Organization of Course

INTRODUCTION

1. Course overview
2. Air Toxics overview
3. HYSPLIT overview

HYSPLIT Theory and Practice

4. Meteorology
5. Back Trajectories
6. **Concentrations / Deposition**
7. HYSPLIT-SV for semivolatiles (e.g, PCDD/F)
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Overall Project Issues & Examples

9. Emissions Inventories
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12. Model Evaluation
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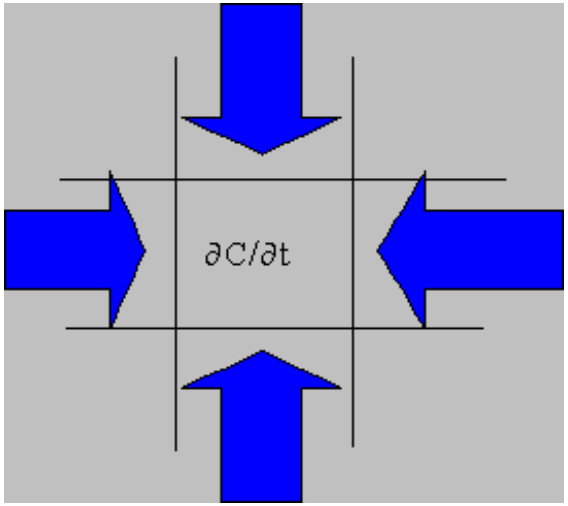
Computational Methods

Eulerian versus Lagrangian

Eulerian Modeling Approach

- Concentrations are computed at every grid cell interface due to diffusion and advection.
- $\partial C/\partial t$ = [advection] + [diffusion] + [source] + [sinks]
- Computationally intensive as each grid cell must be calculated even if pollutants are not advected into the cell.
- Suitable for complex emission and non-linear chemical conversion scenarios.

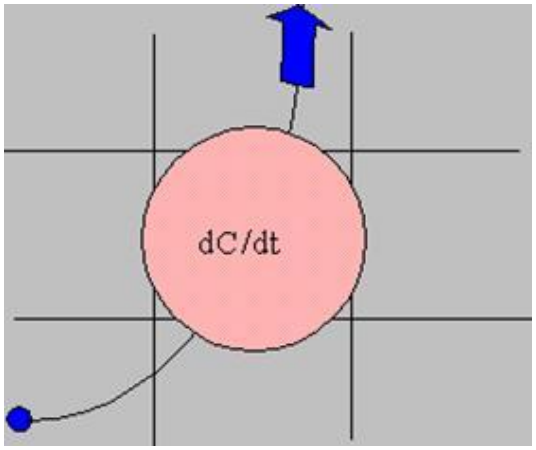


Computational Methods

Eulerian versus Lagrangian

Lagrangian Modeling Approach

- Concentrations computed by summing the mass of each pollutant puff that is advected through the grid cell
- dC/dt = [diffusion] + [source] + [sinks]
- May require thousands of particles to adequately model pollutant dispersion
- Most applicable to point source applications

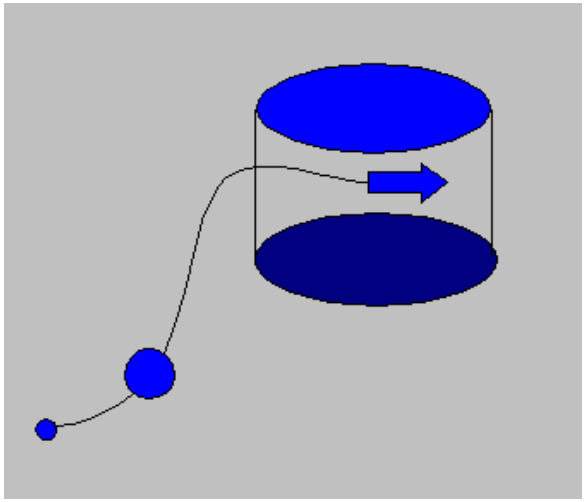


Computational Methods

Lagrangian Puff Model

Puff Model

- Source is simulated by releasing pollutant puffs at regular intervals over the duration of the release
- Each puff contains the appropriate fraction of the pollutant mass
- A puff is advected according to the trajectory of its center position
- The size of the puff (horizontal and vertically) expands in time to account for the dispersive nature of a turbulent atmosphere
- Concentrations are calculated at specific points (or nodes on a grid) by assuming that the concentrations within the puff have a defined spatial distribution

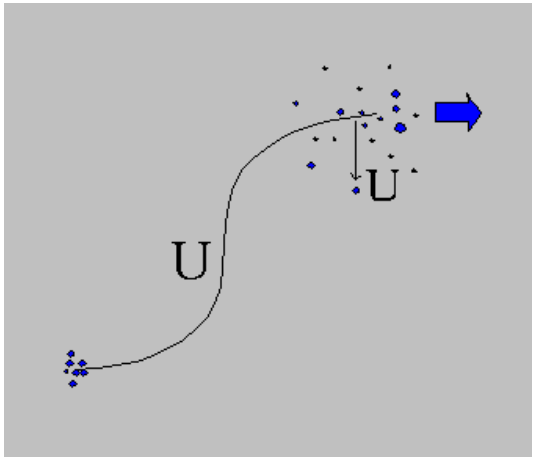


Computational Methods

Lagrangian Particle Model

Particle Model

- Source is simulated by releasing many particles over the duration of the release
- In addition to the mean advective motion, a random motion component is added to each particle at each step according to the atmospheric turbulence at that time
- A cluster of particles released at the same point will expand in space and time simulating the dispersive nature of the atmosphere
- Concentrations are calculated by summing the mass of all the particles in a grid cell
- In a homogeneous environment the size of the puff (in terms of its standard deviation) at any particular time should correspond to the second moment of the particle positions



Particle, Puff, & Hybrid

Definitions:

- Particle: A point mass of contaminant. A fixed number of particles are released and are moved by a wind having mean and random components. They never grow or split.
- Puff: A fully 3-D cylindrical puff (below, left), having a defined concentration distribution in the vertical and horizontal. Puffs grow horizontally and vertically according to the dispersion rules for puffs, and split if they become too large.
- Hybrid: A circular 2-D object (planar mass, having zero vertical depth), in which the horizontal contaminant has a "puff" distribution (below, right). There are a fixed number of these in the vertical because they function as particles in that dimension. In the horizontal, they grow according to the dispersion rules for puffs and split if they get too large.

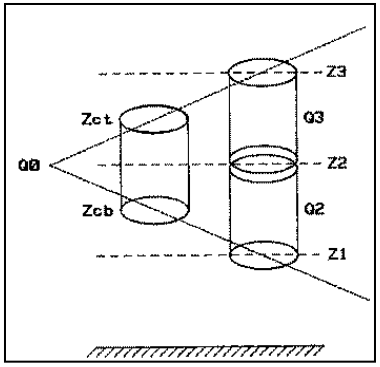


Illustration of how a single particle (Q0) splits due to vertical diffusion into two particles Q2 and Q3.

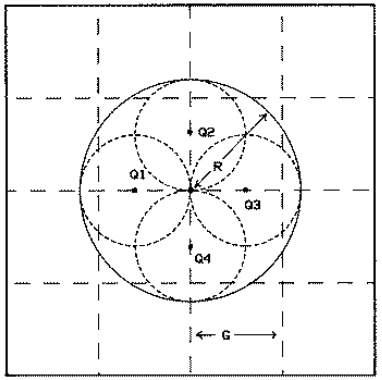
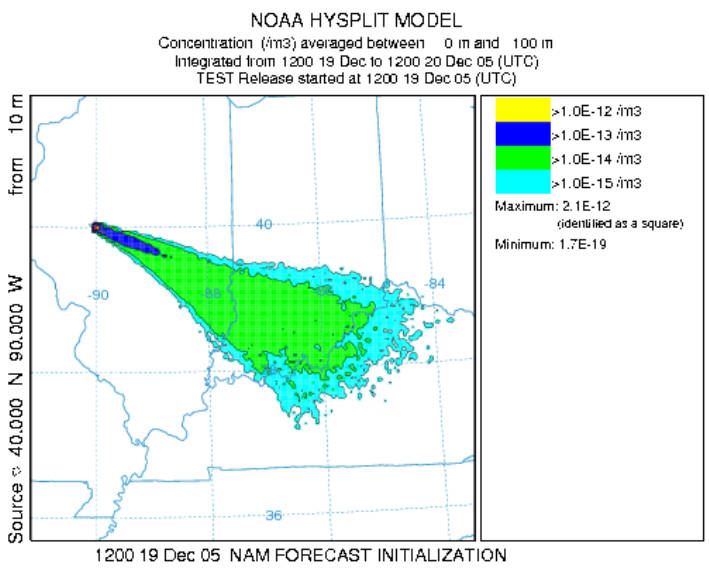


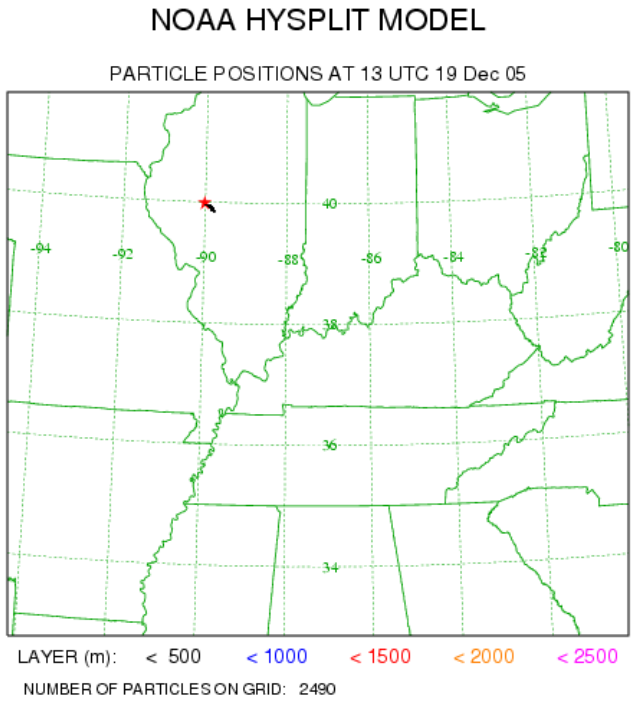
Illustration of how a single particle with radius R splits due to horizontal diffusion into four particles (Q1, Q2, Q3 and Q4) each with radius R/2.

Example of Particle Dispersion

Animation (right) of the 2500 particles that produced the concentration pattern shown below.

Note the higher level particles (blue) moving out ahead of the slower lower level particles (black)





Like “Trajectory HYSPLIT, “Concentration” HYSPLIT can be run

- from the Graphical User Interface (GUI)
- from the Command Line
- from DOS Batch Files

Like “Trajectory HYSPLIT, the CONTROL and SETUP.CFG files are key files, but the contents of these files are different

---

There are many similarities between simulating atmospheric transport and fate with HYSPLIT and simulating trajectories with HYSPLIT… we will do a few examples, but will not go into the depth that we did for trajectories

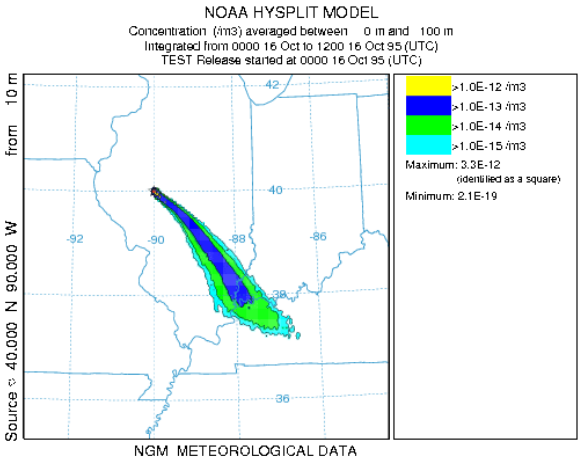
Example Concentration Run from the Graphical User Interface (GUI)

Follow these steps to run the sample concentration case provided with the default installation of PC HYSPLIT

- Start the model by double clicking the HYSPLIT icon on the desktop.
- Click on the green **Menu** button at the bottom of the first screen.
- Click on the **Concentration** menu tab and choose **Setup Run.**
- Click on the **Retrieve** button at the bottom of the menu.
- Click the **Browse** button and find the file **sample_conc** in the working directory.
- Click **OK.**
- Click **Save** to save the configuration settings.
- Click on the **Concentration** menu tab and choose **Run Model.**

  (Note: if a menu pops up says that a SETUP.CFG namelist file was found, choose **Delete file then Run)**
- When the model is complete (**Complete Hysplit** is shown), click on the **Exit** button.
- Click on the **Concentration** menu tab and choose **Display,** then **Concentration** and then **Contours**.
- Click on the **Execute Display** button to display the trajectory in the GSview viewer.

  (Note: as before, if your GSview is not registered, just click **Ok**)
- The resulting concentration pattern should be identical to the one shown to the right.



If a CONTROL file is present in the working directory, then HYSPLIT will read it and carry out a concentration simulation according to this file's specifications

What is in a CONTROL file for concentration simulations?

Lets do another hand's on exercise,

similar to the trajectories that we ran earlier

(…in the same region, for the same time period…),

and we will try to configure the

standard version of HYSPLIT

to simulate the atmospheric fate & transport of mercury

Control File for HYSPLIT Concentration Run

First section: source location, duration of run, and met data to be used

starting year, month, day, hour (UTC) --	08 08 01 00
number of starting locations --	1
lat, long, height (m-agl) for each location --	20.7203 -103.3919 50.0
hours to run (672 = 4 weeks) --	672
vertical motion option (0:data, …) --	0
model top (meters) --	25000.0
number of meteorological data files to use --	3
location of first met file --	c:\hysplit4\metdata\
name of first met file --	edas.aug08.001
location of second met file --	c:\hysplit4\metdata\
name of second met file --	edas.aug08.002
location of third file --	c:\hysplit4\metdata\
name of third file --	RP200808.gbl

Control File for HYSPLIT Concentration Run (continued)

Second section: emissions

Number of pollutants being emitted --	4
4-character ID name --	elem
Emissions Rate (mass per hour) --	0.0
Hours of emission --	0.1
Release start time: year month day hour minute –	00 00 00 00 00
4-character ID name --	HgII
Emissions Rate (mass per hour) --	1.0
Hours of emission --	0.1
Release start time: year month day hour minute –	00 00 00 00 00
4-character ID name --	Hgpt
Emissions Rate (mass per hour) --	0.0
Hours of emission --	0.10
Release start time: year month day hour minute –	00 00 00 00 00
4-character ID name --	Hg2s
Emissions Rate (mass per hour) --	0.0
Hours of emission --	0.1
Release start time: year month day hour minute –	00 00 00 00 00

Control File for HYSPLIT Concentration Run

Third section: GRID for concentration and deposition

Number of concentration grids --	1
Latitude and longitude of grid center --	0.0 0.0
Grid latitude and longitude spacing (degrees) --	0.1 0.1
Grid Extent (latitude and longitude) --	5.0 5.0
Directory for Grid Output File --	.\
Name of Grid Output File --	cdump.bin
Number of elevations for output --	6
Elevations of these output levels --	0.0 200.0 850.0 1550.0 3000.0 4400.0
Sampling Start Time --	00 00 00 00 00
Sampling End Time --	20 12 31 24 60
Sampling Interval (days, hours, minutes) --	00 24 00

This next section is used to define the deposition parameters for emitted pollutants.

The number of deposition definitions must correspond with the number of pollutants released. There is a one-to-one correspondence.

There are 5 entries in the CONTROL file for each defined pollutant.

Control File for HYSPLIT Concentration Run

Fourth section: deposition parameters for each pollutant

(here is for the first pollutant, elemental mercury)

Number of Pollutants Depositing	4
Particle: Diameter (microns), Density (g/cc), and Shape	0.0 2.0 1.0
Deposition velocity (m/s), Pollutant molecular weight (Gram/Mole), Surface Reactivity Ratio, Diffusivity Ratio, Effective Henry's Constant	0.0 200.6 0.0 2.0 0.11
Wet Removal: Actual Henry's constant, In-cloud (L/L), Below-cloud (1/s)	0.11 4.0E+04 5.0E-05
Radioactive decay half-life (days	0.0
Pollutant Resuspension (1/m)	0.0

Control File for HYSPLIT Concentration Run

Fourth section:
deposition parameters for each pollutant
(here we show for all pollutants)

Number of Pollutants Depositing – `4`

elemental mercury (elem)

```
0.0       2.0       1.0
0.0       200.6     0.0     2.0     0.11
0.11      4.0E+04   5.0E-05
0.0
0.0
```

reactive gaseous mercury (HgII)

```
0.0       2.0       1.0
0.0       271.5     1.0     2.0     1.4E+06
1.4E+06   4.0E+04   5.0E-05
0.0
0.0
```

particulate mercury (Hgpt)

```
1.0       2.0       1.0
0.0       271.5     1.0     2.0     1.4E+06
0.11      4.0E+04   5.0E-05
0.0
0.0
```

RGM sorbed to soot (Hg2s)

```
1.0       2.0       1.0
0.0       271.5     1.0     2.0     1.4E+06
0.11      4.0E+04   5.0E-05
0.0
0.0
```

VERY IMPORTANT

- **THE CONTROL FILE HAS TO BE IN EXACTLY THE RIGHT ORDER, and everything must be in the file that HYSPLIT expects to FIND**

- **Many Problems that one might have in running HYSPLIT can be "fixed" if the CONTROL file is fixed**

- ***if you are having problems with HYSPLIT, the first thing you should do is look at the CONTROL file you are using for that simulation…***

Exercise 7:

- open up command prompt
- navigate to c:\hysplit4\working_07

```
cd c:\hysplit4\working_07 [enter]
```

- run conc_run_07.bat

```
conc_run_07 [enter]
```

Note – conc_run_07.bat CALLS conc_set_07.bat

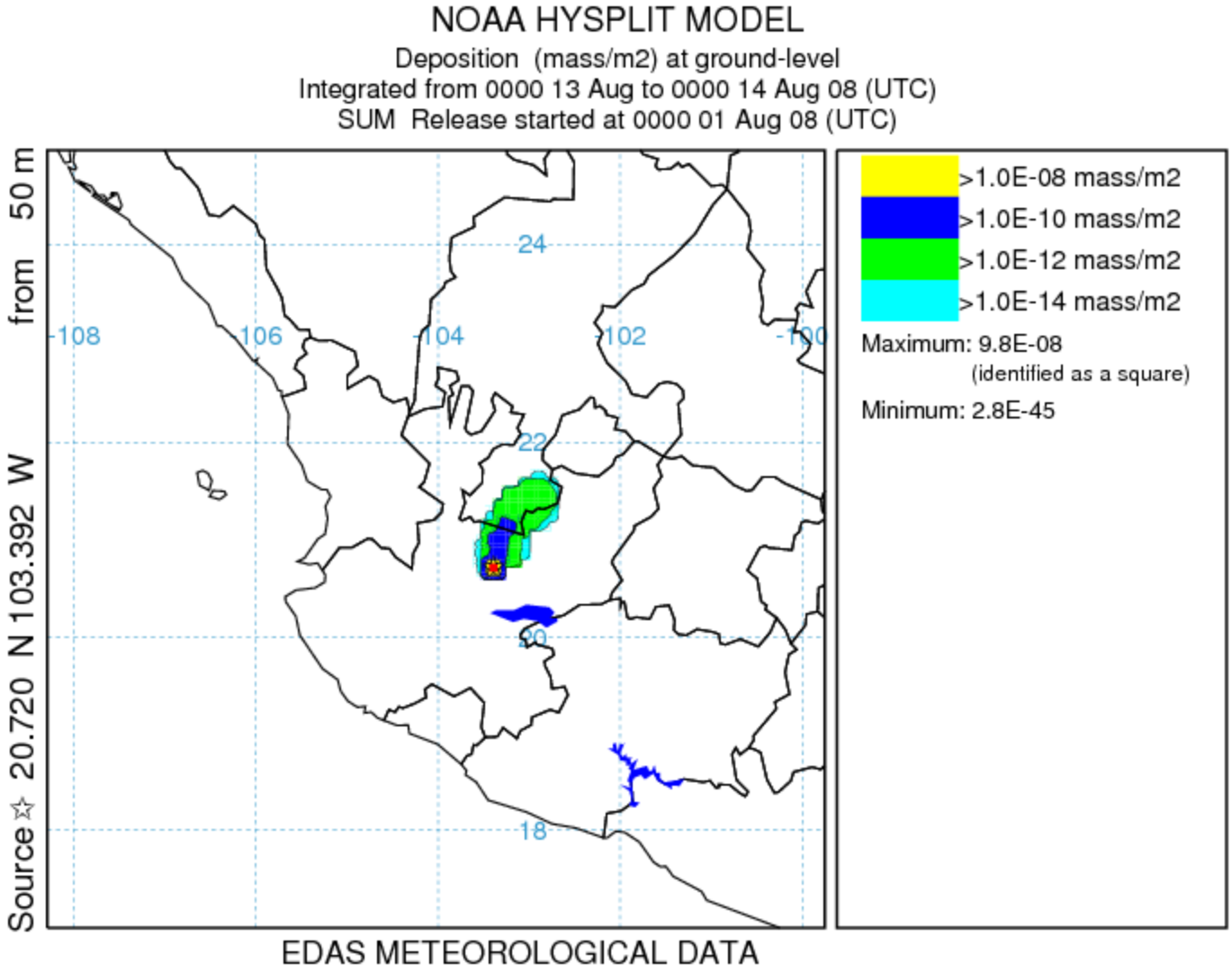
conc_set_07.bat is much more complex than for earlier examples

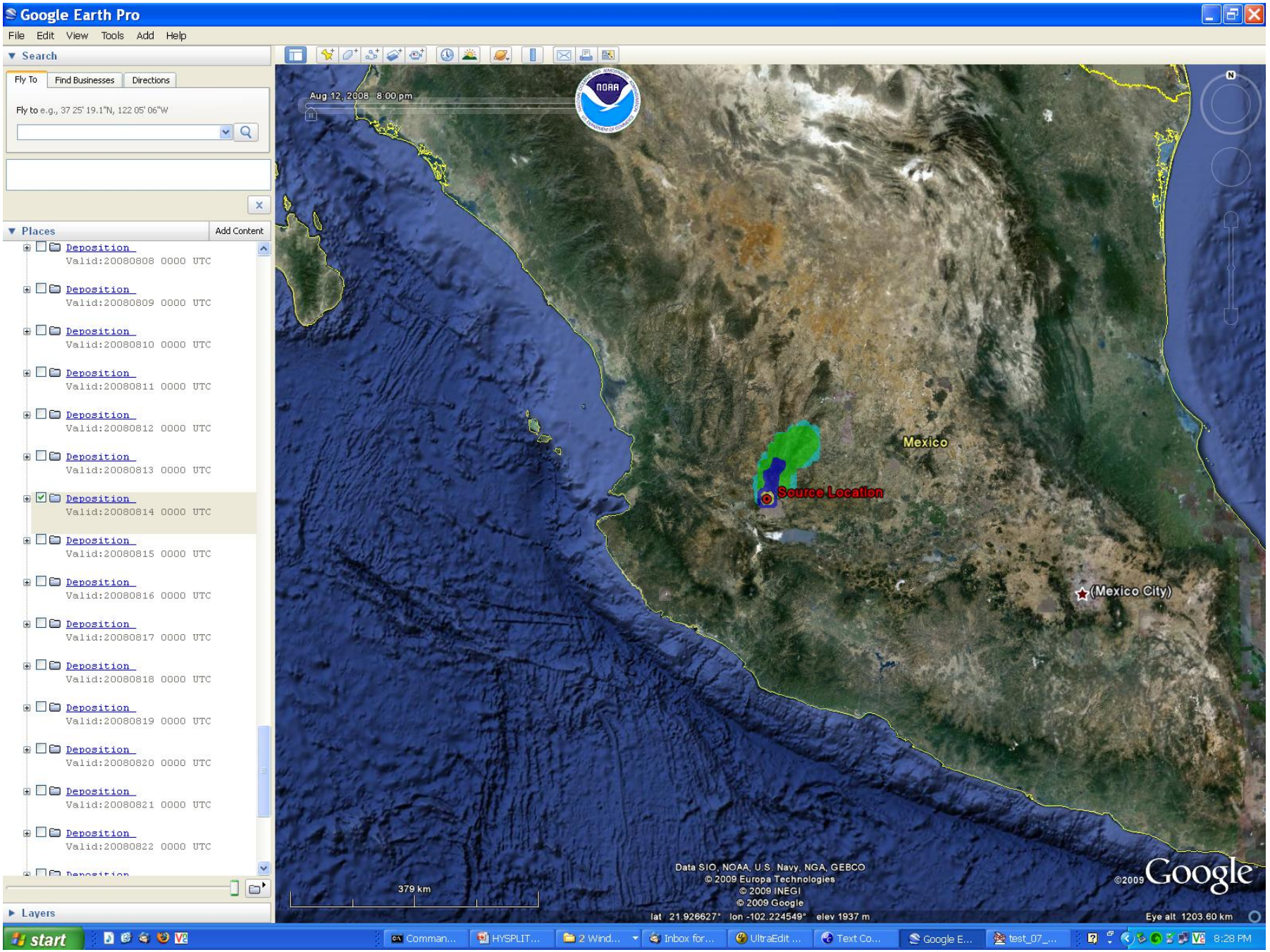
If there is time, we can examine this batch file

```
E:\hysplit4_mdc\hysplit4_hg05\working>concplot
USAGE: concplot -[options (default)]
-a[Arcview GIS: 0-none 1-log10 2-value 3-GoogleEarth]
-b[Bottom display level: (0) m]
-c[Contours: (0)-dyn/exp 1-fix/exp 2-dyn/lin 3-fix/lin 4-set 50-
   0,interval 10 51-1,interval 10]
-d[Display: (1)-by level, 2-levels averaged]
-e[Exposure units flag: (0)-concentrations, 1-exposure, 2-
   threshold, 3-hypothetical volcanic ash]
-f[Frames: (0)-all frames one file, 1-one frame per file]
-g[Circle overlay: ( )-auto, #circ(4), #circ:dist_km]
-h[Hold map at center lat-lon: (source point), lat:lon]
-i[Input file name: (cdump)]
-j[Graphics map background file name: (arlmap) or shapefiles.txt]
-k[Kolor: 0-B&W, (1)-Color, 2-No Lines Color, 3-No Lines B&W]
```

```
-l[Label options: ascii code, (73)-open star]
-L[LatLonLabels: none=0 auto=(1) set=2:value(tenths)]
-m[Map projection: (0)-Auto 1-Polar 2-Lamb 3-Merc 4-CylEqu]
-n[Number of time periods: (0)-all, numb, min:max, -incr]
-o[Output file name: (concplot.ps)]
-p[Process file name suffix: (ps) or process ID]
-q[Quick data plot: ( )-none, filename]
-r[Removal: 0-none, (1)-each time, 2-sum, 3-total]
-s[Species: 0-sum, (1)-select, #-multiple]
-t[Top display level: (99999) m]
-u[Units label for mass: (mass), see "labels.cfg" file]
-v[Values[:labels (optional)] for fixed contours:
   val1:lab1+val2:lab2+val3:lab3+val4:lab4]
-w[Grid point scan for contour smoothing (0)-none 1,2,3, grid points]
-x[Concentration multiplier: (1.0)]
-y[Deposition multiplier:    (1.0)]
-z[Zoom factor: 0-least zoom, (50), 100-most zoom]
```

`-t0` *to get deposition only*


NOAA HYSPLIT MODEL
Deposition (mass/m2) at ground-level
Integrated from 0000 13 Aug to 0000 14 Aug 08 (UTC)
SUM Release started at 0000 01 Aug 08 (UTC)
Source ☆ 20.720 N 103.392 W from 50 m
-108
-106
-104
-102
24
22
20
18
>1.0E-08 mass/m2
>1.0E-10 mass/m2
>1.0E-12 mass/m2
>1.0E-14 mass/m2
Maximum: 9.8E-08
(identified as a square)
Minimum: 2.8E-45
EDAS METEOROLOGICAL DATA


Google Earth Pro
File Edit View Tools Add Help
Search
Fly To
Find Businesses
Directions
Fly to e.g., 37 25' 19.1"N, 122 05' 06"W
Places
Add Content
Deposition
Valid:20080808 0000 UTC
Deposition
Valid:20080809 0000 UTC
Deposition
Valid:20080810 0000 UTC
Deposition
Valid:20080811 0000 UTC
Deposition
Valid:20080812 0000 UTC
Deposition
Valid:20080813 0000 UTC
Deposition
Valid:20080814 0000 UTC
Deposition
Valid:20080815 0000 UTC
Deposition
Valid:20080816 0000 UTC
Deposition
Valid:20080817 0000 UTC
Deposition
Valid:20080818 0000 UTC
Deposition
Valid:20080819 0000 UTC
Deposition
Valid:20080820 0000 UTC
Deposition
Valid:20080821 0000 UTC
Deposition
Valid:20080822 0000 UTC
Layers
Aug 12, 2008 8:00 pm
NOAA
Mexico
Source Location
(Mexico City)
379 km
Data SIO, NOAA, U.S. Navy, NGA, GEBCO
© 2009 Europa Technologies
© 2009 INEGI
© 2009 Google
lat 21.926627° lon -102.224549° elev 1937 m
©2009 Google
Eye alt 1203.60 km
start
8:28 PM

- Optional SETUP.CFG file for concentration/deposition simulation
- If this file is present, with some or all of the parameters specified, HYSPLIT will use the values specified
- For any parameter not specified, HYSPLIT will use DEFAULT values
- If SETUP.CFG not present, DEFAULT values used for all parameters

```
&SETUP
INITD  = 129,
KHMAX  = 9999,
NUMPAR = 4000,
MAXPAR = 4000,
MAXDIM = 4,
QCYCLE = 1.0,
KRND   = 6,
FRME   = 0.1,
FRMR   = 0.0E+00,
KSPL   = 1,
FRHS   = 1.00,
FRVS   = 0.01,
FRTS   = 0.10,
DELT   = 20.0,
TKERD  = 0.18,
TKERN  = 0.18,
TRATIO = 0.75,
MGMIN  = 10,
KMSL   = 0,
CPACK  = 1,
ICHEM  = 0,
DXF    = 1.0,
DYF    = 1.0,
DZF    = 0.01,
PINPF  = 'PARINIT',
POUTF  = 'PARDUMP',
NINIT  = 0,
NDUMP  = 0,
NCYCL  = 0,
KPUFF  = 0,
KMIXD  = 0,
KMIX0  = 250,
SPLITF = 1.0,
FRHMAX = 3.0,
KDEF   = 0,
KZMIX  = 0,
TVMIX  = 1.0,
KBLS   = 1,
KBLT   = 2,
VSCALE = 200.0,
HSCALE = 10800.0,
CONAGE = 48
/
```