PROFESSOR: So, as an aside for more advanced students, let's try to fill in some mathematical details to provide a theory to support or interpret the Lin-Marr hypothesis of disinfection kinetics having to do with the concentration of solutes during drying and their effect on deactivating viruses.

So, to put it in mathematical terms, if we have a certain number of viruses Nv in a droplet, then we'll postulate that d Nv dt is minus lambda v0, the deactivation rate per solute virion collision, times the volume fraction of disinfecting solutes we'll call phi d, which is time dependent, having to do with the size of the droplet, times Nv.

The volume fraction of disinfecting solutes we'll write as alpha D, a constant, times phi s, which is the total volume fraction of solutes present.

And that might be, for example, the fraction of solutes that are sodium chloride or some other salt that might be causing the damage to the virus, as opposed to the mucins or other macromolecules that may be present.

Then we can-- as the droplet is shrinking with a radius R of t, then it's simply the volume of phi s that is getting re-scaled relative to the initial value, phi 0, as R0, the initial radius, divided by R of t cubed.

So that's just simply the changing of the volume.

Now let's recall some of our results from the past earlier part of this chapter having to do with Wells' theory of evaporation.

So, if we consider diffusion-limited droplets, we've shown that the radius of the droplet versus time relative to the initial radius R0 is square root of 1 minus t over tau e, where tau e is the evaporation time, R0 squared divided by d bar, a constant with units of diffusivity, times 1 minus RH, the relative humidity.

Now that predicts pure liquid droplets that shrink all the way to nothing and evaporate away, but, when there's solute present, there's a cutoff, which we've also discussed that gives you an equilibrium stable size of the drop, R equilibrium, relative to R0, which is given by phi s0, the solid volume fraction-- or solute volume fraction initially divided by 1 minus RH raised to the 1/3 power.

By writing that as square root of 1 minus tau over tau e, we can also define the time tau when you reach the equilibrium size by a diffusion-limited evaporation process.

So that's sort of the time to form a stable droplet nucleus.

Now let's start combining all these equations, and we can write what is the volume fraction of disinfecting solutes, phi d of t.

Well, from this equation here, it'll be alpha d times phi s of t, which is phi s0, times this ratio, R0 over R cubed.

So, using this expression for diffusion-limited kinetics, this would give me a 1 minus t over tau e to the 3/2.

And, if we look at the ultimate limit here that they'll get from when it's a solute, when tau goes-- or when t goes to tau, the evaporation time, so when you've reached the droplet nucleus stage, we're left with just alpha d times 1 minus RH.

So that tells us sort of the fraction of solutes which are present as a function of relative humidity, but, also, as a function of time, as drying is going on.

So now let's go back to this dynamical equation.

And let's go ahead and solve it.

So this is a first-order, separable-order differential equation.

So what we can do is write this as minus d Nv over lambda v0.

Nv is equal to phi d of t dt.

So we've put all the N's on one side and the t's on the other side.

And so we can actually then integrate this equation.

And so the integral of dN over N is the natural log of N.

So we can write this as minus 1 over lambda v0 natural log of Nv over Nv0, which is the initial value of Nv.

And, in time, we're integrating from the initial time 0 up to the droplet nucleus time tau of phi d of t dt.

So, substituting our expression right here, we then see that we have alpha d phi s0 times the integral from 0 to tau dt over 1 minus t over tau e to the 3/2.

And we can do that integral and get alpha d phi s0.

And then let's see.

To get the integration variable, we need to have a tau e here and write that as dt over tau e.

And, doing the integral, we would get 2 times 1 over square root of 1 minus tau over tau e minus 1, evaluating at the two limits of integration, taking into account the integral of the-- antiderivative of integrand there is 1 over 1 minus t over tau e to the 1/2 power times 2.

So, putting all this together then, we can write the viability.

So we can write the log of Nv over Nv0 as minus-- we have all this stuff here-- 2 alpha d phi s0 lambda v0, putting the lambda v0 back on the other side with the minus sign.

And then we have times two factors.

So, first, there's the factor, which we know has units of time, which is R0 squared over d bar.

So that's, essentially, kind of a water vapor diffusion time that comes into the evaporation time, tau e.

So that sets the timescale here.

But then what we're really interested in is the relative humidity effect.

So that would be-- let's see here.

So we have this factor, and then we also have the-- let's see.

The 1 minus RH is coming in where?

Sorry, so, 1 over square root of tau, this one is from right here.

That's R over R of tau.

And R of tau is, by definition, R equilibrium.

So it's this factor here.

So we get 1 minus RH over phi s0 to the 1/3 minus 1.

And then we also have this factor of 1 minus RH that comes, yes, from the tau e because the tau e has this sort of basic timescale, but there's also a factor of 1 minus RH that I've included.

So the point of all this theory was to try to understand what is the dependence on relative humidity, which is what I've shown here in white.

And, if you plot this function, then what you find is a function of relative humidity.

Then, if you do here log of Nv over Nv0-- so this is our relative viability of the virus, and the 0 here corresponds to Nv0, the initial-- then, this white function, what this looks like is something, which decays like this.

It kind of reaches a minimum around 80 or in this range from sort of 60 to 80, depending on what the values of this parameter phi s0 is in fact.

And then it goes back up again.

So, basically, we get a shape for the dependence of the relative humanity that nicely matches the experimental data and is consistent with the hypothesis of disinfection kinetics that was postulated by Lin and Marr.