENSSL\_VERSION\}$ .tar.gz
rm openssl- $\{OPENSSL\_VERSION\}$ .tar.gz
mkdir -p  $\{PYTHON\_INSTALL\_DIR\}$ /openssl/usr/local/ssl
mv openssl- $\{OPENSSL\_VERSION\}$   $\{PYTHON\_INSTALL\_DIR\}$ /
cd  $\{PYTHON\_INSTALL\_DIR\}$ /openssl- $\{OPENSSL\_VERSION\}$ 
./config --prefix= $\{PYTHON\_INSTALL\_DIR\}$ /openssl --
openssldir= $\{PYTHON\_INSTALL\_DIR\}$ /openssl/usr/local/ssl
make install
cd -
rm -rf  $\{PYTHON\_INSTALL\_DIR\}$ /openssl- $\{OPENSSL\_VERSION\}$ 
```

Download Python

```
curl -k https://www.python.org/ftp/python/ $\{PYTHON\_VERSION\}$ /Python- $\{PYTHON\_VERSION\}$ .tgz
> Python- $\{PYTHON\_VERSION\}$ .tgz
```

Extract and remove tgz

```
tar -xvf Python- $\{PYTHON\_VERSION\}$ .tgz
rm Python- $\{PYTHON\_VERSION\}$ .tgz
```

Change dir to download Python

```
cd Python- $\{PYTHON\_VERSION\}$ 
./configure --prefix= $\{PYTHON\_INSTALL\_DIR\}$  --with-openssl= $\{PYTHON\_INSTALL\_DIR\}$ /openssl
make install
```

Remove Python download

```
cd ..
rm -rf Python- $\{PYTHON\_VERSION\}$ 
```

Install site-packages

```
cd  $\{PYTHON\_INSTALL\_DIR\}$ /bin
```

Ensure pip, setuptools, and wheel are up-to-date

```
./python $\{PYTHON\_SHORT\_VERSION\}$  -m pip install --upgrade pip setuptools wheel
# Install specific packages
SITE_PACKAGES=(numpy mpi4py)
for i in  $\{SITE\_PACKAGES[@]\}$ ; do
    ./python $\{PYTHON\_SHORT\_VERSION\}$  -m pip install  $\{i\}$ 
```

```
done
cp f2py f2py${PYTHON_SHORT_VERSION}
```

How to run installed Python (can add path or binary to Environment Variables to ease of use)

```
${PYTHON_INSTALL_DIR}/bin/python3.7
```

Windows:

After installing Python, add the following windows paths to the Environment Variables.

Example paths:

```
C:\Users\public\AppData\Local\Programs\Python\Python37;
C:\Users\public\AppData\Local\Programs\Python\Python37\Scripts
```

To do this, open the Control Panel. Open the System Properties window, Advanced tab, and click on the Environment Variables button.

Add the Python installation folder and the Scripts sub folder to the system PATH environment variable.

Numpy, a Python scientific computing package, is required. Not all versions of Python come packaged with numpy. The installation of numpy can be tested by starting Python from a command window and typing the following command:

```
>>> import numpy
```

If numpy is properly linked to Python, no error message is displayed.

If numpy is not installed, it needs to be installed by using a Python package manager such as pip. Open a command window, and type the following command:

```
>pip install numpy
```

If your organization has a proxy server, this might need to be specified also as shown in the following example:

```
>pip install --proxy server.org.name:PP numpy
```

where server.org.name is the proxy server, and PP is the prescribed port number.

MPI

Install Message Passage Interface (MPI) for Python (MPI4PY). This allows GenHysplit to access multiple processors through calls to the MPI interface, allowing the meteorological files to be processed faster than using a single processor. Even if only one processor is used, MPI must still be installed.

Linux:

Install Openmpi version 1.8 or later, which can be found at the following site:

<https://www.open-mpi.org/software/ompi/v3.1/>

Make sure proxy is set up when using a proxy, for example

```
export HTTPS_PROXY=http://server.org.name:PP
export HTTP_PROXY=${HTTPS_PROXY}
export http_proxy=${HTTPS_PROXY}
export https_proxy=${HTTPS_PROXY}
```

where server.org.name is the proxy server, and PP is the prescribed port number

Download and install openmpi

```
curl -k https://download.open-mpi.org/release/open-mpi/v3.1/openmpi-3.1.2.tar.bz2 > openmpi-3.1.2.tar.bz2
gunzip -c openmpi-3.1.2.tar.gz | tar xf -
cd openmpi-3.1.2
./configure --prefix=/usr/local
<...lots of output...>
make all install
```

Windows:

Download Microsoft MPI 8.1 and install both MPI (MSMpiSetup.exe) and the MPI software development kit (msmpisdsk.msi). It is necessary to run both applications.

<https://www.microsoft.com/en-us/download/details.aspx?id=55494>

Version:	Date Published:
8.1.12438	6/16/2017
File Name:	File Size:
msmpisdsk.msi	2.2 MB
MSMpiSetup.exe	5.2 MB

Add the path C:\Program Files\Microsoft MPI\bin to the system PATH environment variable.

After this is done, link mpi with Python with the following command:

```
>pip install mpi4py
```

HYSPLIT

The MACCS-HYSPLIT tools have been tested with versions 927 through 5.0.0. Version 5.0.0 was used for the sample problems below. Later versions of HYSPLIT could produce different

results and/or could be incompatible with GenHysplit. HYSPLIT is a code managed by the Air Resources Laboratory, NOAA. The user should register and obtain an account before downloading the files. A non-registered version also can be used but may not include all the updates available in the registered version. The registration form and instructions can be found at:

https://ready.arl.noaa.gov/HYSPLIT_register.php

Once registered, the ARL webmaster emails instructions for logging into the download page.

The source code or an executable is available for Linux. For Windows, download the registered (not public) version of Windows-based HYSPLIT. No source code is available for the Windows version.

HYSPLIT Sample Problem, Five Days of Data

Follow the instructions in the section Installing HYSPLIT and Other Software above to install software needed to complete this sample problem. The .ccd files generated in this sample problem are used in the section WinMACCS Sample Problem – HYSPLIT Fixed Start Time below.

Download Meteorological Files on Linux

1. Determine directory location for storage of meteorological files. Depending on the number of files, the required storage might be large. The files should be accessible from the location where GenHysplit is to be run. For the sample problem, the total size of the meteorological files is approximately 3 GB.
2. Copy the get_weather_linux.sh and readme_linux.txt files into the meteorological file directory. These files can be found in the included distribution folder, GetWeather.
3. Open get_weather_linux.sh and modify for the sample problem settings as discussed in the readme_linux.txt file. For the sample problem, the modification results in downloading Global Data Assimilation System (GDAS) weather files that contain data on 0.5-degree latitude and longitude increments (0p5) for March 11-16, 2011.
 - a. Modify the value of MET to the desired file storage location
 - b. Modify the value of met_end to "_gdas0p5"
 - c. Modify the value of ftp_loc to "ftp://arlftp.arlhq.noaa.gov/archives/gdas0p5"
 - d. Modify the value of YY to "2011"
 - e. Modify the value of MM to "03"
 - f. Modify the value of DD to "11" "12" "13" "14" "15" "16"
4. Download needed data by typing the following command in the meteorological directory:
>./get_weather_linux.sh

Download Meteorological Files on Windows

1. Determine directory location for storage of meteorological files. Depending on the number of files, the total file size might be large. The files should be accessible from where GenHysplit is to be run. For this test case, the total size of the meteorological files is approximately 3 GB. Create this folder if it does not exist.
2. Copy the get_weather_windows.bat and readme_windows.txt files into the meteorological file directory. These files can be found in the distribution folder GetWeather.
3. Open get_weather_windows.bat in a text editor such as Notepad and modify for the sample problem settings as discussed in the readme_windows.txt file. This can be done either by right clicking on the .bat file and selecting edit or starting the editor and opening the file. Do not double click on the .bat file because that causes the file to be executed. For the sample problem, the desired result is to download Global Data Assimilation System (GDAS) weather files that contain data on 0.5-degree latitude and longitude increments (0p5) for March 11-16, 2011. The new values indicated below should not

contain the quotes. For example, step d below asks to change the YY variable to “2011”. The line should be entered as follows: set YY=2011. There should be no space between the variable and the equal sign or the equal sign and the value.

- a. Modify the value of MET to the desired file storage location. If the path has spaces, enclose the path with double quote marks.
 - b. Modify the value of met_end to "_gdas0p5"
 - c. Modify the value of ftp_loc to "ftp://arlftp.arlhq.noaa.gov/archives/gdas0p5/"
 - d. Modify the value of YY to “2011”
 - e. Modify the value of MM to “03”
 - f. Modify the value of DD to "11 12 13 14 15 16"
4. The data can be downloaded by either double clicking the get_weather.bat file or by running the batch command directly in a command prompt window. This is done by opening the command application (cmd.exe), changing the folder to the location of the batch file, and then typing the command at the prompt as shown:
- ```
> get_weather_windows
```

## Run MacMetGen

1. Determine the folder location for storage of the MacMetGen output files. The folder should be accessible from where you plan to run MacMetGen. MacMetGen is a windows executable. For this test case, the total size of the MacMetGen output files is approximately 180 KB.
2. For the sample problem, copy the MacMetGen input file, sample\_MacMetGen.inp, to a working folder and rename this file met\_fs.inp. The sample file is in the distribution folder \MacMetGen. Detailed information about the format of this input file is described in the document MacMetGen 1.1.0 Users Guide.pdf, released with MacMetGen.
3. Open the met\_fs.inp file in a text editor and modify the sample problem settings. The sample problem is intended to generate a MACCS-formatted weather file using GDAS0p5 weather data from March 11-16, 2011, for the Fukushima Daiichi NPP, for a 16-sector grid with 60-minute time intervals using the dT/dZ stability class method. MACCS requires an input meteorological file with one year of data. As less than one year of meteorological data are provided, the output file repeats the meteorological data until one year is obtained to meet this requirement. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
  - a. Do not modify line 7, retain the value 0 to create the surface data file.
  - b. Modify the path on line 9 to the path and name of the intermediary surface data file for MacMetGen to create.
  - c. Modify the latitude and longitude values on line 11 to “37.4230 141.0329”.
  - d. Leave the value on line 13 as 1, indicating there is one set of meteorological files.
  - e. Modify the first and last dates of interest on line 15 to “20110311 20110316”.

- f. Modify the directory on line 17 to the location of the downloaded meteorological files.
  - g. Leave the value on line 19 as blank, setting the weather file prefix to "".
  - h. Modify the value on line 21 as "\_gdas0p5", setting the weather file postfix to "\_gdas0p5".
  - i. Modify the path on line 26 to the location of the MacMetGen output files with the specified name of the MACCS-formatted weather file.
  - j. Leave the value on line 28 as 60, the number of minutes associated with each line in the output file.
  - k. Modify the number of sectors on line 30 from 64 to 16.
  - l. Modify the value on line 32 to 0 setting the stability class to the algorithm dT/dz.
  - m. Modify the value on line 34 to 9, setting the local time to Japan Standard Time (JST, UTC+9).
  - n. Modify the value on line 36 to 0 to specify the option of using seasonal mixing heights.
  - o. Modify the morning mixing heights on line 38 to "300 300 300 300".
  - p. Modify the afternoon mixing heights on line 40 to "1000 1000 1000 1000".
4. Navigate to the location of the MacMetGen executable in a command prompt. The command is then MacMetGen.exe -i "path\met\_fs.inp", where path indicates relative location to the input file as shown in the following example:  

```
> MacMetGen -i input\met_fs.inp"
```
  5. MacMetGen should then run the sample problem. This can take several minutes. The file currently being processed is shown on the command prompt to help estimate progress.

Four files should be created in the specified output folder: 1) the output surface data file; 2) the MACCS-formatted weather file; 3) a \*.stat file, which indicates the status of the run (should contain "OK" after the run is complete); and 4) a \*.log file, which contains a copy of the input file used and the output shown to the command prompt. The MACCS-formatted weather file can be compared with the "gdas0p5\_dtdz.MET" file included in the Data folder of the project *Gaussian Fixed Start Time*.

## Run GenHysplit

1. Determine the folder location for storage of the HYSPLIT output files. Depending on the number of files, the required storage can be large. The files should be accessible from where Python, OpenMPI (or Microsoft MPI), and HYSPLIT are installed, as well as the meteorological files. For this test case, the total size of the HYSPLIT files is approximately 200 MB, but the total folder size with all intermediate results is 600 MB.
2. Copy the GenHysplit.py, pyhysplit.py, and realization.py files to the folder where you are running GenHysplit. These files can be found in the distribution folder GenHysplit/source.

3. Copy the GenHysplit input files where you want to store the input file. These files can be found in the distribution folder GenHysplit. Detailed information about the format of this input file is described in the document GenHysplit 1.2.0 Users Guide.pdf, released with GenHysplit.
4. For the sample problem, copy sample\_GenHysplit.inp to sample\_problem\_fs.inp. By default, when the input file is not specified on the command line, GenHysplit expects the file to be named test.inp.
5. Open the sample\_problem\_fs.inp file in a text editor and modify for the sample problem settings. The sample problem models radioactive releases to occur each hour from March 11, 2011, to March 15, 2011. Each plume is tracked for a 12-hour period and for a range of 100 miles from the Fukushima Daiichi NPP with default HYSPLIT settings. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
  - a. Modify the directory on line 9 to the location of the HYSPLIT output file.
  - b. Modify the default value on line 11 to 1.
  - c. Delete line 13.
  - d. Modify the directory on line 14 to the location of the downloaded meteorological files
  - e. Delete line 16
  - f. Leave the default values on line 17 as blank.
  - g. Delete line 19
  - h. Leave the default values on line 20 as “\_gdas0p5”.
  - i. Leave the default value on line 22 as 0.
  - j. Modify the directory on line 24 to the location of the HYSPLIT installation folder.
  - k. Modify the directory on line 26 to the location of the HYSPLIT landuse and roughness length folder.
  - l. Leave the default value on line 31 as 1.
  - m. Modify the values on line 33 to “20110311 20110315”.
  - n. Modify the values on line 35 to “141 1 58 E”.
  - o. Modify the values on line 37 to ”37 25 16 N”.
  - p. Leave the default value on line 39 as 0.
  - q. Leave the default value on line 41 as 10.
  - r. The values on line 43 are not used. They can be changed to anything.
  - s. Leave the default value on line 45 as 0.
  - t. Modify the value on line 47 to 12.
  - u. Leave the default value on line 49 as 15.
  - v. Leave the default value on line 51 as 1.

- w. Modify the value on line 53 to 161.0.
  - x. Leave the default value on line 55 as 10.
  - y. Leave the default value on line 57 as 0.5.
  - z. Leave the default value on line 59 as 50.
  - aa. Leave the default value on line 61 as 0.
  - bb. Leave the default value on line 63 as 10.
  - cc. Leave the default values on line 65 as “0.15332 0.28543 0.53138 0.98923 1.8416 3.4284 6.3825 11.882 22.120 41.179”.
  - dd. Leave the default values on line 67 as “1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0”.
  - ee. Leave the default values on line 69 as “0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0”.
  - ff. Leave the default value on line 71 as 2.
6. Execute GenHysplit.

### Running on Linux

For running on a single processor, use the command:

```
mpirun -n 1 python3 <location of *.py files>GenHysplit.py -i <location and name of input file>
```

For submitting a job on to a Linux cluster with a SLURM queueing system with 60 processors, use the command:

```
salloc -n 60 mpirun python3 <location of *.py files>GenHysplit.pyt -i <location and name of input file>
```

### Running on Windows

To view help and to verify that mpiexec has been correctly installed, type the command

```
>mpiexec
```

More help is available with the -help2 command. In this example, the output from the help command is piped into the more function. Tap the spacebar to get the next page of help.

```
>mpiexec -help2|more
```

For running a single processor, the command is:

```
python.exe “completepath/GenHysplit.py” -i “completepath/sample_problem_fs.inp”
```

Where completepath indicates the location of the files needed as shown in the following example:

```
> python "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\GenHysplit.py" -i "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\sample_problem_fs.inp"
```

To take advantage of multiple cores that might be available, open Windows Task Manager to determine the number of cores available. On Windows 10, select the Performance tab. Notice the value of the variable “Cores” in this window. The number of cores is used for the value of n in the mpiexec command. For example, if the number of Cores is equal to 4, the mpiexec command would be as follows:

```
> mpiexec -n 4 python "completpath/GenHysplit.py" -i "completpath/sample_problem_fs.inp"
```

Once successfully finished, the completed set of HYSPLIT output files (.ccd files) is found in the specified directory (line 17 in input file) in the data directory. There should be 120 .ccd files, along with a copy of the input file used and a log file.

## HYSPLIT Sample Problem, One Year of Data

Follow the instructions in the section Installing HYSPLIT and Other Software above to install software needed to complete this sample problem. The .ccd files generated in this sample problem are used in the section WinMACCS Sample Problem – HYSPLIT Weather Sampling below.

### Download Meteorological Files on Linux

1. Determine directory location for storage of meteorological files. Depending on the number of files, the required storage might be large. The files should be accessible from the location where MacMetGen is to be run. For this sample problem, the total size of the meteorological files is approximately 152 GB.
2. Copy the get\_weather\_linux.sh and readme\_linux.txt files into the meteorological file directory. These files can be found in the included distribution folder, GetWeather.
3. Open get\_weather\_linux.sh and modify for the sample problem settings as discussed in the readme\_linux.txt file. For the sample problem, the modification results in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 – December 31, 2015.
  - a. Modify the value of MET to the desired file storage location
  - b. Modify the value of met\_end to "\_nam12"
  - c. Modify the value of ftp\_loc to "ftp://arlftp.arlhq.noaa.gov/archives/nam12"
  - d. Modify the value of YY to "2015"
  - e. Modify the value of MM to "01" "02" "03" "04" "05" "06" "07" "08" "09" "10" "11" "12"
  - f. Modify the value of DD to "01" "02" "03" "04" "05" "06" "07" "08" "09" "10" "11" "12" "13" "14" "15" "16" "17" "18" "19" "20" "21" "22" "23" "24" "25" "26" "27" "28" "29" "30" "31"
4. Download needed data by typing the following command in the meteorological directory:  

```
>./get_weather_linux.sh
```
5. Additional meteorological data are needed for the HYSPLIT file generation. These additional files cover the periods before January 1, 2015 and after December 31, 2015 that are used in HYSPLIT calculations below. They are not needed to generate the MACCS formatted meteorological file.
  - a. For the period before January 1, 2015, open the get\_weather\_linux.sh file and modify the settings as discussed in the readme\_linux.txt file and above. For this period, the modifications should be made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for December 29 – 31, 2014. Then execute the script as discussed above.
  - b. For the period after December 31, 2015, open the get\_weather\_linux.sh file and modify the settings as discussed in the readme\_linux.txt file and above. For this period, the modifications should be made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km

(12) for January 1 – February 10, 2016. Then execute the script as discussed in the Five Days of Data example.

## Download Meteorological Files on Windows

1. Determine directory location for storage of meteorological files. Depending on the number of files, the total file size might be large. The files should be accessible from where MacMetGen is to be run. For this test case, the total size of the meteorological files is approximately 152 GB. Create this folder if it does not exist.
2. Copy the `get_weather_windows.bat` and `readme_windows.txt` files into the meteorological file directory. These files can be found in the distribution folder `GetWeather`.
3. Open `get_weather_windows.bat` in a text editor such as Notepad and modify for the sample problem settings as discussed in the `readme_windows.txt` file. This can be done either by right clicking on the `.bat` file and selecting edit or starting the editor and opening the file. Do not double click on the `.bat` file because that causes the file to be executed. For the sample problem, the desired result is to download North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 – December 31, 2015. The new values indicated below should not contain the quotes. For example, step d below asks to change the YY variable to “2015”. The line should be entered as follows: `set YY=2015`. There should be no space between the variable and the equal sign or the equal sign and the value.
  - a. Modify the value of MET to the desired file storage location. If the path has spaces, enclose the path with double quote marks.
  - b. Modify the value of `met_end` to `"_nam12"`
  - c. Modify the value of `ftp_loc` to `"ftp://arlftp.arlhq.noaa.gov/archives/nam12/"`
  - d. Modify the value of YY to “2015”
  - e. Modify the value of MM to `"01 02 03 04 05 06 07 08 09 10 11 12"`
  - f. Modify the value of DD to `"01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31"`
4. The data can be downloaded by either double clicking the `get_weather.bat` file or by running the batch command directly in a command prompt window. This is done by opening the command application (`cmd.exe`), changing the folder to the location of the batch file, and then typing the command at the prompt as shown:

```
> get_weather_windows
```
5. Additional meteorological data is needed for the HYSPLIT file generation. These additional files cover the periods before January 1, 2015 and after December 31, 2015 that are used in HYSPLIT calculations below. They are not needed to generate the MACCS formatted meteorological file.
  - a. For the period before January 1, 2015, open the `get_weather_windows.bat` in a text editor such as Notepad and modify the settings as discussed in the `readme_windows.txt` file and above. For this period, the modifications should be

made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for December 29 – 31, 2014. Then execute the script as discussed above.

- b. For the period after December 31, 2015, open the `get_weather_windows.bat` in a text editor such as Notepad and modify the settings as discussed in the `readme_windows.txt` file and above. For this period, the modifications should be made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 – February 10, 2016. Then execute the script as discussed above.

## Run MacMetGen

1. Determine the folder location for storage of the MacMetGen output files. The folder should be accessible from where you plan to run MacMetGen. MacMetGen is a windows executable. For this test case, the total size of the MacMetGen output files is approximately 644 KB.
2. For the sample problem, copy the MacMetGen input file, `sample_MacMetGen.inp`, to a working folder and rename this file `met_ws.inp`. The example file is in the distribution folder `\MacMetGen`. Detailed information about the format of this input file is described in the document `MacMetGen 1.1.0 Users Guide.pdf`, released with MacMetGen.
3. Open the `met_ws.inp` file in a text editor and modify for the sample problem settings. The sample problem is intended to generate a MACCS-formatted weather file using NAM12 weather data from 2015, for a fictitious site located at latitude 36.19306, longitude -115.65463, for a 16-sector grid with 60-minute time intervals using the dT/dZ stability class method. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
  - a. Do not modify line 7, retain the value 0 to create the surface data file.
  - b. Modify the path on line 9 to the path and name of the intermediary surface data file for MacMetGen to create.
  - c. Modify the latitude and longitude values on line 11 to “36.19306 -115.65463”.
  - d. Leave the value on line 13 as 1 indicating there is one set of meteorological files.
  - e. Modify the first and last dates of interest on line 15 to “20150101 20151231”.
  - f. Modify the directory on line 17 to the location of the downloaded meteorological files.
  - g. Leave the value on line 19 as blank, setting the weather file prefix to “”.
  - h. Leave the value on line 21 as “\_nam12”, setting the weather file postfix to “\_nam12”.
  - i. Modify the path on line 26 to the location of the MacMetGen output files with the specified name of the MACCS-formatted weather file.

- j. Leave the value on line 28 as 60, the number of minutes associated with each line in the output file.
  - k. Modify the number of sectors on line 30 from 64 to 16.
  - l. Modify the value on line 32 to 0 setting the stability class to the algorithm dT/dz.
  - m. Modify the value on line 34 to -8 setting the local time to Pacific Standard Time (PST, UTC-8).
  - n. Leave the value on line 36 as 1 to specify that mixing heights are written out for each time period instead of using the seasonal mixing height listed below.
  - o. Modify the morning mixing heights on line 38 to “300 300 300 300”.
  - p. Modify the afternoon mixing heights on line 40 to “1000 1000 1000 1000”.
4. Navigate to the location of the MacMetGen executable in a command prompt. The command is then `MacMetGen.exe -i "path\met_ws.inp"`, where path indicates relative location to the input file as shown in the following example:  

```
> MacMetGen -i input\met_ws.inp"
```
  5. MacMetGen should then run the sample problem. This can take between one and several hours. The file currently being processed is shown on the command prompt to help estimate progress.
  6. Four files should be created in the specified output folder: 1) the output surface data file; 2) the MACCS-formatted weather file; 3) a \*.stat file, which indicates the status of the run (should contain “OK” after the run is complete); and 4) a \*.log file, which contains a copy of the input file used and the output shown to the command prompt. The MACCS-formatted weather file can be compared with the “FictitiousSite\_dtdz.MET” file included in the Data folder of the project *Gaussian Weather Sampling*.

## Run GenHysplit

Follow the instructions in the “*Installing HYSPLIT and other software*” section above to install software needed to complete this part of the sample problem. The .ccd files generated in this sample problem can be used in the “*WinMACCS sample problem – HYSPLIT weather sampling*” section below.

1. Determine the folder location for storage of the HYSPLIT output files. Depending on the number of files, the required storage can be large. The files should be accessible from where Python, OpenMPI (or Microsoft MPI), and HYSPLIT are installed, as well as the meteorological files. For this test case, the total size of the HYSPLIT files is approximately 100 GB, but the total folder size with all intermediate results is 300 GB.
2. Copy the GenHysplit.py, pyhysplit.py, and realization.py files in the folder where you are running GenHysplit. These files can be found in the distribution folder GenHysplit/source.
3. Copy the GenHysplit input files where you want to store the input file. These files can be found in the distribution folder GenHysplit. Detailed information about the format of this

input file is described in the document GenHysplit 1.2.0 Users Guide.pdf, released with GenHysplit.

4. For the sample problem, copy sample\_GenHysplit.inp to sample\_problem\_ws.inp. By default, when the input file is not specified on the instantiation line, GenHysplit expects the file to be named test.inp.
5. Open the sample\_problem\_ws.inp file in a text editor and modify for the sample problem settings. The sample problem models radioactive release to occur each hour from December 29, 2014 to February 9, 2016. Each plume is tracked for a 12-hour period and for a range of 100 miles around a fictitious site, for three release heights with default HYSPLIT settings. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
  - a. Modify the directory on line 9 to the location of the HYSPLIT output file.
  - b. Modify the default value on line 11 to 1.
  - c. Modify the directory on line 13 to the location of the downloaded meteorological files
  - d. Delete line 14.
  - e. Leave the default values on line 16 as blank.
  - f. Delete line 17
  - g. Leave the default values on line 19 as “\_nam12”.
  - h. Delete line 20
  - i. Leave the default value on line 22 as 0.
  - j. Modify the directory on line 24 to the location of the HYSPLIT installation folder.
  - k. Modify the directory on line 26 to the location of the HYSPLIT landuse and roughness length folder.
  - l. Leave the default value on line 31 as 1.
  - m. Modify the values on line 33 to “20141229 20160209”.
  - n. Modify the values on line 35 to “115 58 55 W”.
  - o. Modify the values on line 37 to “36 11 35 N”.
  - p. Leave the default value on line 39 as 0.
  - q. Modify the value on line 41 to “10 50 100”.
  - r. The values on line 43 are not used. Can be changed to anything.
  - s. Leave the default value on line 45 as 0.
  - t. Modify the value on line 47 to 12.
  - u. Leave the default value on line 49 as 15.
  - v. Leave the default value on line 51 as 1.
  - w. Modify the value on line 53 to 161.0.
  - x. Leave the default value on line 55 as 10.

- y. Leave the default value on line 57 as 1.0.
  - z. Leave the default value on line 59 as 50.
  - aa. Leave the default value on line 61 as 0.
  - bb. Leave the default value on line 63 as 10.
  - cc. Leave the default values on line 65 as “0.15332 0.28543 0.53138 0.98923 1.8416 3.4284 6.3825 11.882 22.120 41.179”.
  - dd. Leave the default values on line 67 as “1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0”.
  - ee. Leave the default values on line 69 as “0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0”.
  - ff. Leave the default value on line 71 as 2.
6. Execute GenHysplit.

### Running on Linux

For running on a single processor, use the command:

```
mpirun -n 1 python3 <location of *.py files>GenHysplit.py -i <location and name of input file>
```

For submitting a job on to a Linux cluster with a SLURM queueing system with 60 processors, use the command:

```
salloc -n 60 mpirun python3 <location of *.py files>GenHysplit.pyt -i <location and name of input file>
```

### Running on Windows

To view help and to verify that mpiexec has been correctly installed, type the command

```
>mpiexec
```

More help is available with the -help2 command. In this example, the output from the help command is piped into the more function. Tap the spacebar to get the next page of help.

```
>mpiexec -help2|more
```

For running a single processor, the command is:

```
python.exe "completepath/GenHysplit.py" -i "completepath/sample_ws.inp"
```

Where completepath indicates the location of the files needed as shown in the following example:

```
> python "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\GenHysplit.py" -i "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\sample_problem_ws.inp"
```

To take advantage of multiple cores that might be available, open Windows Task Manager to determine the number of cores available. On Windows 10, select the Performance tab. Notice

the value of the variable “Cores” in this window. The number of cores is used for the value of n in the mpiexec command. For example, if the number of Cores is equal to 4, the mpiexec command would be as follows:

```
> mpiexec -n 4 python "completpath/GenHysplit.py" -i "completepath/sample_problem_ws.inp"
```

Once successfully finished, the completed set of HYSPLIT output files (.ccd files) is found in the specified directory (line 17 in input file) in the data directory. There should be 29,376 .ccd files, along with a copy of the input file used and a log file.

## Using the HYSPLIT Model from WinMACCS

### Overview

HYSPLIT is executed independently of WinMACCS. Running HYSPLIT to process a year of weather data is a CPU-intensive process that requires multiple processors to run over a reasonable time (several days). This process must use data consistent with the WinMACCS model settings for the particle bin sizes and the latitude and longitude of the site. The number of particle size bins to be used in WinMACCS, variable NPSGRP, should be equal to the HYSPLIT input for the number of particle size bins and their sizes should be set consistently with the sizes used to determine deposition velocity in WinMACCS. The latitude and longitude defined in WinMACCS, variables Latitude and Longitude, should agree with the values in the HYSPLIT input files. If any of these values are changed in the WinMACCS model, HYSPLIT needs to be run again with the new values. The output files from HYSPLIT are named according to the date and the time modeled. The file extension of the HYSPLIT output files is ccd. For example, 2007122913H001.ccd contains data corresponding to a release that occurs during hour 13 (from 12:00 to 13:00) on 12/29/2007. H001 indicates that the data are for a release height of 10 m in this case.

### Create MACCS-HYSPLIT Files

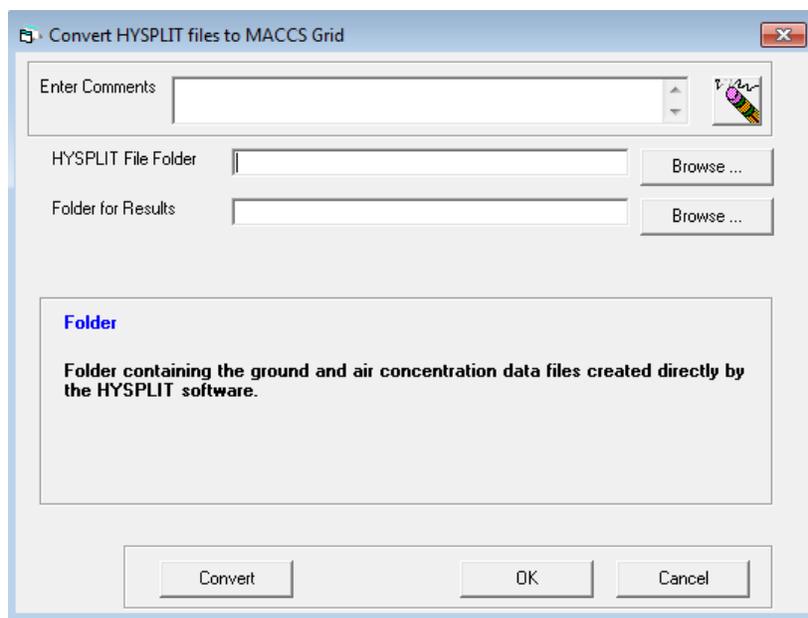
The output from HYSPLIT is organized in a uniform rectangular or polar grid. HyGridConvert, a utility that is bundled with WinMACCS, can convert HYSPLIT data from either a uniform rectangular or polar coordinate system to the nonuniform polar coordinate system used by MACCS. The coordinate system is characterized by the variables SPAEND (defines the outer radius of each ring) and NUMCOR (defines the number of sectors). HyGridConvert is a software tool developed at Sandia and is run from the WinMACCS interface to convert output from the HYSPLIT data files to data files compatible with MACCS. This tool can also be run independently without using the WinMACCS interface.

Before running HyGridConvert, the following variables need to be defined in the WinMACCS interface:

- Latitude
- Longitude
- NUMCOR
- SPAEND

HyGridConvert can be rerun with the same HYSPLIT files if new values are chosen for NUMCOR or SPAEND; HYSPLIT must be rerun if the latitude or longitude of the release location change.

The *Convert HYSPLIT files to MACCS Grid* form is opened by selecting the main menu item *PreProcessing/Create MACCS-HYSPLIT files*. The *Convert HYSPLIT files to MACCS Grid* form opens as shown in Figure 1.



**Figure 1. Convert HYSPLIT files to MACCS Grid Form**

The inputs on this form are folder names that are defined by clicking on the *Browse...* buttons. If either of these folders are on the network, the paths need to be mapped to drive letters in Windows for this process to work correctly. In other words, if the path of the folder starts with a backslash, the drive needs to be mapped using Windows Explorer, so it can be reference as a letter followed by a colon (e.g., X:\my local drive\HYSPLIT output).

The variable *HYSPLIT File Folder* is the folder containing the HYSPLIT result files. These files can be identified by the .ccd extension. All files with the extension .ccd are processed in the folder specified when the *Convert* button is clicked. A set of .ccd files representing a year of data typically occupies about 40-500 GB of storage.

The variable *Folder for Results* is the folder for the HyGridConvert output. It is acceptable to have existing files in this folder. However, when files are created by HyGridConvert with the same name as the existing files, the old files are overwritten. The files output from HyGridConvert are referred to as MACCS-HYSPLIT atmospheric files and have the extension .mcd.

When HyGridConvert is run, a status folder is created in the same folder as the MACCS-HYSPLIT files. This folder is identified by the time of the run, for example Status\_08\_21\_2018\_18\_46\_13 corresponds to a HyGridConvert run that was run on August 21, 2018 at time 18:46:13. This folder contains: 1) the HyGridConvert input file; 2) the

HyGridConvert\_site.inp file; 3) a status file, status.stat; and 4) a detailed output file, status.log. The input file is created by WinMACCS. The status file contains either the character string OK if the execution was error free or an error message from HyGridConvert if an error was detected. Calculation details are saved in status.log.

To aid the user in organizing the MACCS-HYSPLIT files, the concept of a Data Repository was implemented. Because the files typically require 2 to 200 GB for a single year, this feature conserves space by allowing the same set of files to be used by different WinMACCS projects. The Data Repository is a folder that can be specified in the WinMACCS.ini file found in the Program Files (x86)/WinMACCS folder as shown in the following example:

```
REPOSITORY_DIR "D:\WinMACCS Projects\Repository"
```

If this parameter is not defined, it is assumed that the repository is in the following folder located in the user's documents folder:

```
"\WinMACCS Projects\Repository\"
```

HyGridConvert is run when the *Convert* button is clicked. A command window displays the names of the files as they are processed. The status of the run is shown in the WinMACCS Results window. For each release height, there are 8760 files generated by this process for a 365-day year; 8784 are generated for a 366-day year. After HyGridConvert successfully finishes processing, the following line is printed in the WinMACCS Results window:

```
HyGridConvert execution SUCCESSFUL.
```

## Define WinMACCS Parameters

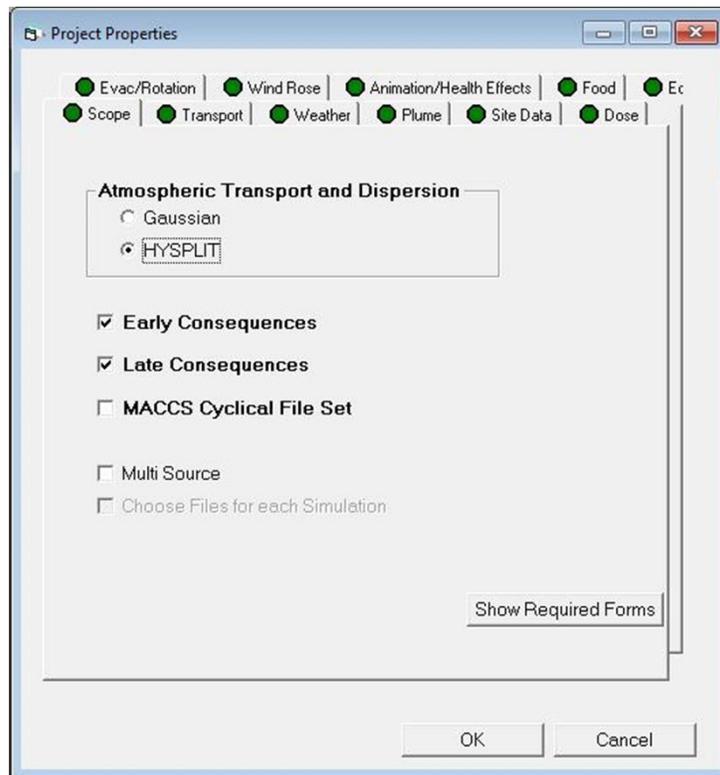
The following steps lead to a WinMACCS project that uses HYSPLIT files to model the atmospheric transport in MACCS.

### Select the HYSPLIT model

The HYSPLIT transport model and the weather sampling method are selected by opening the Project Properties form shown in Figure 2.

- The model is chosen on the *Scope* tab. Select the radio button labeled *HYSPLIT*. Notice that the dispersion model and plume meander model selections are not available on the *Transport* tab when the HYSPLIT model is selected.
- Clicking on the Weather tab, it can be observed that *Constant Weather* (METCOD=4) and *User Supplies 120 Weather Points* (METCOD=3) are not available. Choosing *Fixed Start Time* means that exactly one weather sequence is executed. The other sampling methods, corresponding to METCOD=2 or 5, involve multiple, sampled, weather sequences. *Adjust Mixing Height Based on Time of Day* is not available with the HYSPLIT option.

Clicking *OK* saves the changes.



**Figure 2. Selecting the HYSPLIT model**

### Specify a meteorological file

The MACCS-HYSPLIT files do not contain meteorology data. A MACCS-formatted meteorological file is required for all weather models (METCOD=1, 2, or 5). The meteorology data is needed for the weather sampling algorithms, calculating plume rise height and evaluating the precipitation effects on evacuation speeds. The MACCS-HYSPLIT files and the MACCS-formatted meteorological file should be for the same location and time for consistency. A software product, MacMetGen, is available to create these files.

MACCS supports 15-, 30-, and 60-minute time intervals in the standard (365-day) MACCS meteorological data file. A specific file is selected by opening the *GENERAL/File Specifications/Meteorological File* form and selecting the meteorological file. Clicking OK saves the changes. HYSPLIT data files are in UTC (Greenwich Mean Time). The standard meteorological data file is generally based on a time zone local to the site. This potential difference in time frames between the two files is an inconsistency that can result in an incorrect assignment of weather bins and incorrect calculation of mixing height. This can be fixed by modifying the standard meteorological file to be consistent with UTC and by not using the *Mixing Height Based on Time of Day* option on the *Weather* tab of the Project Properties form (Figure 2). WinMACCS is currently configured to automatically disable the *Mixing Height Based on Time of Day* option when the HYSPLIT is selected.

### Specify location of the MACCS-HYSPLIT files

Specifying the location of the MACCS-HYSPLIT atmospheric transport files created by HyGridConvert is done in WinMACCS by opening the *GENERAL/File Specifications/HYSPLIT Converted Folder* form and defining the location of the MACCS-HYSPLIT files. Unlike other files selected in WinMACCS, such as the site data file, the files are not copied to the project Data folder. Instead, a repository folder is specified that contains the atmospheric transport files. This allows different projects to use the same HYSPLIT data and reduces the storage requirements. MACCS-HYSPLIT files is the path where the MACCS-HYSPLIT files reside and are defined in Table 1.

**Table 1. MACCS-HYSPLIT files variable definition**

| Variable Name       | Definable | Type   | Dimensions | Allowed Values                                                               |
|---------------------|-----------|--------|------------|------------------------------------------------------------------------------|
| MACCS-HYSPLIT files | Yes       | Folder | None       | Legal path on computer, including mapped drives but excluding network drives |

### Specify the site location

Specifying the site location is done by opening the *ATMOS/Weather/Site Location* form. These values are compared with the latitude and longitude written to the MACCS-HYSPLIT files when the user clicks the *Run Simulation* button and before the MACCS simulation is initiated. The two sets of latitude and longitude values must match.

### Define the forms in the HYSPLIT Transport Parameters category

#### *File extensions and lower bounds*

HYSPLIT input parameters specify either a set of release heights or a set of power levels associated with the created dataset. For MACCS to correctly identify the files to use, each set of MACCS-HYSPLIT data files must be identified. This is done by specifying the prefix portion of the file name (ex: H001 is the postfix portion of file 2008010100H001.mcd). Variable HY\_NUMPRE is the number of MACCS-HYSPLIT data file sets and is defined in Table 2.

Variable HY\_PREFIX is a vector of length HY\_NUMPRE and is defined in Table 2. The values determine the expected names of the MACCS-HYSPLIT files. The character string is either in the format Hxxx or Pxxx, where xxx corresponds to three digits. Hxxx represents a release height of xxx\*10m. Pxxx represents a power level of xxx\*0.1MW. For example, H001 corresponds to 10 meters, P050 corresponds to 5 MW.

When more than one release height or power level is used, the variable HY\_LOWER is used to determine when to transition from one set to another. Variable HY\_LOWER is defined in Table 2 and is the lower bound of either the height or the power corresponding to HY\_PREFIX. For example, for a set of release heights of H001, H005 and H020 (release heights of 10, 50 and 200 meters) the HY\_LOWER values of 0, 30, and 100 meters indicate that the H001 file set is to be used for releases between 0 and 30 meters, the H005 file set for releases between 30 and 100 meters, and the H020 file set for releases above 100 meters.

**Table 2. File extensions and lower bounds variable definitions**

| Variable Name | Definable | Type               | Dimensions | Allowed Values                                                                                                                    |
|---------------|-----------|--------------------|------------|-----------------------------------------------------------------------------------------------------------------------------------|
| HY_NUMPRE     | Yes       | Integer            | None       | 1 to 10                                                                                                                           |
| HY_PREFIX     | Yes       | String of length 4 | HY_NUMPRE  | Prefix of MACCS-HYSPLIT data files. The first character must be H (for height) or P (for power) and must be followed by 3 digits. |
| HY_LOWER      | Yes       | Real               | HY_NUMPRE  | [0, 1.0E5] in units of m or MW, depending on whether H or P is used with HY_PREFIX, respectively                                  |

#### *Fixed start time data*

When *Fixed Start Time* is selected on the *Project Properties* form, then only a single weather sequence is run. For either fixed start time or weather sampling, the starting date and time for each weather trial are associated with the plume denoted by MAXRIS, the plume of maximum risk, defined on the *Release Description/Plume of Maximum Risk* form. The variables on the ATMOS/HYSPLIT Transport/Fixed Start Time Data form (see Table 3) are as follows:

- HY\_FIXED identifies the date when the weather sequence begins in UTC. This is entered in MM/DD/YYYY format. For example, “01/31/2008” is a valid string.
- HY\_HOUR identifies the starting hour of the weather trial based on 24 hours in a day in UTC. Hour 1 begins at midnight, hour 2 begins at 1:00 AM, etc.

Information required for the Gaussian and HYSPLIT models when running a fixed-start-time case are similar, but they are specified on two separate forms. An important distinction is that the Gaussian model requires a Julian day and hour; whereas, the HYSPLIT model requires a date and hour. For the purpose of comparing the two models, the user needs to choose these separate

inputs so that they match, accounting for any difference in time zones. For example, the variables ISTRDY and ISTRHR may need to be adjusted to correspond to UTC time when comparing results between the models (e.g., subtracting the difference between the local time zone and Greenwich Mean Time). One caution is that the DAY\_AND\_NIGHT option assumes that the hours in the weather file are local, not UTC.

**Table 3. Fixed start time data variable definitions**

| Variable Name | Definable | Type    | Dimensions | Allowed Values                           |
|---------------|-----------|---------|------------|------------------------------------------|
| HY_FIXED      | Yes       | String  | None       | 10-character string of format MM/DD/YYYY |
| HY_HOUR       | Yes       | Integer | None       | 1 to 24                                  |

### *Weather sampling*

When multiple weather sequences are run (METCOD=2 or 5), with the start date and time determined by the sampling algorithm, a start and an end date are selected on the *ATMOS/HYSPLIT Transport/Transport Dates* form. For the current version of WinMACCS when using any of the weather sampling options, the start day must be January 1, and the end day must be December 31 of the same year for both 365- and 366-day years. However, this requirement is enforced only by MACCS, not WinMACCS.

### *Transport dates*

The transport dates are only required if weather sampling is used. The variables on the *ATMOS/HYSPLIT Transport/Transport Dates* form (see Table 4) are as follows:

- HY\_START is the first date for weather sampling. This is entered in MM/DD/YYYY format. For example, “01/01/2008” is a valid string. Since the weather files used by HYSPLIT are in UTC time, this date is also defined for that time zone.
- HY\_END is the last date for weather sampling. This is entered in MM/DD/YYYY format. For example, “12/31/2008” is a valid string. Since the weather files used by HYSPLIT are in UTC time, this date is also defined for that time zone.

**Table 4. Transport dates variable definitions**

| Variable Name | Definable | Type   | Dimensions | Allowed Values                           |
|---------------|-----------|--------|------------|------------------------------------------|
| HY_START      | Yes       | String | None       | 10-character string of format MM/DD/YYYY |
| HY_END        | Yes       | String | None       | 10-character string of format MM/DD/YYYY |

*Extended time*

The form *ATMOS/HYSPLIT Transport/Extended Time* allows for additional weather days before and after the starting and ending times for weather sampling. This form is required when the HYSPLIT model is selected for all weather options. The variables on this form (see Table 5) are as follows:

HY\_BEFORE is the number of weather days preceding HY\_START, the starting date for weather sampling. The purpose of these additional weather days is to allow for releases that are earlier than the MAXRIS plume segment that is aligned with the selected starting day and hour. For a fixed start time, this is the number of days preceding HY\_FIXED that are supplied.

HY\_AFTER is the number of weather days following HY\_END when using weather sampling. Similarly, this is the number of days following HY\_FIXED when using a fixed start time. The purpose for these additional days is to provide weather for plumes traveling through the grid after the end of the specified time interval, e.g., the end of a year of weather data. The user should choose a value of HY\_AFTER sufficiently large so that the entire release can occur (i.e., to cover the last hour of release).

**Table 5. Extended time variable definitions**

| Variable Name | Definable | Type    | Dimensions | Allowed Values |
|---------------|-----------|---------|------------|----------------|
| HY_BEFORE     | Yes       | Integer | None       | 0 to 2         |
| HY_AFTER      | Yes       | Integer | None       | 0 to 40        |

**Specify model results**

ATMOS results from the simulation are not specific to a plume segment when using the HYSPLIT model. Because of this, a different output request form is used to request Type 0

results. This form can be opened by double clicking on the form name *ATMOS/Output Control/Spatial Intervals* on the Parameters tab. The *ATMOS/Output Control/Spatial Intervals* form is optional. The variables on this form (see Table 6) are as follows:

- NUM0\_HY specifies the number of Type 0 results to be created. For each request, seven results describing atmospheric transport and dispersion are reported. The value is automatically calculated by WinMACCS based on the values of INDRAD\_HY.
- INDRAD\_HY specifies the index of the radial grid element for which results are to be reported. The reported values are for the radial midpoint of the grid element.
- When Report Options are set to CCDF or CCDF & REPORT, the complimentary cumulative distribution function data are reported in the MACCS output file. When set to REPORT or CCDF & REPORT, WinMACCS automatically generates a report over all weather trials based on the quantile values specified on the *Reporting Options* form.

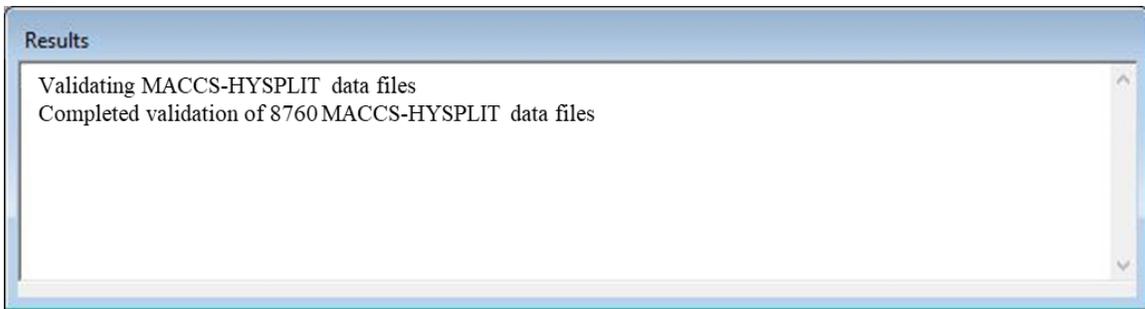
**Table 6. Specify model results variable definitions**

| Variable Name  | Definable | Type      | Dimensions | Allowed Values                    |
|----------------|-----------|-----------|------------|-----------------------------------|
| NUM0_HY        | Linked    | Integer   | None       | 0 to 999                          |
| INDRAD_HY      | Yes       | Integer   | NUM_HY     | 1 to NUMRAD                       |
| Report Options | Yes       | Character | NUM0       | CCDF, NONE, REPORT, CCDF & REPORT |

### Running WinMACCS Using the MACCS-HYSPLIT Model

Clicking the Run Simulation button starts a MACCS calculation. Before MACCS starts, the MACCS-HYSPLIT files are validated against the project settings. WinMACCS reports this process in the Results window. When the spatial grid, number of particle size bins, or the latitude and the longitude settings in WinMACCS are inconsistent with the MACCS-HYSPLIT data files, the MACCS run is not started and an error condition is reported to the user.

WinMACCS also verifies that all the required files are available. The validation step stops if there is a discrepancy between what is expected in the files or if any file is missing. At the end of the validation step, WinMACCS reports the number of files processed provided that all files pass validation. Figure 3 shows the results window after a successful file validation. Table 7 below lists the set of tests done at this validation step.



**Figure 3. Results after successful MACCS-HYSPLIT file validation**

**Table 7. MACCS-HYSPLIT data file validation tests**

| WinMACCS variable                    | Validation                                                                                                                                                                                                 | Remediation if validation does not pass                                                                                                                             |
|--------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| NUMCOR, number of sectors in grid    | Checks that NUMCOR is equal to the value in MACCS-HYSPLIT file header for each file                                                                                                                        | Rerun HyGridConvert                                                                                                                                                 |
| NUMRAD, number of radii in grid      | Checks that NUMRAD is equal to the value in MACCS-HYSPLIT file header for each file                                                                                                                        | Rerun HyGridConvert                                                                                                                                                 |
| SPAEND, radii used to define grid    | For each value of SPAEND, and for each value of RADIUS in the MACCS-HYSPLIT file, validation passes if $ABS(SPAEND - RADIUS) / ABS(SPAEND) \leq 0.001$                                                     | Rerun HyGridConvert                                                                                                                                                 |
| NPSGRP, number of particle size bins | Checks that NPSGRP is equal to the value in MACCS-HYSPLIT file header                                                                                                                                      | Rerun HYSPLIT with a consistent value for the number of particle size bins or modify number of particle size bins in WinMACCS to be consistent with HYSPLIT results |
| Latitude, site latitude              | LAT is the latitude written to the MACCS-HYSPLIT file and Latitude is the value in WinMACCS. Validation passes if $ABS(Latitude - LAT) \leq 0.01$ , which corresponds to approximately 1 km at the equator | Rerun HYSPLIT. Location of data site being modeled is not consistent with HYSPLIT results                                                                           |
| Longitude, site longitude            | LONG is the longitude written to the MACCS-HYSPLIT file and Longitude is the value in WinMACCS. Validation passes if $ABS(Longitude - LONG) \leq 0.01$ , which corresponds to approximately 1 km           | Rerun HYSPLIT. Location of data site being modeled is not consistent with HYSPLIT results                                                                           |

One additional note on validation is that WinMACCS may not validate additional HYSPLIT results required by MACCS that depend on how the deposition flags are set for the various chemical groups. Commonly, MACCS is used to model N aerosol bins for most chemical groups as depositing by both wet and dry deposition, except for one chemical group, the noble gases, which do not deposit either by wet or dry deposition. With this choice, one additional HYSPLIT result is needed to capture the transport of the non-depositing noble gases, i.e., HYSPLIT must create N+1 distinct air and ground concentration fields. Possibilities that are rarely used are to

allow some chemical groups to deposit by dry deposition but not by wet deposition or to allow some to deposit by wet deposition but not by dry deposition. To capture all combinations of dry and wet deposition,  $2*(N+1)$  distinct HYSPLIT results are needed. Both MACCS and HYSPLIT accommodate all these possibilities and MACCS requires HYSPLIT to have quantified the correct deposition behavior; however, WinMACCS does not validate these additional variations. WinMACCS only validates that the number of aerosol size bins match.

As WinMACCS is checking the HYSPLIT files, if any are missing, the MACCS run is not started. In this case, HYSPLIT might need to be run to create the missing files, followed by running HyGridConvert to convert the HYSPLIT output into MACCS-HYSPLIT files. The required MACCS-HYSPLIT data files by weather sampling method are shown in Table 8.

**Table 8. MACCS-HYSPLIT data files required by weather sampling method**

| Sampling Method                    | Files Required                                                                                                                                                                                                                                          | Example                                                                                                                                                                                                                                                                                          |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Fixed Start Time (METCOD = 1)      | 24 files associated with a weather day defined in WinMACCS variable HY_FIXED, plus files associated with HY_BEFORE days before HY_FIXED and HY_AFTER days following HY_FIXED. A complete set of files is expected for each value of variable HY_PREFIX. | HY_FIXED = "06/01/2008"<br>HY_BEFORE = 1<br>HY_AFTER = 2<br>Exactly one value of HY_PREFIX, and HY_PREFIX[1]="H001"<br>There must be 24 files/day *4 days, or 96 files, starting with 2008053100H001.mcd and ending with 2008060323HY001.mcd                                                     |
| Weather Sampling (METCOD = 2 or 5) | 24 files per day for all days in the interval defined by WinMACCS variables HY_START and HY_END, plus files associated with HY_BEFORE days before HY_START and HY_AFTER days following HY_END                                                           | HY_START = "01/01/2008"<br>HY_END = "12/31/2008"<br>HY_BEFORE = 2<br>HY_AFTER = 15<br>Exactly one value of HY_PREFIX, and HY_PREFIX[1]="P050"<br>There must be 24 files/day * (2 days + 366 days + 15 days), or 9,192 files, starting with 2007123000P050.mcd and ending with 2009011523P050.mcd |

### MACCS-HYSPLIT Model Results

Basic air and ground concentration results are available when using the HYSPLIT atmospheric transport option. These are analogous to the results that can be obtained for the Gaussian plume segment option, but not identical. For example, the concept of a plume centerline does not exist in the HYSPLIT model, so centerline is replaced by peak, which has the meaning of the maximum value around the compass at a distance corresponding a circle at the center of a ring. Table 9 provides a description of the Type 0 outputs that are created when using the HYSPLIT transport model.

**Table 9. Type 0 outputs when using the HYSPLIT transport model**

| Result                                                     | Description                                                                                                                                                       |
|------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Peak Ground-Level Air Concentration (Bq·s/m <sup>3</sup> ) | Peak (around the compass), time-integrated, ground-level, air concentration for the selected radionuclide at the requested distance (i.e., peak value of $\chi$ ) |
| Peak Ground Concentration (Bq/m <sup>2</sup> )             | Peak (around the compass) ground concentration for the selected radionuclide at radionuclide exit time at the requested distance (i.e., peak value of $D$ )       |
| Total Peak Ground Concentration (Bq/m <sup>2</sup> )       | Peak (around the compass) ground concentration for all radionuclides at radionuclide exit time at the requested distance                                          |
| Adjusted Source Strength (Bq)                              | Inventory of the selected radionuclide at radionuclide exit time accounting for decay and deposition                                                              |
| Ground-Level Chi/Q (s/m <sup>3</sup> )                     | Peak (around the compass) time-integrated, ground-level, air concentration for the selected radionuclide divided by the initial source (i.e., $\chi/Q$ )          |
| Radionuclide Arrival Time (s)                              | First time at which a non-zero ground-level air concentration of the selected radionuclide crosses the midpoint of a ring                                         |
| Radionuclide Exit Time (s)                                 | Last time at which a non-zero ground-level air concentration of the selected radionuclide crosses the midpoint of a ring                                          |

## WinMACCS Sample Problem – HYSPLIT Fixed Start Time

### Locate HYSPLIT Data

To generate the HYSPLIT files needed for this project, follow the steps in the previous section, HYSPLIT Sample Problem, Five Days of Data, to create the five days of HYSPLIT files before running the problem in WinMACCS.

Sample output files from the GenHysplit program (the program that runs HYSPLIT to create atmospheric transport results) are provided in the distribution folder \Sample Problems\HYSPLIT\_files\_fixed\_start. These files have an extension “.ccd”. It is not necessary to run GenHysplit (and hence HYSPLIT) if the provided files are used.

Sample output files from the HyGridConvert utility (the program that converts the output from GenHysplit to the MACCS input format) are provided in the distribution folder \Sample Problems\MACCS\_files\_fixed\_start. These files have an extension “.mcd”. It is not necessary to run GenHysplit (and hence HYSPLIT) or HyGridConvert if the provided files are used.

### Create Project

Start WinMACCS.

Select *File/Open Project* from the main menu. Open the project file *Gaussian Fixed Start Time.mxd*.

Select *File/SaveAs Project* from the main menu. Enter *HYSPLIT Fixed Start Time* in the *Project Name* text box. Click *OK*.

### Select the HYSPLIT Model

Select *Edit/Project Properties* from the main menu. In the *Project Properties* form on the *Scope* tab, change the *Atmospheric Transport and Dispersion* option from *Gaussian* to *HYSPLIT* (see Figure 2). Click on the *Weather* tab. Notice that *Fixed Start Time* is selected. Click *OK* to save.

### Define the MACCS-HYSPLIT Variables

HyGridConvert was used to generate a set of input files (.mcd) for use in this sample problem. The .mcd files contain air and ground concentrations interpolated onto the MACCS grid. These .mcd files can either be used directly for the sample problem or as comparison files after following the process below.

If it is necessary or desired to create .mcd files from the .ccd files, do the following:

Select *PreProcessing/Create MACCS-HYSPLIT files* from the main menu.

Click the *Browse ...* button next to *HYSPLIT File Folder* text box and select folder containing GenHysplit output (.ccd) files.

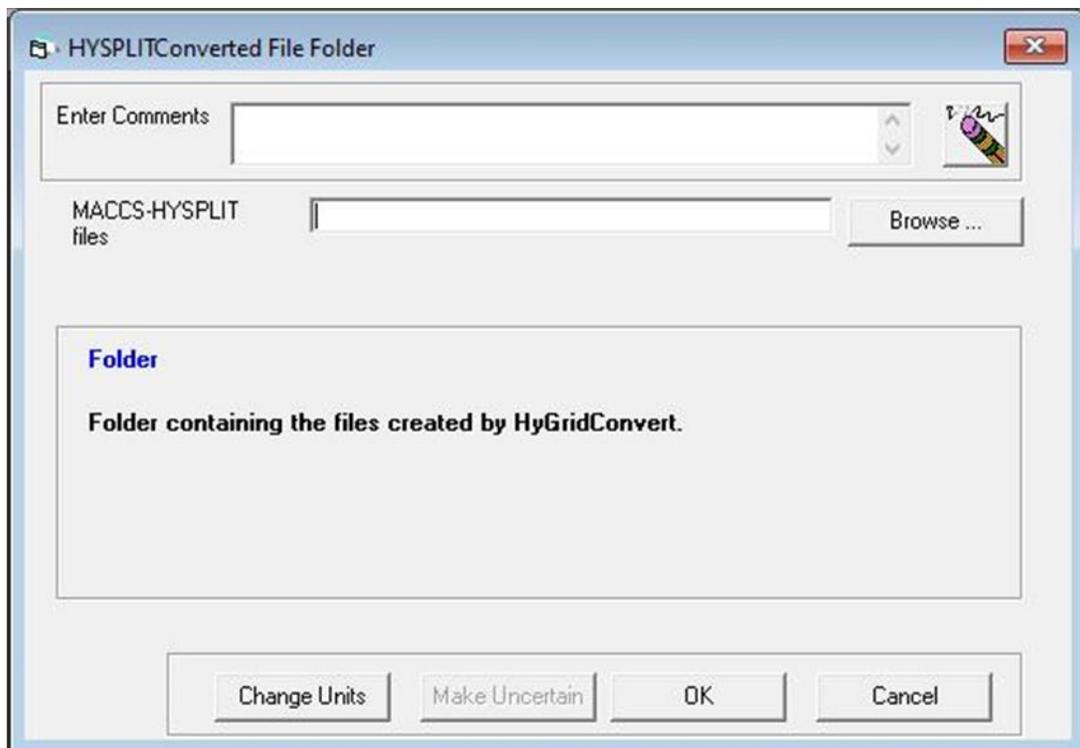
Click the *Browse ...* button next to *Folder for Results* text box and select folder where you wish to store the desired MACCS input files (.mcd).

Click the *Convert* button. This begins the conversion process and can take a few minutes.

After the conversion is complete, answer *Yes* to have this folder automatically linked to this project. If this is done, there is no need to manually link this folder using the form *GENERAL/File Specifications/HYSPLIT Converted Folder*.

#### Specify the location of the MACCS-HYSPLIT files

This may not be necessary if the folder was linked from the form *PreProcessing/Create MACCS-HYSPLIT files*. Sample .mcd files have been included in the distribution folder \Sample Problems\MACCS\_files\_fixed\_start. To use the provided files, click on the plus sign next to the *GENERAL/File Specifications* entry. Double click on the form named *HYSPLIT Converted Folder* (see Figure 4). Click the *Browse ...* button next to *MACCS-HYSPLIT files* text box and select the folder containing the set of MACCS input files (.mcd) to be used in this calculation. Click *OK*.



The image shows a software dialog box titled "HYSPLITConverted File Folder". At the top left is a folder icon and the title. At the top right is a close button (X). Below the title bar is a section for "Enter Comments" with a text input field and a vertical scroll bar, and a pencil icon to the right. Below that is a section for "MACCS-HYSPLIT files" with a text input field and a "Browse ..." button to its right. Below the input fields is a larger text box containing the text "Folder" and "Folder containing the files created by HyGridConvert." At the bottom of the dialog are four buttons: "Change Units", "Make Uncertain", "OK", and "Cancel".

**Figure 4. Form to define location of MACCS-HYSPLIT files**

Indicate the prefixes for the MACCS-HYSPLIT files and when to use them

Open the form ATMOS/HYSPLIT Transport/File Extensions and Lower Bounds. Fill in the grid as shown in Figure 5 and then click *OK*. Figure 5 specifies that all releases above ground level (0 m) are to be treated using a file(s) ending in H001, which represents a release at 10 m. Multiple release heights can be represented by specifying multiple files sets with different endings. For this sample problem, only one set of files were generated.

File Extensions and Lower Bounds

Enter Comments

HY\_NUMPRE

|   | HY_PREFIX | HY_LOWER |
|---|-----------|----------|
| 1 | H001      | 0        |
|   | *         |          |

4 to 4 Characters ; Row bounds: [1, 10]

Hxxx, where release height is xxx\*10 m, or Pxxx where power level is at xxx\*0.1 MW. Example: H100, P050. Values should be either all be Pxxx or Hxxx. Example file in a set: 2008010200H100.mcd corresponds to MACCS-HYSPLIT data for January 2, 2008 at 0 hours at 1000 m.

Change Units    Make Uncertain    OK    Cancel

**Figure 5. Fixed Start Time Sample Problem File Extensions and Lower Bounds**

Define time intervals

Open the form ATMOS/HYSPLIT Transport/Fixed Start Time Data. The weather file was developed with only six days of data and using UTC time (see section, HYSPLIT Sample Problem, Five Days of Data). Therefore the day was set as day 1 and hour 7 in the Gaussian Fixed Start sample problem. For the HYSPLIT Fixed Start sample problem, we set day to the actual date, 3/11/2011 and the hour in UTC time, which is hour 7. Fill in the grid as shown in Figure 6 and then click *OK*.

HYSPLIT Fixed Start Time Data

Enter Comments

HY\_FIXED 03/11/2011

HY\_HOUR (-) 7

**10 to 10 Characters**

The date when the weather sequence begins in MM/DD/YYYY format.

Change Units Make Uncertain OK Cancel

**Figure 6. Fixed Start Time Sample Problem HYSPLIT Fixed Start Time Data**

Open the form ATMOS/HYSPLIT Transport/Extended Time. Fill in the form as is shown in Figure 7 and then click *OK*. The values in Figure 7 indicate that no weather is specified prior to the starting day and 4 days are specified following the starting day. This allows releases to occur for a maximum of 5 consecutive days.

Extended Time

Enter Comments

HY\_BEFORE (d) 0

HY\_AFTER (d) 4

**Integer [0, 40] days**

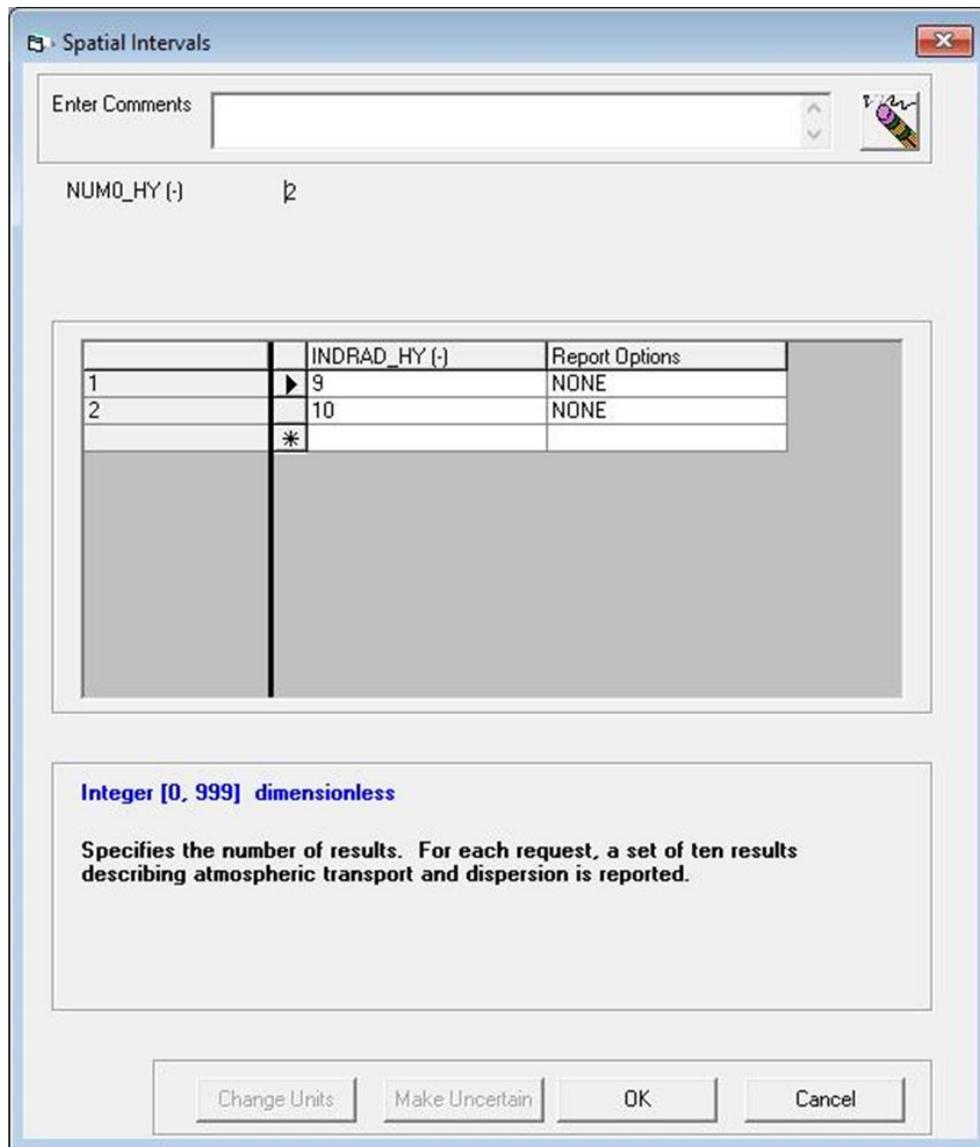
**Number of weather days after HY\_END if using uniform, nonuniform or stratified weather sampling. Number of weather days after HY\_FIXED if using the Fixed Start Time model.**

Change Units Make Uncertain OK Cancel

**Figure 7. Fixed Start Time Sample Problem Extended Time**

Define ATMOS output quantities

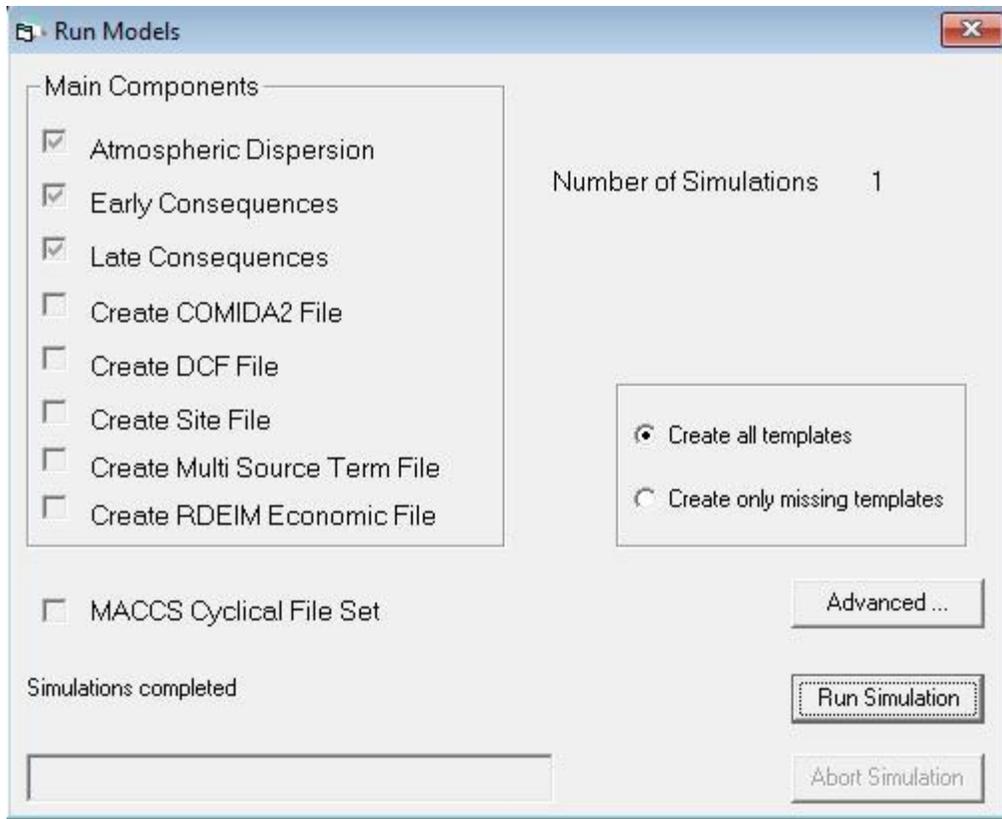
Open the form ATMOS/Output Control/Spatial Intervals (see Figure 8). To mimic the same output locations used in the Gaussian Fixed Start sample problem, fill in the form as is shown in Figure 8 and then click *OK*.



**Figure 8. Fixed Start Time Sample Problem Spatial Intervals**

### Run the MACCS-HYSPLIT Model

Select *Execute/Run Models* from the main menu. Click the *Run Simulation* button (see Figure 9).



**Figure 9. Run Models form**

Running the simulation generates a Model1.bin and Model1.out file in the Output folder. Comparing the Model1.out file with the “HYSPLIT Fixed Start Time.out” file included in the Output folder of the project *Gaussian Fixed Start Time* allows a user to determine differences between their setup and this sample problem.

The output files from GenHysplit used in this calculation were created using a Linux operating system running HYSPLIT version 5.0.0. There could be differences in the results when the version of HYSPLIT is different or when HYSPLIT was run under a different operating system.

## WinMACCS Sample Problem - HYSPLIT Weather Sampling

### Locate HYSPLIT Data

To generate HYSPLIT files for use with this project, follow the steps in the previous section HYSPLIT Sample Problem, One Year of Data to create one year of HYSPLIT files before running the problem in WinMACCS. WinMACCS can then be used to convert the “.ccd” files using the HyGridConvert utility, as discussed in section WinMACCS Sample Problem – HYSPLIT Fixed Start Time above.

Sample output files from the GenHysplit program (the program that runs HYSPLIT to create atmospheric transport results) and processed through the HyGridConvert utility (the program that converts the output from GenHysplit to MACCS format) are provided in the distribution folder \Sample Problems\MACCS\_files\_weather\_sampling. These files have an extension “.mcd”. It is not necessary to run GenHysplit (and hence HYSPLIT) or HyGridConvert if the provided files are used.

### Create Project

Start WinMACCS.

Select *File/Open Project* from the main menu. Open the project file *Gaussian Weather Sampling.mxd*.

Select *File/SaveAs Project* from the main menu. Enter *HYSPLIT Weather Sampling* in the *Project Name* text box. Click *OK*.

### Select the HYSPLIT Model

Select *Edit/Project Properties* from the main menu. In the Project Properties form on the Scope tab, change the Atmospheric Transport and Dispersion option from Gaussian to HYSPLIT (see Figure 2). Click on the Weather tab. Notice that Uniform Bin Sampling is selected. Click *OK* to save.

### Define the MACCS-HYSPLIT Variables

Specify the location of the MACCS-HYSPLIT files

On the *Parameters* tab of the *Project* window, click on the plus sign next to the *GENERAL/File Specifications* entry. Double click on the form named *HYSPLIT Converted Folder* (see Figure 4). Click on text box next to the words *MACCS-HYSPLIT files*. Note that a comment appears in the area below this text box describing the required input. To satisfy this input requirement, click the *Browse ...* button next to *MACCS-HYSPLIT files* text box and select the folder containing the set of MACCS input files (files with the extension .mcd) to be used in this calculation. Click *OK*.

A set of input files (.mcd) have already been created using GenHysplit (which runs HYSPLIT), and a utility that can be run from WinMACCS called HyGridConvert. When the spatial grid definition is changed (WinMACCS variables SPAEND or NUMCOR), HyGridConvert needs to

be run to recreate the .mcd files. If the site location (Latitude or Longitude), the number of aerosol size bins, or the aerosol sizes change, HYSPLIT must be rerun.

The sample .mcd files can be found in the distribution folder \Sample Problems\MACCS\_files\_weather\_sampling

Indicate the MACCS-HYSPLIT files and when to use them

Open the form ATMOS/HYSPLIT Transport/File Extensions and Lower Bounds (see Figure 10).

The release height and the power used in the GenHysplit calculation are encoded in the file name. The calculation can be based on either height (using H in the HY\_PREFIX variable) or power (using P in the HY\_PREFIX variable), but not a mixture of both.

The variable HY\_LOWER determines when the associated files are used. Notice, the units of HY\_LOWER are in meters in this example because files with an H in the postfix portion of their names (H001, H005 and H010) are used. For this sample problem, H001 (representing a release height of 10 m) is used for release heights in the range of 0 to less than 30 m. H005 (representing a release height of 50 m) is used for release heights from 30 to less than 75 m. H010 (representing a release height of 100 m) is used for heights greater than or equal to 75 m.

Fill in the grid as is shown in Figure 10 and then click *OK*.

File Extensions and Lower Bounds

Enter Comments

HY\_NUMPRE      3

|   | HY_PREFIX | HY_LOWER |
|---|-----------|----------|
| 1 | H001      | 0.       |
| 2 | H005      | 30.      |
| 3 | H010      | 75.      |
|   | *         |          |

**4 to 4 Characters ; Row bounds: [1, 10]**

**Hxxx, where release height is xxx\*10 m, or Pxxx where power level is at xxx\*0.1 MW. Example: H100, P050. Values should be either all be Pxxx or Hxxx. Example file in a set: 2008010200H100.mcd corresponds to MACCS-HYSPLIT data for January 2, 2008 at 0 hours at 1000 m.**

Change Units    Make Uncertain    OK    Cancel

**Figure 10. Weather Sampling Sample Problem File Extensions and Lower Bounds**

Indicate the dates to use in the model

Open the form ATMOS/HYSPLIT Transport/Transport Dates (see Figure 11). The software expects 24 files for each day to be present in the *MACCS-HYSPLIT files* folder for each value of height or power specified on the *File Extensions and Lower Bounds* form. This analysis is for the year 2015. Fill in the form as is shown in Figure 11 and then click *OK*.

HYSPLIT Transport Dates

Enter Comments

HY\_START

HY\_END

**10 to 10 Characters**

**The first day of possible weather in MM/DD/YYYY format.**

Change Units Make Uncertain OK Cancel

**Figure 11. Weather Sampling Sample Problem HYSPLIT Transport Dates**

Open the form ATMOS/HYSPLIT Transport/Extended Time (see Figure 12). The software expects 24 additional files for each value of HY\_PREFIX times the number of days in HY\_BEFORE plus HY\_AFTER. For this sample problem, MACCS-HYSPLIT files for two days prior to 2015 and 40 days after 2015 were generated. Fill in the form as is shown in Figure 12 and then click *OK*.

Extended Time

Enter Comments

HY\_BEFORE (d) 2

HY\_AFTER (d) 40

**Integer [0, 2] days**

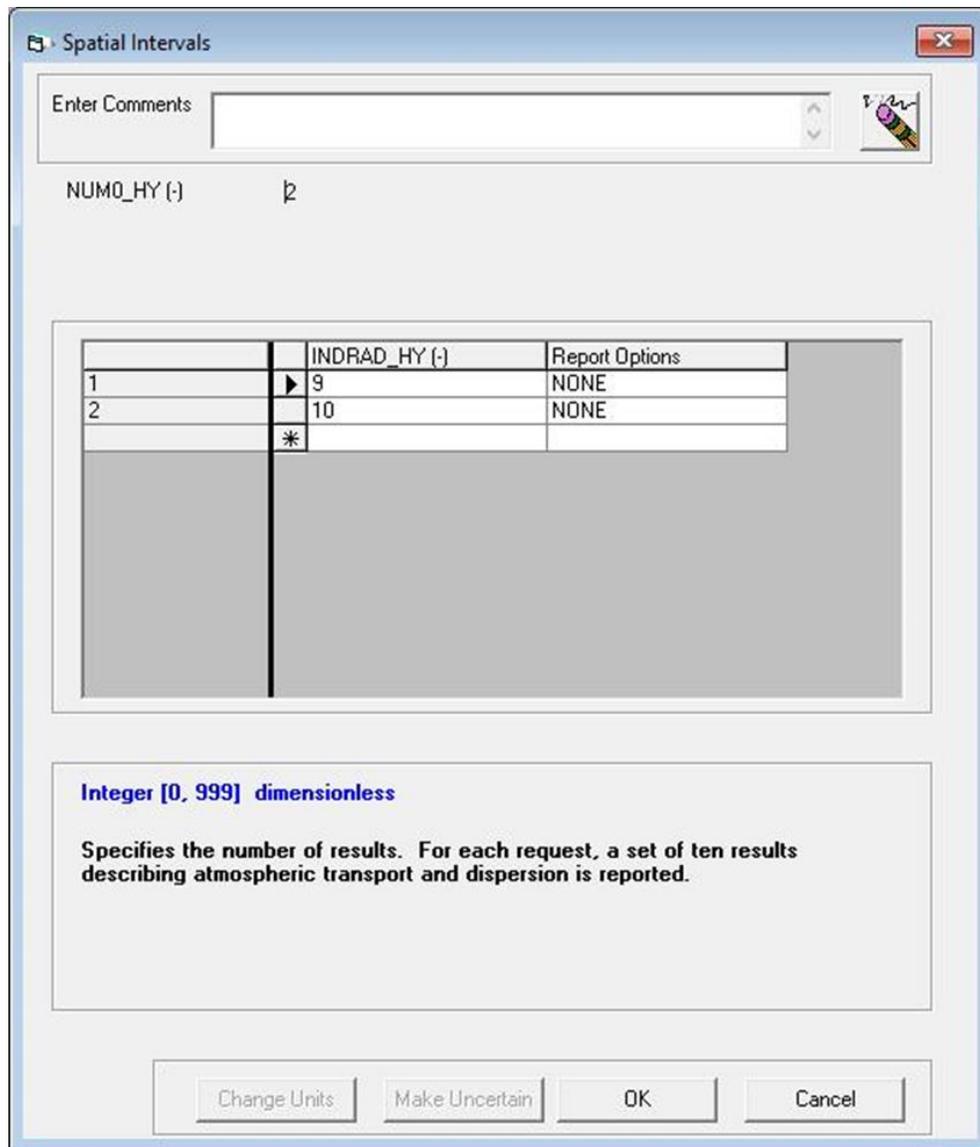
**Number of weather days preceding HY\_START if using uniform, nonuniform or stratified weather sampling. Number of weather days preceding HY\_FIXED if using the Fixed Start Time model.**

Change Units Make Uncertain OK Cancel

**Figure 12. Weather Sampling Sample Problem Extended Time**

Define ATMOS output quantities

Open the form ATMOS/Output Control/Spatial Intervals (see Figure 13). To mimic the same output locations used in the Gaussian Fixed Start sample problem, fill in the form as is shown in Figure 13 and then click *OK*.



**Figure 13. Weather Sampling Sample Problem Spatial Intervals**

### Run the MACCS-HYSPLIT Model

Select *Execute/Run Models* from the main menu. Click the *Run Simulation* button (see Figure 9). This should generate a Model1.bin and Model1.out file in the Output folder. Comparing the Model1.out file with the “HYSPLIT Weather Sampling.out” file included in the Output folder of the project *Gaussian Weather Sampling* allows a user to determine differences between their setup and this sample problem.

The output files from GenHysplit used in this calculation were created using a Linux operating system running HYSPLIT version 5.0.0. There could be differences in the results when either the version of HYSPLIT is different or when HYSPLIT was run under a different operating system.