>>Jackie: Hi, everyone. Welcome and thank you for joining us today for the Membrane Topology and Morphology for Fouling Control Webinar as part of the NAWI webinar series. Before we get started today, I am going to just go over a few quick housekeeping items related to WebEx – the platform we're using today. This webinar is being recorded and a recording will be made available afterward on the NAWI website. If you have any questions during today's presentation or at the end, we will have a Q&A session at the very end of the presentation.

You can submit any questions through the Q&A box in your WebEx panel – should be at the bottom of your screen, likely the bottom right. Please, note that there is both a Q&A panel and a chat panel. We ask that you submit all questions through the Q&A panel so we don't miss anything. If you have any technical difficulties during today's webinar, you can also let us know through that Q&A portal and we'll do our best to help you get those resolved. With that, I'd like to hand things over to the deputy task area lead for modeling and simulation. Deb, are you there?

>>Deb: I am. Thank you so much, Jackie. So, I'm Deb Agarwal from Berkley Lab. Did you want to say something else, Jackie?

>>Jackie: No. I think with that, we're good for you to go ahead and introduce today's speaker.

>>Deb: Okay. I want to thank everybody for joining this webinar. We've got a wonderful speaker today – Doctor Battiato. Oh. Sorry. I butchered that.

Ilenia, you're gonna have to forgive me on that one. So, she's got a background in physics, in engineering, in computational science, and did her Ph.D. at San Diego – University of California San Diego. She's done her postdoctoral training in physics at the Max Planck Institute in Germany, and she's also been in the mechanical engineering department at Clemson and San Diego State, and she is now at Stanford University in the Energy Resources Engineering Department, and her research interests lie in theoretical computational fluid mechanics and transport processes in porous, medium, multiscale, and hybrid computational methods, effective medium theories, and multiphase flows. And before I turn it over to Ilenia to give her talk, I want to also remind folks that the next seminar – NAWI seminar – that's about modeling and simulation will be in a month on May 3rd at the same time, and that will be Erin Wilson of Idaho National Labs, and that will be speaking about a speciation-based solution model emerging from solvent driven aqueous separations. I'll remind you of that at the end as well, but I just wanted to also put that up front in case people leave early. So, with that, I'd like to turn it over to Doctor Ilenia.

>>Ilenia: Okay. Thank you, Deb. Thank you for the introduction. And yeah, you didn't butcher my name. It's okay. So, I just want to make sure you can see my screen just fine.

[Crosstalk]

So, if I – okay. So, first of all, thank you very much for the opportunity to speak at the seminar, and today, I'm going to present some work that we have done sometimes a few years ago under a different funding. It was NSF funding and now, we are using, actually, some of the tools developed in that specific project to further enhance our working membranes in the context of NAWI. So, here, I'm going to talk about rough or wiggly membrane topology and morphology for fouling control.

I'm going to go fast in the intro so that we can possibly spend more time on the technical part. I do not have to define to this audience that water availability – equitable availability and access to potable water – is key to development, however, we know that there is too little and too soon.

We see on the left the blue planet, but then, if you essentially kind of collect all this water in three different bubbles – can you see my pointer? Yes? No? Maybe?

>>Deb: Yes.

>>Jackie: Yes.

>>Ilenia: Thanks. So, then, you know, what you would see here is that this large sphere is all the water in the ocean – ice caps, lakes, river, groundwater and so on and so forth – even in the water you _____ your dog and your tomato plants. In the middle sphere, it's the liquid freshwater – so, groundwater, lakes, and swamp water, and rivers – and then, in this super tiny bubble is water in lakes and rivers.

So, it's immediately obvious that a lot of water is in the oceans and this is just a quantitative assessment of that very trivial observation, and therefore, one clear way to be able to access and to provide more potable water is through desalination.

So, now, this is a pie diagram of different techniques that I used in desalination and we see that reverse osmosis membrane has a good share in terms of water potabilization.

So, what is reverse osmosis? So, generally speaking, it's a process by which if you put a semi-permeable membrane and you technically push really hard, then the pores of this membrane are so small that essentially, the solid dissolve in the water will be stuck on one side of the membrane while the water molecule will go through. And this is just a picture that shows actually how small these pores in these membranes are. In the back, you see a red blood cell that is in the characteristic size of six micron and the reverse osmosis membrane pore – and this is not in scale – it's essentially three orders of magnitude smaller. In the middle, you see just the size of a bacteria.

So, quickly, what is osmosis? Well, if again we have two solutions – one concentrated solution – you have solvent – let's say water and then salt, and then, on the other side, we have a less concentrated solution. And if you put a semi permeable blend where the membrane is essentially permeable to water but not to the salt, then the system will try to reach equilibrium – so, to reach equal concentration on both sides. But since the

membrane is semipermeable just to the water molecule, then, what you're gonna observe is the flux of solvent from the left to the right. Now, in reverse osmosis, the process is essentially the opposite.

You practically apply a force – you push really hard – to really reverse the process and to take the system completely out of equilibrium. So, you want, essentially, to create a highly concentrated solution on one side and then, freshwater on the other side. And you can imagine that this will require a good amount of energy to be applied to the system to keep it out of equilibrium.

And so, one common problem with reverse osmosis membrane but also other types of separation processes is fouling.

This is just a quick schematics of how fouling works. Again, it's very intuitive. We are now looking at the membrane from the top. At the bottom, here, we have wastewater so, it's the feed side – the dirty water – which we want to purify. If you push this water – this feed water – parallel to the membrane, then you would have permeate flux _____ to the membrane surface.

And you know, if the membrane is clean, then, of course, you would have a clean water flux that then you would collect and you know, put somewhere. But then, the problem is that since – again, the feed side is loaded with salt or other substances. Then, in the process of generating a clean water flux, then you would build some foulant on the membrane which would lead to a local impairment of oxide. So, you hear that the arrow is a little bit smaller and so, whatever the membrane has cleaned, then you can still reach the maximum flux, but where the membrane if foul then, of course, you can achieve complete – like, full clogging, right? And so, the problems associated with foulant are twofold and they're kind of – the face to face of a coin.

On one hand, it creates immediately permeable flux impairment – so, it decreases the permeate flux that you can potentially have from an otherwise clean membrane, but at the same time, increase in energy input. So, if you want to, again, push through the same amount of water, you can possibly still can, but you have to operate system at a much higher pressure, which means that you are increasing energy input, and the increasing energy is in the use of the operation of these systems, of course – it's something that you would like to avoid both for financial reasons, but also for really environmental reasons, right?

And so, the question of controlling fouling is an old question and there is no single answer. And the reason that there is no single answer is because the system is multi-scale, as it is outlined here – and you can literally try to affect the outcome at different scales. So, you know, we can operate at the chemical level where, essentially, we would like – where potentially, you could modify the interaction force between the membrane and the foulant – the foulant molecule – at the nanoscale, right? Or you could try to do modifications on the surface of the membrane – so, for example, patterning it in some

way or form. And this – we will refer to this type of treatment as topological modification, topological alteration of a membrane.

So, this type of alterations are at the micron millimeter scale, but then, you can also do it at a much larger scale – for example, by looking at the separator. You can do modification of membrane shape or separator morphology at the system scale, which is at the centimeter scale.

And so, when people – you know, engineers or scientists – try to alter the system – an engineering system performance, they – the first place they look for inspiration is generally nature. And so, if we think about topological modification of a membrane to, again, alterate microscopic properties, then the immediate thing that comes to mind is the lotus leaf, where you can see that by it changing the pattern of the surface of this material, you can alterate wettability. And this is a clear implication for the membranes, because ultimately, you would really like things to stick less, right?

And so, this, in other context, has been done. There has been, you know, in the past 20 years, a lot of studies in how to pattern surfaces to achieve different surface properties that are desirable. These are applications to drive reduction in laminar and turbulent flows, but some similar studies have actually been performed in the context of membranes where certain membranes were actually fabricated with some micro patterns on top, and it was observed that, in fact, under certain conditions, you could decrease fouling. And this is just one of the studies that are available. There are many more.

Another possibility's again, to alter the spacer – morphology. So, it's that, let's say, of having membrane channels that are classic or rectangular shape, one question could be, "Okay. What if we do morphological modifications of the spacers such that the morphology of the channel changes on a much larger scale, like the meandering of a river?"

And so, also, this has been investigated and some benefits have been observed – and here, I provide the reference.

Now, the question that we started asking actually emerged from the fact that there didn't seem to be an overall agreement of when and what technique would be helpful in fouling. So, certain studies reported very clear advantages by doing given modifications, but other studies did not seem to necessarily agree on that conclusion. And so, what really – what we started wondering was, "Okay. How do we do – does this depend on dynamic condition?" So, yes, we can do morphological or topological modifications, but does the performance of this type of modification actually depend on the dynamic conditions in which we operate the system?

And if that's the case, how can we formulate a problem in a way that is holistic and that can allow us to assess, in the same framework, whether it's best to do, let's say, rough or wiggly? And so, the general question was, "Okay. How do we, essentially, create a framework that allows us to evaluate the structure – structural changes – either

morphological or topological – at different scales and evaluate them at the macroscopic scale in a fair way?"

And so, there are different approaches. Of course, the classic approach is to do trial and error. You come up with a design, you fabricate it, you run experiments, you record your results, and then, you go through an iteration schemes and then, based on your knowledge, experience, intuition, you design something new and then, try to see whether the performance is better or not. And so, the advantage of this approach is that it's true, which is something that should definitely not be underestimated, and it's fun, but the drawback is that it is expensive because you need to have a person there doing these experiments. So, it's an investment of human capital but, at the same time, it's also slow converging because the iterations are always just – and actually possibly different from the previous one.

And technically, you have a much higher chance of converging to a local optimum rather to a global optimum, depending on where you start, right?

So, the other approach is to use computational tools, right? And the clear advantage is that it allows you to span larger parameter space automatically. You don't have to have a person look at the screen while the simulations run. The drawback is that it can become computationally expensive in then it requires experimental validation. In our case, we really did not have a choice because we are not experimentalists, and so we kind of move towards the second option, and we – immediately, it was obvious to us that there were a number of challenges that had to be addressed for us to think about the problem in a way that was meaningful.

So, first of all, we needed to account for full coupling of flow, solute bulk transport and foulant surface concentration. We had to account for all dynamical feedbacks between these three different physical processes, and so, the coupling couldn't be just one way, but it had to be a two-way coupling between these processes. We wanted to predict system-level quantities – pressure drop and permeate flux – because these are the quantities that then we can use for validation against experiments, but we also wanted to try to predict the spatio-temporal evolution of the fouling pattern and try to do that we or no fitting parameters with a kind of underlying scientific hypothesis in our group that if you got the physics right, then you shouldn't be spending a lot of time calibrating the model once you got your parameters right.

And these predictions, in different conditions, should be essentially parameter free. And so, there are a number of models that have been developed and I'm just gonna broadly talk about two categories. So, there are approaches that include the modeling of flow, solute, and fouling. The advantage is that, you know, they do couple flow and transport, right? So, you do you have full coupling, but often times, the fouling is just modeled in terms of concentration, polarization, not as a surface concentration – so, not as a different quantity than concentration polarization. So, generally, the idea in these models is that if we can get a very accurate distribution of the concentration field in the bulk and we can properly represent concentration polarization, then we would be able to know roughly

where fouling is, because they're strongly correlated, right? But we do not technically distinguish between them. Other approaches have looked actually at modeling fouling separately and as a surface concentration, but the approach was simplified in terms of removing the coupling between these physical systems, which can be a challenge, especially in the presence of hynolinear systems like the one we are looking at.

And so, what we proposed was a model where really, our primary objective was to retain the temporal dependance – so, just looking at steady state configuration, but really looking at the full evolution of the flow field and the fouling field. We wanted to see where the fouling started initiating, because that can be used – this knowledge can be used for design. And then, our primary interest was to separately model surface concentration for the foulant and bulk concentration for concentration polarization and account for the full coupling between the hydrodynamics and the foulant onset. In particular, we wanted to model what – the picture that I showed you before – where you have full feedback between the deposition of the fouling at a certain location and a concurrent decrease of the flux because of, essentially, clogging or because of this layering effect. And so, what we did was we just used the _____ equation to model the flow field, then, a standard _____ diffusion equation to model the bulk concentration, and then, essentially, the way we propose to model this coupling between hydrodynamics, bulk transport, and surface concentration was through the boundary condition on the membrane.

So, I would like to emphasize that in our model, the membrane represents the boundary, but it also represents the location where the coupling between all these physics occur. In particular, this is the boundary condition that we propose so, this is the flux – the permeate flux. This is the class osmotic term that you would have and drive the flow through the membrane. But then, we have kind of a penalty term that is related to the local surface concentration of the foulant. So, if you increase the surface concentration in the foulant locally, you are essentially decreasing the volume, the flux.

But changing the flux – that changes the boundary conditions for the flow field. And so, that's how the feedback loop is implemented. And then – I mean, these are classical equations that I've – boundary conditions that is generally used to , you know, model again the flux through the membrane in terms of the bulk concentration, and then, to model the kinetics of the foulant accumulation on the membrane. And so, in this model, essentially, as I briefly mentioned, we account for time evolution. We account for full coupling through that additional term in the boundary condition for the permeate flux that allows us to explicitly distinguish concentration polarization from surface concentration of foulant.

So, it fully couples the flow field, concentration, foulant deposition, and it links the flux reduction with foulant accumulation on the membrane. So, the quantities of interest that we looked at were, first of all, the definition of what a non-foulant membrane surface is. And so, the way we define it numerically is the location on the membrane where the concentration – the surface concentration of the foulant is thresholded according to a given criteria, okay? So, if surface concentration is lower than some kind of value, then

we consider that non-fouled. And then, based on this definition, we can define the permeate flux as – the total permeate flux – as just the surface integral on the membrane surface that is not fouled, and then, of course, we have a pressure drop in the channel, which is the driving force.

The first thing that we did was to essentially validate the model. We did it by using an unsteady measure from previously published work and fouling patterns. So, here, you see the experimental measurements of the dots and then, the solid line is the prediction. Here, you see, in red – well, whatever color this is – anyway – magenta, maybe – okay. I'm not colorblind.

So, this, with the numerical simulation. So, we were able to capture both the temporal dynamics of a very pretty long-time scale, temporal scale, and the spatial dynamics in steady state.

So, we started with looking – we wanted also to validate the fouling pattern. That was one of the critical parts we were interested in so, we went back to the study that was previously published by another group and what we did – they provided pictures of the fouling.

We extracted the geometry of each spacer and then, essentially, what we did – we run the simulations and then, we did the comparison in this pressure drop flux type of diagram where the experiments are the black symbols, and these are the measuring errors. And then, our numerical simulation is really the corresponding symbol, but in red. So, we were pretty happy with these predictions as well. So, then, in terms of global measurement, we did well.

The question was – could we predict, actually, the fouling pattern? So, what we did was to first proceed with image processing of the images – of the experimental images that were given to us for this different fouling pattern. The R1 is essentially the rectangular classical shape of a channel. Then, what we did was to convert this image into a grayscale to extract, essentially – to correlate intensity – color intensity – to surface concentration and then, by thresholding it, we obtain this fouling pattern for different morphologies. And then, we compared the data and the model.

So, the data are the red plots while the model predictions are the blue plots, and you see that we can actually capture these isometric tales in these fouling patterns and the peaks and drops of these wiggly channels. So, so far so good.

But still, though, we absolutely had no idea how to assess the performance of – concurrently – of membrane topological and morphological modifications within the same framework. So, how do we know when one is better than the other, they're both equally good? How do we make an assessment that it's good for design and engineering these membranes in real systems? And so, what we understood it was needed was a couple of things. So, we need shared quantities to optimize and then, a shared design and decision variables.

And so, we took a step back and we said, "Okay. Let's go back and let's look at the straight channel case and let's start to build – to define dimensionless numbers that can help understand what are common parameters, regardless of what type of modifications you can make." And so, first of all, we needed something related to the performance of the membranes and so, we know that permeate flux is one of the critical elements to assess performance, but also pressure drop. And so, we define two dimensionless numbers – the Sherwood and the Bejam number, which are corresponding the non-dimensional counterpart of the total permeate flux and the total pressure drop. So, technically, we would like to maximize – for each configuration, we would like to maximize the Sherwood number and minimize the Bejam number.

And then, of course, there are expected dimensionless numbers like the Reynolds Number, Peclet Number, the Darcy Number, and the _____ number that represent the reactivity – you know, these absorption reactions that control the dynamics of the foulant accumulation.

So, then, if you non-dimensionalize your system, you get what you get and then, we started looking, actually, and it was still too complex so, we could understand nearly anything and so, we said, "Okay. Let's try to see what happens in the long-time scaling limit."

And what we wanted to do is to identify the relationship between pressure drop and permeate flux when the system reached equilibrium in the long-time limit. And so, we wanted to essentially calculate some function like this, right? And we actually were able to derive this analytically in this limit, and the tool – the derivations are in the paper, but what really matters are like, two main points. At steady state, what we saw is that the chevron number can be written as a function of Bejam number only plus all these other dimensionless numbers that are intrinsic represent – that are fixed, right? They don't depend on operation conditions.

It's the geometry or the permeability of the membranes and stuff like this. But then, the other important point was essentially that there was somebody missing from this. We would have expected an explicit dependance on Reynolds number, but we didn't find it. And so, that suggested to us that maybe Bejam and Sherwood number had the same scaling in terms of Reynolds number and that is why it is up from this derivation.

So, once you have an analytical solution now, you can look at a lot of different things and so, we started actually looking at asymptotic behavior of the Sherwood number in terms of the Bejam number for different values of the Bejam number – so, the two classical limit. What happens if Bejam goes to zero? What happens if Bejam goes to zero? What happens if Bejam goes to infinity? And so, what we found is that two limits actually are different and then – so, we know, essentially, how the Sherwood number scales.

And the reason why this scaling is important is because now, we can use this scaling to actually try to understand how this overall filtration performance index scales, right? So,

what we did was to define this filtration performance index as a ratio between the Sherwood and Bejam. It includes, again, these two factors that we care about – membrane permeate flux and the pressure drop – and, by knowing the individual scaling of this Sherwood number as a function of Bejam number, we could know the scaling of this performance index, which is ultimately what we would like to maximize.

And so, this is just how the scaling of this performance index looks like for different values of the Bejam number, and this is just the plot so, there is nothing there.

So, now that we have that, we start having like, a little bit of a context in which to analyze these different morphologies, right? So, first of all, what we wanted to do was to validate that analytical scaling that we had found, right? Because if the analytical scaling is correct, then we could use – literally use the performance index in these representation in terms of Bejam and Sherwood number as a common ground to analyze membranes with different modifications at different scales. And so, what we did was to essentially develop synthetic examples. So, we looked at morphological modifications – so, wiggliness; membranes with wiggly channels – 10 different configurations where the M0 is the straight channel.

So, the M type of modification is the morphological modification – the wiggly one – then, we considered three topological modifications – so, where we have pattern to the surface of the membrane with pillars of different sizes and heights and stuff like that. We considered three modifications where the pillars are aligned and three modifications where the pillars are staggered, and then, we considered three hybrid patterns where we combine both morphological and topological modifications.

And so, we started running simulations. This just shows how the surface concentration of the foulant looks like so you can start guessing where the foulant is going to start accumulating these different configurations.

And so, some observations that I would like to make before we proceed is that the previous analysis provides like, a first step, although still incomplete framework to study membrane performance. And why is that? Why it is? So, it is useful because we have, somehow, a way to – we have a shared objective, which is this membrane performance index, but still, we have an issue. In presence of topological or morphological alterations of the membranes, additional length scales are introducing the problem.

And in our dimensionless numbers – so far defined – we have absolutely, whatsoever, accounted for this aspect, which is the most important thing, right? And since the input velocity and the length scales associated with the membrane alteration are the primary decision value – because the input velocity's the operation condition – and the length scales are essentially the design characteristic of our membrane, we wanted an explicit dependance of the filtration performance index E on the Reynolds number, and this Reynolds number had, somehow, to include these additional length scales that could allow for morphological and topological modifications.

And so, that's what we did. We kind of defined – out of a hat, practically – these dimensionless scales. So, this ratio – I'm going to go back just to the figure that shows the geometry.

So, the first ratio is the ratio between the shortest distance between the sides of the membrane with essentially – with this inlet distance, and then, the second is just the depth of the membrane minus *H* side the height of these features – of these topological features. So, this is some kind of dimensionless numbers that allows us to describe the topological pattern, right? So, we see that there is no topological alteration. H* is equal to zero and this is equal to one. So, this value can change between zero and one. So, once we define that these length scales associated with these alterations of different scales, then we essentially redefine the dimensionless Reynolds number as a rescaled classical Reynolds number where we included these length scales, okay? And then, we essentially checked whether this plotting data against this Reynolds number could tell us a little bit more.

So, here, I'm plotting again the Sherwood number, which is the dimensionless permeate flux, and the Bejam number, which is the dimensionless pressure drop, as a function – so, in the inset, there's a function of the classical Reynolds number, and this is for all the geometry. So, what you see is that if I plot it against the classical Reynolds number without accounting for any of these scales, all the data are scattered – so, not useful. But if we use now this rescaled Reynolds number, at least in some regions, it's for some values of the Reynolds number, I get a collapse. So, I can actually infer the scaling between this Sherwood number and these dimensionless – these Reynolds*. And the same happens for the Bejam number.

We also see that our hypothesis – that the reason why, in an analytical solution, there was no explicit dependance of Sherwood number and Bejam number because their scaling was the same with the Reynolds number seems to be true. So, they both scales with Reynolds square.

So, once we have that, we actually validate our analytical scaling with whatever the numerics tell us, and what we see here is that this is the analytical scaling that we found, and these have the numerical simulation. So, what we see is that the analytical scaling that we derived is actually accurate of a certain value of the Bejam number. Now that we have confirmed this scaling, we can now do what we really care about, which is actually try to understand this dimensionless performance index in terms of this Reynolds number for all different geometries, right – topological and morphological modifications.

So, I would like to emphasize that where we are here – it's we did what I, in the beginning, said was the problem, right? So, we needed a shared optimization target, which is now this index performing index, and then, we needed a shared parameter, right? And this one now is a shared optimization parameter – design parameter – because now, this include both topological and morphological modifications. So, it allows us to evaluate different things in the same framework.

So, with this, essentially, what we did – sorry; these are all the simulations together. What we did – we extracted the best performer for each category at each Reynolds number and then, essentially, we came up with this plot.

So, again, this is a plot of the dimensionless performing index as a function of this rescaled Reynolds number. So, the blue – dark blue represents the "do nothing" option. So, this is the straight channel without any type of modification. The middle blue is morphological challenges – so, where we do the wiggly channel – and then, the light blue is the topological modification – so, where we add roughness – engineered roughness – to the membrane. And so, what we see is that we have actually three different regions.

The first region to the left – for lower Reynolds number – shows that the best performer between morphological and topological modifications of the membrane is actually wiggliness. So, if you do wiggly channel, globally, you gain – sorry – globally, you gain – both in terms of pressure – of decreased pressure drop and increased permeate flux. Instead, the topological modification actually is worse than do nothing option, and the explanation is actually quite simple. Imagine that you have very low Reynolds number – so, very slow flow, right? So, everything is very viscous.

Then, you have a lot of shear stress, right? So, essentially, all the pressure drop comes from the shear stress. But then, you essentially – by adding bumps to the surface, you are increasing the surface and so, you are dramatically increasing the shear stress, but you're not gaining anything in terms of reduced permeate flux, because since the flow is slow, it also accumulates a lot of foulant. So, you literally – you better do nothing rather than adding patterns if you do not have the right combination of Reynolds number and topological features. So, then, there is a transition region and then, there is the last region where if you, on the other hand, are operating at higher Reynolds number – or at least a combination of Reynolds number and modifications that are compatible – then, the topological modifications perform better in terms of morphological changes.

And again, this is also intuitive. If you image having a wiggly channel where flow is really fast, you may expect that, because of the wiggliness, you lose – you have very strong resistance to flow and so, you have to use a lot of energy to push the flow through. But the decrease – the local decrease in fouling is not able to counterbalance the amount of energy that you are inputting to overcome, essentially, this wiggliness, right? And so, at higher Reynolds number then, topological modifications are expected to work better. So, with this, I would like to conclude.

So, what we did was to develop a modeling framework for fouling in the reverse osmosis membranes, which is fully coupled, so we won't account for these three different physics and is also unsteady. The solver has been validated and then, we kind of introduced this concept of – well, we used this concept of filtration performance in terms of this dimensionless Sherwood and Bejam number as a possible way to analyze systems that can be technically very different, and we also introduced a modified Reynolds number that allow us – this is the design parameter, right? It includes both the morphological and topological design – so, the static part of the dynamic part of the design. So, includes the

topology and morphology, but it also includes the velocity field, right? The input velocity.

And then, we did numerical validation and showed that this Reynolds* represents – seems to represent – a good – you know, appropriate scaling variables for all 114 numerical value simulations that we run. We demonstrated that these curves – these performance Reynolds* curves – can actually be used to both identifying best performing designs within each modification type – so, morphological modification or topological modification – as well as combined design – like, hybrid designs. And then, these are really the last two comments that I made – that at lower Reynolds*, morphological changes improved the overall membrane efficiency over the benchmark and topologically, altered membranes – so, the bumpy ones. But for higher Reynolds number, the situation is reversed. The topologically altered design are superior to all morphological design. So, the surface roughness seems to be able to significantly reduce fouling while only moderately increasing the pressure drop.

So, with this – so, now, currently, we are using SUMS and incorporate new capabilities. We are in the context of NAWI so, now we are really looking at incorporating turbulent effects through simulations and also, we have also included density variability and _____ parameters to account for essentially, effects of concentration on density. We have also generalized this model to – this SUM – to model the in the systems and so, this is exciting work and hopefully, I will have further updates. So, with this, I am done. Thank you.

>>Deb: Thank you, Ilenia. I think that – so, there's one question so far from Leon. "Is there a major distinction between biological fouling and inorganic scaling in your analysis?"

>>Ilenia: So, unfortunately, the only way, at the moment, we can account for different types of fouling is through the coefficients, right? These – can you still see my – let me –

>>Deb: Yes. We can still see your slides.

>>Ilenia: So – and I'm rolling through them, right? Or do you see them –

>>Deb: Yes.

>>Ilenia: Okay. So, the only way, at the moment, that we can account for this is just by changing the coefficients in the modeling equations. We have no implemented alternative models to model different types of fouling. We do not have, honestly, the knowledge to do that. But if anybody – you know, so, here. So, the only way we can change the type of foulant is by changing, essentially, these coefficients – K1, K2, and A0.

We have not done an extensive study on seeing what type of foulant is best represented by this model so, if it's only a matter of choosing the right parameters or if you really did

like, a different equation. But I would love to have this conversation if you have knowledge on this.

>>Deb: Thank you. And I noticed on your slides where you showed the image from the actual fouling versus what you had in the simulation – that there was significant amounts of sort of random bits of fouling that happen outside of the places where your simulation expected.

>>Ilenia: Yes.

>>Deb: Is that just such a small amount that there's no point in trying to represent any of that or is that worth trying to add some sort of a randomness feature to this?

>>Ilenia: No. This is an excellent point. So, I would argue that of course – that the objective should be to try to get things as realistic as possible because it's very hard to make an assessment of how important that layer – those little bits are. You know, _____ – it's convenient, right, if I say, "Ah, yeah, they don't matter at all, right?" So, my preference would be that we would be able to capture those.

Now, I like the idea of adding roughness. I always balance – when we do modeling, I always try to balance model complexity with results, right, in the sense that the moment you start adding complexity, you need to add parameters, right? And then, you need to add calibration effort and *dadada.* So, it would – I think it would be interesting to look and see whether this threshold between model simplicity and predictivity still balances out. Yeah. It could be an interesting thing to look at.

In terms of validate, the only way I can tell you whether it matters or not is in terms of validation, right? So, if adding this would increase the match by a given percent and that percentage is relevant in design, then I think it should definitely be done. But we will know our _____ so, probably, we should do it and then see if it was worth the effort.

>>Deb: So, we have another question. "Can the model be extended to capture things like hot spots?"

>>Ilenia: Well, so, can I have a clarification about what – I have a certain idea about hot spot, but in a different context. What do you mean by "hot spot"? It's like, just localized, you know, concentration? Localized area where concentration may be really high, things like that?

>>Deb: Localized high flux.

>>Ilenia: Localized high flux. Well, the argument is that if the physics is correct, then you don't need the generalization. This should be seen from the model. This is my argument. So, I believe that the model should already be able to do that.

But do I – unless we do localized measurements from experiments, this is purely speculative, right? But the model is the model, right? So, it predicts what's inside. And to model hot spots, you do not need additional physics, right? This is not additional physics. It's just the same physics where, you know, for whatever reason – be it geometry, be it coupling and *dadada,* there is strong variations of flux.

So, I think the model should already be able to do that, and I would love to know whether there are data that we can use to try to validate even that aspect.

>>Deb: Okay. Thanks. So, we have another comment/question. "It's counterintuitive that roughness can reduce scaling. Clearly, this is not the case in thermal processes."

>>Ilenia: So, the way I think about roughness – so, it all depends, right? And that's why – so, I cannot comment on thermal processes so, I'm sorry. We can have a separate discussion there. I would like to know more what you mean by that. So, in terms of this specific context, right?

So, you can think about – so, roughness – it all depends. It depends on the flow field, right? If the flow feed is fast enough, you can imagine that you can create the _____ zones beside the posts, right? And so, you can essentially have just localized fouling in very small locations behind the posts or behind this pattern, and if the flow is pretty fast, then, essentially, you would create a very localized patch of foulant right behind. But if you play around with the density of this pillars or whatever structure, then, essentially, you'll know where the fouling will be and how much the wake – how big the wake of this fouling will be.

So, if you can control the _____ zone beside these pillars, then to me, it's not counterintuitive. At low speeds? Yes. At low speeds, you know, you wouldn't be a winner. You would do worse, right?

Because you have further deceleration of the flow. And what we saw is that essentially, fouling – accumulation of fouling is anti-correlated with shear stress, right? So, the way I think about fouling and flow is that if I can locally increase the shear stress on the surface of the membrane, I will decrease fouling. So, I just have to create a fluid field that has a shear stress, because then, you would have a sweeping effect. So, I don't know if that answers the question.

>>Deb: Thank you. And I guess I have a follow-on one on that 'cause I guess I'm curious. Would it make a difference if the membrane was different behind the pattern, right? If you proposed that the fouling all – the deposition all happens right behind the post, then let's say I was able to manufacturer a membrane that had – that assumed that, therefore, it didn't make it porous or able to transmit, you know, right behind the post. Would that change the equation?

>>Ilenia: Well, it would – just the change – so, essentially, the only thing you would change is your domain, right? So, you have to account – so, in these particular

simulations, our posts were not permeable, okay? They were just impermeable posts. And so, because of that, the boundary condition on the post is like, no slip so, you do not have anything. So, it will not change anything.

It will just change, literally, the setup of your simulation. It will not change your equations. In collaboration with David Logner and Scott Hosson at the Clemson, we are actually generating membranes with some patterns where the patterns are permeable. And so, in that case, of course, you know, things change, right? But for this specific simulation, the posts were impermeable. But it doesn't have to be that.

You can have parameters that are spatially varying, right? And this is ultimately what would be very nice – like, to essentially have a membrane where – assume that you decided the pattern work for that specific configuration. Maybe, at eh inlet, you can have a certain pattern. In the middle, you can have a different pattern and at the end, you can have a different pattern. So, you can do heterogeneity in pattern topologies and, you know, depending on how you want to alter the flow field locally at different locations along the membrane. So, everything is possible, but the formulations would be the same.

>>Deb: So, I guess one last question on validation. Now that you've come up with these results, have you had a chance to then try and predict a best pattern and then test that membrane?

>>Ilenia: No, we have not done yet. We were supposed to be doing it. We ran out of time. No. We are actually – so, we did not do – we did not get to the point of doing like, complete optimization – like, you know, spanning, really, the entire parameter space diligently.

What we did was to essentially come up with a pattern that had a specific feature. We essentially wanted to create a reversible pattern – reversible to flow – such that you do not have to stop the operation to clean the membrane. So, you would use just the continuous flow and you reverse the flow to clean it, alternatively, along different path so that you don't have to stop operation. And so, it was not optimized based on this performance index, but it was optimized based on, you know, the idea of not stopping operations. And they are actually – now, at Clemson, you know, they have manufactured it and now, we are in the process of seeing whether our simulation can, in fact, predict.

We call it "Tire Thread". It's like, essentially, chevrons like this. So, they are symmetric, whether you flow this way or that way, and you can alternatively clean up, because of local shear stress, certain channels depending on which direction you flow. So, but yeah, we haven't done that. We are in the process of.

>>Deb: Okay. So, one last quick one. "Have you looked at different treatment options beyond the backward flow that can impact the fouling?"

>>Ilenia: No.

>>Deb: Okay. So –

>>Ilenia: We just –

>>Deb: – we're reaching – sorry – we're reaching the end of our hour and I want to thank everybody for joining and for the excellent questions and Doctor Battiato – I think now I've got it – for this excellent presentation and for this nice research. And I want to remind everybody – the next of the seminars on modeling and simulation topics is going to be May 3rd, and that will be Erin Wilson from the Idaho National Laboratory. And that will be a speciation-based solution model emerging from solvent driven aqueous separations. That will be at 11:00 Pacific, 2:00 PM Eastern as well, just like this one. So, thank you, everybody, and if you have further questions, please, feel free to reach out directly to Doctor Battiato and ask those questions. Thank you so much.

>>Ilenia: Thank you. Bye, everybody.

>>Deb: Bye-bye.

[End of Audio]