Up to this point all the concentration simulations that we have done assumed an inert non-depositing gaseous tracer. However more realistic simulations are possible and we can make some simple assumptions about transforming pollutants from one to another, or the deposition, either wet or dry, for particles and gases. These are the components we will look at in section 11.

Let's start with the simplest case of a linear mass conversion. Before we get started on this, let's create a baseline simulation from which we will be making changes. Again as before, we will use the surface level CAPTEX concentrations as a baseline for doing our comparisons. To get started press reset to ensure that we do not have any leftover components or variable set within the graphical user interface. And then retrieve the surface level CAPTEX simulation that was set up in the beginning of the concentration section. And if you recall that was named captex_control.txt. It was a 68 hour simulation using a North American Regional Reanalysis data. And we can do the same for the name list file, the captex_setup.txt file.

And at this point I would suggest two changes. We're not going to be running very long. We can do most of these examples by just doing a 25 hour simulation, essentially eight three hour samples. So change the run time to 25. And since we are not going to be running such a long simulation, we can run with fewer particles. So go to the advanced menu and set menu #4, the release number limits, to 20,000. And this configuration will become our

baseline for doing the transformation and deposition simulations. Let's run the model and confirm that the results are what we want.

When it completes, let's open the display and we will keep this relatively simple, we will convert to picograms, but we will let the program draw its own contour intervals. But let's save the output file name to a unique name, for instance, the base case. And let's execute display, and we will get eight frames, and in this last frame you should have a picture that looks like this with a peak concentration of 9000 picograms per cubic meter. And this file would be located, of course, in the hysplit4/working directory, plot_base.ps.

So now to do transformation, the simplest approach, now HYSPLIT does contain some complex chemical conversion modules. These are separate executable programs that can deal with sulfate chemistry, or ozone chemistry, but both of those are beyond the scope of this tutorial. But here we will deal with a simple transformation. In this case the transformation is defined as a rate, in terms of fraction per hour. The default is 10% per hour, but obviously you can enter any number you desire. And the way that is computed, is the mass removal is determined by this dimensionless number, which is the conversion rate times the time step, the integration time step. So over this time step, that beta times the mass that's contained in a particle is what is removed each time step. If the beta number is very small, then this computation is used, if the beta is larger

then we need to use the exponential equivalent. When beta is very small these two terms are equal. Now this is the removal fraction from mass one, but correspondingly mass two also then gains this value, what is removed from mass one is applied to mass two.

And there is also a correction factor called the molecular weight correction factor. An example of why you may want to define this is, for instance, doing a simple transformation of SO2 to SO4. If we define this transformation at 10% per hour, each time step of that transformation is not just the 10% of mass that's converted from here to here, but it also picks up an additional two oxygen molecules going from 2 to 4. And that is what needs to be corrected for in the molecular weight correction factor. So the difference in molecular weight between SO2 and SO4 is essentially 1.5.

How do we define this transformation? It's a relatively simple process. We go to, first the pollutant menu, so the main menu bar here, and let's define instead of one pollutant, we will define two pollutants. You have to define two, I mean you have to define more than one pollutant, if you're doing transformations, obviously. Of course species one is still the PMCH that we are releasing and this menu is populated, of course, by the values from menu one when you first define the second pollutant. So we will correct this and let's just call this pollutant two for now, and it will have no emission, and no duration of emission. Now we could define an emission rate for this pollutant as well, but we want all the mass that's being

transformed into pollutant number two to come from pollutant number one. Now we don't have to change anything else, that's really all we need to do in this menu.

The next step is we have to go to the advanced configuration setup for concentration and we go to in-line chemical conversion modules, that is menu number 10. And in menu number 10 we can define conversion of species one to species two. As I said the default is 10% per hour, .1, you can put a different number in here, and then you need to do a save. And before I do the save I want to emphasize that normally the default, when you define multiple pollutants in HYSPLIT, is that each pollutant is emitted on its own particle. So originally we released 20,000 particles for this baseline calculation, but now when we define two pollutants, what will happen is that 10,000 particles will be released on PMCH and 10,000 particles will be released on the pollutant number two. So if we were to do chemical transformation of pollutant one, the PMCH to pollutant number two, they would have to be defined on the same particle, the transformation cannot occur on different particles, because in this Lagrangian computational mode, one particle doesn't really know where any of the other particles are. So unless we were to create a new particle each time step at the location of the original, the one that's being transformed, that would be the only way to do that, but that would also be computationally very inefficient. So what happens when you define a conversion of species one species two, this parameter, this single particle mass dimension is automatically set to two. I

don't have to set it to two, that number here, but it does that automatically. And that tells HYSPLT that for each particle, it can have more than one mass dimension. So we can release 20,000 particles, but each particle that's being released will have two dimensions in the mass index. So regardless of whether I change this number or not, they will be changed automatically to two, because of this conversion rate being set.

Now this type of process, where you are converting from mass on one species to another species, on the same particle, really only works if both of those particles have the same dispersion and transport characteristics. As an example, if a gas were to be transformed to a very large particle, that has a large settling velocity, we can't really treat the dispersion of a gas and a rapidly settling particle on the same computational particle. We would have to have different transport pathways for each one, and each would have to be on its own particle. So this chemical conversion really only works properly when both species have the same transport and dispersion characteristics. So let's save, save, and run model.

I don't know if you noticed, when we started the simulation, it mentioned that simple species conversion was enabled. Now we can do display. Let's call this simply plot_chem, and we can leave everything else alone, and this is now, I should say we are plotting PMCH. If we were to do the same thing for the other species, pollutant two, execute. So let's take a quick look at what we're seeing here. If I were to go back and look at the

numbers that are being plotted, and it's kind of summarized here for you. Let me make this a little smaller. Let's go back to the beginning and this is pollutant two, and you can see we start out with the maximum concentration is 47000, and as we go on in time, it's 47000 again, and then 38000, and so on, 36000, 25000, 15000, 12000, 8000. If you were to go to the original, the PMCH calculation, the one that's being transformed from, go back and generate this one. You can see we start out at 200000, and then 70000, 41000, and so on. The numbers that are defined here in this table are the results that you should be getting for the peak concentrations.

And so in this case, the PMCH is the original, and the pollutant two is one being transformed to. If you had no conversion going on, the pollutant two column would always be zero and we would be getting results similar to the base calculation. And you can see the base calculation with no transformation. And you can see that if you add these two together, you are getting a number that's very similar to the base. So you have a rapid decrease here and it is more rapid than the base case because of the transformation to pollutant number two. While on the pollutant number two side, we have a balance between the reducing concentrations due to dispersion and increasing concentration due to the transformation from PMCH.

Obviously the PMCH does not transform, nor deposit, we're just using this as an example of how to do this

calculation. And the last point I'd like to make is that when we did this calculation, it automatically, the graphical user interface, generates this CHEMRATE.TXT file and that is what HYSPLIT reads, which defines the transformation of pollutant 1 to pollutant 2 at the rate of 10% per hour. And in this case there was no molecular weight correction factor, which was one. You can define multiple lines here and HYSPLIT will process the conversions one record at a time, if you have multiple pollutants defined. And in that situation you would have to go into the menu and define, you would have to define in the name list, the MAXDIM value, which is what we saw in the graphical user interface in the advanced menu in terms of the dimension, on how many mass dimensions are permitted on a single particle. So that number would have to be changed if you're running more than two, and you would have to do that yourself through the menu or through editing the name list file.

So this concludes the discussion of simple transformations.