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.

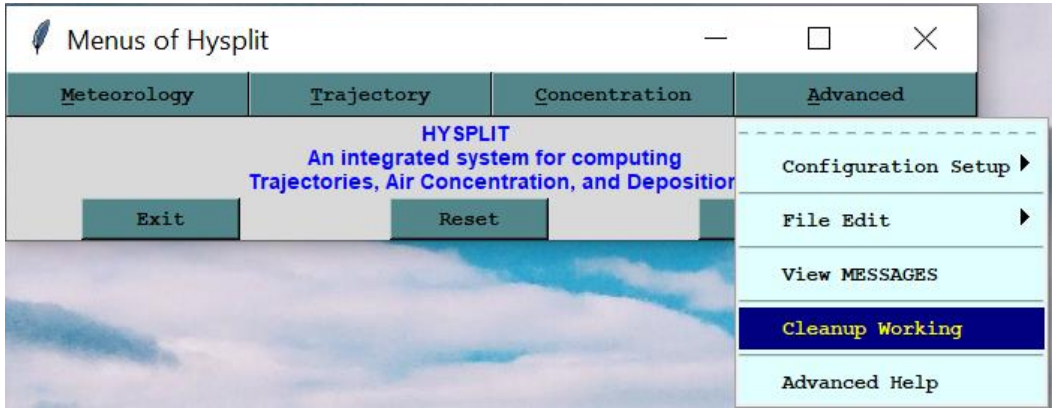
Go to **ADVANCED→CLEANUP WORKING**

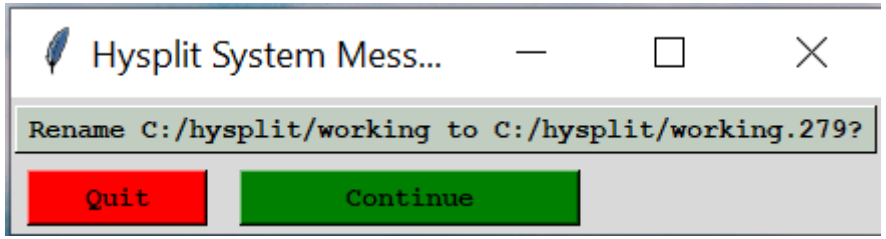
It will then ask you if you want to continue.

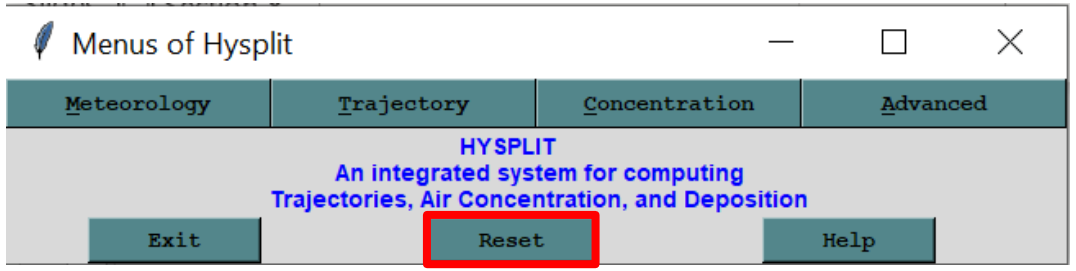
Click **CONTINUE.**

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.

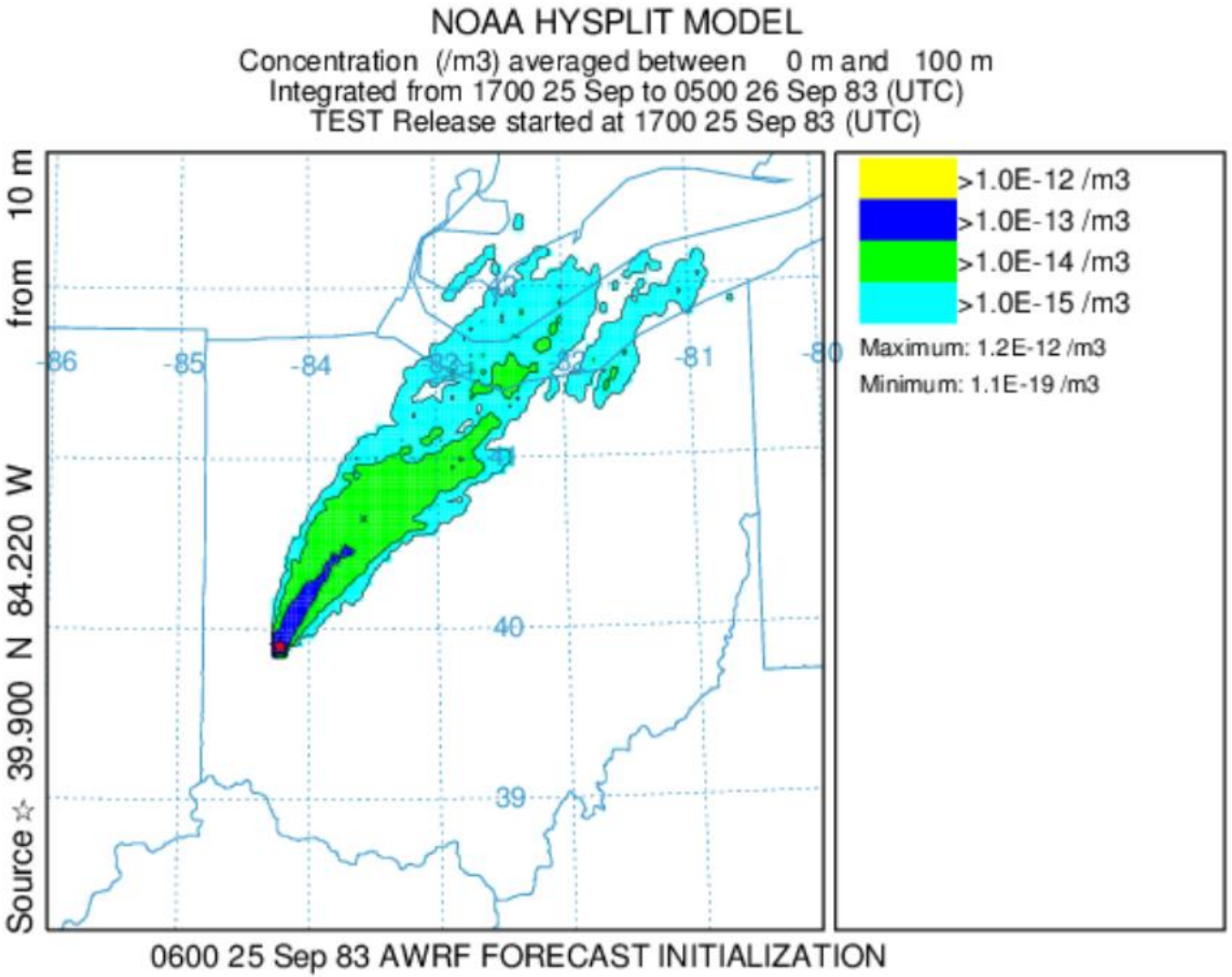
Now, re-open *hysplit* and hit **RESET** on the bottom to change all settings back to default.





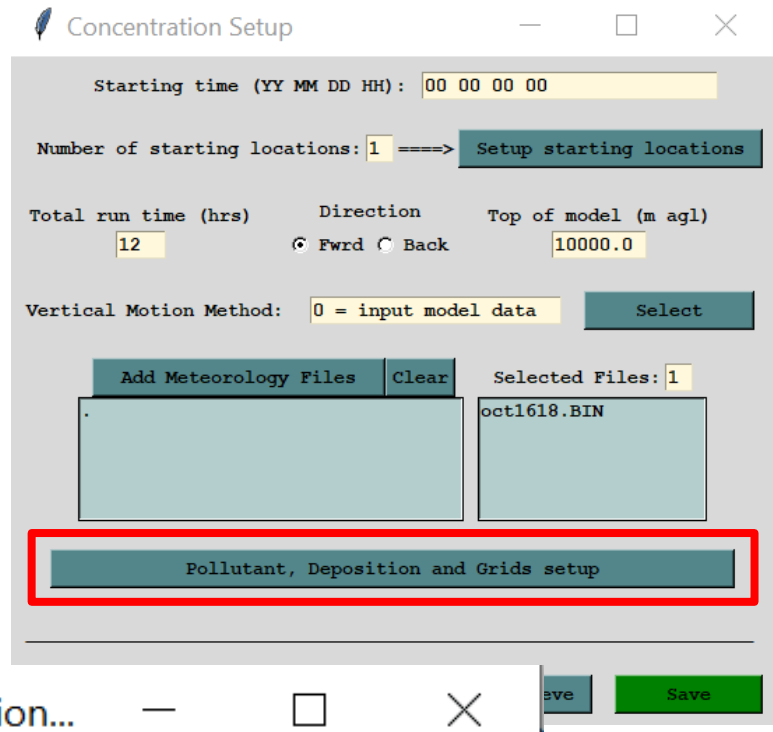


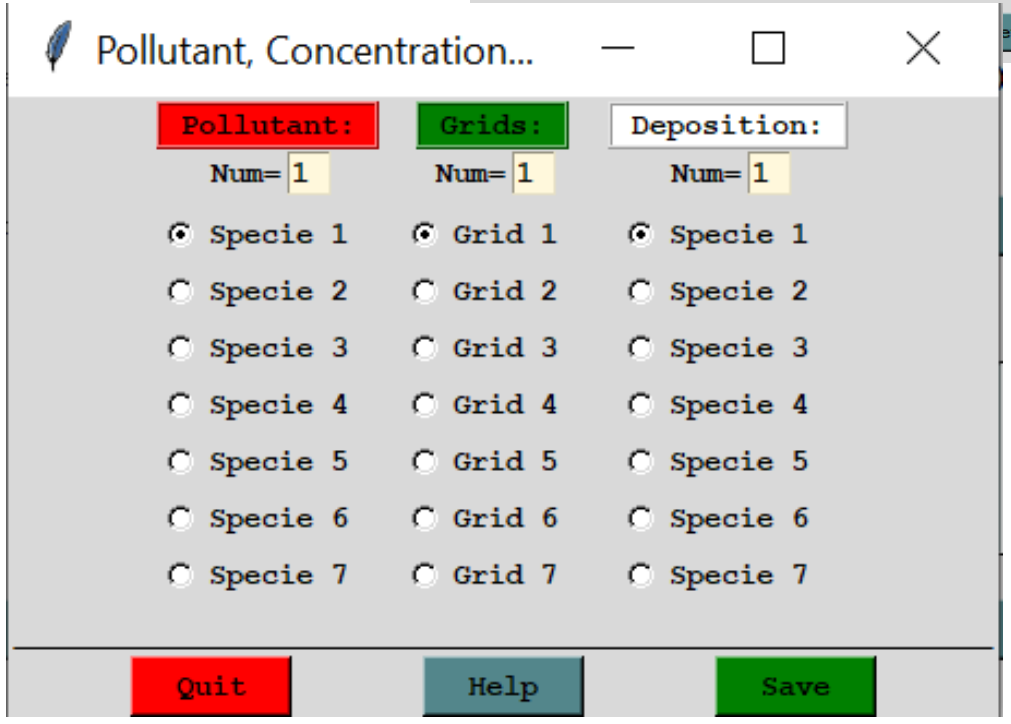
CONCENTRATION



CONCENTRATION - SETUP

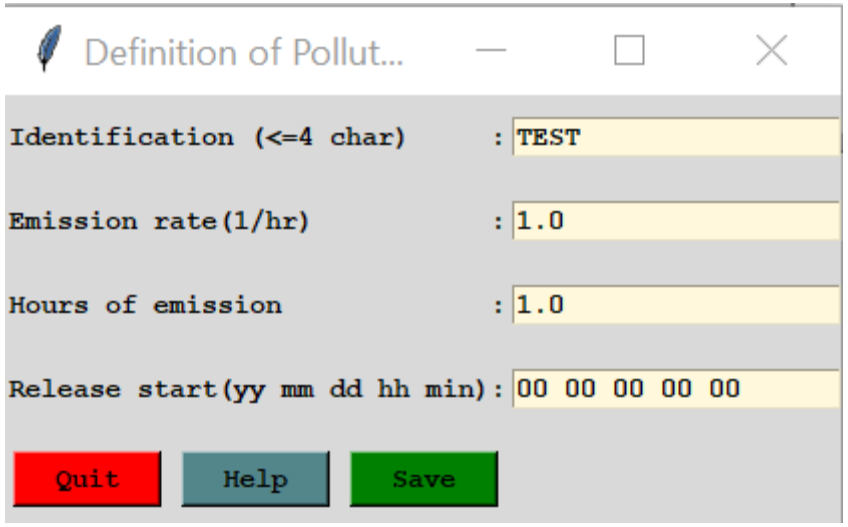
- Very similar inputs compared to *Trajectory*.
- Additional menu for **POLLUTANT, DEPOSITION** and **GRID** set up.
- You can specify more than one pollutant and its deposition properties as well as multiple grids.



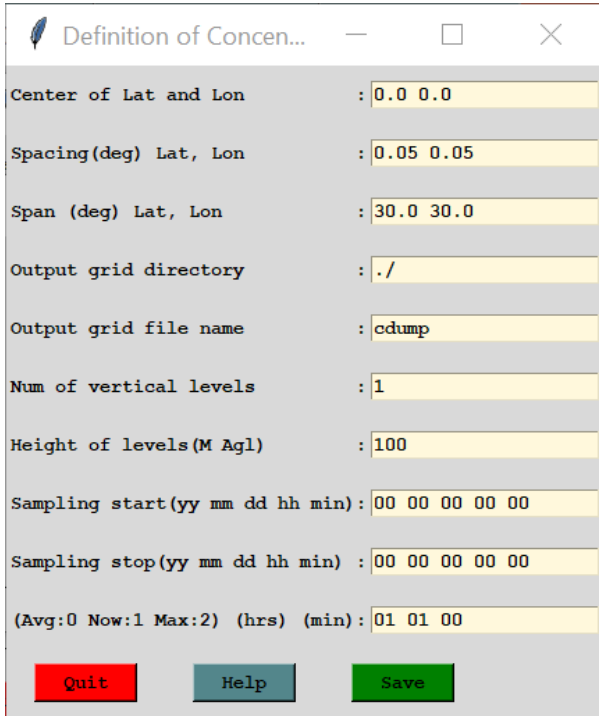


CONCENTRATION - SETUP

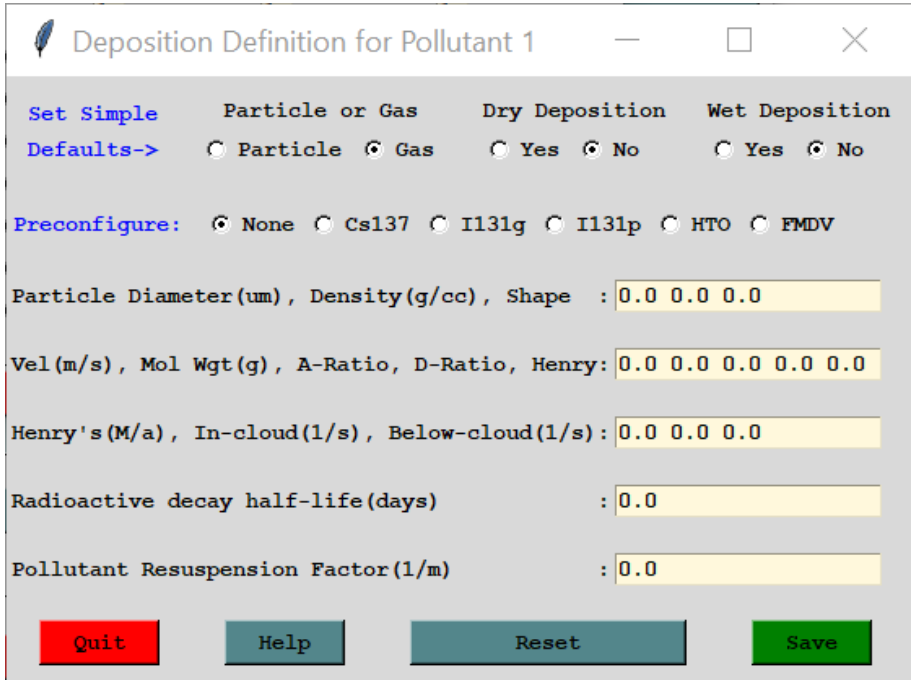
POLLUTANT OPTIONS



GRID OPTIONS



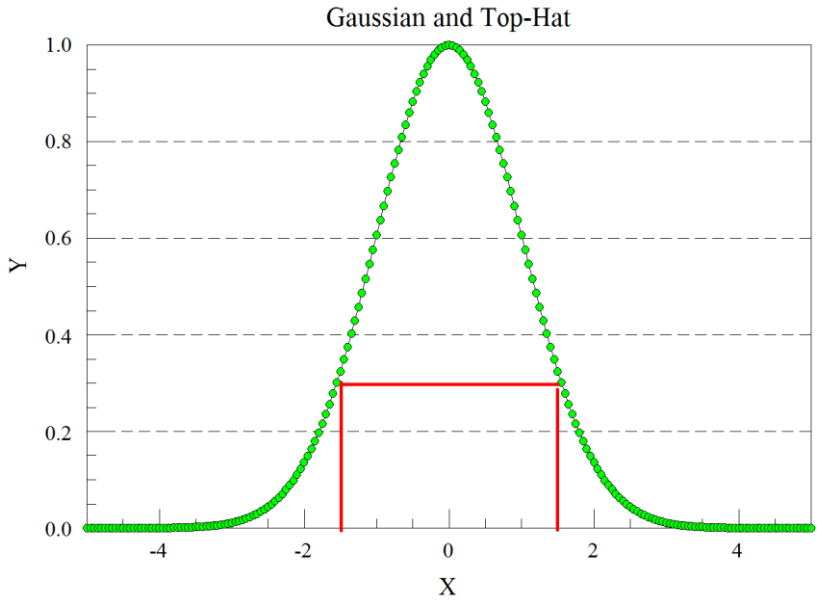
DEPOSITION OPTIONS



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):

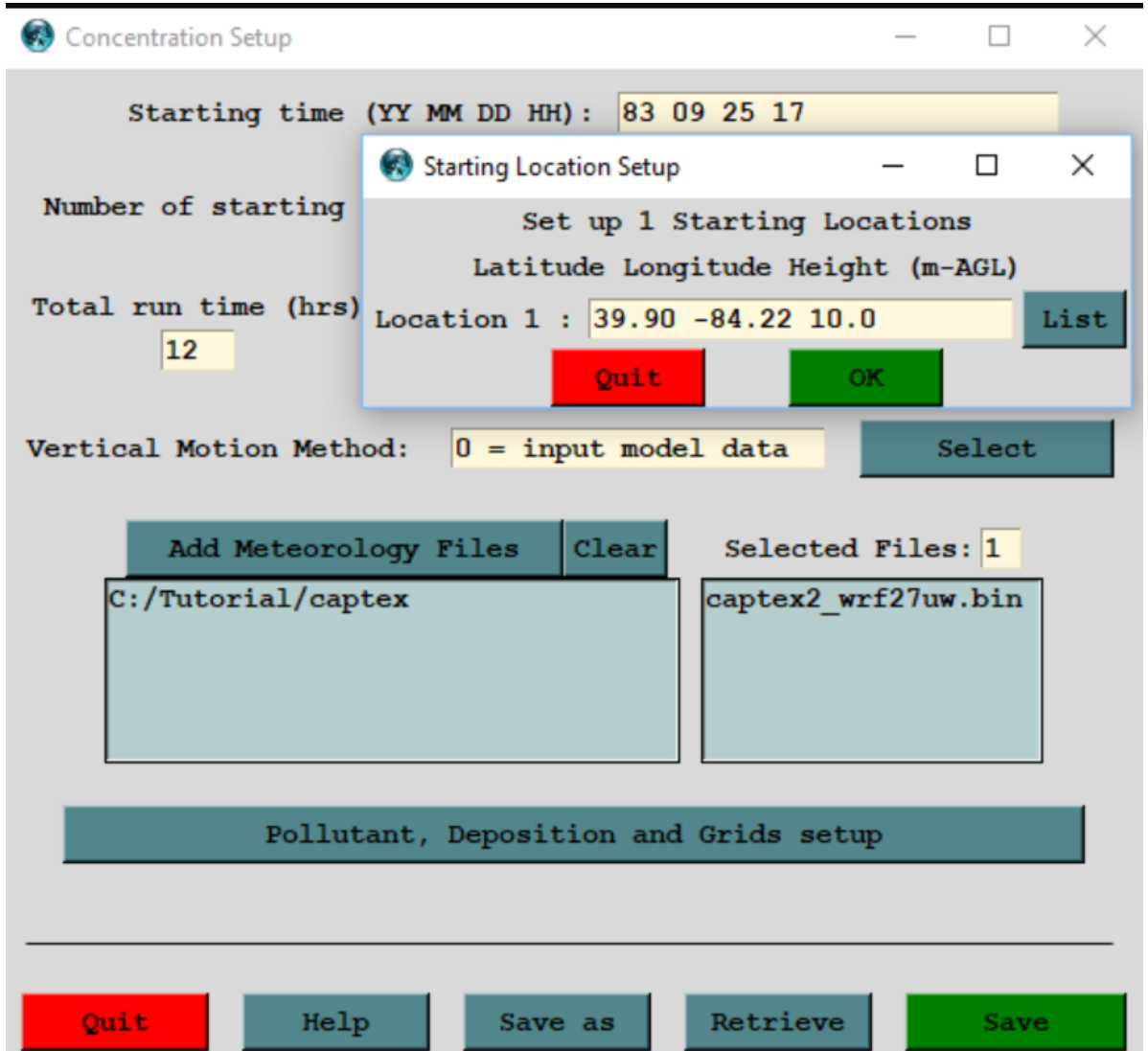
- Six 3-hour releases of perfluorocarbon (C7F14) tracers: four in Dayton, Ohio and two in Sudbury, ON
- Samples collected at 84 sites, 300-800km from the release over 3-6 hour averaging periods for 48-72 hours
- Aircraft also collected data for short time periods (6-10 mins): the lowest level was 914m MSL and the highest was 2134m MSL
- More information can be found here: https://journals.ametsoc.org/view/journals/apme/56/8/jamc-d-16-0345.1.xml

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→CONCENTRATION→CONTOURS** and except the defaults by clicking **EXECUTE DISPLAY.**



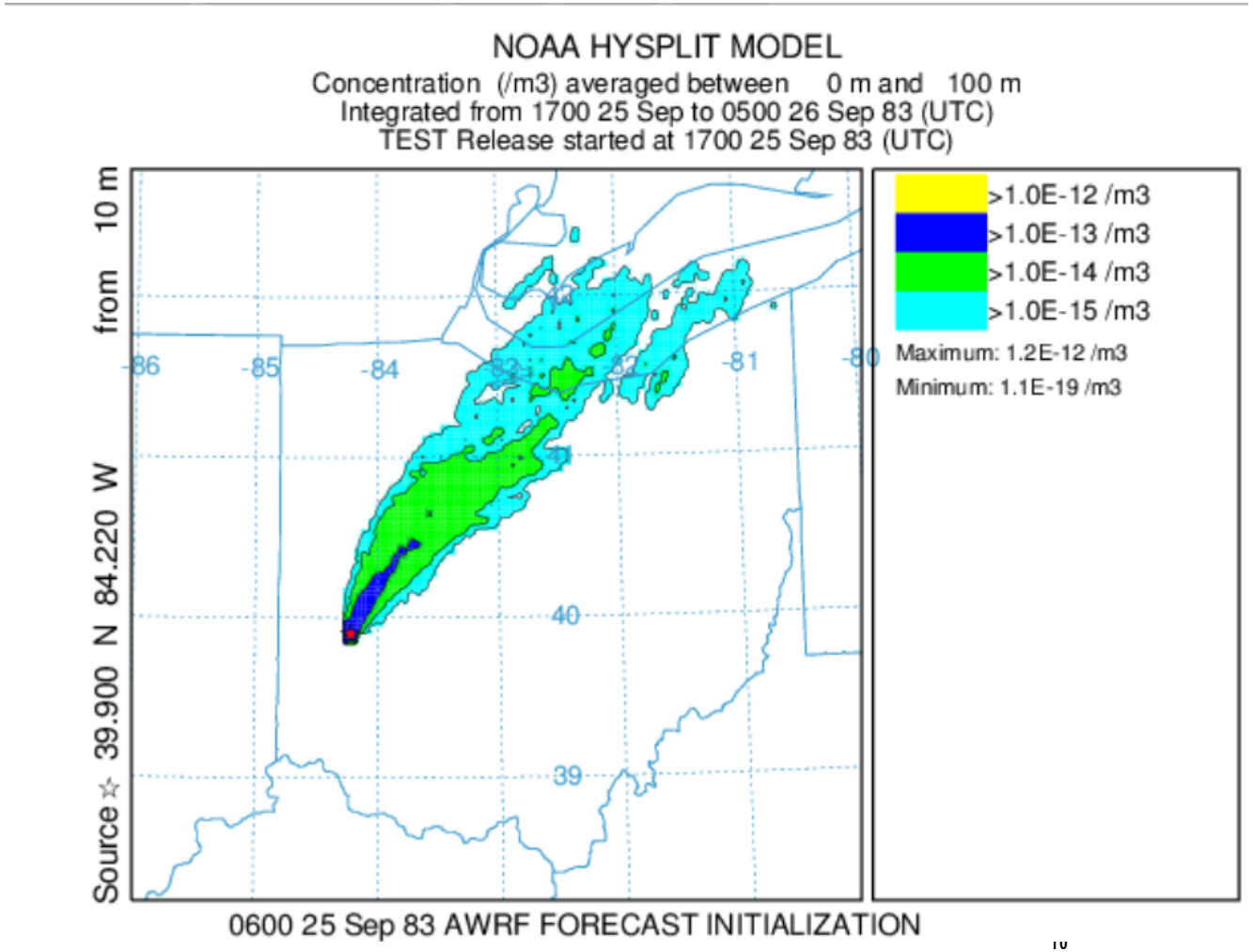
CONCENTRATION – SIMPLE SCENARIO

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 $1x10^{-12}$ to $1x10^{-15}$.

If one particle (mass = 1/2500) were contained in a grid cell of volume 5x5x1 km ($2.5x10^{10}$ 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 PARTICLE

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

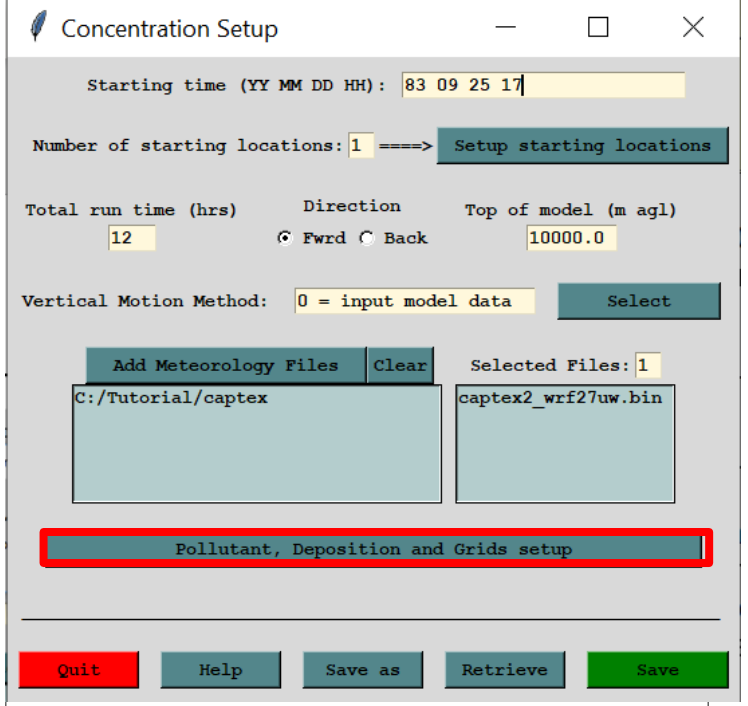
Go to **CONCENTRATION→SETUP→POLLUTANT, DEPOSITION AND GRIDS SETUP.**

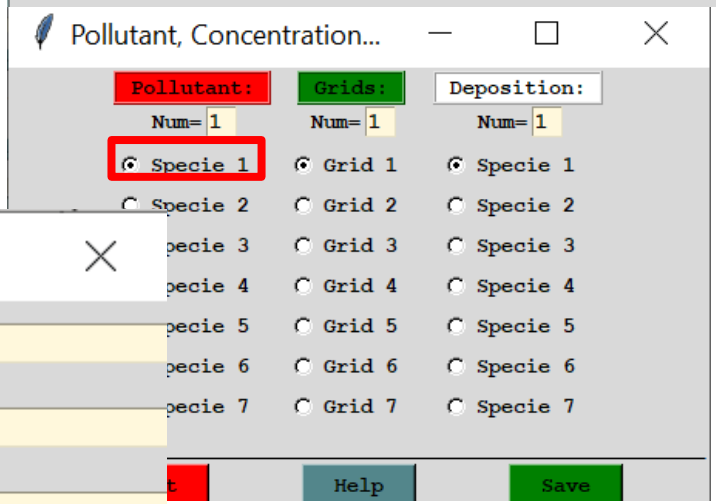
Next, click on **SPECIE 1** under **POLLUTANT** (there will only be one for this case).

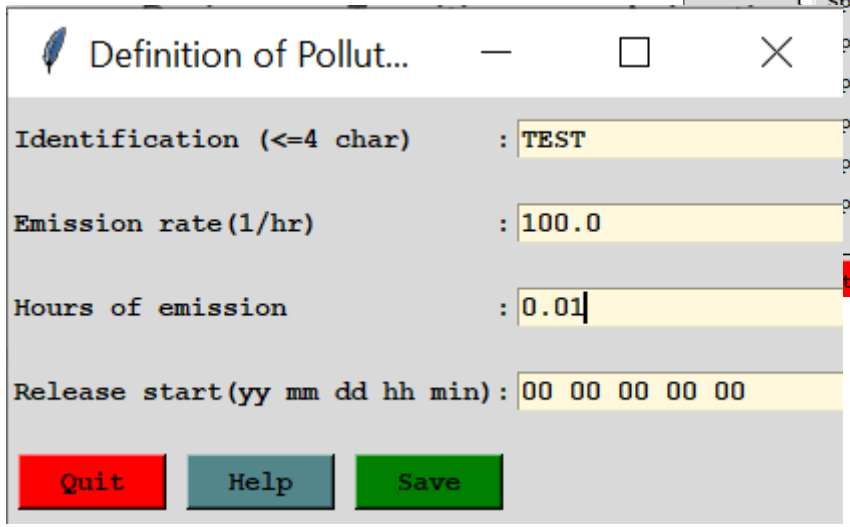
We will be changing the **EMISSION RATE** and **HOUR OF EMIISION,** but not the overall volume. All mass is now released on one time step though.

Make the changes as shown here.

Hit **SAVE.**





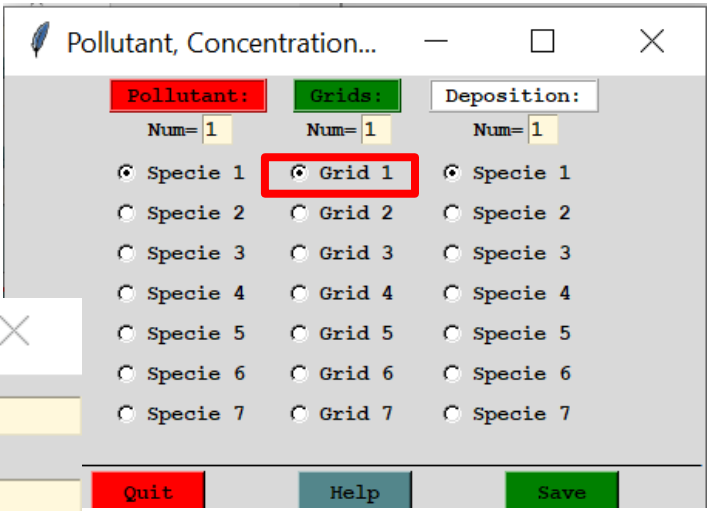


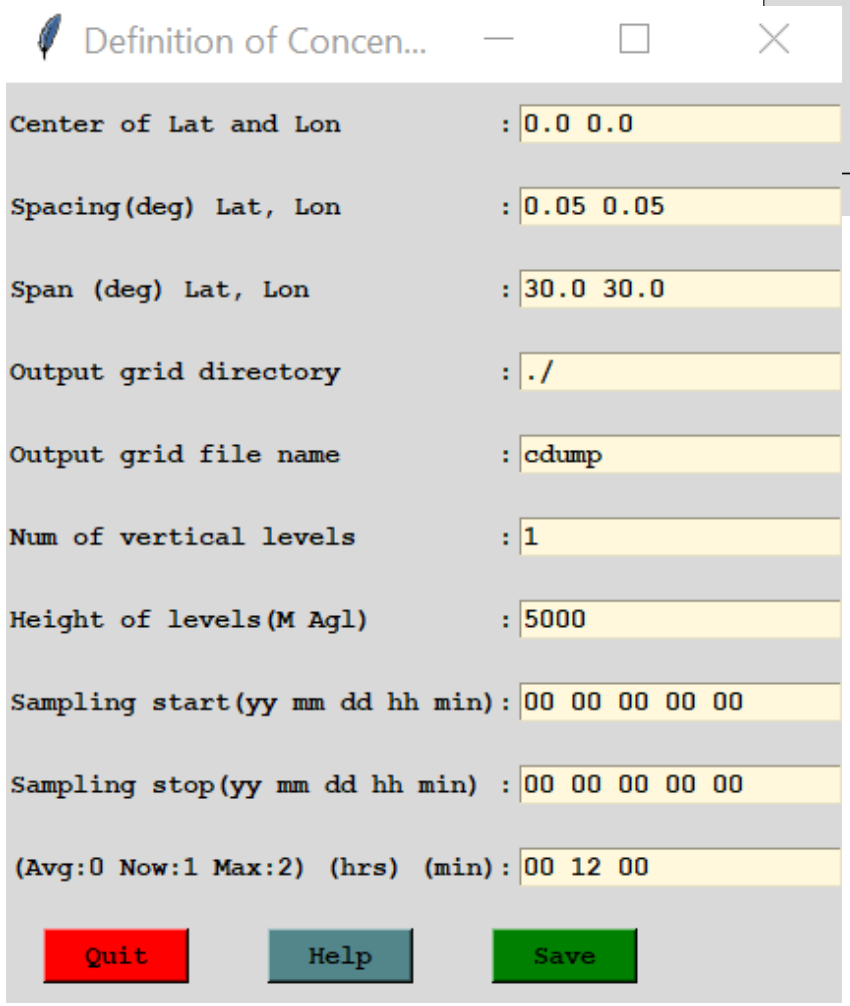
CONCENTRATION – SINGLE PARTICLE

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

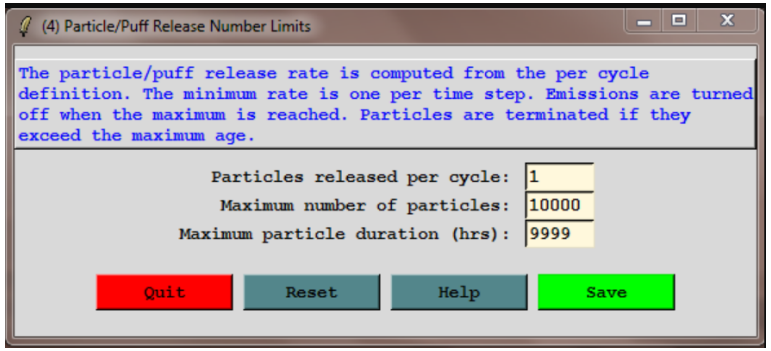
All we are changing here is the height of the levels to make sure we have a large enough domain to track the single particle.

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





CONCENTRATION – SINGLE PARTICLE



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

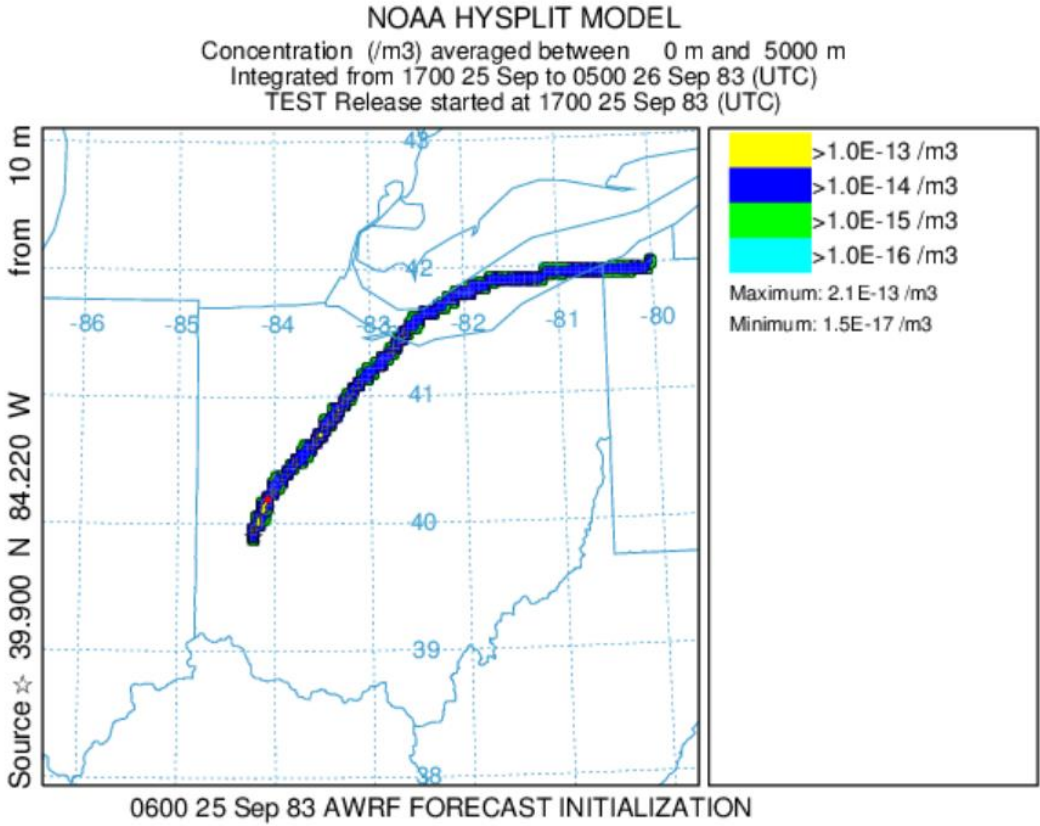
Go to **ADAVANCE→CONCENTRATION→MENU #4**

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.



CONCENTRATION – SINGLE PARTICLE

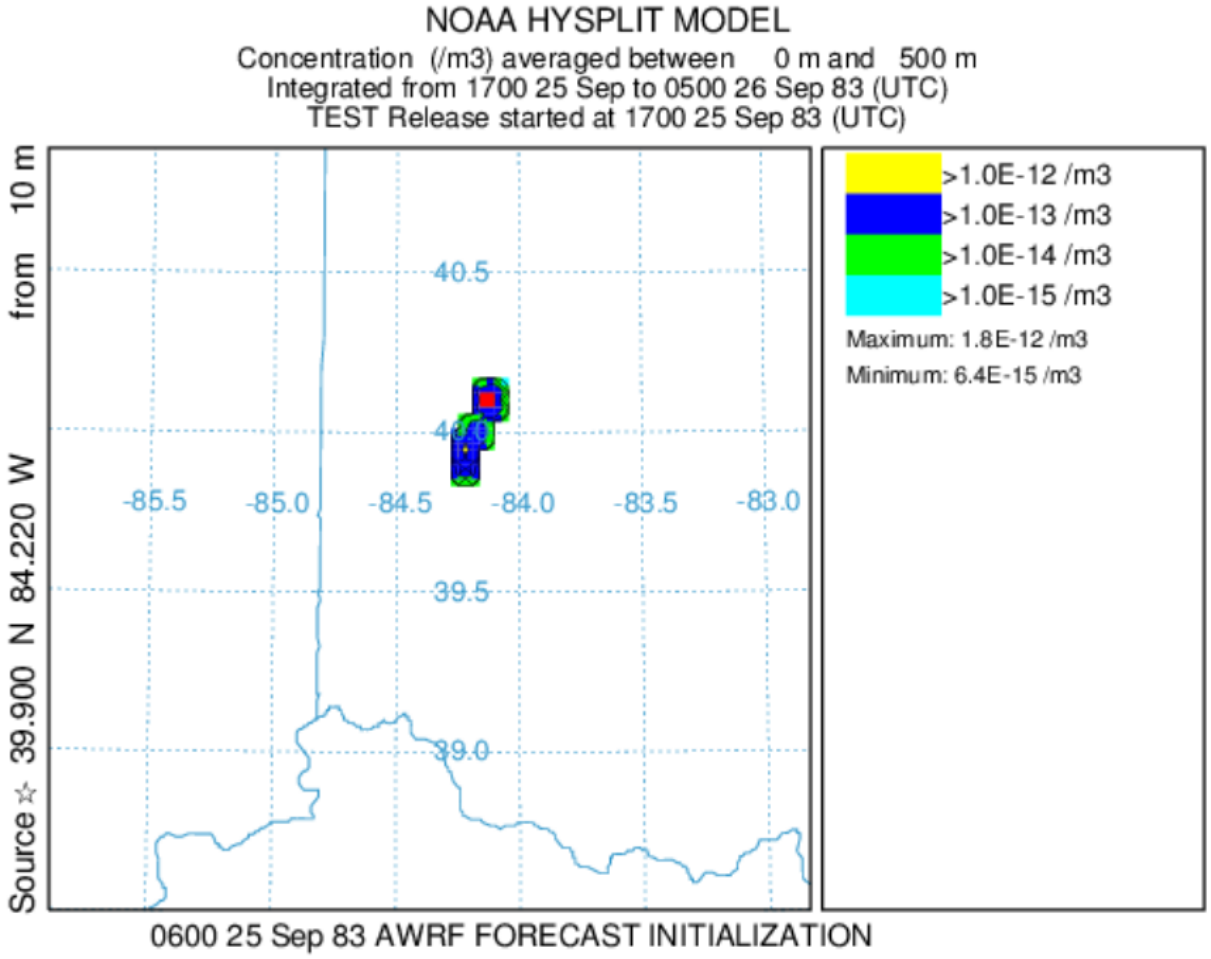
But what if we didn't model as high of a domain?

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.



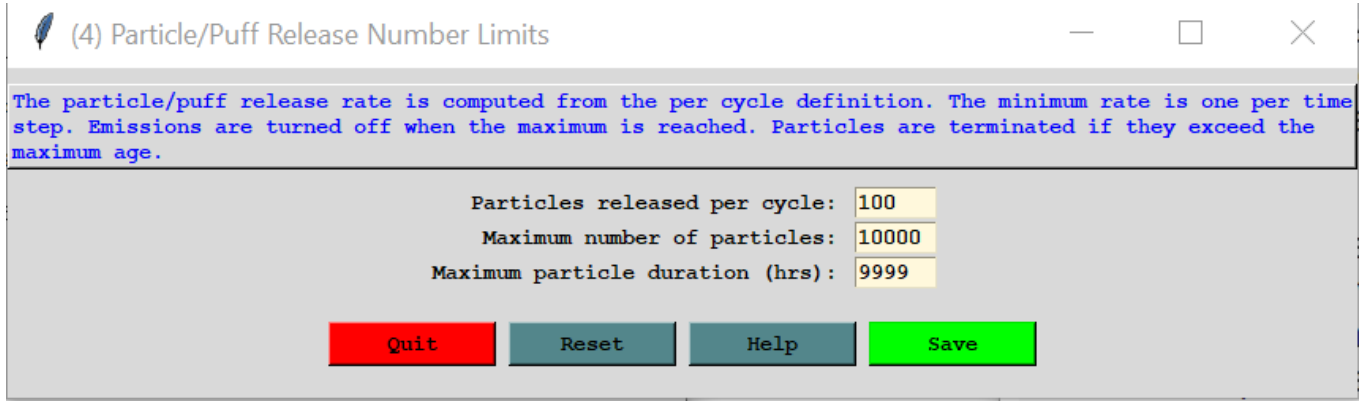
CONCENTRATION – MULTIPLE PARTICLES

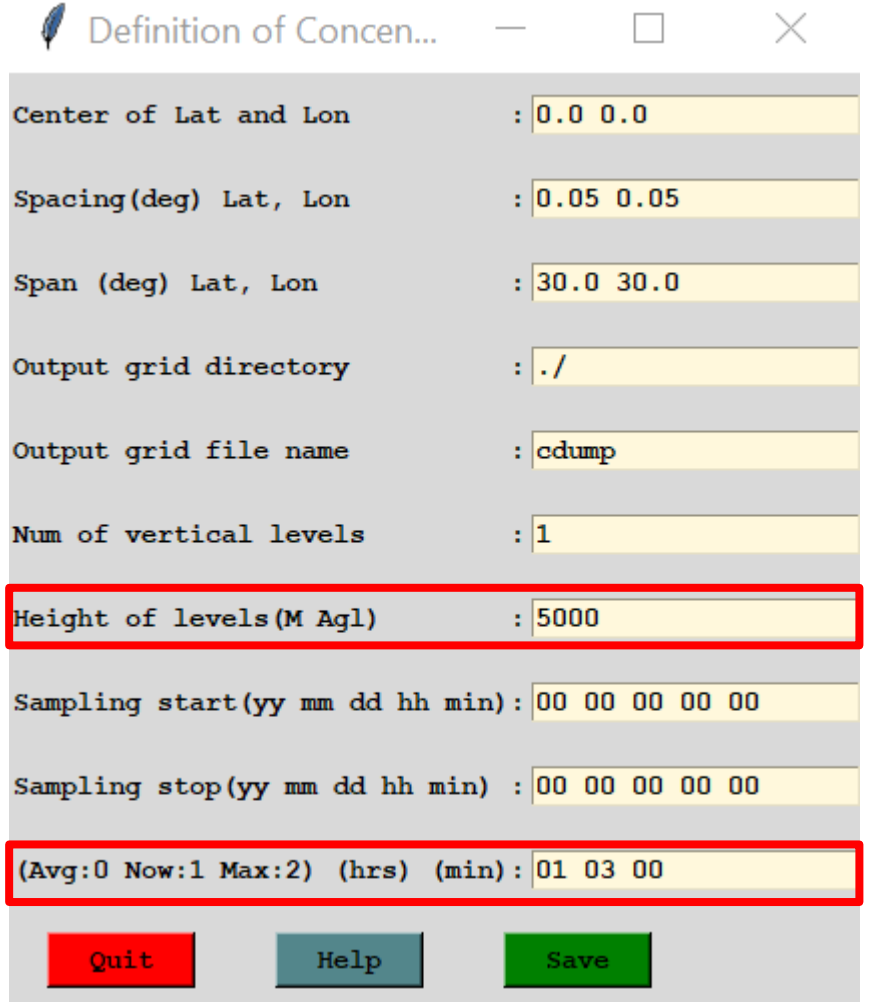
We will now model multiple particles.

First change the **HEIGHT** back to **5000.**

Then we will change the **AVERAGING** time to every **3** hours.

Next, go to: **ADVANCED→CONCENTRATION→MENU #4** and change the number of particles from **1** to **100.**





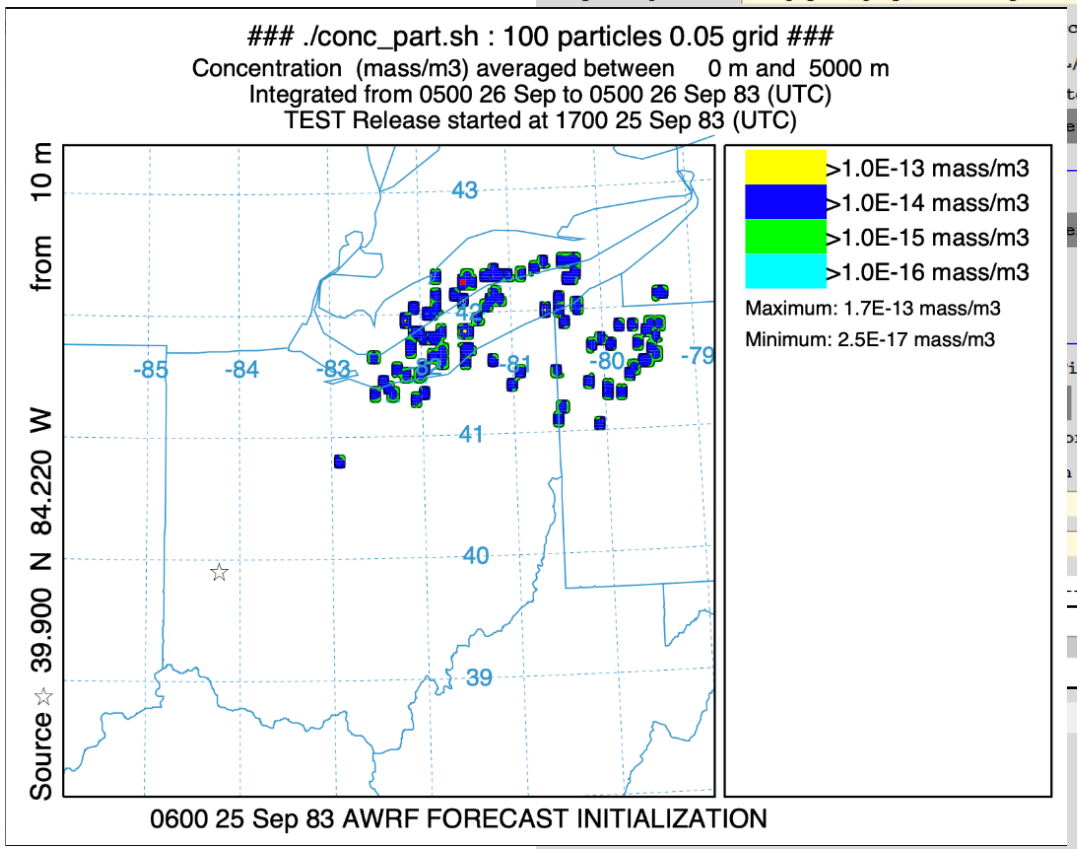
CONCENTRATION – MULTIPLE PARTICLES

RUN the model.

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

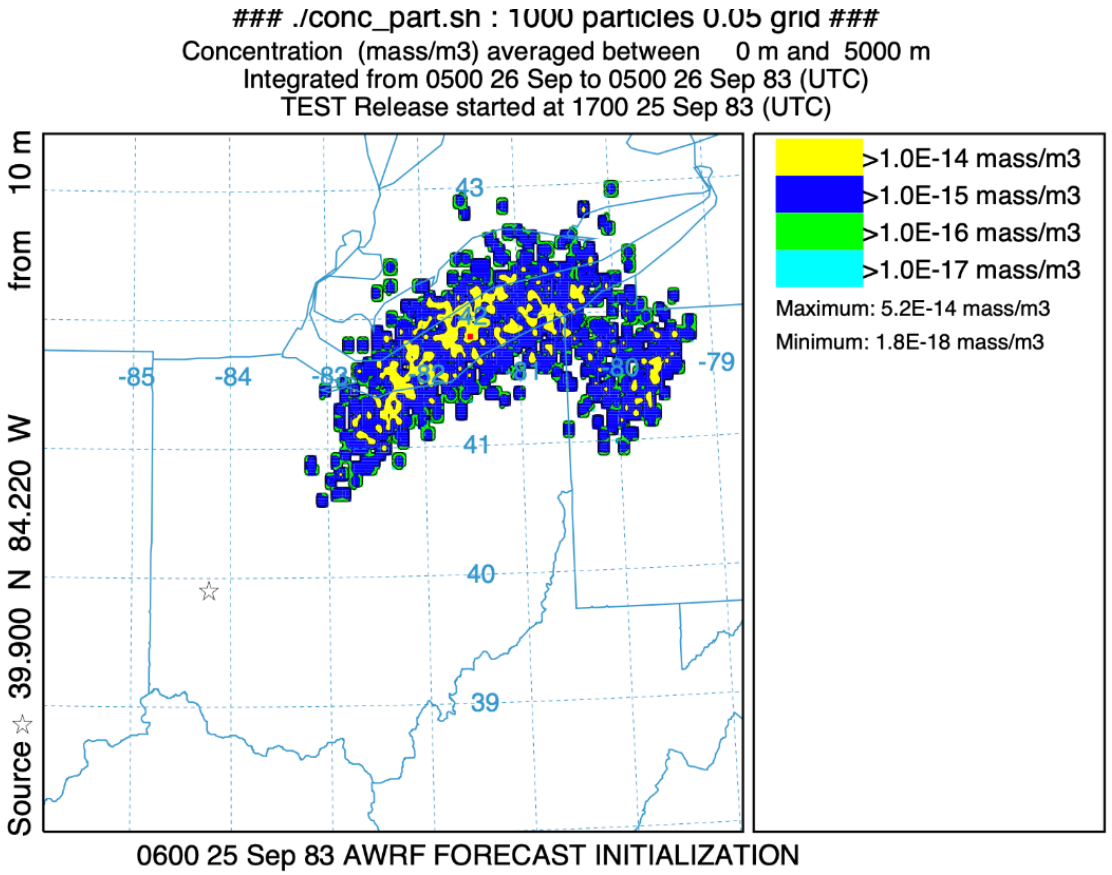
You should have four images load onto your screen (for every 3 hour period over 12 hours).

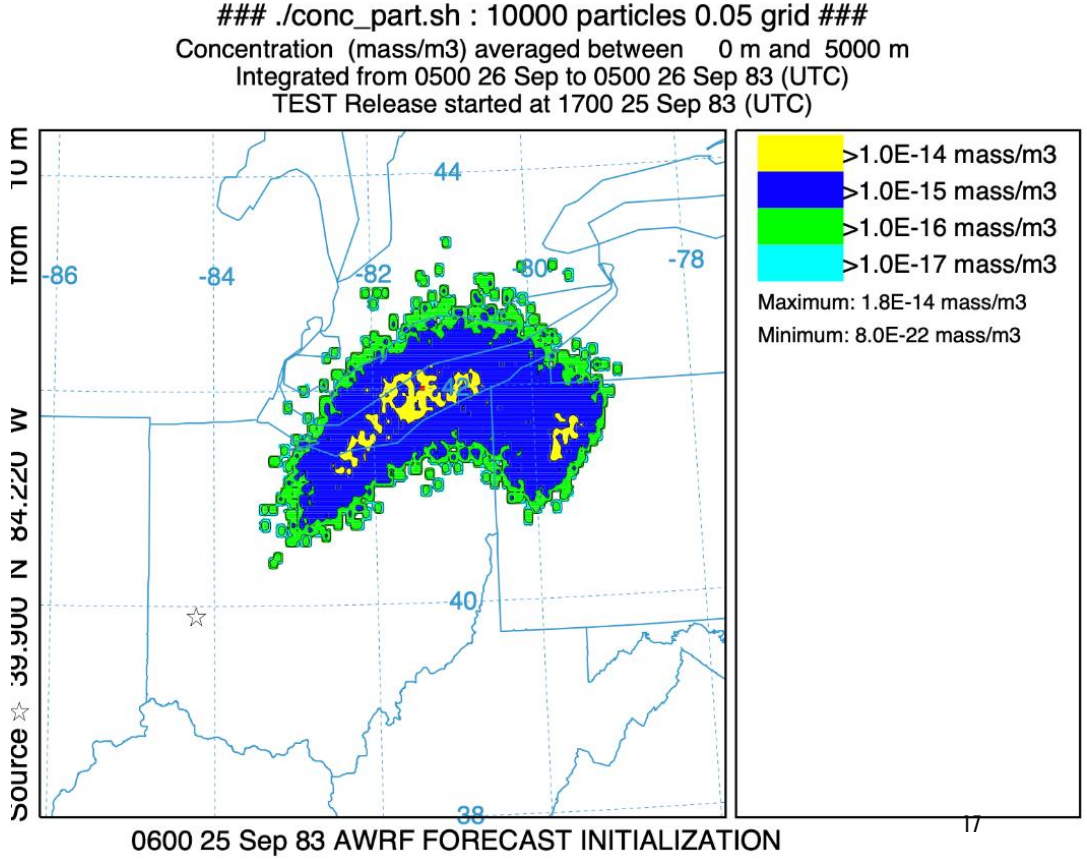
We still do not get a good plume from this, lets try 1000 and 10,000 particles as well.



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: https://www.arl.noaa.gov/documents/reports/arl-224.pdf

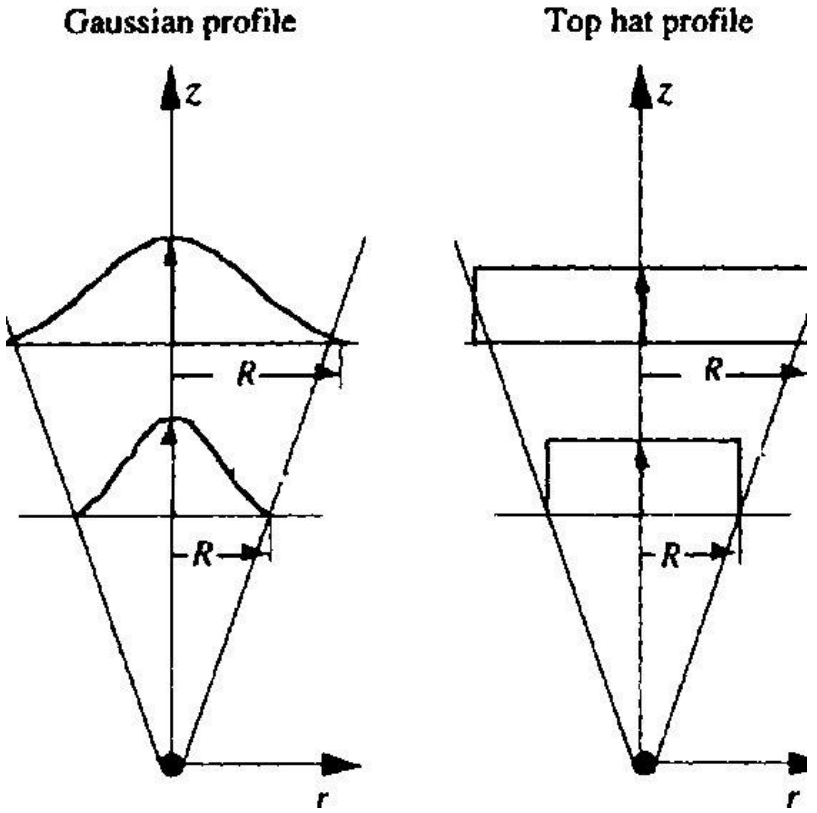
TOP HAT VS GAUSSIAN

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.

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

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

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

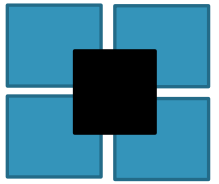


*Top-Hat used more often because less complex computing and just as accurate as Gaussian downwind of source. Gaussian only more accurate right at source.

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 $P(x \pm 0.5\sigma h, y \pm 0.5\sigma h)$.
- A large **Gaussian** puff splits into five smaller puffs when $3.0\sigma h > Lh$. 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.



*σh 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.

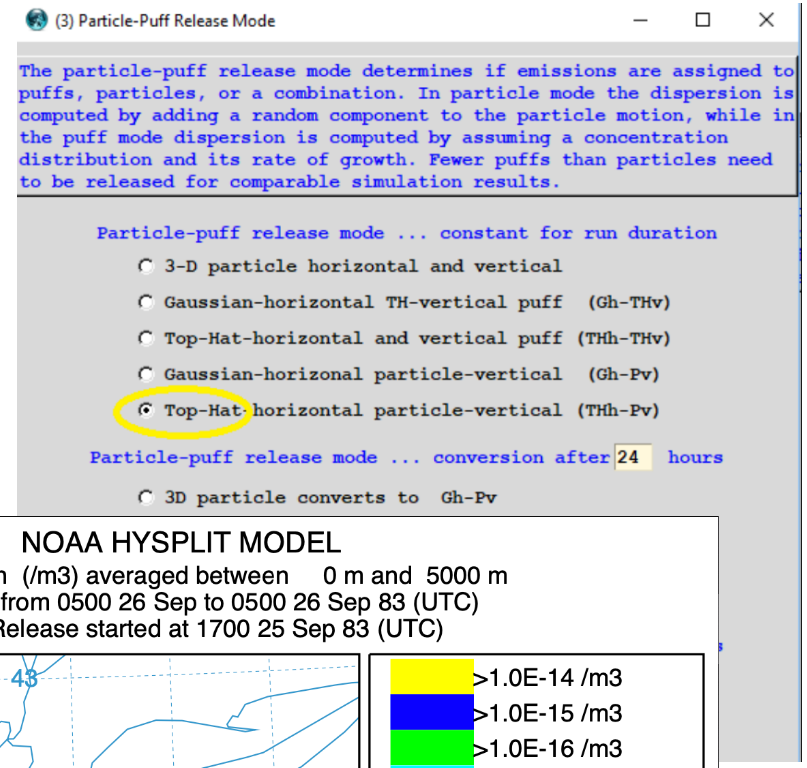
CONCENTRATION – TOP HAT

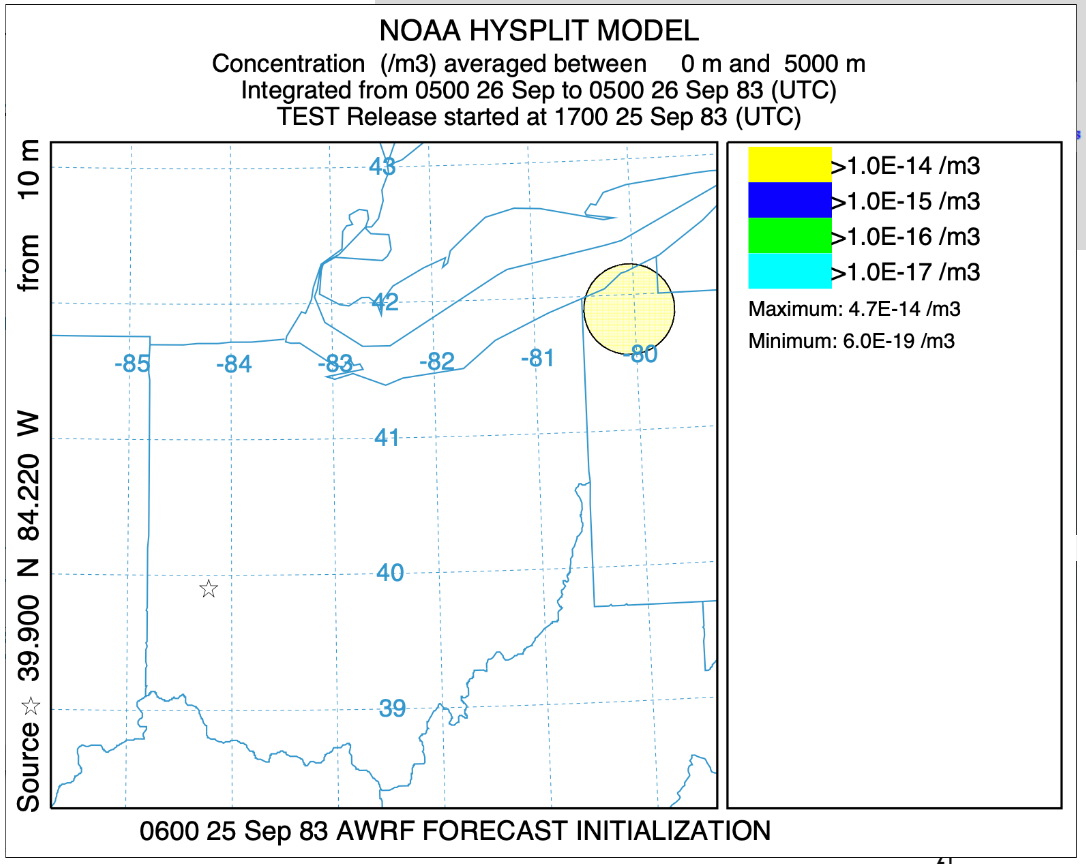
Go to:
ADVANCED→CONCENTRATION→MENU #3

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.





CONCENTRATION - GAUSSIAN

Go to:
ADVANCED→CONCENTRATION→MENU #3

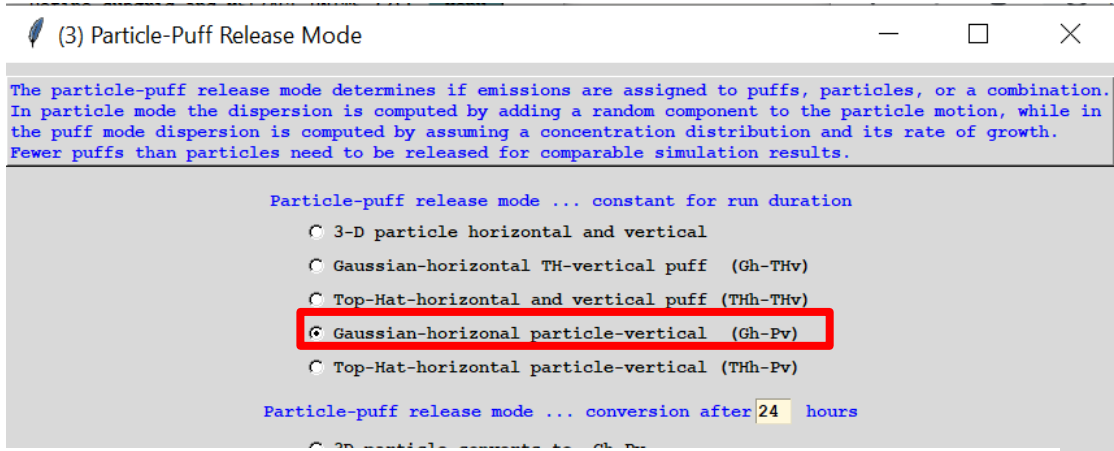
We will select the **GAUSSIAN-HORIZONTAL PARTICLE-VERTICAL.**

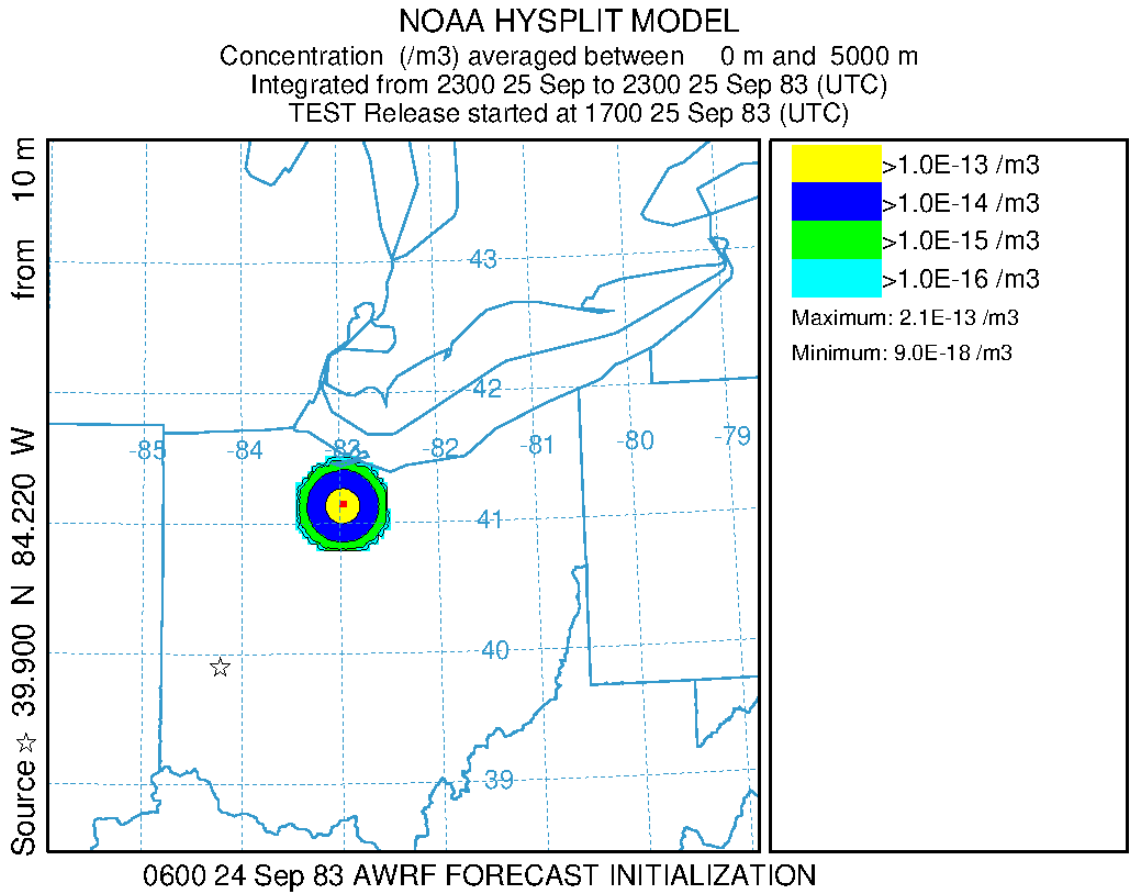
RUN the model and display the output in **FRAMES** as we did before.

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.





CONCENTRATION - HYBRID

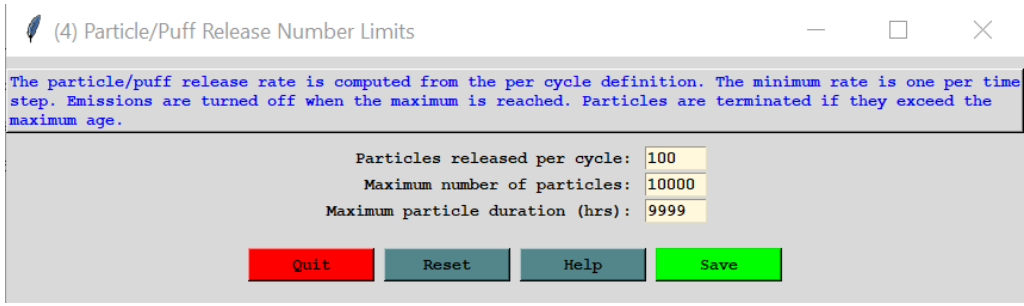
One advantage of *hysplit* is its ability to model horizontal dispersion with puffs, but the vertical mixing is treated as individual particles. Otherwise growing vertical puffs would have to split very frequently to simulate the boundary layer wind shear.

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.

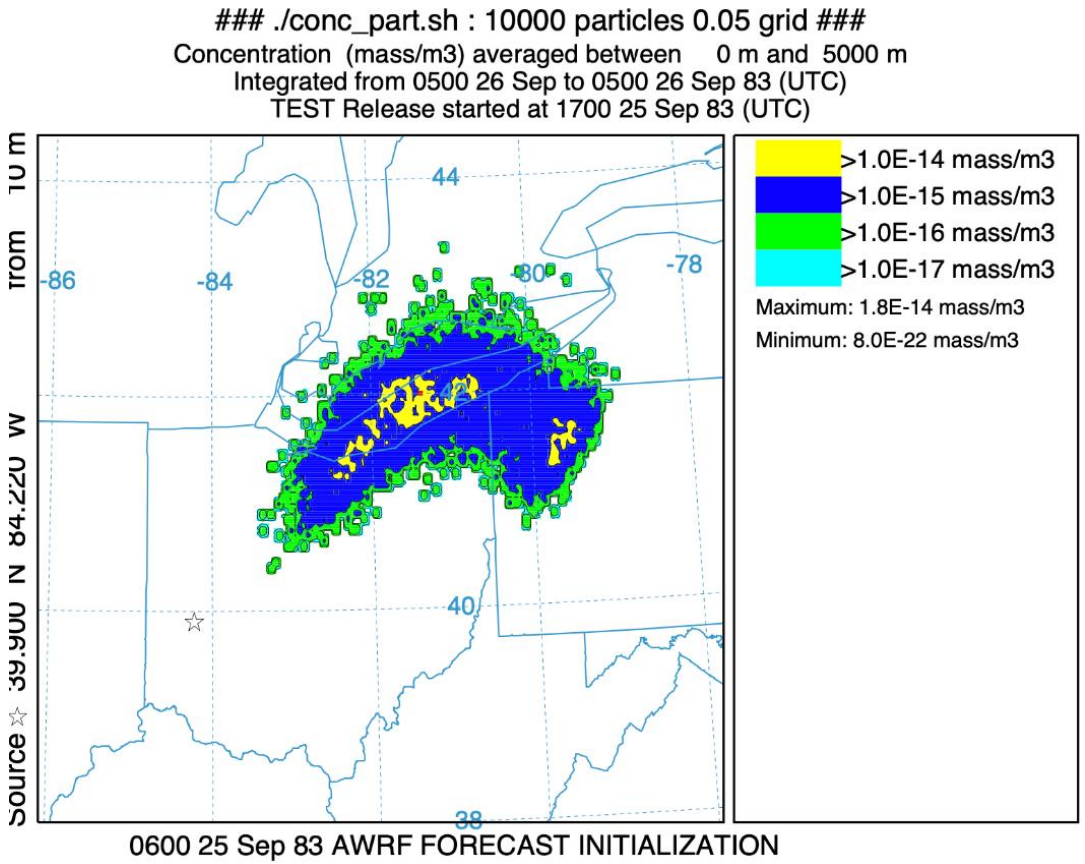
We can see this by changing the particle count to 100 through:
ADANVANCED→CONCENTRATION→MENU #4

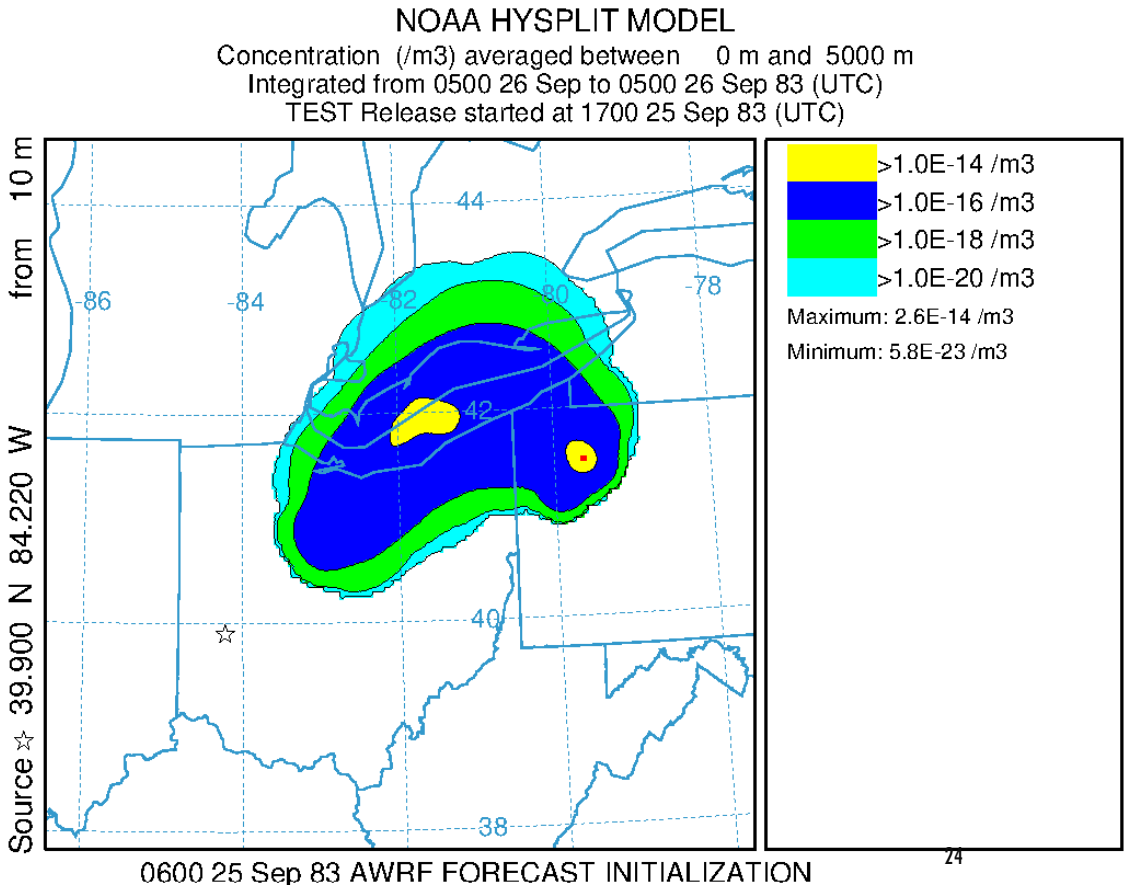
*Keep plume as Gaussian-Horizontal with Particle-Vertical



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-prediction and can only be addressed by increasing the value of MAXPAR.