Normally when we compute air concentrations we compute it as a mass divided by volume, but we can also look at mixing ratios, either volume or mass mixing ratios.

The basic calculation starts with the perfect gas law. So when we started working with the CAPTEX data, we always worked with measured air concentrations and calculated air concentrations that were in grams per cubic meter or picograms per cubic meter for convenience. However, the original that were reported by the laboratory, the analysis laboratory for the experiment, were in volume mixing ratios, that is liters of pollutant per liters of air. For convenience these were converted to concentrations.

The first step in this, as I mentioned, is the perfect gas law. And that tells us that the conversion, the mass to volume conversion, is really just dependent upon the molecular weight of the pollutant, and we are treating it as an ideal gas. That is there are 22.4 L per mole of that gas. And using that conversion, and you can go through the algebra here, this is the gas constant, temperature, and pressure, to get the volume per number of moles. And you can see that to get units of pollutant in grams per cubic meter or mass per cubic meter, we simply take the concentration in volume units times the molecular weight, times the constant here that we determined, this 44.64 moles per cubic meter, that is essentially the inverse of this.

The second step is how to convert concentration, that is the volume mixing ratio, to air concentration. So for instance, using this simple equation that was derived from the perfect gas law, we can just substitute the values for the PMCH tracer. So the tracer concentration in grams per cubic meter, so that is the first term here, this is grams per cubic meter, but we've broken it up into picograms and the conversion factor from grams to picograms equals the pollutant concentration in liters per liter. I'm following again this example here, but in units of femto liters but with the conversion of between liters and femto liters, times the molecular weight of the PMCH, that is 350 grams per mole, times the conversion factor. And we find that to convert from femto liters per liter, which is the unit reported by laboratory to pg/m^3 (picograms per cubic meter) we need to multiply by 15.6. And so this is the same process you would use to convert any of the other tracers that were used that have different molecular weights to g/m^3 or pg/m^3.

Now the option, there is an option in the model to permit you to do some of these conversions automatically. And that is we can divide the output, so before the concentration, normally the concentration would be output in mass per cubic meter, mass per cubic meter of air. However there is an option where we can divide the output concentration or the output concentration by the air density. That is, we divide. If we look at units of kilograms, we divide the kilograms of pollutant for cubic meter of air by the density of air, that is the kilograms of air per cubic meter, that results in a mass mixing ratio of kilograms of pollutant per kilograms of air. And then to get a volume mixing ratio, we rely on the fact that for an ideal gas the liters of the pollutant per mole is the same as the liters of air per mole, so this essentially drops out, and then the only thing that matters is the ratio of the molecule weights between air and the pollutant. That is this ratio. So by multiplying that ratio by the mass concentration, the mass ratio here, we can get the concentration in volume mixing ratio. So we can convert from mass mixing ratio, which is output by HYSPLIT if we set the flag to divide by air density, we can get, converted the output to volume mixing ratio, which is the units that were reported by the laboratories, by simply dividing by the ratios of the molecular weights. So this conversion for the PMCH tracer which has a molecular weight of 350, would simply be the ratio of 29, which is the molecular weight of air, divided by 350, so that's in liters per liter, times a conversion to femto liters. And so to get output in femto liters per liter, if we have concentrations reported in kilograms, that is kilograms per kilogram, that would be the multiplier. If the mass units were grams rather than kilograms, we divide by thousand, and so the final conversion factor would be 8.3×10^{10}.

So this process is really, there are really only two steps of this process, and that is we set the flag and the model output would be in kilograms of pollutant per kilogram of air and then we need to convert the model output to liters per liter by just multiplying by the molecular weight, the ratio of the molecular weight, molecular weight of the air versus the pollutant. And then the rest of the conversions are just to either go from grams to kilograms or femto liters or liters. So I will let you, you can work these numbers through on your own, it might be a bit easier than following this verbally. But the bottom line is this would be the conversion factor that we would use in the example.

So let's go back and recalculate the aircraft example that we have just done previously, or if you don't have it, you can load the configuration. But before, if you are continuing on, we should remove the LAGSET file from the working directory, so that we do not do that again, that is the Lagrangian dynamic sampling. Now you can start by going to set up and if you are not continuing on, you can find the aircraft sampling CONTROL file in the tutorial/files directory, and you should retrieve that, by the way, yes, OK. And you should do the same for the name list. And if you are continuing on you should retrieve the name list because we did make some changes.

And really the only thing that needs to be done is to go to the conversion menu, and we have, and you have the option of dividing the output mass by air density, so that will be summing the mass mixing ratios to get the average mass mixing ratio as the answer. And also we should set maybe the border labels, so that we get something that looks correct. Let’s put PMCH tracer and the mass units will be femto liters and this will be per liter. And we should be able to just, let me just check to make sure that everything else is okay. We are doing a one hour average about this at flight level of 914 meters and we run model.

And notice the message that we are doing this division by air density and then we're going to do the display. And we will look at the 1000 m level and as I mentioned we should have the multiplier here which will take us from kilograms, kilograms per cubic meter, to femto liters per liter, and that was 8.3E+10 and I can leave the label field empty because we are using an over-ride. And let's set the contours to something reasonable, 2000, +1000, +500, +200, +100, and let's execute display.

And you can you can see 2000, 2300 was approximately the peak concentration, in femto liters per liter, and we happen to have the original measured data file. If you look in the CAPTEX report, everything is in femto liters, and that does exist in the CAPTEX directory. We call it, just for this example actually, data_orig; these are the measurements that were made in femto liters. And, so we can plot that by adding that file. So you can see that we are getting the peak of about 2000 near the center region here where the peak was actually measured. And in this would be in the same units, of course, as the original measurements were made.

So the question you might have is well why would I want to do this rather than just doing a single conversion at the end or as we did in many of, or all the other examples, where we actually had converted the native data in femto liters to grams per cubic meter. And the reason is that we are not assuming, when we do this calculation, we are not assuming a fixed density for air. So that the previous conversions were all done using a fixed value for the air density, probably at standard temperature and pressure.

Whereas, in this calculation, you are doing the conversion dynamically, based on what the actual temperature and pressure was at the level that the sample was collected. So it really all depends upon your application. In the CAPTEX application, these data were all converted to a reference temperature and pressure and therefore we can use a single conversion factor. But if you are using uncorrected data, then you may want to use the local values that apply at the measurement time.

This whole discussion goes well beyond the scope of configuring HYSPLIT and has more to do with how observational data are processed for other purposes. And it is best as a user that you need to understand the origins of your data and how they are prepared before you do something with it.

And this concludes the discussion of volume or mass mixing ratios.