HYSPLIT

The Hybrid Single-Particle Lagrangian Integrated Trajectory model

OVERVIEW – DAY 2

Cleanup

Part 3: Concentration

- Set-up
- Equations
- Case Study
- Apply
 - Simple Scenario
 - Single Particle
 - Multiple Particles
 - Puffs

CLEANUP

Before we begin, we will clean out our working directory.

Go to ADVANCED→CLEANUP WORKING

It will then ask you if you want to continue.

Click **CONTINUE**.

Hysplit will then close and if you go to your hysplit folder, there will be the new folder you just created and your working directory will be empty.

Now, re-open *hysplit* and hit **RESET** on the bottom to change all settings back to default.



CONCENTRATION



Concentration Setup \times Starting time (YY MM DD HH): 00 00 00 00 Number of starting locations: 1 ====> Setup starting locations Direction Total run time (hrs) Top of model (m agl) 12 • Fwrd C Back 10000.0 Select Vertical Motion Method: 0 = input model data Add Meteorology Files Selected Files: 1 Clear oct1618.BIN Pollutant, Deposition and Grids setup Pollutant, Concentration... Х Pollutant: Deposition: Grids: Num= 1 Num= 1 Num= 1 Specie 1 • Grid 1 Specie 1 C Specie 2 O Grid 2 C Specie 2 C Specie 3 O Grid 3 C Specie 3 C Specie 4 O Grid 4 C Specie 4 C Specie 5 O Grid 5 C Specie 5 C Specie 6 C Grid 6 C Specie 6 C Specie 7 C Grid 7 C Specie 7 Quit Help Save

CONCENTRATION - SETUP

- Very similar inputs compared to *Trajectory*.
- Additional menu for POLLUTANT, DEPOSITION and GRID set up.
- •You can specify more than one pollutant and its deposition properties as well as multiple grids.

CONCENTRATION - SETUP

POLLUTANT OPTIONS

Ø Definition of Pollut	- 🗆 ×
Identification (<=4 char)	: TEST
Emission rate(1/hr)	: 1.0
Hours of emission	: 1.0
Release start(yy mm dd hh min)	: 00 00 00 00 00
Quit Help Save	

GRID OPTIONS

Ø Definition of Concen	- 🗆 ×
Center of Lat and Lon	: 0.0 0.0
Spacing(deg) Lat, Lon	: 0.05 0.05
Span (deg) Lat, Lon	: 30.0 30.0
Output grid directory	: ./
Output grid file name	: cdump
Num of vertical levels	: 1
Height of levels(M Agl)	: 100
Sampling start(yy mm dd hh min)	: 00 00 00 00 00
Sampling stop(yy mm dd hh min)	: 00 00 00 00 00
(Avg:0 Now:1 Max:2) (hrs) (min)	: 01 01 00
Quit Help	Save

DEPOSITION OPTIONS

🖉 Depositio	on Definition for Pollu	tant 1			\times
Set Simple Defaults->	Particle or Gas O Particle ⓒ Gas	Dry Dep C Yes	osition • No	Wet Dep C Yes	oosition • No
Preconfigure:	• None C Cs137 C	1131g C	1131p C	нто С р	MDV
Particle Diame	ter(um), Density(g/co	e), Shape	: 0.0 0.	0 0.0	
Vel(m/s), Mol	Wgt(g), A-Ratio, D-Ra	atio, Hen	ry: 0.0 0.	0 0.0 0	0.0
Henry's(M/a),	In-cloud(1/s), Below-	-cloud(1/	s): 0.0 0.	0 0.0	
Radioactive de	cay half-life(days)		: 0.0		
Pollutant Resu	spension Factor(1/m)		: 0.0		
Quit	Help	Reset	t	s	ave

CONCENTRATION - EQUATIONS

Concentrations in Hysplit are determined in three different ways:

- 1. 3-D Particle: $\Delta c = m (\Delta x \Delta y \Delta z)^{-1}$
- 2. Top-Hat: $\Delta c = m (\pi r^2 \Delta z)^{-1}$
- 3. Gaussian: $\Delta c = m (2 \pi \sigma_h^2 \Delta z)^{-1} \exp(-0.5 x^2/\sigma_h^2)$

Notes:

- Different schemes can be used for vertical and horizontal motion at the same time. The motion of the horizonal determines the method in which the concentration is calculated.
- •The incremental concentrations are added to each grid cell or node each advection time step for all particles or puffs that intersect that point.
- •The final average concentration is the incremental sum divided by the number of time steps in the concentration averaging period.



CONCENTRATION — CASE STUDY

We will be using data from the Cross Appalachian Tracer Experiment (CAPTEX):

- Six 3-hour releases of perfluorocarbon (C7F14) tracers: four in Dayton, Ohio and two in Sudbury, ON
- Samples collected at 84 sites, 300-800km from the release over 3-6 hour averaging periods for 48-72 hours
- Aircraft also collected data for short time periods (6-10 mins): the lowest level was 914m MSL and the highest was 2134m MSL

•More information can be found here: <u>https://journals.ametsoc.org/view/journals/apme/56/8/jamc-</u> <u>d-16-0345.1.xml</u>



CONCENTRATION — SIMPLE SCENARIO

•Go to **CONCENTRATION→SETUP RUN**.

•Change all the inputs to match the CAPTEX scenario, as we've done before for the trajectory case.

*Note to add in new meteorology, make sure to **CLEAR** the existing files first.

•Then, go to CONCENTRATION→RUN MODEL.

•Lastly, go to **CONCENTRATION** → **DISPLAY** → **CONCENT RATION** → **CONTOURS** and except the defaults by clicking **EXECUTE DISPLAY**.



Pollutant, Deposition and Grids setup
Quit Help Save as Retrieve Save

CONCENTRATION — SIMPLE SCENARIO

The concentration pattern represents the average particle mass in each grid cell divided by the cell volume.

The plot shows 12-hour averaged contours of concentrations from 1×10^{-12} to 1×10^{-15} .

If one particle (mass = 1/2500) were contained in a grid cell of volume 5x5x1km ($2.5x10^{10}$ m3), then the air concentration would be about $1x10^{-14}$ units m⁻³.

The concentration here though is averaged so the lower concentrations here are due to reduced residence times.



CONCENTRATION — SINGLE PA

We will keep the same setup as previously. Howeve we will now edit the Grids menu.

Go to CONCENTRATION -> SETUP -> POLLUTANT, **DEPOSITION AND GRIDS SETUP.**

Next, click on SPECIE 1 under POLLUTANT (there w only be one for this case).

We will be changing the **EMISSION RATE** and **HO OF EMIISION**, but not the overall volume. All mass now released on one time step though.

Identification (<=4

Emission rate(1/hr)

Hours of emission

Release start(yy mm

Quit

Make the changes as shown here.

Hit **SAVE**.

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CONCENTRATION — SINGLE PARTICLE

Next we will change the **GRID** settings. Click **GRID 1**.

All we are changing here is the height of the levels to make sure we have a large enough domain to track the single particle.

Hit **SAVE** to close all menus and go back to the *hysplit* home.

Definition of Concen... : 0.0 0.0 Center of Lat and Lon : 0.05 0.05 Spacing(deg) Lat, Lon Span (deg) Lat, Lon : 30.0 30.0 Output grid directory : ./ Output grid file name : cdump : 1 Num of vertical levels Height of levels (M Agl) : 5000 Sampling start(yy mm dd hh min): 00 00 00 00 00 Sampling stop(yy mm dd hh min) : 00 00 00 00 00 (Avg:0 Now:1 Max:2) (hrs) (min): 00 12 00 Quit Help Save



CONCENTRATION — SINGLE PARTICLE

Lastly, before running the model we need to ensure it is only including one particle, not its default of 2500.

Go to ADAVANCE→CONCENTRATION→MENU #4

Change **2500** to **1**.

Click **SAVE** to exit everything.

Now **RUN THE CONCENTRATION MODEL** and display the results as **CONTOURS**, accepting all defaults as we have before.

You should see a narrow plume similar to the trajectories we've modelled.

NOAA HYSPLIT MODEL Concentration (/m3) averaged between 0 m and 5000 m Integrated from 1700 25 Sep to 0500 26 Sep 83 (UTC) TEST Release started at 1700 25 Sep 83 (UTC)

Ε

10

from

≥

84.220

z

39.900

Source 🜣





CONCENTRATION — SINGLE PARTICLE

But what if we didn't model as high of a domain?

Go back to the **GRIDS** menu and change the height to **500**.

RERUN the model and plot the results as contours.

For this situation, a single particle is insufficient for a realistic simulation.

- •Particles that mixed to the upper-levels of the boundary layer travel at faster speeds.
- •Winds aloft also tend to be more clockwise than those at the surface.



CONCENTRATION — MULTIPLE PARTICLES

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	Ø Definition of Concen	- L X
	Center of Lat and Lon	: 0.0 0.0
We will now model multiple particles.	Spacing(deg) Lat, Lon	: 0.05 0.05
First change the HEIGHT back to 5000.	Span (deg) Lat, Lon	: 30.0 30.0
Then we will change the AVERAGING time to every 3 hours.	Output grid directory	: ./
Next, go to: ADVANCED	Output grid file name	: cdump
and change the number of particles from 1 to 100.	Num of vertical levels	: 1
(4) Particle/Puff Release Number Limits – 🗆 🗙	Height of levels(M Agl)	: 5000
ne particle/puff release rate is computed from the per cycle definition. The minimum rate is one per time tep. Emissions are turned off when the maximum is reached. Particles are terminated if they exceed the aximum age.	Sampling start(yy mm dd hh min): 00 00 00 00 00
Particles released per cycle: 100	Sampling stop(yy mm dd hh min)	: 00 00 00 00 00
Maximum particle duration (hrs): 9999	(Avg:0 Now:1 Max:2) (hrs) (min): 01 03 00
Quit Reset Help Save	Quit Help	Save

A

CONCENTRATION — MULTIPLE PARTICLES

RUN the model.

Go to the CONCENTRATION→DISPLAY→ CONTOURS and make sure to click the option for FRAMES before you click EXECUTE DISPLAY.

You should have four images load onto your screen (for every 3 hour period over 12 hours).

We still do not get a good plume from this, lets try 1000 and 10,000 particles as well.



CONCENTRATION — MULTIPLE PARTICLES

At 10,000 particles we have a much better plume shape. However, it is still much coarser than our test case. Although this case only had 2500 particles it was averaged over 12 hours instead of the 3 hours we used here. The model needs to sample a sufficient number of particles over the averaging interval and concentration grid size to ensure robust results. The ratio of these two should be such that the air concentration is not sensitive to the particle release rate (determined by trial/error).



CONCENTRATION - PUFFS

Instead of following thousands of individual particles, we can follow a mean trajectory and model the growth of the horizontal (and vertical) distribution. This is known as a **hybrid** approach. This can done by two methods in *hysplit*:

- 1. Top-Hat: concentration is zero outside and a constant average value inside.
- **2.** Gaussian: follows a normal distribution over a range of 3σ .

All **vertical dispersion is modelled as **Top-Hat** (or particle). However, **horizontal** dispersion can be **either**.

More info: <u>https://www.arl.noaa.gov/documents/reports/arl-224.pdf</u>

TOP HAT VS GAUSSIAN

Incremental concentrations for **Top-Hat** and **Gaussian** puff are computed at the center point of each grid cell. Only puffs that intersect this point will be summed. In contrast, a 3D particle can be summed anywhere. Volume is a combination of the puff radius and cell height.

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

And the standard deviation (σ_u) is used to calculate horizontal puff growth rate and initiate splitting:

$$d\sigma_h/dt = \sigma_u$$

*Top-Hat used more often because less complex computing and just as accurate as Gaussian downwind of source. Gaussian only more accurate right at source.



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PUFF SPLITTING

What happens when a puff expands to cover several meteorological grid points?

- **Top-Hat** puff splits horizontally into four puffs, each with 25% of the mass, when $1.54\sigma h > Lh$. These new puffs are located at P(x±0.5 σh , y±0.5 σh).
- A large Gaussian puff splits into five smaller puffs when 3.0σh >Lh. The center puff gets 60% of the mass while the outside 4 puffs get 10% each. All of which are located similar to the Top-Hat, but with a plume in the middle.
- $^{*}\sigma h$ is the puff horizontal standard deviation.
- *Lh is the meteorlogical grid spacing.
- In order to keep array dimensional space, the model also has several rules for merging and removing puffs as a function of standard deviation.





(3) Particle-Puff Release Mode

The particle-puff release mode determines if emissions are assigned to puffs, particles, or a combination. In particle mode the dispersion is computed by adding a random component to the particle motion, while in the puff mode dispersion is computed by assuming a concentration distribution and its rate of growth. Fewer puffs than particles need to be released for comparable simulation results.

Particle-puff release mode ... constant for run duration

C 3-D particle horizontal and vertical

C Gaussian-horizontal TH-vertical puff (Gh-THv)

C Top-Hat-horizontal and vertical puff (THh-THv)

C Gaussian-horizonal particle-vertical (Gh-Pv)

Top-Hat horizontal particle-vertical (THh-Pv)

Particle-puff release mode ... conversion after 24 hours

C 3D particle converts to Gh-Pv



CONCENTRATION — TOP HAT

Go to: $ADVANCED \rightarrow CONCENTRATION \rightarrow MENU$ #3

We will select the **TOP-HAT-HORIZONTAL PARTICLE-VERTICAL**.

Next go to **MENU #4** and change the particle release number back to 1.

RUN the model and display the output in **FRAMES** as we did before.

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Gaussian-horizonal particle-vertical (Gh-Pv)

C Top-Hat-horizontal particle-vertical (THh-Pv)

Particle-puff release mode ... conversion after 24 hours

CONCENTRATION - GAUSSIAN

Go to: ADVANCED → CONCENTRATION → MENU #3

We will select the GAUSSIAN-HORIZONTAL PARTICLE-VERTICAL.

RUN the model and display the output in **FRAMES** as we did before.

Here the circular structure is only conserved for 6 hours before it splits.

The area covered after 12 hours though is still much less than the multiple particle case.

If the center point of either type of puff passes over a sampling location, the integrated concentration at that point will be the same.



0600 24 Sep 83 AWRF FORECAST INITIALIZATION

CONCENTRATION - HYBRID

One advantage of *hysplit* is its ability to model horizontal dispersion with puffs, but the vertical mixing is treated as individual particles. Otherwise growing vertical puffs would have to split very frequently to simulate the boundary layer wind shear.

Modelling the change in dispersion with time can greatly speed up computation time compared to tracking individual particle trajectories.

Hysplit's default though is to compute 3D particle trajectory, so it is up to the user to use other approaches.

We can see this by changing the particle count to 100 through: **ADANVANCED CONCENTRATION MENU #4**

*Keep plume as Gaussian-Horizontal with Particle-Vertical



CONCENTRATION - HYBRID

Comparing the hybrid approach (right) and the 3D particle (left), we see that this approach is satisfactory. However, depending on your application of *hysplit* it may not suffice. ***Look at the concentration ranges



CONCENTRATION — PUFFS SPLITTING

First, change the particle count back to 1 and running the model.

We can view the splitting process by going to: **ADVANCED** VIEW **MESSAGES**

Looking at the second right most column we can see the number of puffs. In this case the puff splitting took place at **83 09 25 22** or **5** hours into the simulation.

Here, we see we started with 1 particles and the splitting goes: 5, 7, 17, 29, 65, 113, 237. *Recall the splitting occurs for $5^{(#)}$ of splits).

Why? Not all puffs grow at same rate and some may leave domain, so it is difficult to quantify the amount of puffs at each Δt .

*There is a limit to the amount of puffs though in a given simulation (MAXPAR) and the model will slow down and eventually terminate as it approaches it. This could result in a substantial concentration under-predictior and can only be addressed by increasing the value of MAXPAR.

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