

## MITOCW | MITRES\_10\_S95F20\_0104\_300k

PROFESSOR: So let's look at a little more detail at the equilibrium size of respiratory droplets that are emitted during breathing, or coughing, or speaking.

And the key idea is that these droplets are not pure liquid.

As explained in the wells curve, pure droplets that are small enough will shrink completely and evaporate.

However, these droplets contain a significant amount of solutes.

And those solutes, in the case of mucus coming from your lungs or from your vocal cords, your nasal pharynx, are full of proteins and other macromolecules, carbohydrates.

And also there are always in bodily fluids plenty of dissolved salts such as sodium and chloride or calcium or potassium ions.

Also, in saliva, many of these species are present, although it's not quite as thick of a liquid.

And of course, virions as well will find themselves in here, and it also constitutes solutes.

So the idea is that we don't just have a pure liquid.

So there is some initial volume fraction of solute in the liquid.

And in addition to that, most of these liquids -- sorry, the solutes I should say are charged and thus hygroscopic.

What that means is that, of course, the salt, those ions are literally charged species, but also the proteins and other macromolecules that many charge residues and sites along the molecule, which attract water.

And essentially, there is a layer of bound water solvating all of these species I just mentioned, including the virus.

So I'll just sketch that there's lots of bound water, which is surrounding each species, including the virus.

There's essentially a layer of water mostly around these molecules here and other species.

So it's solutes plus the bound water that's coming from solvation of these molecules in liquid.

So that water is pretty firmly attached.

And even if you dry the material, a lot of that water will still be left over.

It takes a significant amount of energy to remove it.

And so if we think that -- if we describe there is initial volume of the droplet  $V_0$ , and a radius  $R_0$ , so let's say it's initially a circular droplet, there is an initial amount of solid,  $V_s$ , which is  $\phi_s^0$  times  $V_0$ .

So there's a certain amount of solutes in there which cannot be removed.

So the water can evaporate, but the solutes will not.

So let's think a little bit about what the consequences of that are.

So let me do a brief derivation here for looking at the thermodynamics of this system.

And the key idea is just to get to the final result.

I don't want to dwell on the details of thermodynamics.

But an important concept here is the relative humidity of the air.

So there's moisture in the air.

There's water vapor.

And it's at a certain level.

So we often write that  $\rho_h$  for relative humidity.

And that can be defined as the concentration of vapor, water vapor in the air relative to the vapor concentration that would be in equilibrium with pure liquid.

So when the concentration water vapor gets high enough, eventually you start to nucleate water droplets.

And you start to have condensation water.

That's essentially how rain forms from the clouds.

So that's that ratio.

So relative humidity is telling you how close you are to basically having, water liquid water come out of the air.

OK, now, the relative humidity also tells us something about how far you are from that phase transition point.

And there's a very simple approximation.

I'll put approximate here.

We can also write that this is -- scales with, and is -- can be in fact close to the liquid volume fraction in equilibrium inside the drop.

So that'll be the water volume fraction of water liquid inside the droplet.

At least you can see here in this relationship when this volume fraction is one -- in other words, we have pure water -- then the relative humidity is 100%.

OK, and on the other hand, when you have, let's say, only 50% water, over here, that's like having relative humidity 50%.

This can be derived by more careful consideration of the ideal entropy of mixing where essentially this term here is take into account the excluded volume and the fact that all the sites in this droplet are not available for the water.

So they're being excluded by all the solutes and the bound water that are present.

And similarly, we have a buildup of free energy in the bulk as well.

So basically, this comes from some thermodynamic considerations of equilibrium between water vapor and water liquid.

We can write this as 1 minus the volume fraction in equilibrium of the solid.

OK, now the thing is that we can now write this.

So if we multiply through, we can write this as  $1 - RH$  -- so what is the volume -- so when we get to equilibrium, this droplet is going to change its shape.

It's going to reach a new shape, which we're going to calculate our new volume,  $V_{\text{equilibrium}}$ .

And so what this would be  $V_{\text{solid}}$ , which is  $\phi_s^0 V_0$  divided by  $V_{\text{equilibrium}}$ .

So it's going to be new volume,  $V_{\text{equilibrium}}$ , which will be achieved then.

And then we'll end up with the equilibrium volume fraction.

So if I take these equations here, and I solve, I get a fundamental result, which is that the equilibrium volume of the droplet relative to the initial volume is equal to, well, we have put this on the other side.

That'll be  $(1 - RH)$ .

And we divide that out.

And we find that it's the initial volume fractions solutes divided by  $(1 - RH)$ .

That is our key result. And let's plot what this looks like.

So if we plot the relative humidity on the horizontal axis, from 0 to 100%, so at 100%, the water vapor is saturating the air.

And you would start to nucleate and condensed water liquid from that.

At 0, the air is completely dry.

And there is essentially no water vapor present.

So that's the range.

And typical comfortable rooms have a relative humidity around 50%.

This is a typical number.

And let's plot on this axis the equilibrium volume.

It could also be the equilibrium radius because I should say that if there are spheres, that this is also equal to  $R_{\text{equilibrium}}$  divided by  $(R_0)^3$ .

So I can also take a cube root of this.

And I would have the ratio of radii.

So we would know if we started a certain radius, what's the final radius.

OK, so we can talk about volume.

We can talk about radius.

So here is the initial size of the drop.

And somewhere down here is  $V_s$ , which is the solute volume, which is  $\phi_s^0 V_0$ .

Now what is this value?

It depends on the kind of liquid.

So saliva is mostly water with some salt and a few other molecules.

But in saliva, the volume fraction  $\phi_s^0$  is 0.5% in saliva.

OK, so that's just gives you a sense.

So this is quite far down, right?

But then, if you look in mucus, it depends which mucus you're talking about.

But the mucus that comes from the lungs or from the pharynx, it can vary.

But what has also been measured in droplets that are emitted by breathing is that this can range anywhere from 5% to 10%.

So a fairly significant amount of the volume of the droplet is containing all these molecules and the bound water around that.

Now we know that because mucus is very sticky.

It's a non-Newtonian fluid.

It doesn't maintain a nice round shape even.

It can have a regular shape.

It flows slowly.

It has a high viscosity.

And that's because it has a large amount of these hygroscopic solutes.

So mucus might be a little bit higher up.

But in any case, what you then find is we can sketch different regions of this plot now.

So this curve this formula drive here, when the relative humidity is zero, we start here.

So that's saying when there's no water in the air, you completely dry the droplet.

And you're left just with the molecules, the solid molecules, and possibly the bound water around it, depending on how dry the air actually is.

And then it rises up and blows up at 100%.

So when you get to 100%, then droplets are getting really large.

And if you actually hit 100%, then you can't really speak of an equilibrium size because you'll just start to get lots and lots of water.

So that's that limit.

And so now we can look at three different regimes of the kinds of droplets that we'd expect to see.

So down here at 0% or close to zero, we have a dried droplet nuclei as they're called in the public health field.

These respiratory aerosols, if they completely dry out, and you're left with just these solutes, then that's called a droplet nucleus.

So it doesn't necessarily mean it's a nucleus for phase transformation as we use that term in, say, engineering or in physics.

But it's really just refers to the core of just the hydrated solutes.

So if I could sketch what that looks like, that would be-- for example, all those molecules I just sketched there might be condensed into some little blob, which, by the way, could include a virion.

In fact, it could even be just one virion if that were all that were in there.

And you would have a little bit of bound water around it.

But you essentially have a dried up blob of just the solutes.

OK, and so that -- and then, of course, the smallest volume you can get is just the initial solute volume that you started with, plus the bound water.

On the other end, if we are near 100% relative humidity, then the fact that these are hygroscopic solutes, which like to have water near them, will form as a nucleation site to actually cause more and more water to grow and be absorbed into this droplet.

And not only do the droplets not shrink, as predicted by the Wells curve for a pure liquid, but they can actually grow.

So if the size here is small enough to begin with, let's say it were a several-micron droplet to begin with, but it contains a lot of solutes, and we're at very high humidity, actually the particle can grow.

So over here, we could end up with an even larger droplet than we started with where now because the humidity is so high, and we have the same number of molecules in there that I sketched before, that's more dilute now.

And there's maybe a virus or a virion here and there.

And of course, there's also some salt.

But basically, the droplet is growing.

So here we have hygroscopic growth and also we have what's called deliquescence, which refers to water that's absorbing around these salt molecules and even causing some other molecules or charges on these macromolecules to dissolve into solution because it's more and more water present and it can solvate more species.

And so whereas hygroscopic growth refers to water being absorbed into a more solid-like framework, you can also be generating more aqueous solution, which is deliquescence.

So basically, the droplet can actually grow.

And that would be like when you're here, let's just say.

And this might be when you're here.

And then, of course, when you're at 50% relative humidity, you can see the droplet has shrunken but not all the way down to the initial solute volume fraction, but something larger.

And in fact, if the relative humidity is 50%, you end up at exactly twice the solid volume fraction.

So if the solid volume fraction of mucus is 10%, you may end up with a droplet that is maybe 20% of the volume.

So maybe it looks something like this.

OK, and so we have a little bit of shrinking going on.

And maybe there's even a virus in there as well.

But there is still plenty of water.

And so you can see also now the value of having solutes in mucus in terms of making the virions more viable and more easily transmittable because they hold onto the water.

So that the virion is in a stable environment.

So that when it ends up being inhaled into someone else's lungs that it can then more easily diffuse out of that region and infect the host cells.

In contrast, if you have a nearly pure liquid that the virion is in, let's say pure water or even saliva, which is actually mostly water, then the droplet will shrink by a factor of 100.

And it might be just literally a virion with a [couple of ions] just enveloped with a tiny bit of water.

And maybe that, in some cases, would be not as viable of a situation for the virions.

So basically the mucus fragments are likely to be the more common source of the aerosols that will stay in the air and remain infectious.