Now that we've optimized the configuration for the base case, we will go back and look at some of the calculations that are involved that influence the dispersion of the individual particles. However, before we go into that, let's just briefly review the calculation that's involved. Remember that the only difference between the dispersion case and the straight trajectory calculation, that we did in the beginning sections, is that the trajectory calculations use the three dimensional velocity fields from the meteorological data to compute the mean particle trajectory. When we do an air concentration calculation, where we also look at the dispersion of those individual particle trajectories, we are adding an additional turbulent component to the mean trajectory or the mean particle movement. In the case of the three dimensional particle calculation, we are adding a turbulent component to the mean velocity. And that turbulent component was derived from the random number generated by the computer times a turbulent statistic. And the same turbulence statistic was also used to compute the rate of puff growth. So it’s either used for particle dispersion for the 3-D particle calculation or puff growth for the puff calculation. It's the same velocity, turbulent velocity statistic.

So in essence what we want to know is how does the model determine what that turbulence statistic is and those are the turbulence parameterizations. Effectively what needs to be done is that the meteorological model computes mean components for the winds, for temperatures, and various, and the various meteorological

state variables. From those mean state variables, we need to determine what the corresponding turbulence values would be. And there are several computational approaches to address this.

In the first approach, we use the equations from Kanthar-Clayson, where we are explicitly predicting the turbulent velocity in the vertical and the two horizontal directions. And this turbulent velocity is the, is equivalent to the standard deviation, so if you take the square root of this quantity, you get Sigma-W or Sigma-U. What it is is the instantaneous velocity minus the mean velocity squared, square root. And the functional forms that we use are related to the friction velocity, the height above ground, and the depth of the boundary layer. And so you can see that there's an explicit relationship between the three turbulent component velocities. And this is the default method, so if you select no other option then HYSPLIT will use this.

The second approach uses the equations of Beljaars-Holtslag and this is slightly different, in that we are computing a diffusivity for heat, which is based on again height, the depth of the boundary layer, as well as a stability parameter. And the stability parameter is also a function of the friction velocity, which is a measure of the momentum transfer in the atmosphere, the Monin-Obukov length, and the convective velocity scale. And this diffusivity then is converted to a standard deviation of the vertical velocity, this turbulence parameter based on the length of the Lagrangian time scale. The Lagrangian time

scale is the time it takes for the correlation, for the turbulence, to be uncorrelated. In HYSPLIT we typically assume a few hundred seconds for the vertical component and approximately an hour for the horizontal component. And then we assume that the horizontal turbulence, both the U and the V components, are equivalent to the vertical. Note that this implies, this implies equal partition between the vertical and horizontal components. The other approach implies a specific relationship between the horizontal and vertical components. And in the third approach, we can override the partition by assuming a diffusivity in the horizontal that is related to a deformation of the velocity field. So the more the velocity field is deformed, that is the gradients in the north-south, how does the gradient in the north-south velocity change in the east-west direction and so on. The more the deformation the more turbulence is assumed within that grid cell and that can be used to change the partition with the other approaches.

And a fourth approach, which we will discuss in the next section uses the turbulent kinetic energy. So some meteorological models predict turbulent kinetic energy directly and if that field is available, we can use it. So we do not have to explicitly compute W prime, U prime, or V prime, it is actually computed by the model.

The reason for having these different options is that not all meteorological models have the same data available; some will have flux components, some will not. If they have to be computed, then there is less accuracy than if

the flux components were provided as part of the meteorological model output. Normally you don't have to make this decision, HYSPLIT will make the decision for you automatically based upon the data that are available to it. As I mentioned, the default is this Kanthar-Clayson approach, and the reason we're going to go through just the options here is so that you can see the effect on the plume calculation when we just choose these different options. And normally you would not be making these choices except in the context of computing an ensemble, a dispersion ensemble, where would be looking at different realizations by changing the model physics.

So to actually do the calculation using different methods, let's go ahead and open up the set up menu, and we're going use the configuration that we had previously optimized for this aircraft sampling case. And if you're not continuing on from the previous section, let's go ahead and retrieve that, which was called conc_case_control.txt and for the name list file, retrieve conc_case_setup.txt. Okay, save. So normally the menu that you would look at is menu number seven, which configures the turbulence method. And you can see that and in the vertical turbulence, the default is undefined, and by undefined that means there is no selection here, and the model will select the optimum one, with the assumption that the default will be the Kanthar-Clayson. So if I were to save, and this is going to give you the same result as before. And then display, and it case you didn’t delete the display from the last run, make sure you set the map a little bit off to the east. We're going to show just the upper level, 1000

meters, where the aircraft sampling occurred, we're going to have the multiplier to get picograms, and we are going to force the units, at 80%, save, and this should be identical to the result you had in the last section for optimization. Notice the peak being 31,000. We did forget to plot the measured data and that was, as you recall, data_case.txt. We'll see that the next time.

Now as a result of this run, if you look at messages, the name list variable that was set for the turbulence method is KBLT, and we need to find this here, and you can that, it is defaulting to zero, which is undefined. But we do know that once the model configures, the PBL mixing scheme is set to two, which is the Kanthar-Clayson. Now let's explicitly set Kanthar-Clayson, like so, and save, save. Exit, display, and you get the same result, now is the measured data of course. And if we go to the MESSAGE file, we now see KBLT set to two and of course the PBL mixing scheme is still two.

Now let's say we want to try the Beljaars-Holtslag approach, those are questions, advanced, number 7, select this, save, save, run, and display. And you can see that the plume is slightly more narrow and we do have a much higher peak concentration, almost double, so it did have an effect. And if we look at the MESSAGE file, you can see that the KBLT parameter is now set to 1, and the PBL mixing scheme which is essentially the same thing, it's the KBLT parameter, but it is the result of, after the model, when you start HYSPLIT, it evaluates the meteorological data, it may change the mixing scheme.

In this case it was the same.

And the last option, we're going to do the deformation. And we want to do the deformation with the Kanthar-Clayson, so save, save, exit, and display. And now you can see even a more narrow plume. Now we know of course, going in the narrow direction, because we have the answers, is not correct, and that is why the default is the Kanthar-Clayson in this approach. The model will select that. But there're other situations, where some of these different approaches might prove a better solution. It's beyond the scope to go into that at this stage and in fact it is area of an uncertainty as to which approach might be best. In part it depends on the meteorological data that you have, on the particular meteorological circumstances. But the main reason why we were going through this here, is to demonstrate the kind of variability that you might get, and later on when we look at concentration ensembles, selecting different physics options, is one of the ways we generate ensemble members. And in some ways, these are all valid solutions and they have some probability of being the correct solution. So when you do ensembles, this can add to that range of possible answers.

And I would also want to add that when you're doing these kind of configurations, remember the help file is always there and it can provide some discussion as to the options that are available to you, the parameters that are being changed, and there is a place in the User's Guide where it gives you a summary of all the name list variables. So

you can review what the model is doing and what the different options can provide for you in terms of different types of output.

And this concludes.