

To conclude the introductory section on air concentration calculations we will do an exercise. In one of the previous sections of the tutorial, we started with one particle, and then increased to 100, 1000, and then 10,000. And you probably did not notice, but the maximum concentrations changed with each simulation. For instance, in the 100 particle simulation, the concentration, the maximum concentration, at this red point, was  $2.6 \times 10^{-13}$ , while in the thousand particle simulation, it was about half of that,  $1.3 \times 10^{-13}$ , while in the thousand, or 10,000 particle simulation, the maximum was half again, at  $7 \times 10^{-14}$ . Although we did not show the hundred thousand particle calculation, which takes quite some time, the maximum concentration only decreased by 10%.

So the question is, since we already have a sense that the concentrations from a model simulation are sensitive to the particle number, and that is related to the concentration grid cell size. What would happen if we were to make the concentration grid a little bit coarser, perhaps from .05 to .10°? At what point would the change in maximum concentration stabilize? When would we get the same result?

To get started you have to do the exact same thing that was done in the previous tutorial and load the CONTROL file and the setup file that you had saved and make those changes with a different grid resolution. So at this point you could pause the tutorial and wait and restart it when you want to see the answer.

Okay the solution would be, let's open up the, I'm going to press reset first, and then open up the set up, and retrieve the configuration that we had saved previously, which was conc\_test\_control.txt and before we click on save, these are 12 hour simulations, from Dayton. We need to change the grid resolution to 10 km instead of 5 km and we should also change the output interval to every three hours. Those are the same changes we had made in that previous section. Save to close all these menus. And we need to do something similar for the advanced, configuration, concentration, and we're going to open up menu #4 and we're going to run with 100 particles.

This'll be the first test and then run model, with the setup file. And let's look at the result. Let's go to the end of the calculation and you can see that the maximum concentration is  $8.6 \times 10^{-14}$ , you should write that down. Let's do this again, now for 1000 particles. All you need to change is the configuration, 1000, save to close, run model, display. Let's go to the end. You can see there's a slight change,  $6.4 \times 10^{-14}$ . It is almost the same result as before. And for completeness, let's go ahead and run the 10,000 particle simulation. Save to close, run model, and display. And let's go to the end, and you can see the maximum is 6.7, so it's actually gone up a little bit. So effectively we're getting the same answer with 10,000 particles as we are with 1000 particles, which is also very close to the 100 particle simulation. Going from 100 to a 1000 particles was about a 25% change, going from 1000 to 10,000 particles, was a 5% change.

And comparing this 1000 particle simulation with the 10,000 particle at the finer grid, we are getting about the same result. So this is the 1000 particle simulation with 6.4 at the 10 km grid, but the previous 5 km, the difference in the max is about 9%, but we're seeing a very similar structure and concentration.

So what actually can we infer from these results? So what happens, this is a very simplified example of what we just had seen. Let's assume we have three different simulations, each one using a different number of particles. In the first, 6 particles, then 12, and then 24 particles. And these particles are distributed about the plume as you can see here, the red dots, will give you a representation of these particles, after some time downwind. And the little blue box here represents a concentration grid cell. So if I were to compute the maximum concentration that's observed, in this case the total mass of these particles is one, the maximum concentration, since only one particle is sampled, in this case it would be once  $1/6$ . But in the case of 12 particles, we're now sampling three particles in the box, but each particle only contains a mass of  $1/12$ , so the total the maximum concentration would be essentially  $3/12$ . Now we increase the particle number any further, double it again, and we now have 24 particles, each one having a mass of  $1/24$ , and now the same grid cell samples six particles, but as you can see the maximum concentration would be the same as the previous simulation. Because when we went from the 12 to 24 particle simulation, the

sampling box, the sampling grid cell size, is adequately representing the distribution of the particles that we have, you know, between six and 12. The density was still sensitive to the number of particles, because we were under-sampling, if you will. But as we go beyond 12, we can keep increasing the density, the particle density in the grid cell, but it's not going to change the concentration, because the contribution of the individual particles goes down.

So it's just something to remember when you are configuring the model and you are trying to decide what the optimal particle number might be. Fewer particles give you faster results, but also more noisy results, and sensitivity to the size of the grid cell and location with respect to the plume.

And this concludes exercise number seven.