GenHysplit 1.2.0 User's Guide

July 14, 2020¹

1. Introduction

This document describes the design of GenHysplit 1.2.0 and provides usage instructions. GenHysplit collects input values and generates a set of output files of deposition and air concentrations using the HYSPLIT code. The output files can then be used to model potential consequences. GenHysplit is configured to model the transport of a normalized release over a one-hour period. Multiple aerosol sizes are tracked in the same calculation, each with individual transport properties. Furthermore, released aerosols and gases can be specified to deposit by any combination wet and dry deposition processes, including neither wet nor dry deposition.

The HYSPLIT model is a complete system for computing simple air parcel trajectories as well as complex dispersion and deposition simulations. The initial development was a result of a joint effort between the National Oceanic and Atmospheric Administration (NOAA) in the U.S. and Australia's Bureau of Meteorology. HYSPLIT can use most weather data sets. HYSPLIT can be used with NOAA weather data sets that provide sufficient spatial and temporal resolution to define representative wind fields and assure that meteorological variability is accurately captured.

2. Code Structure

GenHysplit 1.2.0 is written in Python3. Python 3.3 or higher is required, as that version contains all the required python packages needed for GenHysplit. The GenHysplit code (GenHysplit.py) includes multiple modules for organization of the data structures. The modules defined in the source folder are:

• realization.py

This module contains information for each 'realization', which is a combination of each specific weather day, hour of release and release height or plume energy. The realizations also have several methods associated with them that are invoked as well. These include a 'run' method, which acts as a main function call for each realization.

• pyhysplit.py This module contains the initialization configurations and options associated with HYSPLIT. It also contains routines to create HYSPLIT input files based on the parameters set for the realization.

¹ Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2022-10314O

3. Assumptions

The following are assumptions that are hardwired into GenHysplit:

- 1. Each weather file is HYSPLIT compatible and has a filename that contains the year, month, and day in the format YYYYMMDD, where YYYY is the year of the weather day, MM is the month of the weather day, DD is the day of the month for the weather day. Furthermore, all filenames within the same weather data set have the same prefix and postfix. The complete file name is defined by the prefix and postfix character strings added to the date portion.
- 2. Polar output grids are divided into 128 equal sectors, with equal spacing between radii (in km).
- 3. Rectangular output grids have equal spans and spacing (in km) in the North, South, West and East directions about an origin.
- 4. The earth is a sphere with a radius of 6,378.1 km (used to convert from latitude/longitude to km).

These assumptions can easily be changed in the source code if they become obsolete or invalid.

4. Running the Code

GenHysplit is written in Python3. Typing 'python3 GenHysplit.py' in the source directory starts GenHysplit, assuming that there is a valid 'test.inp' file in the current directory. To change which input file is used, the '-i' option on the command line can be used to specify a file with a different name. If a GenHysplit run is interrupted, the '--restart' option can be used to continue. Invoking this option causes GenHysplit to check to see if a realization has already completed and, if so, skip to the next realization instead of recalculating the realization. GenHysplit is setup to use OpenMPI to take advantage of using multiple processors. Typing 'mpirun -n xx python3 GenHysplit.py' in the source directory runs the case on xx processors (if they are available).

5. Input Files

The default input file name for GenHysplit is 'test.inp' (which can be under a different name if the –i command line option is used). The GenHysplit input file contains information on where other required files and programs are located. These required files are:

- Weather file directory(ies)
- HYSPLIT directory
- HYSPLIT landuse and roughness length directory

The input file also contains the input values that control the weather days, grid definitions, release definition, run time, output frequency, and aerosol parameters. The specific format of the input file is discussed in Section 7.

The weather days are specified in the input file by defining consecutive date ranges. For each group, the first and last day in the date range are listed in the input file. A single day can be selected by setting the first and last day of the group to be the same. For example, to request weather days in the months of March, April, and May of 2015, the first day should be set to 20150301 (March 1, 2015) and the last day should be set to 20150531 (May 31, 2015).

The concentration grid is defined by specifying the output grid type and size, base grid size and spacing, and the surface-layer height used for ground-level air concentration calculations. The base grid size determines the distance from the release location to the edge of the base grid in each direction. The base grid spacing determines the size of the grid cells in the base grid, which generates a rectangular grid with Δx equal to Δy that are equal to the set spacing, or a polar grid with 128 equal sectors and Δr equal to the set spacing. The height used for ground-level air concentration calculations determines the vertical grid spacing.

The number of grids used in the simulation is determined by comparing the base grid and the output grid. The base grid size and spacing are repeatedly multiplied by two until the output grid size is reached or exceeded. This generates multiple grids, with increasing extent and spacing. Setting the base grid size equal to the output grid size results in a single grid with the base grid spacing. For example, if the output grid type and size was set to rectangular and 100 km, the base grid size was set to 10 km and the base grid spacing set to 1 km, this results in five grids, with the following attributes:

- 1) 20 km by 20 km with 1 km spacing
- 2) 40 km by 40 km with 2 km spacing
- 3) 80 km by 80 km with 4 km spacing
- 4) 160 km by 160 km with 8 km spacing
- 5) 200 km by 200 km with 10 km spacing

For a polar grid type with the same grid parameters, this also results in five grids, with the following attributes:

- 1) 10 km radius (20 km diameter) with 1 km spacing between radii, 128 equal sectors
- 2) 20 km radius (40 km diameter) with 2 km spacing between radii, 128 equal sectors
- 3) 40 km radius (80 km diameter) with 4 km spacing between radii, 128 equal sectors
- 4) 80 km radius (160 km diameter) with 8 km spacing between radii, 128 equal sectors
- 5) 100 km radius (200 km diameter) with 10 km spacing between radii, 128 equal sectors

The release definition is determined from the latitude, longitude, plume rise approach, release heights list, plume energies list, and horizontal area for the release. The latitude and longitude specify the release location. Two plume rise approaches are available, release heights or plume sensible energy rates. Specifying the plume rise approach of release heights, causes GenHysplit to use the values in the release heights list as starting heights for the release location. Specifying the plume rise approach of plume energy release rate causes GenHysplit to use the values in the plume energy release rate causes GenHysplit to use the values in the plume energies list as inputs to HYSPLIT, which then in turn calculates an initial release height based on the plume energy and the meteorological data at the time of release. A value of zero horizontal area denotes that the release is from a point source, while values greater than zero denote that the release is from a horizontal area source.

The run time value determines the duration of the simulation after the one-hour release. The output frequency value controls the amount of temporal resolution in the output files. To ensure the output files contain matching output times, sixty (number of minutes per hour) must be evenly divisible by the output frequency (e.g., 1, 2, 3, 4, 5, 6, 10, 12, 15, 20, 30, 60).

Aerosols are represented in the HYSPLIT simulation by Lagrangian particles or Gaussian puffs. When using Gaussian puffs, HYSPLIT requires the output concentration grid to be rectangular. The aerosol parameters in the input file denote the number of Lagrangian particles/Gaussian puffs used to represent each aerosol size for each release. The sizes, densities and deposition velocities of each of the aerosols are also defined in the input file. The number of aerosols is calculated from the number of entries in the aerosol size section. The number of density and deposition velocity entries needs to match the number of aerosol sizes. An aerosol size of zero is used to denote noble gases, which are non-depositing. A deposition velocity of zero causes HYSPLIT to determine the deposition velocity as a function of size and density using a resistance model.

The deposition configuration in the input file denotes which cases are to be evaluated. Three configurations are available. Configuration #1 uses the defined aerosol sizes and includes dry and wet deposition in the calculation. This results in N air and ground concentration fields, where N is the number of aerosol sizes. Configuration #2 includes the calculations in Configuration #1 and adds one additional calculation of an aerosol that has neither dry nor wet deposition (i.e., it is non-depositing). This results in N+1 air and ground concentration fields. Configuration #3 includes the calculations in Configurations #1 and #2 but doubles the number of calculations by including calculations of aerosols that have dry, but no wet deposition and aerosols that have wet, but no dry deposition. This results in 2(N+1) air and ground concentration, N fields that account for only dry deposition, one field that only accounts for wet deposition, and one field that accounts for neither dry nor wet deposition. Both MACCS and HYSPLIT model wet deposition independently of aerosol size, so modeling wet deposition without dry deposition results in a single set of air and ground deposition fields.

6. Output Files

The output binary files for GenHysplit are 'YYYYMMDDHHXXXX.ccd' files, where YYYY is the year of the weather day, MM is the month of the weather day, DD is the day of the weather day, and HH is the hour of the release. The XXXX is either Hhhh, representing a fixed release height, at a height of hhh times 10 m or Pppp, representing a rate of release of plume sensible energy of ppp times 0.1 MW. These files are located in the 'data' directory of the specified output directory. GenHysplit also keeps all the intermediate files for each realization in a directory unique to that realization with the name YYYYMMDDHHXXXX.

7. Input File Contents and Valid Ranges

The input file format, along with examples are shown below in Table 1.

Line Number	Expected Input	Example
1 to 7	Seven Comment lines	<pre>! ! ! An input file for a GenHysplit run ! ! ! ! ! ! ! File Information ! !</pre>
8	Comment	! Output Directory
9	Output Directory (Valid directory)	/scratch/djclayt/ADT/GenHysplit/testing/test
10	Comment	! Number of meteorological data sets
11	Number of Meteorological Data Sets (Integer > 0) [n]	2
12	Comment	! Meteorology directory for each data set
13 to 12+n	Meteorology Directory (repeated for each data set) (Valid directory)	/scratch/consequence/meteorology/nam12 /scratch/consequence/meteorology/gdas0p5
13+n	Comment	! Weather file prefix for each data set
14+n to 13+2n	Meteorology Prefix (repeated for each data set) (text, may be blank)	
14+2n	Comment	! Weather file postfix for each data set
15+2n to 14+3n	Meteorology Postfix (repeated for each data set) (text, may be blank)	_nam12 _gdas0p5
15+3n	Comment	! Are the meteorology files generated with the stn2arl utility (0=no, 1=yes)
16+3n	Meteorology file type (0 = not generated with stn2arl utility, 1 = generated with stn2arl utility)	0
17+3n	Comment	! HYSPLIT Directory
18+3n	HYSPLIT Directory (Valid directory)	/projects/rpsls/hysplit/hysplit.v5.0.0
19+3n	Comment	! HYSPLIT Landuse and Roughness Length Directory

Table 1. GenHysplit Input File Format

Line Number	Expected Input	Example
20+3n	HYSPLIT Landuse and Roughness Length Directory (Valid directory containing landuse and roughness length information)	/projects/rpsls/hysplit/hysplit.v5.0.0/bdyfiles/bdyfile s0p1
21+3n to 23+3n	Three Comment lines	! ! ! Run Information ! !
24+3n	Comment	! Number of groups to run
25+3n	Number of Realization Groups (Integer > 0) [x]	1
26+3n	Comment	! First and last day for each group [YYYYMMDD]
27+3n to 26+3n+x	First day of group [white space] last day of group (repeated for each group) (YYYYMMDD, where YYYY is the year of the weather day, MM is the month of the weather day, and DD is the day of the weather day)	20080101 20080101
27+3n+x	Comment	! Release Longitude [degrees minutes seconds direction (W or E)]
28+3n+x	Release Longitude (degrees minutes seconds direction (W or E), separated by white space)	70 51 5 W
29+3n+x	Comment	! Release Latitude [degrees minutes seconds direction (N or S)]
30+3n+x	Release Latitude (degrees minutes seconds direction (N or S), separated by white space)	42 53 53 N
31+3n+x	Comment	! Varying heights (=0) or varying power (=1)
32+3n+x	Option to specify varying heights or varying power, value must be 0 or 1	0
33+3n+x	Comment	! Release Heights [m] (truncated to increments of 10 m, max=9990 m)
34+3n+x	Release Heights (m) (Numbers > 0, separated by white space. Values are rounded down to increments of 10 m with a maximum of 9990 m. Values are ignored if varying plume energies option selected.)	10
35+3n+x	Comment	! Heat release [MW] (truncated to increments of 0.1 MW, max=99.9 MW)

Line	Expected Input	Example
Number		
36+3n+x	Plume Energies (MW) (Numbers > 0, separated by white space. Values are rounded down to increments of 0.1 MW with a maximum of 99.9 MW. Values are ignored if varying release heights option selected.)	0.1 2.05 5.64 30.06
37+3n+x	Comment	! Release horizontal area [m2]
38+3n+x	Release horizontal area (area source term, m^2 , Number >= 0)	0
39+3n+x	Comment	! Run time after release [hr]
40+3n+x	Run time after release (hr) (Integer > 0)	6
41+3n+x	Comment	! Time increment for concentration output [minutes]
42+3n+x	Time increment for concentration output (min) (Integer that evenly divides into 60 > 0)	15
43+3n+x	Comment	! Output Grid Type (0=rectangular, 1=polar)
44+3n+x	Output grid type (0 = rectangular, 1 = polar)	1
45+3n+x	Comment	! Output Grid Size [km] (distance from release location)
46+3n+x	Distance from release location to maximum output grid span (km) (Number > 0)	1610.0
47+3n+x	Comment	! Base Grid Size [km] (distance from release location)
48+3n+x	Distance from release location to maximum base grid span (km) (Output Grid >= Number > 0)	10
49+3n+x	Comment	! Base Grid Spacing [km]
50+3n+x	Base grid spacing (km) (Base Grid >= Number > 0)	0.5
51+3n+x	Comment	! Height for ground-level air concentration calculations [m]
52+3n+x	Height for ground-level air concentration calculations (m) (Number > 0)	50.0
53+3n+x	Comment	! Modeling Approach (0=Lagrangian particles, 1=gaussian puffs)

Line Number	Expected Input	Example
54+3n+x	Modeling approach (0 = Lagrangian particles, 1 = Gaussian puffs)	0
55+3n+x	Comment	! Number of particles/puffs per aerosol size per minute
56+3n+x	Number of HYSPLIT particles per aerosol size per minute in simulation (Integer > 0)	10
57+3n+x	Comment	! Aerosol sizes [microns]
58+3n+x	Aerosol sizes (microns) (Numbers >= 0 separated by white space)	0.15332 0.28543 0.53138 0.98923 1.8416 3.4284 6.3825 11.882 22.120 41.179
59+3n+x	Comment	! Aerosol densities [g/cm3]
60+3n+x	Aerosol densities (g/cm ³) (Numbers >= 0 separated by white space, correspond to the same sequence defined in the aerosol sizes section)	1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
61+3n+x	Comment	! Deposition velocities (m/s) [0=internal calculation]
62+3n+x	Aerosol deposition velocities (m/s) (Numbers >= 0 separated by white space. Values correspond to the same sequence defined in the aerosol sizes section.)	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
63+3n+x	Comment	! Deposition configuration (1=wet and dry, 2= configuration 1 + neither wet nor dry, 3= configuration 2 + both no wet and no dry)
64+3n+x	Aerosol deposition configuration (1 = dry and wet [base case], 2 = configuration 1 + the case with neither dry nor wet, 3 = configuration 2 + the cases with either no dry or no wet)	2