Multiphysics Depletion & Chemical Analyses of Molten Salt Reactors (2023 GIF Pitch contest) Dr. Samuel Walker, INL, USA (2nd Place Winner of the 2023 Pitch Your Gen IV Research Competition)

Berta Oates
Welcome everyone to the NEXT Gen IV International Forum webinar presentation. I am Berta Oates. I am your host. Today's presentation on Multiphysics Depletion & Chemical Analysis of Molten Salt Reactors will be presented by Dr. Samuel Walker.

Doing the introduction today is Dr. Patricia Paviet. Patricia is the Chair of the Gen IV International Forum Education and Training Working Group. She is the National Technical Director of the Molten Salt Reactor program for the Department of Energy, Office of Nuclear Energy.

Patricia.

Patricia Paviet
Thank you very much Bertha. Good morning. Good evening, everyone. It's a pleasure to have with us Dr. Samuel Walker today. He is one of the winners of the 2023 'Pitch your Gen IV' research competition.

He's a research and development Staff Scientist in the Advanced Reactor Technology & Design Department of Idaho National Laboratory. He earned his Ph.D. in Nuclear Engineering from Rensselaer Polytechnic Institute in 2021 where he worked developing mass transfer modeling approaches for insoluble fission product transport in Molten Salt Reactor systems.

His graduate work was funded by NEUP from DOE, a Fellowship that he was awarded in 2017. His current work at INL focuses on coupling NEAMS tools for multi-scale and multiphysics analysis of advanced reactors with a heavy focus on MSR multiphysics.

His expertise lies in modeling chemical species transport phenomena in molten salts used in fission and fusion systems. Applications of his work include source term and safety analyses, multiphysics core and system design, chemistry control system modeling, and novel MSR safeguard approaches.

So, thank you very much, Sam, for being here with us today. And without any delay, I give you the floor. Thank you so much.

Samuel Walker
Thank you so much, Patricia. I really appreciate the introduction. Just making sure that everybody can hear me and see my laser pointer.

So, yeah, I just wanted to say it's an honor for me to be able to speak here at the Gen IV international forum. I think I first learned about GIF about maybe 10-11 years ago, about the same time I learned about molten salt reactors. And so it's really exciting that I get to come here and speak about some of the research I've been doing over during my Ph.D., but also in the last two years at INL. And it kind of makes me think about this saying that we overestimate what we can accomplish in two years, but we underestimate what we can accomplish in ten. This is exciting to see ten years down the road, how far I've come.

I'll just give a brief outline of the talk. The big idea is what I've coined Depletion-Driven, Spatially-Resolved Thermochemistry & Chemical Species Transport in MSRs. In order to really get an idea of why this is important, though, we are going to do, I call it short but we're going to do a pretty detailed history view of the molten salt reactor experiment, specifically looking at some of the multiphysics liquid fuel issues that arose during the molten salt reactor experiment.

Next we're going to look at the nuclear energy advanced modeling and simulation. That's the NEAMS framework that the DOE has put together in the United States for MSR analysis. And then we are going to look at some of the specific application studies of this framework that we've been working on over the last two years, really looking at multiphysics depletion of MSRs and this chemical species transport analysis. And then lastly, we are going to just briefly look at some ongoing and future work that we are doing this year, and hopefully we'll start in next year as well.

So before I jump straight in, I just wanted to highlight some of the collaborators that I do work with, because no work is truly done in a vacuum I would say. So, listed here are some of the primary people that I work with at Idaho National Laboratory. Mauricio Tano, Abdalla Abou-Jaoude, Parikshit Bajpai, and Rodrigo de Oliveira. These are four kind of the modeling and simulation MSR specific folks at Idaho National Laboratory. And it's been great to work with them, especially Mauricio Tano, who is a key person that I work with on a daily basis.

And then I also want to just highlight Ryan Stewart and Odera Dim at Brookhaven National Laboratory. We have an ongoing safeguards project with them. Thomas Fuerst, who is also a tritium expert at Idaho National Laboratory, and Olin Calvin, who is someone that we worked with in the past that participated in some of the work that I am going to be showing here.

And then lastly, the mentor. So Wei Ji at Rensselaer Paulo Technic Institute was my advisor during my Ph.D. And right now my current manager is Gerhard Strydom, who is the NTD, the National Technical Director in the US for gas cooled reactors. So I get a different perspective from the gas-cooled people on a monthly basis to keep me balanced from my MSR bent.

So why molten salts? This is the first question that everyone should ask. Why do we actually care about molten salts? And there are several reasons why I care about them and why other people are really getting excited about molten salts over the last ten years specifically. And two of the big reasons are enhanced passive safety for molten salt reactors and the enhanced economic opportunities that come with using molten salts. So looking at the passive safety aspect, molten salt reactors, they can operate at low pressures, typically one to five atmospheres. You don't need as much of a pressure containment system like you are required to have for light water reactors. They also operate at low fuel temperatures. And so, when you use a solid fuel, you have very large temperature gradients because at the very center of your solid fuel all the way up to your cladding and coolant, there's this huge temperature gradient that forms. But with molten salts, you actually have a very low fuel temperature because the temperature of the fuel and your coolant are at the same temperature. So you also have prompt negative temperature coefficients where you will have – if your fuel cell heats up in your core, it pushes the fuel cell out of your critical configuration in the core, which actually decreases your power and then you'll oscillate until you find the new power. You also have this idea of using emergency drain tanks where we can have a freeze plug that can melt, and then it will drain your whole system into a non-critical configuration here in these dump tanks.

As far as economic opportunities go, even though you have a very low fuel temperature, your coolant temperature though which can be used for electricity generation is actually very high. And it's high enough that you can actually use it as process heat too for other industrial applications. You can also possibly look at medical isotope production, depending on how you would want to set up your reactors and also the different, I guess, safeguards or licensing concerns that would be applicable here, but that's definitely a possibility. You also have fuel cycle flexibility, so you can use the thorium uranium fuel cycle or the uranium plutonium. And because you also have this capability, you also have the ability to control your neutron spectrum quite a bit. And so you can have different sorts of reactors where you want to have a breed and burn or just have a very specific experimental reactor to do a certain task. You have a lot of flexibility in how you design your system.

So just a quick history view, or I'll say it's quick, but I take a long time, so I'm going to try to make sure I keep my time focused here. The molten salt reactor experiment was the second molten salt reactor that was built, but it was the most famous, I would say. And this was operated at Oak Ridge National Laboratory. And this was in the 1960s at Oak Ridge. And this was really under Alvin Weinberg, who was the brainchild that kind of pushed this work forward. It used uranium tetrafluoride fuel. But future work after this really laid the groundwork of what they call the molten salt breeder reactor, which they envisioned to have thorium fuel and to breed uranium as a thermal breeder. And so that also comes with a lot of challenges, but also comes with a lot of benefits using a thermal spectrum to breed fuel. But this really was a proof of concept, and it began a new way of considering how to do nuclear energy. So it's a very old concept of, but it's a challenging one, technically. And so it kind of got shelved for several years, but it's coming back in the last ten years with a passion. And so we are going to see if we can tackle some of these technological challenges to increase the technological readiness level of this reactor and bring it to market in the next ten years.

So what I focus on in my work and how I contribute to MSRs is really looking at depletion driven thermochemical effects and chemical species transport. So we're going to have this kind of loop that I have here of a molten salt reactor in general. This is just a little figure that I put together, and we're going to be looking at some of the different effects that happens in this MSR. So the first one that you can really happen, because it's a fluid dynamic fuel system, you can have some of the efficient products or particulates that form in your salt. They can precipitate due to Redox reactions. So the Redox reaction is something – the Redox potential of the fuel salt is something that I'm going to go into detail more, but really it's going to determine whether different elements in your fuel salt are stable as a fluoride or chloride, or whether they are going to precipitate as a gas or as a noble metal. You also have corrosion that can happen. This is also largely dependent on your fluorine or your Redox potential of a fuel salt. But it's also temperature driven as well. So you have soluble particle generations due to corrosion that you want to account for and limit in your system. You can also have – sometimes you might have bubbles in your system that you'll need to account for. Whether these were accidentally introduced or purposely introduced to clean out your system, you can have particle deposition on these interfaces. And so you want to understand the mass transfer of material to bubbles that are either extracting material on purpose or are just present in your system.

You also have deposition of insoluble particles, so you can have plating out of different noble metals in different areas in your reactor. And a lot of these are going to be decaying, and so they're going to be providing a heat source. And so you will want to know what that heat source is when you need to cool the reactor in case you have to drain it or something like that.

And then lastly, a lot of these reactors have an off-gas system. And really what this means is that you have a free surface here where the fuel salt can expand into this void. And also, if you want to extract bubbles or volatile gases to increase your neutron economy, like if you want to extract xenon 135, then you are going to have this interface. And so particle deposition on this interface can really complicate things, whether you are forming a kind of foam or a surfactant effect here, you want to take this into account.

Really, my work can really be focused in looking at Redox potential control to mitigate corrosion. That's a very important aspect of the molten salt reactors. Shown here on the right is actually a nickel cage. And inside of this nickel cage is a beryllium rod that you really can't see. But this is what they use in a molten salt reactor experiment to control the Redox potential. You'll see this kind of deposition here on the nickel cage. And this is actually iron and chromium deposits that reduced onto the surface here because the beryllium was reducing the fuel salt. So beryllium was dissolving into the fuel salt to reduce the overall system. And it was any corrosion products that were in the system were then plating out here. And so we want to be able to model this and understand how to control the chemistry of molten salt reactor, especially if we go through high burnups.

There's also the idea of looking at off-gas system control. So we want to understand what sort of source terms are coming into the off-gas. Because if your off-gas system fails, I think studies have shown that that really is where you're going to have the most radionuclides that could be released into the environment. And so we want to calculate what that would be here.

And then lastly, this is super important for material accountancy. And so this is as far as safeguards and methodologies and how to apply this, and also the decay heat aspect, this is where thermochemical effects and chemical species transport are really invaluable.

So we are going to talk about some of the fluid fuel issues in MSRE. And I mentioned the Redox potential. And so we are going to dive a little bit deeper into that. So this right here is a graph from the molten salt reactor experiment of the U4 to U3 ratio. So this is a way of measuring the Redox potential, basically. So this shows you how much of your fuel is going to be in your tetrafluoride state as opposed to your trifluoride state. And as we see that we go through burn up, this ratio is increasing in the molten salt reactor experiment and then has these sharp decreases. I'll talk about those in a second. But typically here, depletion is an oxidizing event. And the reason why that is it's oxidizing is because most of your fuel in your system is UF4. And so you have an oxidation state of 4+ here that you need to replace basically whenever you fission one uranium atom. But the problem is, most of your fission products are not as thermodynamically stable as the uranium in your system.

And so, instead of replacing your cation charge of 4+, you are actually typically only replacing about 3+ in your fission products. As so, as this continues, then you are going to have a cationic deficiency, and your flooring potential will increase. And so, rather than having UF3 in your system, you are going to have more and more UF4. And if this keeps increasing, then you're going to have corrosion at the walls, which is shown right here in this kind of equilibrium reaction that happens in the molten salt reactor, where you have chromium in your wall that's going to be reacting with your uranium tetrafluoride to form your uranium trifluoride. But you also have this chromium fluoride that forms as well. And so, this will increase. As you increase your UF4 concentration, you're going to increase your chromium fluoride in your system. But also, if you let it keep going forever, then once it has eaten up all your chromium, or maybe the iron or nickel in your wall, then you'll also have UF5 and UF6 that can form which are gaseous forms of uranium. We don't want to let this get too far carried away with depletion. We want to actively control it so that we can replace the cationic deficiency with material that we choose to put in there rather than the material from the wall because we don't want our walls to just be eaten away.

So, how would we do this? And this is what they did in the molten salt reactor experiment. But like I said, the chromium and the iron are kind of naturally controlling the Redox potential through corrosion. But you don't necessarily want to rely on corrosion to control your Redox potential. Right? So beryllium, which is one of the base salts in the molten salt reactor experiment, is one of the key components there. They would add excess beryllium into your system to then reduce your uranium fluoride back down to uranium trifluoride. So that way you can control that Redox potential. So these steps here, these giant decreases here are when they would insert beryllium rods into the salt, and then they are actively reducing that UF4 to UF3 ratio.

So there's a lot of different options of how you might want to control this. This is just one of the options of controlling the Redox potential. But it's really based upon the thermodynamics and the thermochemical aspect of your composition of your fuel salts. And so this is a table of electrode potentials here showing different elements in your FLiBe salt and how soluble they are. So really, if you look at the first one here, lithium, which is one of the base elements here, it's going to be the most soluble and the most reducing element in your salt.

But then you have your rare earths that are extremely soluble. And then as you come down here, you have beryllium and then your uranium. But if for some reason, your potential is not being controlled by the chemical activities of your uranium 4 and uranium 3 here, which is what is happening in the molten salt reactor experiment, and you can reduce it with beryllium, then you do have chromium that becomes more thermodynamically favorable than uranium or beryllium. Or not. I shouldn't say it's more thermodynamically favorable, but it becomes – as your chemical potential increases here, then you do have a higher amount of chromium and iron will enter into your system. And so you want to actively keep your chemical potential down in this range where uranium is the most, is just at the very end of what's stable there. And that way you can prevent a large amount of corrosion from occurring.

So that's one aspect is controlling Redox potential, and that's something that we're going to look at later. Another phenomenon that really affected the multiphysics behavior of the molten solar reactor experiment was the liquid gas interface phenomenon, which is what I touched on earlier. And so this is the loop of the molten salt reactor experiment. This is your core. You come up through the riser, yeah, up here through the outlet of the core, and then it comes up here into this pump. So there's a centrifugal pump here that then goes out to the heat exchanger and then down an elbow, and then through the downcomer and back through.

But a very important part, which is the pump hole right here, is blown up here on the right, and this is that liquid gas interface that existed in the molten salt reactor experiment. So here's your centrifugal pump that's sucking up, and then pushing out your salt. But not shown here is a small discharge line, or a bypass line, I should say. It's not technically a bypass line, it's a recycle line I guess you can say. So off the discharge line, there was another line that would come out and come and enter this torus up here, this toroid I should say. And it was about 50 gallons per minute, so about 5% of your flow, and so some of it will be diverted and then shot through this helium atmosphere, and then fill up part of the pump bowl. And so here inside the pump this is where most of the fuel salt is cycling. But then outside of the pump, in the pump bowl, there was a certain amount of fuel salt that was building up here, and then it would slowly be sucked back down underneath the skirt and re-entering the primary loop. They use this to try to extract the volatile gases through this liquid gas contactor, the spray tower. The jets here coming down would cause a lot of turbulence here on this interface. There's a lot of entrainment of helium bubbles that would occur here. Most of these bubbles would go back up to the surface and pop, and the gases that were here would then be diffused and then taken out through a gas line. But some of these bubbles could go deeper down, closer towards this skirt, depending on certain operational parameters, and we'll talk about that shortly where actually some bubbles did get sucked under the skirt and into your primary loop, and we'll look at that. So that was not necessarily planned for or anticipated. Well, they did anticipate that it was a possibility, but they thought that they had done a good enough job of designing this where that wasn't going to happen, but it still happened.

You also have this overflow pipe that is here inside of this molten salt reactor or inside of this pump bowl. And so if this fuel salt got too high, then we go over this pipe and be drained into this kind of an overflow tank. That tank could be repressurized at some times, and then force the fuel salt back in. But this was there in case there was a huge reactivity transient, and you have a lot of fuel salt expanding and then needs to go somewhere. So that's what that was for.

Then you also have the sample cage here which is where the beryllium rod was put in. This was like a catch all, do all aspects of the molten salt reactor experiment. And because all these effects were very close together, some of them interacted with one another, and we'll talk about that. So they were very smart how they designed this. But at the same time, perhaps we need to separate some of these aspects up so that they don't interact in the same way that we saw in the molten salt reactor experiment.

So like one of those that I was mentioning was the circulating void that could happen. And so, as you might anticipate, it was very affected by the fuel pump speed of the pump. And so if you turned up the pump speed too high and you have very fast rpms, then this would suck those entrained helium voids down into the skirt a little bit faster, and you would have the circulating void effect. So if you turned down your pump speed to 900 rpms, then you would have hardly any pump, any void, any circulating helium in your system. And so, yeah, definitely that's one of the key aspects of why they were circulating voids.

But here is actually the effect that would have on your multiphysics. So, if there was some helium bubbles that got sucked into your loop, then you would have these little power blips, which is what is shown here. These are power blips from circulating voids that they were like, hey, what's going on? Why is our power fluctuating? And then they realized that they were sucking these voids into the system. And you have a slight temperature increase due to the reactivity insertion event there.

There's one more thing here, though, that we do need to talk about, and that is the surfactant effects that they are hypothesized to have occurred in a molten salt reactor experiment to explain another phenomenon that they saw. So, during the U 235 runs of the molten salt reactor experiments, this is when the fuel was mostly using enriched U 235. That was the first set of runs, runs 1 through 14. They really didn't see that much overflow into the overflow tank. I'll just go back real quick. So, yeah, so they did not see a lot of fuel cell expansion, where you have a lot of salt entering the overflow pipe. But in the U 233 run, so here they shut down the reactor for a period of time. They swapped out the fuel. So they took the U 235 based fuel salt, they fluorinated it, extracted the uranium, and then they reloaded it with U 233 enriched salt, just to see if they could run it using U 233. And then they reloaded it into the system here. And then they did something that we talked about earlier that we showed. They reduced the salt, just like they did in the U 235 runs. They added beryllium. Now, when they started adding beryllium though, the reactor started behaving very differently. And so the ingestion of the waste significantly increased, so there was more bubbles being sucked into the reactor, because after they had reduced it with beryllium, and also you had a lot of salt overflow rates. So this is a fuel salt transfer rate in pounds per hour into the overflow tank. And so suddenly, after you add in some beryllium, then you get these huge amounts of salt that's being extracted from the reactor into the overflow tank. And so the idea here is that the beryllium, whether it's reducing the corrosion products, because that's what was hypothesized, is that there were a lot of corrosion products actively in the fuel salt. Still, after they had swapped out the fuel salt, they didn't quite control the chemistry as well as they had hoped. And so there was a lot of iron and chromium in the system. And so as these are being reduced and depositing on this interface, then it's creating a surfactant effect, where it's decreasing your surface tension, and it's kind of like – I don't know if you've made oatmeal, but this is definitely like the ability of longer lasting bubbles and this frothy aspect is hypothesized to have occurred. And so this is part of the reason why you have this overflow phenomenon where it's kind of bubbly and you have a lot of salt that is then building up, whether it's in these frothy bubble formations, kind of. So that's what is hypothesized it would happen. They couldn't really recreate this effect afterwards and follow on experiments, but there's definitely something happening here with the beryllium affecting the performance of this interface. And this is very interesting, and we need to investigate this further.

So that's kind of why these different multiphysics liquid issues is really what sparked my interest. And I definitely think that we want to really understand them and control them so that we can have a very well-behaved reactor. So, yeah, we use the chemical species tracking problem formation then to model a lot of these different effects. And this is really important for containment. So we really want to know where do the radionuclides go. Right. If you have cesium iodide at an interface, how much cesium iodide is going to be vapor and be extracted into your off-gas system. This is important for heat removal, right? So if you have a lot of these noble metals that are depositing, especially if they are depositing in different areas, how much builds up there and what sort of heat source terms do you have because of these fission products in different areas?

It's important for reactivity because we looked just back at some of the different effects that can happen. But it's also important for your neutron precursors, right? If some of them are thermodynamically unstable or extracted, then it's going to affect your reactor beta effective corrosion. That's one of the biggest aspects here. And then safeguards, really looking at where does our significant, our special nuclear material end up? And if there is any hold up or if there's any sort of funny business happening with the uranium in your fuel salt, whether people are explicitly trying to plate it out by over-reducing the salt with beryllium, or whether they are doing different sort of divergence scenarios, we can use all of this information to really tell us whether the reactor is behaving normally or whether some diversion scenario is happening. So how do we tackle this chemical species tracking problem? And our approach that we've been using at Idaho National Laboratory is really to develop approximate or wrong models, albeit useful models. Every model is wrong, but some are useful. So the idea here is that we're trying to develop useful models that capture these multiphysics effects. We want to verify that they are numerically implemented correctly, right, because the computer tells you exactly what you tell it to do. And so if you tell it to do something wrong, then it will give you the wrong answer. And so you definitely want to verify that what you thought you told the computer to do is what it's doing. But that's just half the game, right?

The most important aspects moving forward really are testing and validating them against separate physics experiments and then using them to inform integral effects, test designs moving forward, and validate our multiphysics models.

And so we have an exciting reactor that's coming online in the next two years at Idaho National Laboratory. That's the molten chloride reactor experiment. And so that's going to be the first chloride reactor, but it's also going to be the first molten salt reactor that we've made in a long time. And so we are excited to use that to validate a lot of these models that we are developing right now.

So we are using the NEAMS tools or the NEAMS toolkit, which is what the DOE has been kind of building up over the last 10 years to model advanced reactors. And these are the suite of tools that we use. We use the MOOSE framework, which is an open-source finite element and now finite volume kind of environment, to be able to model all of these partial differential and ordinary differential equations and then couple them together.

And so some of these codes are listed here that we use for MSRs. NEK-5000 is like a CFD code that's very high fidelity. And Griffin is our neutron transport code, that's also a very high-fidelity capability. And then walking down our fidelity, kind of our fidelity ladder I would say, we have Pronghorn, which is our coarse mesh thermohydraulic solver, which is what I use primarily just because it gives me the ability to look at the whole reactor system and also resolve it with a certain amount of fidelity that captures a lot of these chemical species' transport properties, but it can still run with reasonable time.

And then going further down, you also have SAM, which is the System Analysis Module. So that's like if you want to look at the system level of your reactor with your second and third coolant loops as well. And then as far as fuel performance and thermochemistry, we have Bison and Thermochimica. And so I'll talk more about these, because these are the ones that we really use a lot that we've coupled into the MOOSE framework that we're able to use to do a lot of the thermochemical analysis of our molten salts.

So this is the framework that we put together over the last year. And really, like I said before, Griffin is what we use to look at our neutronics and our depletion of our fuel salt. Pronghorn is what we use for our thermal hydraulics and our species transport. So if you want to – yeah, so Griffin is going to give us, with its depletion capability, it's going to give us a 0D inventory of our nuclides. And so it's like it's solving the Bateman equations, you know, so it's just an ordinary differential equation in time. But Pronghorn here. If you actually want to track specifically the whole partial differential equation of different nuclei, then we can put that species equation into Pronghorn and really understand how specific elements are behaving in our system. And then Thermochimica is our chemical equilibrium calculations and speciation.

So Griffin provides our power distribution to Pronghorn. Pronghorn then would give us our temperature precursor and advection of different spatial source and sink and removal rates for 0D inventory calculation. And so we can use this to inform our spatially resolved depletion aspect. Pronghorn also gives the temperature pressure, and then if we are tracking certain element spatial distributions in our system, certain nuclei that we want to resolve spatially, then we can use Thermochimica then to give us spatially resolved thermochemistry of the reactor. And so this would then give us Redox potentials and vapor pressures and chemical speciation that occurs, that then would feed back into our species transport model here.

And then if you do want to do long transients, then you can couple just Thermochimica and Griffin. And this will really give you kind of a 0D analysis, but you are able to inform your 0D analysis with higher fidelity models of the extraction rates of different nuclides. And so, yes, that's kind of our big framework, the three primary codes that we've coupled and are using right now at this time.

I do want to highlight that most of Pronghorn here, well, I'll get to that in just a second. So we'll first just look at depletion driven thermochemistry and this is the 0D aspect of it. So, as I said, Thermochimica is what we are using to solve for the equilibrium thermochemistry of the system. So this is an open-source Gibbs Energy Minimizer, and it's developed by Markus Piro and his team. And Markus has recently moved to McMaster University. But here's a link for access to Thermochimica. And I will say that we have this ability now within MOOSE. So MOOSE is open source. You can download it and start running with it immediately. Then very quickly, you can activate the Thermochimica aspect within MOOSE, now that it's coupled and wrapped. And so, very quickly, you can start to run Thermochimica within MOOSE and start to do a lot of the same analysis that I'm doing here.

But Thermochimica can only really be used with a good database. And so that's why I want to talk about the molten salt thermodynamic database, thermochemical, the MSTDB-TC. This is developed by Ted Besmann and his team at South Carolina University and Oak Ridge National Laboratory. And here's the link for this database. And I would say that he's been working very hard over the last several years to have a very comprehensive database for both fluorides and chloride salts. And it's really impressive what he's been able to put together. So that's what our work has been leveraging to take this database and then look at the different phase diagrams that are predicted for the element and pressure and temperature effects that we see in our molten salt reactor.

So this is just the first study looking at this, the Redox potential control of molten salt fast reactor during depletion. Now, I should say that the molten salt fast reactor, this is just a kind of proof of concept of this idea. So, I know that you wouldn't necessarily want to actually use beryllium to reduce the fuel salts in the molten salt faster reactor design, because it's a fast reactor and you don't want to moderate your neutrons too much. But, yeah, this is just kind of an idea of similar to the molten salt reactor experiment, using beryllium to reduce our fuel salts in time. So we are going to be looking at the corrosion product nickel, though. We want to see how much nickel is going to be formed if we don't control our Redox potential with depletion. And then if we do want to control it, we can put in like a PID control system where we are actually controlling our flooring potential within a certain range by actively dipping in a certain amount of beryllium to maintain a steady Redox potential.

So, this is just our 0D model looking at what the foreign potential does through depletion. And what we see here is that as we are going through depletion, we do see this steady increase in our Redox potential, but then suddenly we have this fast increase and then slow down here. And so this really is showing us that the U4 to U3 ratio which is controlling the Redox potential here, is then no longer controlling the Redox potential. So it's no longer the chemical activity of uranium that's controlling it. When it quickly increases and then slows down here, this is actually it's switched to a new Redox buffer that's controlling the Redox potential. This range right here is actually due to our nickel corrosion. So this is very similar graph here, because this shows the amount of the moles of nickel in your system.

And so when it's a reduced system, you have hardly any nickel in your molten salts. But as depletion and fission is ongoing and you are not actively controlling it with beryllium, then you have a large amount of nickel that builds up. Now, the Redox potential continues to increase because nickel is not as thermodynamically stable as beryllium. So that's why this is going to exhaust your nickel eventually, and then it will continue to rise. We don't want to see this nickel corrosion occurring, so we want to actually control it. The blue line here is actually where we put in beryllium into our system. We can see that, yes, using the PID controller, and we are controlling how much beryllium we're putting into the salt, we can control the

Redox potential to keep it roughly stable in our system. And so then, the amount of corrosion products then that are formed are very minuscule because we were actively controlling the chemistry.

This also has an impact on the volatilization of species. This is kind of the next step, looking at your iodine or your cesium in your system. And so, we see that cesium iodide vapor formation is something that is expected, but it's very miniscule because iodine and cesium are pretty soluble in your reactor if your fluorine potential is well controlled. So that's what these guys are showing here. The green and the red here is our Cesium 137, which is whether it's being controlled – yeah, the green and the red are the cesium, whether they are being controlled or not controlled, and so we don't see a huge effect on the cesium. But what we do see is iodine volatilizes when your fluorine potential increases. And that's because iodine is also in the same group as fluorine here. And so as your fluorine potential increases, so will your iodine potential increase. And so we have a significant increase in, like, iodine that will end up in the off-gas system. So when you are not controlling it, your Redox potential, then you can have 31% of iodine 131, just as an example, ending up in your off-gas system. But if you are controlling it, then you have a very small fraction of your total iodine ending up in your off-gas system.

So if you want to look at source term, or if you are wanting to use some of these off-gas signals as measurements in safeguards analysis, you really need to understand what the fluorine potential is doing so that you can predict how your off-gas system will behave. So next, we are going to just keep moving along and look at spatially resolved thermochemistry. So this is really looking at Pronghorn and Thermochimica coupled. And so we want to look at some spatial resolution of our system now. And I will say that Pronghorn, which is also most of Pronghorn is actually what we call the Navier Stokes module in MOOSE. And so, if it's a module with MOOSE and it is completely open source, there's only one or two things in Pronghorn, like some friction correlations that are not open source. But if you wanted to take this off the shelf and start running your Navier Stokes models using MOOSE and then coupling with Thermochimica, this is something that everyone can immediately download and start doing tomorrow.

And actually, I think – oh, yeah, I did mention here. So what we do here is this is our open-source model of the molten salt fast reactor that's on the virtual testbed. And so if you go to this link here, this is like a list, and a conglomeration of all these open-source advanced reactor designs that use NEAMS tools. And so, very shortly actually, this specific thermochemical aspect of the molten salt fast reactor model will be uploaded. And so you can go on there and download it yourself and start to play around with things that's based upon this work right here.

But, yeah, we want to really look at the spatial resolved corrosion and Redox potential control for the MSFR. And so this is our temperature in our RZ model of our MSFR model. And so if you envision this being reflected here and then revolved around the other side, it's here, it's a 2D RZ model of our system, and this is our pressure distribution for our model that we just took off the VTB.

And then we actually want to start to look at – maybe we are adding beryllium at a certain place, and so we are going to be looking at the actual transport of the beryllium in our system and then the corresponding effect that it has on our fluorine potential. And so I have a little video here that I'm just going to show, which will try to highlight the effect of adding beryllium. So we are adding beryllium here at the bottom, and it starts to cycle through the reactor and slowly build up in our system. And that's the beryllium reducing our extra beryllium coming into the system. And this is the effect that it has on the fluorine potential. So you see that it's reducing the fluorine potential. The red is a higher fluorine potential, and the blue is a reducing effect from the beryllium, changing the composition of our fuel salts. If we wanted to actually look at beryllium reduction transients, we can do that. Or if you want to have some sort of novel fueling or novel Redox control analysis, then this gives you the ability to look at those transients. So this is just kind of a proof of concept, but we are looking at validating this work moving forward. Let me see if I didn't mix anything.

Oh, yeah. So we also see that if you have any sort of nickel corrosion product in your system, which is shown here, this is some NIF2 that formed due to the high temperatures in the core. And as we are reducing it here with our beryllium, then the NIF2 decreases, and it's actually, we'll be swapping that NIF2 into just solid nickel. So you can see that reduction of corrosion products also happening.

Then we really want to look at the whole picture, right. We want to look at depletion-driven spatially resolved thermochemistry. So we want to couple our spatially resolved chemistry, but we also want to incorporate our depletion steps into how that actually changes our overall chemistry of the system at a small-time scale, but also at a large time scale, where we can take large depletion steps.

So Griffin and Pronghorn calculates the multiphysics steady state solution and our fission source, temperature and pressure. So this just shows you what our steady state multiphysics solution of our model will be. And then Griffin and pronghorn depletion then calculates our 0D nuclei concentration, which is what I mentioned before. But this is also incorporating the effect of nuclei flow on altering our reaction rates, right, because you have a lot of these species that are in a flux and then out of the flux and back into a flux. And so when we couple these together, we'll have to modify our reaction rate in our Bateman equations to actually account for that effect.

But we also have Pronghorn species tracking, so then we can actually, we'll have a 0D for like well mixed nuclei that are homogeneous in our reactor, where there is no real spatial distribution. We can just use our 0D calculation from Griffin. But if we want to use – if we are tracking explicitly the whole partial differential equation where there is spatial resolution of certain nuclei, then we can then take the spatial aspect from Pronghorn and the 0D aspect from Griffin and then merge these two to get an accurate estimate of how the thermochemistry is also changing, whether it's well mixed or whether there's spatialized chemistry because of certain nuclei being in different areas of your reactor.

And then lastly, the Thermochimica really gives us that elemental distribution calculation speciation. So this will tell us, yeah, how much cesium iodide is actually in a vapor phase and how much is being extracted, and then that feeds back into our depletion and our species transport equations. So this is just kind of a high-level look at some of the effects that we have here. And so we mentioned this earlier, the chemical species volatilization, but now we could see it in 2D. And so this is the fluoride potential of your salt at beginning of life. And so it's very reduced, it's very happy. And then this is your ideal. This is your iodine, like stable iodine gas that's in your fuel salt. And so it's very, very small, the amount of iodine gas that's either in the vapor or that's in the stable gas phase if there's xenon that's present also as well. And so you have a very small amount of gaseous iodine in your system.

When we move forward to 2 MW day per kilogram of uranium burn up, then we see that our Redox potential has drastically increased because we have not been actively controlling it. And our stable iodine gas is increased by six orders of magnitude. So we have a lot of volatilization of iodine that's occurring here. And this shows you where that volatilization would be happening. So it can also inform where you might want to put in off-gas system to collect different things.

And then we can look at cesium iodide here. So your cesium iodide is, this is before burnup, and this is after burnup. And so it increases by roughly two orders of magnitude but it's not drastic. Your cesium and iodine are kind of – it's not as affected by the fluorine potential as opposed to, say, your I_2 gas. And so here, this is I_2 in your system that's very, very limited at beginning of fuel salt, at the beginning of life of your reactor. And then as we go through depletion on our fluorine potential drastically changes. So does our iodine gas. So this is ten orders of magnitude increase here of I_2 gas formation. And so you can kind of start to look at these effects and see the spatial aspect of them as well.

And then this is our corrosion model. This just looks at – the nickel that's in the system is very small, and it's only in the very highest temperature. The NIF_2 is only at the very highest temperature areas of your reactor. But here, when we go through depletion, then it's not just the temperature effects affecting the hot and cold leg affecting your corrosion. You also have your fluorine potential drastically increasing that corrosion that will be seen.

All right, so I think I have just about maybe 10-15 minutes left. So this is our fourth study that we looked at. And rather than using thermochemical equilibrium where we assume that the reaction at the interface is instantaneous, and that we assume that it's there is no limiting factor as far as how quickly material can react. We actually want to look at the kinetics of corrosion or kinetics of Redox reactions. And so this would then be used – this would be done using the Poisson-Nernst Planck equation that we've worked and implemented into Pronghorn as well.

And so this could really look at diffusion of materials to the interface and then the actual Redox reaction that occurs, and then the concentration profiles of these different species to actually determine what the Redox current or the corrosion current would be at the interface.

So, using the Poisson-Nernst Planck equation, it's basically the species transport equation. But we also have the electrostatic, I guess, component of our diffusion that's also included here. And we also want to solve for our electrochemical potential. So, we have these two equations that were solved. Right now, this equation is kind of Jerry-rigged where we assume a certain potential. But in the future, we might want to actually use Thermochimica to tell us what that thermochemical potential would be in the bulk and then we can couple these two more adequately. But right now, we are just using the Nernst equation, which also will give us that thermochemical potential, but it will only give us that for one reaction, basically. And so, we have to model these reactions explicitly, whereas using

Thermochimica, it will naturally do all that, gives energy minimization for us to tell us what that thermochemical potential be in the bulk.

But as far as the corrosion current that happens at the interface, we use the Butler-Volmer equation. And so that's this beast down here. I know it looks pretty bad but it's not that bad. It just shows basically the likelihood of the reaction going in the forward direction or backward direction, depending on what our Redox potential is and our concentrations at the interfaces of our reducing product and our oxidizing product. So, yes, that's what the Poisson-Nernst Planck equation is and Volmer equation, how we couple them to do this corrosion kinetics modeling.

So the next step then is really model verification. So, we use the method of manufactured solutions to develop our simple solutions to this numerical problem that we are putting in. This is kind of just an erroneous equation that we put in to verify, as opposed to using the full equation there. But, yeah, we can then verify that yes, we did put this into the computer correctly, and we have a second order convergence. So that's good. And then we actually want to validate it, though. And so this is a molten salt loop at Oak Ridge that is referenced here. We took the data from this loop where we have a hot leg and a cold leg of this salt loop. In the hot lake, we see that we do have corrosion occurring where chromium and iron are being leached into the salt. And in the cold lake, we actually see that we do have a deposited layer here. And so in the hot leg, maybe the iron is soluble at that state because the temperature difference. But then in the cold leg, it's no longer soluble, and it's actually plating out and creating a deposition layer. And so we want to see if we can actually recreate some of this data. So, using the PNP model, we do see that we have reasonable good agreements here. So, this is the penetration length of the material. So this is showing you how much material is kind of lost as we – the experimental data versus our predicted data. And this is the actual concentration here. So, the chromium concentration here shows that the distance, like how deep into the wall does the chromium actually exist or whether it's depleted. And so we see that most of our chromium does leave the system, but our iron here in the hot leg, it is leaving the system which is shown here because it's 50 or 60% of the iron at different lengths into the material, but here we also see deposition in the cold legs as well. We are able to capture both those effects using the PNP model. We are pretty happy that we got this to work, and we are enhancing this capability right now, this fiscal year.

So, lastly, just some ongoing work, because I think I am coming close to my time here. Currently, this year we are also putting in two phase flow capabilities within Pronghorn. So that way we can actually start to model some of these circulating voids and the effects that they have on our reactivity. And so, this is like the molten salt reactor experiment, and we have the temperature distribution in our MSRE model, or RZ model of the MSRE. And then we also have like a void distribution that is generated here by fission gas. In reality though, we've modified this and we have like the pump hole [ph], and we'll have an insert here of helium bubbles that then cycle through the system. And we can then model our transport of gaseous species to that void and look at how much like, say, xenon 135 is extracted or different, different effects of that interphase mass transfer effect.

So that's currently ongoing. And so that's something that is coming up right now. Oh, yes, this is just a little video here showing the reactivity insertion transient of the power density here, cycling, and then we have the temperature increase in our fuel salt. And then correspondingly, we have our void that is also starting to form and then diffuse and be transported through the loop. So that's something that we have ongoing right now. A new aspect that I'm really excited about, so I do want to just talk about this briefly, is we have an ongoing project with the Advanced Reactor International Safeguards engagement project program. And so, this is the ARISE program out of NA241. So this is really looking at safeguards and how we can apply these in an international aspect. And so, what we are looking here is the multiphysics chemical species forensics of analysis that we can do using this chemical species transport. So right now, we are setting up these multiphysics models that have both the 0D aspect, so we can do these long term transients to see what extraction of material would kind of affect our different signals that we want to measure, whether that's an off-gas signal or a thermochemical signal or delayed neutron precursor reactivity signal. We can use both our 0D models and our high fidelity RZ models to understand what material should be expected in different areas that sensors could then measure. And that will tell us what nominal reactor operation is and then whether misuse is actually actively occurring.

And right now, we have a partner with Brookhaven National Laboratory. They are using machine learning to then take all this data that we generate and to really define what that nominal behavior is and then also to look for possibly new signatures that we, like the human eye can't really understand. So, the machine learning model will really start to look at all these different nuclei to identify new signatures that we can see. And so yeah, it's a very exciting project. So, in the next couple of months we should have some more, more concrete results coming out and we're going to be doing a lot of publications looking at what we find.

But there's definitely like this electrochemical reduction that could happen. And so this is, say, you are trying to control your fuel salt, but you over reduce your fuel salt, whether that's on purpose or accidentally, you have this plating out of uranium. And so we want to be able to model that, whether that's held up in the system or whether it's intentional.

And then lastly, this is some future work that I really want to – we're actively looking for funding and collaborators on this, but this is looking at liquid breeding blanket tritium modeling. So the idea is we can use our Griffin Depletion model to really get our idea of how much tritium is going to be generated from our lithium 6 in a fusion system. So, this is as far as fission, this is now looking at fusion tritium breeding blankets for fuel generation. And so, we'll be able to look at how much tritium is generated. We'll be able to look at the chemistry control of that breeding blanket using Thermochimica. Right. So it's the same process. As your lithium is depleted, then your fluorine potential is going to change, and you want to be able to control that actively. But you also want to account for whether your tritium is T2 or whether it's TF. We want to look at that. And then the tritium diffusion would be – inside of the salt would be that a species transport would be done using Pronghorn. And then as far as actually diffusing through materials or whether you are using different sort of extraction like a vacuum sieve, or different sort of diffusion aspects would then be handled through with TMAP8 with the solids. So we are coupling all these together to give a very good analysis of our liquid breeding blankets.

So yeah, that's something that we are ongoingly looking for funding and collaboration aspects with. So that's something that I think would be a great application of this work moving forward. So lastly, I just want to have some acknowledgments and funding collaborators. I definitely want to thank Patricia Paviet for funding a large part of what we saw here today through the MSR campaign. So, a lot of the coupling and the analysis work is really taking what the NEAMS tools people are producing, and then that feedback between the actual application people like me where we are trying to model new aspects, that iteration is very valuable. And so, we are super thankful to her for all of her support of this work and then the applications of it going forward, which are so many.

I also want to thank Logan Scott and Bego Barrado and the entire ARISE team for their support of this new project that I'm working on, and hopefully we'll have some new publications on that coming out very soon. And then lastly of course, the collaborators, Mauricio Tano, being the main one that I work with on nearly a daily or weekly basis here at Idaho National Laboratory. So with that, thank you for your attention and I'll take some questions. I do want to say that I'm super thankful for everyone listening to this talk and we're always looking for collaborators. So please reach out whether you want to use these tools as modeling and simulation people or whether you are an experimentalist. We are very excited to work more with experimentalists and to have more collaborations so we can actually validate a lot of these tools, whether we are designing experiments or validating them after the fact. This is something that we really want to continue our work with. So, with that, thank you so much…

Berta Oates
Thank you. Thank you, Dr. Walker. There are a few questions that have come in. Well, questions continue to come in. We're going to take a quick look at the upcoming webinar presentations. Again, you have invitation announcement flyers in the handouts pane where you can download and share these with any of your colleagues who may be interested. In May, a presentation, it's a panel discussion, a joint GIF/IAEA presentation on regulatory activities in support of SMRs and advanced reactor systems. In June, Directed Energy Deposition Process of Corrosion Resistant Coating for Lead-Bismuth Eutectic Environment. And in July, Online Monitoring Development in Support of the Nuclear Fuel Cycle.

I am going to turn off the laser if that's possible here. I am also giving you organizer rights, so you should be able to see these questions. Also, you can undock your questions pane and then it'll size – you know, drag and drop like any Microsoft products so that they are not one font. You'll be able to increase the, the size of that square.

Samuel Walker
Perfect. Yeah, I can see them now.

Berta Oates
Now, first. The first question I guess, is a comment. Need to study free seals more. Passive free seals are very unlikely to be proven reliable, especially over the long-term operation predicting release and reach full potential is challenging. MSRE used manually operated, not passive free seals.

Samuel Walker
No. That's a very, that's a very excellent point from Ed. It's always good to know a name, to know a face, I should say as well. Yeah, that's something that is definitely, you know, that's just a generic concept that different people and different reactor vendors are going to have to look at. But that's something that it's a very good aspect that we could probably look at more here. Looking at whether we

are looking at the freezing of the salt and modeling the active or passive free seals. That's very interesting to a good potential further research opportunity going forward. Let's see, you need to study negative temperature coefficient of MSRs more. Heating up pushes out fizzle and negative reactivity effect, but also pushes out absorbers, coolant fertile vision products and positive reactivity addition due to salt heat up.

Yeah. So we see that using our models as of now, we can see both the initial negative effect, but we also see the positive reactivity effect as well. So, you have this kind of oscillating effect that happens there. So, that's a very good point that you highlight there. Was the loop void calculated from power oscillations or directly measured. So, this loop void that I just showed. Oh, sorry, let me see here, this is 655, so this will be compared for the MSRE. So this loop void was calculated from the power oscillations. Yes, that is exactly how they determined what they thought the void was in the salt inside the loop, basically. So, they did not have a way of measuring how much gas was cycling through the MSRE. So, no, yeah, basically they determined from the power oscillations what they thought the void size was.

Use this system of codes to analyze free seals chemical, thermal, and structural effects. As temperature changes, chemical build up draws a noble metal settling on top frozen surface, hardening, radiological, thermal changes of frozen salt, time to melt, time to full flow on heat up, time to drain fuel. That's Ed. Yes, yeah, definitely. I will take – these are all aspects that we could possibly look at. And I will need to – I'll copy this comment for future work here. But yeah, because this is definitely something that we can start to look at, especially the salt freezing and looking at as the composition of our fuel salt changes, how that changes our melting and our freezing point of our solution, that's something that we can definitely look at. And reactivity, you know, maybe accident scenarios where we are overcooling our salt in some areas. So.

All right, in fast reactors, beryllium dose may be limited by spectrum effect. Redox may also change by radiolysis intensity, such that beryllium dosing may have varying benefits leading to similar experience of BWR with hydrogen chemistry. Can this limit be modeled? So may be limited by spectrum effect. Yeah, that's a good aspect. Right. I did highlight that. Whether you would want to use beryllium or not in a fast reactor to control your Redox potential, we can actually model that. So, we could – say you actually have the real MSFR fuel salts that does not have any beryllium initially, but you actually do want to slightly dope it with beryllium and then look at the neutronic effect of that to see, oh, no, where our breeding ratio is no longer where we want it to be and our K effective is not really. Yeah, we can, we can look at that effect basically. Right now we haven't actually done it, but that's definitely easily done. I shouldn't say easily done. I mean, it will take a little bit of work, but like a couple of weeks to months of focus on it. But yeah, the coupling and the framework is there. So all you have to do is really set up the problem, basically.

So that's, that's a very good question to look at that. You could also look at other metals that you would want to use to reduce your salt. So maybe you don't want to use beryllium, you want to use something else. But, yeah, that's definitely something we could look at. When the reactor is under emotions due to either quakes or ship motions, rapid transients with non-equilibria prevail. Do you plan to extend your model in the future under motions due to earthquakes or ship motions or rapid transients, will non-equilibria prevail? Yeah, it's a good question whether non-equilibrium will prevail. Oh, I see. He's saying that thermochemical equilibrium is no longer valid here. Yeah, so that's like what we do with Thermochimica where we assume that the reaction rate – where like the actual Redox reaction is instantaneous. It would be like an engineering assumption that we are making there that it is in equilibrium. But if you wanted to actually look at the actual kinetics, that might be more important for something where you have like a ship rocking, like you mentioned, then yeah, you could definitely use like the Poisson-Nernst Planck equations with the Butler-Volmer. That would give you maybe those transient analyses a little bit better to see how fast different effects are happening. But everything else, like the species transport and the neutronics and everything is time dependent. So yeah, the only real assumption there is that there's thermochemical equilibrium at every time step, which is what Thermochimica is doing, as opposed to modeling the kinetics explicitly. But yeah, the transport and everything would be ideal for those kinds of transients in ship-rocking.

Is it possible to track high aggressive elements such as tellurium transport? Yes, yeah, we can definitely look at – that's actually we have some models looking at tellurium right now, and I should say I forgot to mention that we have a project that's funded right now where we are looking at trying to validate a lot of these models using the molten salt reactor experiment. So that's some of the limited fission product data that we have, whether it's off-gas measurements or noble metal depositions or fission products within our graphite. So, we are trying to actually use these codes and capabilities and validate them against this limited data that we do have available.

And part of that is also like hitting that Redox potential increase. We want to look at – we have our depletion model with what we think the fission products are building up in the fuel salt. And then we want to look at how that fluorine potential can be recreated with MSRE. But yeah, an important aspect of this is tellurium. Right now, tellurium is not within the MSTDB-TC. So we would have to make some chemistry assumptions about how tellurium behaves. But we can definitely look at tellurium transport and how it's reacting, where it ends up. Like we can look at where it ends up in the reactor. As far as how it's reacting with where it ends up is the question that we'll have to look a little bit more carefully at. We could make some assumptions using the PNP model as far as kinetics goes. But yeah, not having it in the database really limits us. So, we'd have to make some conservative analysis guesses of how tellurium will be behaving at this time.

And also, if you want more information on tellurium, then we can always ask Ted Besmann, and say, hey, we want this element in our database to really understand how it's going to be behaving with all the other elements in our soup of elements. Right.

Not a question. Just want to thank you for your insightful presentations. Thank you so much.

All right, here's another question from Victor. Another name I know, not a face, but a name. Did you model tellurium intergranular cracking? No, I have not modeled that in this situation. And I think I previously touched upon the tellurium transport. I will say that we have another person that I did not mention here. I have not had the chance of working with him yet, but he is a postdoc out of Michael Tonks' group, who is. I think Michael Tonks is at Florida University, at Florida still. So he does phase field modeling. And so he would actually – so this new student, Chaitanya. Sorry, he's not a student, he's a postdoc. He is a new postdoc, and he's probably going to become a full-time staff very soon at INL. And so he's doing the phase field modeling effect of molten salts. And so, we want to take his models that he's developing, Chaitanya's models, and couple them with our Thermochimica and species transport capability to really get an idea of that multiscale aspect of corrosion as well, where we have delirium intergranular cracking and looking at the phase fields and then stepping that out to the actual species transport of it to the interface. So that's something that's definitely exciting. But we need to find more funding going forward to really get that multi-scale aspect really resolved well. How do you control Redox or for U free salt? So Redox potential control for U free salt is not as important I would say maybe, if that's what they are like, just fly [ph] salt with no fission products, no uranium concentration changing. Right. It's just fly [ph] salt and you want to control it. So you could do the same thing with beryllium. But then there's a great paper by Jong [ph] that talks about the three primary methods of controlling the Redox potential. So you can also fluorinate it. You can use like a – you can sparge it with HF gas to control the ratio of fluorine that way. And you can also use like a soluble buffer. So you could maybe put some – you could dope your salt with something else that then would maybe it's like europium 3 to europium 2, and that would control the chemical potential of the fluorine by the chemical activities of those two in relation to each other.

So, yeah, there's also other ideas that I've had that I think would be great as far as refueling and active chemistry control of your system. So I am looking at those right now and I hope to maybe publish something on that going forward.

So, does Thermochimica take into account the solubility of beryllium zero in fact. Yes, that's what we're doing there. So, basically, I have beryllium in the system, and I have thermochemical equilibrium between the beryllium that is in a solid state and the amount that's actually in the fly of salt. And so then we can – and then we assume that's instantaneous reaction. Right. So let’s say, yes, I have so much of these elements in this certain cell, and then it will tell me how much is going to be beryllium fluoride. Beryllium has different forms. There's not just BEF2, but there's also the not – I can't exactly say the right chemical term here, but, yeah, there's other forms of beryllium in the salt. Right. There's different complexes that it can form. And so, yeah, so it determines how much beryllium is soluble and how much is still solid.

So when we make that calculation, then we transport the soluble amount away from that interface, and it will continue to do that until the beryllium is – if I leave the beryllium in there, then it will continue to do that until the beryllium is then no longer – it's like the beryllium in the – yeah, basically, they're at equilibrium with each other. So that transient will continue until the beryllium is no longer being added into the fuel salts or maybe other things are being extracted, like uranium are plating out. So, until the fly of this is perfectly happy, the beryllium will continue to dissolve into the salt.

Are you looking to expand the application of coupled codes you presented to other reactor coolants, such as liquid metal fast reactors? That's a really good question. We can definitely do that right now with, like, the Pronghorn and the Griffin aspect, the Navier Stokes model for species transport. So you could use these same models to do source term analysis of SFRs. The thermochemistry aspect, probably not so much just because – I mean you could, but you would need to have the correct database for the liquid metal. And I am not sure how important those effects are as opposed to molten salt reactors, where they are very important. The thermochemical aspect of fission product behavior is very important in a molten salt, as opposed to maybe diffuse, just because the concentrations are higher because it's in the fuel salt. But I suppose like diffuse fuel failure, where you have certain species in the sodium that would be soluble, as opposed to gaseous in the sodium.

So, yeah, I would definitely say that the species transport aspect is totally there, but the actual chemistry or analysis, that aspect you would need to really look at that in more depth. So, thank you for your brief presentation. Thank you for your comment.

In the MSFR there's no beryllium in the fuel salt. Yes, that is true. And this was just kind of an example of looking at using beryllium to reduce it. But, yeah, like I said, the neutronic aspect of that is not favorable, and so you do not want to thermalize your neutrons. So, yeah, I totally see that. And you would need to use a different reducing metal. Whether you could use lithium, I mean you could definitely try but there are some concerns there as far as lithium is even more reducing than beryllium. And so, you could really over reduce your salt easily with lithium. So, you'll have to look at that a little carefully.

Hello. Thank you for your very interesting presentation. Could you explain why do you expect cesium iodine to be gaseous as its boiling point is 1280 C? Thanks. So, yeah, when I say that the cesium iodine is gaseous, I am really talking about a very small amount of the vapor pressure that's actually. So, it's a very tiny amount that is the vapor pressure that would form, that would then if there is a gas phase present, a very small amount will still, just due to entropy, will end up in the gas phase. So that's what Thermochimica is trying to try to take out of the database that it's processing. But, yeah, but you don't have like a stable cesium iodine gas phase, but you do have a very small amount of vapor pressure that would enter a gas phase that does exist. Like, say, you have a stable xenon gas phase, you will have a small amount of different species that end up in that gaseous phase.

Ranga from OPG, are you going to consider binary and ternary molten salt mixtures? If yes, do you have any potential candidate for simulation? Right now, the binary molten, ternary molten salt mixtures, that's what the MSTDB-TC is doing. So it takes both binary and ternary phase diagrams and then collects all this data together so that they are self-consistent. That way you can see how even in more exotic 5, 6, 7, 8 mixtures of salts, how the different elements should behave given their basis functions in their binary and ternary configurations. So, a better person to ask would be Ted Besmann to really understand how the MSTDB-TC is put together and the different assumptions that are made to understand how those elements are interacting in the fuel salt.

But yeah, this work is really trying to, given that we trust MSTDB-TC, that they are accurately putting everything together, this is what we expect should happen in a large system. Is it true that material science is the biggest barrier to entry for MSRs? If corrosion is such an issue, with what materials will the impellers in the pump and the thin tubes in the heat exchanger be made of? That's a good question. And it's definitely a bigger picture question. I would say that corrosion doesn't have to be an issue if you can control the Redox potential. But if you have large thermal gradients, it's unavoidable at some point. Right? And when I say large thermal gradients, like you have a very high temperature region in the core, and then maybe you are a very low temperature region somewhere else after the heat exchanger. So, if you have a very large difference there, then you will have just natural hot leg corrosion and cold leg deposition that's happening, even if your Redox potential is being controlled. But what materials will the impellers or the heat exchanger be made of? That's a very good question, and I don't know if I can answer that. But I believe that the MSRE use Hastelloy N for both of those materials. I'm pretty sure. Don't quote me on that, but that's something that can be researched. But I do know they use a lot of Hastelloy N in general, like a nickel-based alloy. But it's possible, though, if you want to not push certain limits to maybe bring the temperature down a little bit and use more off-the-shelf materials, as long as you are adequately controlling your potential, like I mentioned earlier, and you don't have a huge thermal gradient. So that's kind of my, just my off-the-cuff answer to that question.

Another Ranga from OPG. Thermal degradation of molten salt is an important issue. How can this be modeled, oh, how can this be included in your modeling? So, thermal degradation of molten salt. Not exactly sure what you mean by thermal degradation of molten salt. So, forgive my ignorance there. But I do know that as the salt goes through burn up, you will have a lot of fission products that will build up in your fuel salt. But as far as degradation, thermal degradation, I am not exactly sure.

Like maybe the heat transfer coefficient changing or something, I'm not sure exactly. Are you planning to use nitrate salt in your modeling process? No, not now, but like a nitrate sulfur, like solar salts I think is what you're talking about. That's definitely something that you could do. I believe that the MSTDB-TC has enough of the different binary and ternary models there to also have some of those solar salts that would be used for that modeling or for that purpose.

Right, for heat storage. So, I definitely think that's possible. But I'm not planning on doing it or at least right now, I'm not planning on doing that. I'll say that.

Hello, and thanks for your presentation. Can you model gas bubble generation from atoms to respectable sized bubbles? What tools should be used for that? Thanks, Antoine. So, yes, we technically could do this from atoms to respectable size. Yeah. So say you don't have a helium void in your reactor, and say you just have the xenon gas that is formed. So Thermochimica will – if you tell it that you have xenon, it will look at how much xenon you will need before you have a stable gas phase that's present. So then it would say, yes, your xenon is either dissolved in your salt or no, it's actually an unstable gas phase, depending on your pressure of your system that you specify. So, it's definitely possible to say your xenon is either dispersed in your fuel salt or whether it's actually at significant concentration where you have a stable gas phase present. And then as far as the bubble size, we're looking at the void modeling that we did put in there. We'll have mass transfer of xenon to interfaces. And so, you could have probably – I would imagine you'll have heterogeneous nucleation of gas bubbles. So, you'll have xenon transport to a surface where the concentration will build up, and then you would have a bubble that could form at the interface and then probably detach from the surface. Or if it's graphitic, then it will go into the graphite pores. Right.

But that's definitely something that we can start to look at using these models. The two-phase flow aspect is new, so we are working on that right now. But that's something that, whether you have a presence of a void or not, we want to be able to model, so that's a very good point.

And then lastly, did you look at the chemical and neutron effects of minor actinides in the fuel salt? Is the database from Ted Besmann, complete on this subject. Thanks for your presentation. So we do have some actinides in the salt, the neutronic effects. Not all of the actinides are there. I shouldn't say that. So, I know that you have thorium, plutonium, and uranium that are in the database right now. As far as the minor ones, I don't think there are that many that are there. So, you'll definitely need to reach out to Ted to ask him more information about that and when we could expect that coming in. I will say this, though, about database formulation, is that every time you add a new element, and you want to keep the entire system self-consistent, that it becomes incredibly more difficult each element that you add to your database. And so, it's no minor feat to add in anything. Right. So right now, I think he has like 16 or 17 elements in both the fluoride and chloride systems. And they take data from all over and they evaluate it and then they integrate it into this database. And so it's a lot of work, but I think, yeah, it's a huge problem. And so at some point you have to make certain assumptions maybe of how certain actinides would behave. And then you can use surrogates with the existing data that you do have, assuming that will behave similarly to another one, another actinide that you do have data for.

And then lastly, how would you control Redox potential in chloride salts? Thanks. So this one, similarly, you could do a reducing metal, whether you use sodium itself, but you do have to be careful. But that's just my off-the-cuff thinking is that you would use, you could also probably sparge it as well with like a hydrogen chloride gas. But that's just based upon the same idea of taking from the fluoride salt and applying it to the chloride salt. So that's just my off-the-cuff answer. Well, thank you so much. I think I got through them all right at the end of the hour or so.

Berta Oates
That was fantastic. Thank you very much for sharing your expertise and your passion. Your energy is just something that comes through. It's incredible to listen to your enthusiasm, and I really do appreciate what you bring to the table. Patricia, are you still – do you have any last-minute thoughts? I know that you have to hop off right at the top of the hour, which is where we're at.

Patricia Paviet
Yeah, I'm still there. I'm still there Berta. I was looking at the website for Ted, Professor Ted Bessman, that I could put in the chat. Yes, got it. Not sure I can do that, Berta. It's all live. I'm trying to see how I can share that with the people who are here. So, I see the chat box, Berta. You know, I'm gonna send it to you, Berta, right now. This is the link. We talked a lot about Professor Ted Bessman and the database that he's developing. So he has a website, and I send it to Berta. Berta, do you see it?

Berta Oates
I do.

I am sharing it now. It should be showing.

Patricia Paviet
Okay, very good. Okay. Very good Berta. Thank you so much. Really excellent presentation Sam. Congratulation again on being one of the winners of the 2023 ‘Pitch your Gen IV’ research competition. I am confident that we have a nice workforce, future leader of tomorrow. It's always nice to see that we have new people

coming in and juniors and the enthusiasts. And the number of questions. I didn't count them, but Bravo. When you have a lot of questions like that, and you are able to answer to the best of your knowledge. So, thank you very much.

Samuel Walker
I was just going to say that, if anybody has any more follow-up questions, feel free to email me, because I always like to interact with people and especially develop new collaborations, so.

Patricia Paviet
Yes, exactly. Yes, exactly. So, Berta, did you share the website with everyone?

Berta Oates
I did. I do believe it's now posted.

Patricia Paviet
Okay, very good. So, I think we're good. Thank you so much, Sam. Again, thank you very much, Berta, for putting everything together. And we see each other next month for the GIF/IAEA joint webinar presentation. So that would be a panel session a bit different than what we are doing. So thank you, everyone. Thank you, Berta. Thank you, Sam.,

Berta Oates
Bye-bye.

Samuel Walker
Thank you. Bye.

END
