Molten Salt Reactors Taxonomy and Fuel Cycle Performance

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Berta Oates
Welcome everyone to the next GEN IV International Forum webinar presentation. Today's presentation on Molten Salt Reactors Taxonomy and Fuel Cycle Performance will be presented by Dr. Jiri Krepel. Doing the introduction today is Dr. Patricia Paviet. Dr. Paviet is the Group Leader of the Radiological Materials Group at Pacific Northwest National Laboratory. She is the National Technical Director of the Molten Salt Reactor Program for the Department of Energy, and she is also the Chair of the GEN IV International Forum Education and Training Working Group. Patricia.

Patricia Paviet
Yes. Thank you very much, Berta. Good morning everyone. Good evening. It's a pleasure to have Dr. Jiri Krepel with us today. He is a senior scientist in Advanced Nuclear System Group of Laboratory for Scientific Computing at the Paul Scherrer Institut in Switzerland. He earned his Ph.D. in 2006 at the Czech Technical University, Prague, and the Helmholtz-Zentrum Dresden-Rossendorf in Germany for his thesis entitled Dynamics of Molten Salt Reactors. At PSI, he is responsible for fuel cycle analysis and related safety parameters of GEN IV reactors. Dr. Krepel is the Coordinator of the PSI MSR research, represents Switzerland at the GIF MSR project. He has recently been nominated Chair of the GEN IV International Forum MSR Provisional Systems Steering Committee. He has experience in the neutronics of liquid-metal and glass-cooled fast reactors and in neutronics and transient analysis of thermal and fast MSRs. Jiri, without any delay, I give you the floor. I am really, really happy. Sincerely, thank you so much, Jiri, for presenting this webinar for us today.

Jiri Krepel
Okay. Thank you, Patricia. Thank you very much for kind introduction, and I am really glad to see so many people from all around the world following this seminar.

I would like to start with two disclaimers. One is that I am typically trying to pass too many information. I hope you will be not really too over-flooded by it. The second one is that almost exactly 2-1/2 years ago, I did the first seminar for this GIF webinar series about thorium and uranium cycle comparison in many reactors.

This presentation is kind of a buildup or a continuation of that presentation, so you may have a look later. It explicitly focuses on MSR and MSR performance. I have divided it into seven parts. Firstly, I would like to mention the definition and taxonomy of molten salt reactors, then looking a little bit of cross-sections and reactor physics. Next would be definition or a kind of discussion of five neutronics performance parameters. Then looking on breeding capability and core size and [Unclear] from that is the breeding in open cycle, so-called breed and burn cycle, and then defining the burnup for liquid fuel which is not so obvious. The last part is a little bit detached. It's about radionuclides distribution and release during accidental conditions. I will also mention three publications during this presentation, which are more or less the source of all the information, and you can have a look later.

The definition of Molten Salt Reactors, I adopted from the IAEA-TRS report, which is still in preparation. I think it's not yet final version released. The definition says that MSR is any reactor where molten salt has prominent role in the reactor core. It can be fuel. It can be coolant. It can be moderator. This status report from IAEA is one document, which I used for preparing this presentation, and I tell you preparing this document and preparing the taxonomy for this document was very interesting, a collaborative work with many international colleagues. Knowing that it can be fuel coolant or moderator, there is a high flexibility what you can do with MSRs. It's not a single concept. It's an entire category of reactors.

The taxonomy was necessary, and we agreed, or we converged to something like three major families. The decision was not about, let's say, neutron spectrum or the type of salt or fuel cycle you use, but we kind of converged to something, which is rather like technological.

The three major classes are graphite-based molten salt reactors where there is graphite and salt, and it profits from the fact that graphite is compatible with the salt; homogeneous molten salt reactors where there is more or less nothing in the core, it's just the salt; and heterogeneous molten salt reactors where you have some structural materials, which is separating liquid fuel from another material. You can subdivide further these classes into families and types. For instance, for the graphite-based molten salt reactor, you have fluoride salt cooled reactors, so reactors where the fuel is embedded in graphite matrix, and the salt is acting only as a coolant. Then, you have the graphite moderated molten salt reactors, so reactors where the fuel is diluted in the salt and graphite is acting only as a moderator.

In the homogeneous MSRs, you can divide it into two families according to the salt type. You have homogeneous fluoride fast MSRs and homogeneous chloride fast MSRs. The types are defined by the fuel cycle type, and for fluoride it is thorium breeder or more or less plutonium-containing reactor, which covers both, enriched uranium burning and transmutation more or less. For chloride, you have a breeder, but you can also breed and burn reactors. At that time, when we prepared this taxonomy, there was no transmuter with the chloride salt. It's not mentioned here, but of course you can think about more types.

For heterogeneous MSRs, there is a non-graphite moderated MSRs, which needs structural material to separate the moderator, which is not compatible with the salt. And there are heterogeneous chloride fast MSRs, profiting from the fact that with fluoride salts, you can get quite hard spectrum, and you can probably afford to lose some neutrons on the structural material and dedicated coolant. Of course, liquid fuel gives you enormous flexibility, so there is also category or class of others, and these are typically obsolete or minor concept. I can read them, it's directly cooled MSRs, it's subcritical MSRs, hybrid moderator MSRs, chloride salt cooled fast reactors, frozen salt MSRs or hybrid spectrum MSRs or heterogeneous gas cooled MSRs. Those are not really followed, and those are typically obsolete. For each of the six major families, I have an extra slide characterizing a little bit.

For the fluoride salt cooled reactor, you can say that the type definition is based on the fuel, if it is pebbles or if it is solid fuel, which is not moving like prismatic or compacts. The primary heat exchange in this case takes place in the core because the fuel is solid and the salt is a dedicated coolant. It uses TRISO-particles in the graphite matrix. From neutronic performance perspective, it's a converter, you cannot reach breeding. For leakage utilization, it can use reflector. Typically, there are no blankets in this case. Then, for illustrative, for kind of picture how it may look like, I typically take a concept, which I found in the literature, which is the oldest one. Maybe, it's not always the same, but typically it's the case.

For characteristics, I would like to mention here that the coolant salt should be probably lithium fluoride beryllium difluoride, because the beryllium has a certain moderation power, and this salt has therefore a negative density effect. If you would use another salt, probably you may end up with positive effects. The specific fuel density is very low in some designs. You might have volumetric waste, volumetric spent fuel. The core can be transparent for neutrons because of that.

The second family are more or less graphite moderated MSRs. In this case, they are divided by the fuel cycle type. You have thorium breeder or uranium converter. The primary heat exchange takes place out of the core because the heat is converted by the fuel salt and the actinides as the fuel are diluted in that salt. Typical salt used here is lithium fluoride beryllium difluoride or even lithium fluoride alone. You don't need structural materials because graphite is compatible with the salt, and you can operate such a reactor as a breeder or converter.

You can achieve breeding in thorium cycle, of course only, and for leakage utilization, you can consider not only reflector but also multi-zone core like in the case of MSBR or even blankets. For characterization, the specific fuel density typically is higher than in fluoride salt cooled reactors, and the graphite lifespan is limited by its irradiation because there is no fuel inside. It's not limited by burnup. It's just lifespan due to irradiation of graphite. Hastelloy vessel is protected by the graphite, so it has a longer lifespan. If you want to breed, you may need to swiftly remove fission products and even protactinium.

Let's go to the third family. It's homogeneous fluoride fast MSRs. The types here are defined again by the fuel cycle type. It can be thorium breeder or converter or burner. Since the actinides are diluted in the salt, again, the primary heat exchange takes place out of the core. There are no structural materials. It's homogeneous. The core is just filled by the salt. It can act as a breeder. It's slightly more relaxed neutron economy. You don't need so fast fission product separation like in the MSBR in the thermal breeder, but still you need to do it. In this case, there is no graphite protecting the vessel, so you may need to regularly replace the reactor vessel. You don't use beryllium in this case because beryllium is a moderator, but the lithium fluoride, which you use also has certain moderation power. It is fast reactor, but it is the softest fast spectra, I can imagine. At the same time, it has low transparency for neutron, so you can end up with possibly quite compact cores.

Next, the second homogeneous are the chloride fast MSRs. Again, types are defined by fuel cycle. It can be a breeder in uranium-plutonium cycle or even breed and burn. I don't mention here thorium cycle; I will come to it later. Again, actinides are diluted in fluoride salt, so the heat exchange takes place out of the core. For leakage utilization, we use blanket or reflector. The first design I found in the literature is from 1956 in this case. Again, you have the same issue as in homogeneous fluoride fast MSRs, the vessel is irradiated by neutron, so you may need to replace it very frequently. Compared to lithium fluoride, which I mentioned earlier, in this case you have typically sodium chloride, and there is kind of absence of scattering or moderation power in the salt. These reactors can be quite transparent for neutrons. As a consequence, you have very hard spectrum, but also you may have a very large reactor.

The fifth family are non-graphite moderated molten salt reactors. Here, it is a little bit more complicated to discuss because the types definition is by the moderator state, you can have solid or liquid moderator. For the liquid moderator, let's name heavy water or sodium hydroxide from the two startups from Denmark. It's not easy to conclude if the primary heat exchange takes place in the core or not because in some cases you can decide that the moderator will act as a heat exchange medium. In some cases, you can say, "No, I will still use salt," as a medium, which is converting the heat out of the core.

Breeding in these reactors is questionable because you really rely on the neutron economy of the structural material, which is separating the fuel from the moderator. The example here is from 1954 from the kind of scoping period where people looked on many different designs. Of course, in this case, the limited lifespan is of the separation materials, of the tubes, which are in the reactor, and the tubes or the material also determines the neutronic performance.

The last family are heterogeneous chloride fast MSRs. In this case, you put the salt into fuel pins, and it's surrounded by dedicated coolant. Salt typically does not have heat exchange function, even though you can decide other way, but since you put the fuel in pins, you don't want to pump the salt extensively. Again, typically rely on sodium fluoride or other fluorides. You can breed. You can use it as a converter. Breed and burn is questionable; theoretically possible, but questionable. In this case, probably, this is not the oldest design, but I picked up this because it's a Swiss design from 1972 where the fuel salt was cooled by blanket salt actually. Again, lifespan of separation material reducing the neutronic performance, but possibly may provide some scattering, so maybe it may result in smaller course. Nonetheless, I cannot say from my own experience, because for the heterogeneous MSRs, I have the least experience from the six families, and it is because the design data for these reactors are typically not available. It is much easier with graphite moderated reactors or homogeneous reactors than with these heterogeneous reactors.

Now, let's have a look, what materials can be used in these reactors, in these six major families. They are identified in four groups of materials like water-like; hydrogen, deuterium, oxygen; or liquid metals or gases or salts including two isotopes of lithium, beryllium, fluorine, natural magnesium, chlorine 35/37, natural potassium, calcium. Okay, sodium was already included in the liquid metals. I had a look on cross-section, so typically on capture cross-section, which you can see here. In this plot, the color scheme is selected so that the brown curve, typically, you see it's lithium 6, indicates a high capture, and the edge kind of middle capture rate is lithium 7, so whatever is above lithium 7 is brownish, and once you are below lithium 7, you get to green theme, and dark green is low capture. The capture cross-section was determining the color scheme. If you look on scattering cross-section, you see that there is no correlation between capture and scattering. The colors are really, really randomly distributed here. You can also see that they have different shapes. The capture cross-section is strongly evolving with the energy of neutrons, whereas scattering cross-section has certain plateau there.

It's very hard to discuss and analyze this chart, so what I did, I have averaged the cross-sections in two energy ranges, in energy range of 0.1 eV and in an energy range of 0.1 MeV. If you do this averaging, what you obtain, for instance, for the thermal scattering is this chart. Here, I would like to say that the order of the nuclides is selected so that the most scattering is on the top, it's hydrogen, but the color, which is representing capture is still preserved. To discuss a little bit more, how these materials can moderate, of course, you need also to include the logarithmic decrement of energy ξ, and I did the product of these two to define or to generate something like moderation power. You can see microscopic moderation power, which is not really a classical definition.

If you look on this moderation power, you see that hydrogen is the best. Yes, it's really by one order better than everything else. Deuterium is the second with more or less 10 times lower moderating power and beryllium almost 20 times lower moderating power. Surprisingly, number four is chlorine 35, but we don't use it as a moderator, and the reason is simple because it has a tremendous capture cross-section. The first from this perspective is lithium 6. We are typically enriching lithium to get rid of lithium 6, whenever lithium is used in thermal spectrum, even in fast, I would say, and typically the chlorine is also enriched, if you want to improve your neutron economy.

Now, you can have a look on moderation power in fast neutron range. It's a fairly similar chart as in the thermal range, but I would like to point out here that, for instance, fluorine is a more strong moderator in the fast energy range. It's not only a moderator, but kind of the moderation power in fast energy range is higher. The same is valid for lithium and for magnesium, and the reason is that there are resonances of scattering cross-sections, which are increasing actually the average cross-section. This is the reason why, for instance, lithium fluoride, it's not a moderator, but it's suppressing the spectrum. Then, you can have a look on fast capture where, okay, lithium 6 is outstanding, it's really capturing a lot. Other materials are, let's say, okay-ish. Of course, again, chlorine certified is questionable, but it's comparable to lead.

You can use these data, and you can kind of conclude which new guys [ph] are moderators, of course, you know all of the moderators, and which nuclides have suppressing fast neutron spectrum. Here, I would like to point out fluorine or lithium 7 or magnesium, which nuclides can be used for breeding in terms of spectrum, typically all moderators, but not hydrogen because of its higher capture, and which can be used for bidding in fast spectrum. Here you exclude moderators, and in case of fluorine you can do that, but you get really soft fast spectrum.

I have another slide about other materials. I will not spend much time here. Just mentioning that nickel, which is often used in alloys, has roughly twice higher capture cross-section than iron. Silicone, which is sometimes together with carbon silicon carbide foreseen for kind of a good economy neutron core is quite good from capture perspective and scattering perspective.

I wanted to characterize in this presentation actually these reactors from reactor physics perspective, but once again we have six families. We have fluoride salt cooled reactors. We have graphite moderated MSRs, homogeneous fluoride fast MSRs, homogeneous chloride fast MSRs, then non-graphite moderated MSRs, and heterogeneous chloride fast MSRs. It's not straightforward to do that, and I will do it very briefly just making a bullet-wise list of features or issues.

I would like to mention double heterogeneity, which is relevant for the first family. This first family is kind of cross breed of HTR and MSR. It has the same issue as HTR. Next one is the graphite limited lifespan and positive temperature effect, of course, for graphite moderated MSRs. You can have positive coolant and blanket density effect in the systems where there is a dedicated coolant. You can have large migration area, typically in graphite moderated reactors or in reactors with chloride salts. Fuel volumetric heat up and homogenization, this is valid for all reactors where there is liquid fuel. Power level determination and peaking in the core is the opposite, it's in the reactors where you have either solid fuel or liquid fuel in pins where the heat exchange surface is determined by the pin geometry, and you have issue of the power peaking.

Local overheating and excessive burnup, it's valid for reactors with liquid fuel where you can have stagnation zones or a little bit of fuel salt enclosed by structural material. Fission products circulation or you can say this famous delay neutron rift, again for all reactors where the fuel is extensively circulated or pumped through the reactor. Removal of gaseous and non-soluble fission products, typically, it is applied because it helps to improve neutron economy, but it also has some impact on the core layout and so on. Protactinium 233 longer half-life, it has roughly 11 times longer half-life than neptunium-239. In some cases, you really need to separate the protactinium from the reactor so that you can let it to decay outside of the neutron flux to reduce its parasitic capture. Limited structural material lifespan, more or less in all families you face it more or less.

Here, I would like to mention that after this IAEA report about molten salt status, the second report I really rely on is the Molten Salt Reactors and Thorium Energy. It's the second edition of a book, which is in preparation. I am not sure even if I could present what I do just now because I am more or less presenting some outcomes of this book. It should be the chapter four about reactor physics, but I use it as a kind of chance to advertise this book.

There are five neutron performance parameters where the first foremost is breeding capability. If you think about it, it's straightforward. It's more or less indicating how many neutrons can be captured on uranium-238 or thorium-232. It's nothing else than that. How many neutrons you can waste or lose being captured on these two materials? The reason why we are typically – and enriching uranium is the exact opposite. You want to reduce the capture of uranium. You want to reduce breeding if you are enriching your fuel. It also depends on the reactor type, so it's not fully so straightforward.

It's about neutron economy, and I would like to name for MSR here that you can avoid structural materials in many families, so it can help your neutron economy. The second parameter is achievable burnup, and it's limited by fission products parasitic neutron capture and of course fuel irradiation stability. It depends on initial reserve of fissile material, so it may be much better in the breeders. Here, I would like to name the radiation stability of the salt. It's not limiting you. You are limited by the other factors. Now, initial fissile mass as the third parameter, of course, again determined by neutron economy and spectrum type. Sometimes, if it is not a breeder, you need to hire initial excess of fissile material to reach higher burnouts.

Here, I would like to name online refueling and removal of some fission products, which is also relevant for the achievable burnup, of course. Fourth parameter is means of criticality maintenance. The change of actinides and build up fission products results in reactivity oscillations and the compensation needs may differ between reactors. You have liquid fuel, so you have chance to reshape or drain the fuel from the reactor in ultimate case. The last one is transmutation capability. Roughly speaking, it's neutron costs and speed of synthetic actinides fission. Of course, here you also need compatibility of the fuel with synthetic actinides. This may be the big advantage of MSRs, if they would be used as transmuters, that there is absence of fabrication step and solubility of the respective actinides is kind of limiting factor here. From these five, of course, the breeding capability is the most important, and all five depends on neutron economy.

Neutron economy is also determining four reactor classes based on breeding capability. Burner as the first one more or less avoids fertile materials like uranium-8 or thorium-2. It has the lowest neutron economy from this perspective, and it's meant for burning of synthetic actinides. Converter typically like light water reactor or denatured MSR use enriched uranium and the discharge fuel finally contains more or less the same amount of plutonium as of uranium-5. In breeders, I will speak here about uranium-plutonium cycle as on the illustration, you preserve the fissile mass. You discharge fuel, which has the same fissile mass as the initial fuel and you profit from this only in case you really recycle the fuel. Then, in case you have really excellent breeder, which is overbreeding, you can even operate it in breed and burn mode where you load fuel from depleted or natural uranium, and you discharge fuel with a lot of plutonium, and in average the core is critical.

Now, for the purposes of the next few slides, I need to do a small detour [ph] to nuclear physics because irradiation of thorium-2 and uranium-8 results in kind of irradiation chains. I would like to show you nuclide chart, and I would like to point out that there is kind of a repetitiveness of actinides properties with a period of two protons and four neutrons. If you look on the nuclide chart, you can see that thorium-2 and uranium-8 are at the same position from the stability line, and this is probably the reason why we have them as primordial actinides on the earth. For plutonium-244, which would be the next one, it was nearly possible to be primordial nuclide, but unfortunately the half-life and the age of Earth didn't allow it.

Now the irradiation trajectories or chains are very similar for these two nuclides, but there is one big difference. In thorium chain, at the position of uranium-5, you have uranium-5 at certain position which has a very long half-life and decaying by alpha decay. At the same position in uranium-8 chain, you have plutonium-241, which is decaying very, very fast with beta minus decay. This is the major difference between these chains. Second thing or third thing I would like to point here is, in general, there are more nucleons in uranium chain. In general, all the elements have slightly shorter half-lives, but for the same reasons typically also produce more neutrons per fission.

I spoke about neutron balance, and I don't have time to go in real detail, but neutron balance has components. One is neutron leakage. Second is, let's say, parasitic neutron absorption on non-fuel materials. Then, you have the neutron balance of the actinides itself. I really like the very famous Eta-2 neutron balance as an indicator of breeding. But if you look in detail on it, you need to introduce correction factors to see the reality. You should account for fast fission of the fertile material. You should account for parasitic neutron captures on the daughter product. In case of thorium-uranium cycle, you should consider parasitic neutron captures on uranium-4 and its daughter products.

The last term also includes the parasitic neutron capture on protactinium, which leads to uranium-4 and its daughter product. This is the neutron balance you can do, and the reason why you can do it so nicely is that – or why I could do it so nicely is that I was doing it for equilibrium state. I had equalized composition of uranium-8 and thorium-2 irradiation chains, and you can do this balance in many different ways. This was first, and the second one is you just do Nu-2. You take all the neutrons you have from fission. You subtract two neutrons because you need one for fission, one for breeding. Then, you have fast fission on the fertile, and then you have capture of actinides as a kind of correction factor and end-to-end reaction as extra neutrons.

You can do also like neutrons per fission, and you can subtract the neutron costs of fission. For instance, if you fission uranium-3 and you know it's coming from thorium-2, it costs you two neutrons; if you would fission uranium-5, it will cost you four neutrons. The last is the simples [ph], more or less the neutron balance of thorium irradiation chain. It's nothing else than the famous D-factor of thorium-2. I will not discuss what is D-factor; you can have a look in the literature. But more or less it's the neutron cost to burn certain nuclides together with its daughters.

I did enumerate these neutron balances for the first four families because I don't have much data for the fifth and sixth, for the heterogeneous MSRs. There is also migration length in the table. You can see the first line, and you can see really that chloride salts are really transparent for neutrons and the same is valid for FHR in case of pebbles. I will not waste time here going to details, but I will show the first balance, the Eta-2. If you would just do Eta-2 without any correction, you would get something, which is ranging from 0.18 to 0.31, neutrons per fission. It looks very nice for thermal spectrum, but then you need to introduce the corrections.

For instance, in the case of FHR, you see that from 0.25 you drop down to 0.06 neutrons because of parasitic absorptions of higher nuclide. Very often some people present paper about breeding and they say, "Yeah, it can breed," but the statement is valid for a fresh core or is valid for the first few cycles. It's much different if you go for the second, third, fourth cycle and you build up the higher actinides. The second balance, of course, you end up with the same numbers, but you start from Nu-2, which is less accurate than Eta-2. Firstly, with the correction factor, especially with the capture of actinides, you get the right numbers, and then the fission costs, again the same results and D-factor is roughly the same result.

With one click, I will change these numbers from thorium cycle to uranium cycle, and what you can see immediately here is that there is much deeper flow. The neutrons are more or less – the balance of neutrons is negative in all thermal reactors, and it's much stronger positive in fast spectrum, and the H [ph] when it is becoming positive is between MSFR with FLiBE and FLi salt. Whenever you have beryllium in the salt, you cannot breed in uranium-plutonium cycle; when you remove beryllium, you can theoretically.

You can make it graphical to make it easily digestible. Obviously, uranium-plutonium cycle is quite good or excellent when you are in hard spectrum. Thorium cycle is more balanced, therefore you can potentially breed in thermal spectrum. Graphite moderated reactor only can breed in thorium cycle. For fluoride fast MSR, you have kind of equal performance and almost epithermal spectrum. For chloride fast MSRs, you can go for both reactors. But you can already now see that the neutron balance, the excess of neutrons in thorium cycle is almost half of that one of uranium cycle, and this will have big consequence on the core size, and the breed and burn mode is only possible in uranium plutonium cycle.

The other parameters, I will just go swiftly through it because I don't have anything equally elaborated. For achievable burnup, I would like to point out that it's mainly a question of ratio between fission products and fissile actinides. If you have a reactor, which is breeder in thermal spectrum, you have a lower reserve of fissile actinides, you are much more sensitive to fission products. In fast spectrum on the other hand, if you have more than 10% of fissile actinides, you can, of course, afford 10% of fission products much easily than in thermal spectrum where you have 1% or 2% of fissile material and

10% of fission products, which represent five5 to 10 times more of something absorbing than something fissile.

The initial fissile mass again, here is only the specific density of fissile nuclides in these MSR examples. Of course, in the terminal spectrum, typically you have less actinides and from these actinides lower percentages fissile, you can really have a much lower initial fissile mass in these reactors.

For means of criticality maintenance, I don't even have an illustration, it's quite boring slide, but okay. You have liquid fuel. You can remove fission products. You can add actinides. You can use unusual reactivity control methods because the salt is liquid, you can expel the salt by kind of empty cylinders to tune the reactivity. For accidental conditions, you can even think about kind of overflow systems and so on.

For transmutation capability, as the last parameter, typically you should have a look on radiotoxicity balance if you are in open cycle or on reprocessing losses. But you can also have a look on speed or pace of transmutation which is proportional to the cross-section, and of course, the cross-section is always higher in thermal spectrum. You can also have a look on neutron costs. How many neutrons it costs? I have an example here for plutonium-242, and you see that in thermal spectrum it consumes one neutron to get rid of one atom of plutonium-242 and in fast spectrum it almost produces one neutron for the same because of the fissile daughters, which are in the chain of plutonium-242.

I will again look on the breeding capability, but a little bit more realistic cases. In my previous presentation 2-1/2 years ago, I was already showing this slide where we looked on five different fluoride salts and six different moderators, and the outcome was kind of a parametric study where we changed the salt share. On X-axis, there is salt share in the core, and on Y-axis, there is a channel radius, kind of heterogeneity study. What you can see here is that lithium fluoride is neutronically the best salt that heavy water and beryllium are really good moderators. You can more or less forget hydrogen, if you would like to breed, and graphite is nothing special, just it is the only one which is compatible with the salt. You can directly use these results, which didn't include the structural materials for separation of the moderator.

If you would include it, for instance, in the beryllium or heavy water case, you would get curve like this where the full line is the original performance and the dashed lines are for three different separating materials. Obviously, the only thing which works is silicon carbide or carbide-carbide composites. I am joking on this slide usually that purely from neutronic perspective, we can design heavy water boiling MSR.

Let's have a look for fast reactors. For homogeneous fast MSRs, similar study, five fluoride salts, three chloride salts, and analysis of the performance. This is a very convoluted chart. It is based on one of the reactivity balance method, but what we can see here is that from chloride salts the enriched sodium chloride is the best and from fluoride, again, it's lithium fluoride. The beryllium, because it's moderating, really does not help in the fast reactors. The actinide fluorides, the last column, I kind of neglect because the melting temperature of that would be probably too high.

The same for uranium cycle, looks similar, but the reactivity axis for enriched sodium chloride salt is much higher. This is also the reason why you think about breed and burn. You can also operate it with natural chlorine. There are four almost equal salt for fluoride. But, of course, the question is, if you can at all operate it because of the limited plutonium trifluoride solubility?

Now, let's have a look at the core size. If you would compare it directly with classical sodium and gas cooled reactors, which are shown here, the homogeneous fluoride salt-based fast reactor would be roughly a bit like this, the blue square. In uranium-plutonium cycle, it will be slightly bigger, and if you will stay by uranium-plutonium cycle and switch from fluoride to chloride, you will get more or less the same performance. The difference between five and six in size is small, but it is by chance because in chlorides the core is really transparent and profits from really, really high k-infinity of the salt, whereas in fluorides the core is kind of scattering neutrons and the k-infinity is much lower. So, by chance they are almost equal.

If you would change to thorium cycle and fluorides, you have lower k-infinity, and the transparency makes the core really big. For comparison, this is the size of MSBR designed Oak Ridge, but here the salt content in the core was only 13%. It's not the same as a homogeneous reactor fully filled by salt. You can also do kind of criticality line using the Fermi barcode theory because you know the migration length, and on this slide, you can see the position of uranium-plutonium cycle and thorium-uranium cycle.

If I just skip to another slide, it shows you that whenever you have a fast spectrum, uranium-plutonium cycle is performing much better, provides you much smaller reactor, and the edge where it is changing is somewhere around MSFR with lithium fluoride salt. These two points are more or less on the same spot. If you put beryllium in the salt, if you have FLiBE there, you cannot at all breed with uranium-plutonium cycle, only with thorium cycle.

The core size also depends on the breeding gain you wish. I was showing the core size for breeding gain zero so [Unclear] breeding reactors. If you would like to have lower breeding or higher breeding, of course, you must change the core dimension respectively. Thorium cycle is much more sensitive for that, you may need to exchange the core size more than in uranium-plutonium cycle, of course.

I have still three topics to speak about, so I need to a little bit speed up.

There is also self-sustaining breeding option in open cycle, which is called the breed and burn. In solid fuel case, you load assembly, which is from depleted uranium, it is traveling or reshuffled through the reactor, and you discharge the most burnt assemblies, and the core is critical because in average there is enough plutonium. In liquid fuel case, you will load the same depleted uranium with salt and what you have in the core is in case of single fluid its average composition, you are discharging average composition, not the most burnt composition. Of course, this may change if you have multi-fluid, but you still discharge the average composition in the last volume. There is something like fuel residence time distribution, and the average burnup of the salt more or less is a function of this residence time and of course also the fission products share is a function of the reprocessing or removal of fission products.

For that breeding, you can define a simple criteria because the fuel or the salt you are discharging includes fissile material and your conversion ratio and your burnup must be so that the fissile material you are discharging is an excess. You will not miss it. You are discharging fuel, which includes excess of fissile material. To achieve that, same example, if your conversion ratio will be 1.2, you need to reach burnup, which is five times higher than the fissile share. If you have fast reactor with 10% fissile actinides, you need to reach 50% burnup with conversion ratio 1.2 so that the fissile material discharging is just breed [ph] excess. This makes the breed and burn a little bit challenging, and it's always question of the core size because you would really like to minimize leakage.

Here, I have curves for equilibrium, k-infinity. If you simulate this breed and burn on infinite lattice, you can see that thorium cycle is nearly impossible, in mixed cycle maybe, and for uranium cycle it is possible, and the more actinides you manage to pack in your salt, the better is the performance. Of course, the smaller is then finally your core, but the question is if chemistry and the melting temperatures allow for something like very packed actinides in the salt.

You can then compare the core size for closed fuel cycle and breed and burn open cycle. Because you need to utilize the leakage more in the breed and burn cycle, of course, you end up with bigger cores.

I wanted to also speak a little bit about the burnup definition, and let's start with solid fuel reactor where it is, I hope, straightforward. If you have a burnup, which is defined like gigawatt base per ton of heavy metal, you integrate the power you produce and you divide it by the mass of actinides, you load it to the reactor to produce that power. You can also define it as a FIMA percent, you integrate the fission rate and you divide it by number of actinides atoms you loaded to the reactor. Both definitions, I hope, are quite straightforward. The fission product sharing the core is more or less equal to burnup if you express it in the FIMA percent units. It's straightforward and relatively easy to understand. In liquid fuel, it's a little bit more complicated, and you can define the burnup as a differential property. You can divide the current power of the reactor with mass of actinides you are refilling to the reactor in case of stabilized operation.

If you do this in FIMA percent, it's fission rate divided by atomic concentrations or total number of atoms you are refilling to the reactor. You can approximate this a little bit by the balance of actinides or balance of fission products, but it's much more complicated. You can also have integral definitions, more or less where you do integrate these properties, but in that case you need to account also for the initial actinide mass you loaded in the core. Obviously, these two definitions will differ between each other and they also differ from the definition from solid fuel.

I have now two examples, what it can cause, so first of all, that the share of fission product is not equal to the burnup in FIMA percent. I showed curves showing the k-infinity evolution as a burnup for the breed and burn reactor. You can see it again here in this chart as a function of differential burnup, but you can plot it also as a function of fission products share in the core. One of the first publications we did about breed and burn was including this information. It was the curve as a function of fission products share in the core, and if you replot the same curve for the differential burnup, if you account for the fact that fission products are removed from the core, you get slightly different profiles.

Another point I have here is that if you have stabilized operation for a long time, the integral and differential definition will converge to each other. Here, I have more or less an integral definition of burnup for breed and burn reactor, and you will see that it starts at zero because the initial mass of actinides in the core is tremendous. It takes a long time that you see some reasonable integral burnup, but the longer you operate the reactor the more it converges to the differential burnup. This was kind of a theoretical intermezzo.

I am coming to the last part of my presentation, which is a little bit detached from the rest, and it's about radionuclides distribution and release during accidental conditions. As I mentioned, molten salt reactors may profit from the fact that you are removing fission products from the reactor. And I pick up as an example here the EVOL and MARS benchmarks, which was based on the MSFR core developed in Europe on simplified geometry of this core. This core is based on lithium fluoride carrier salt typically in thorium cycle and has a blanket. There are two major reprocessing streams. There is a removal of gaseous and volatile fission products with cycle time of 30 seconds and then the reprocessing of the fuel salt with a cycle time of 450 days. I would like to stress here that zirconium with proton number 40 is not included in the gases and volatile fission products. It's not really removed by bubbling.

If you simulate this reactor, then you can get a distribution of radiotoxicity, let's say, normalized per 1 cubic meters of salt and after 200 years of operation of such a reactor. It's immediate radiotoxicity after shutdown, so it may change within minutes or hours. But immediately after shutdown the major component of radiotoxicity is in off-gas system. From this 15 presented decay chains of fission products or actinides, more or less in 13 cases the major component is in the off-gas system. Only in two cases, it is in the core. First case is the rank 11 where it is caused by protactinium and thorium-3 decay and rank 14 where even though it's probably fission products, which are not removed by off-gas system. There is not much left in the fuel salt, but once again this is immediately after shutdown.

What we did in that study is that anyway assume that you have a fuel salt, which can be spilt. As simplified containment was considered and an idea that there is some leak of salt and all the fuel salt was spilt to the bottom of the containment and that it was heated up by decay heat in 2 hours to 1500 K, and now we try to simulate what will be released from that spill. For that, we used MELCORE loosely coupled with GEMS. GEMS is thermo-dynamics code providing the properties of compounds to MELCORE, and it relies on the HERACLES database for that case.

We needed to update a little bit, the HERACLES database includes some new species and to have something which can calculate the activity coefficients and provide it to MELCORE.

I have three slides of examples of the results. The mass released as a function of fluorine content. The middle chart is for stoichiometric case. The left one is where you have 1% less fluorine and the right one for 1% more of fluorine. These three charts are only for actinides, actinide species, and you can see that there is quite strong dependency typically for uranium pentafluoride and thorium trifluoride. Thorium trifluoride, that is, less fluorine is dominating. When there is more fluorine, it's almost not there, and the opposite is for uranium pentafluoride. When there is less fluorine, it's almost not there, and when there is more fluorine, it's dominating. The same was obtained for fission products, but the dependency there on the, let's say, redox potential of fluorine content was not so strong.

You can process the result, and you can also look on released activity in Becquerel in form of aerosols on the left and vapors on the right.

Ultimately, you can then conclude what is your major carrier of radiotoxicity, and what we find out in that case the major carrier is zirconium. Now of course, the question is, zirconium tetrafluoride, it has higher vapor pressure, why it is at all in the salts still, why it doesn't leave the salt so to off-gas system? This is a kind of open question and could be that if you change the simulation of the off-gas system that this radiotoxicity component will be not evaporating from the fuel salt, but it will be present rather in the off-gas system.

This was a part, which does not really fit the overall frame of the presentation because it was not so much related to the fuel cycle. But the removal and reprocessing of the salt, of course, it's strongly influencing the fuel cycle performance, and often if you want to create your own design, what you do, you include some coefficients of removal and often these parameters may be not realistic. This was probably the message related to the fuel cycle.

Okay, that's all I prepared for today. I hope that it was understandable and not really too fast, and I hope you will have some questions.

Berta Oates
Thank you, Jiri. Before we move to questions, we will take a quick look at the upcoming webinar presentations in February; Safe Final Disposal of Spent Nuclear Fuel in Finland; in March, Advanced Reactor Safeguards and Materials Accountancy Challenges; and in April, a presentation on Overview of Nuclear Graphite R&D and Support of Advanced Reactors.

There have been questions regarding the handouts, and I apologize for the formatting. It has been pointed out that the sizing was incorrect, and there are some garbled characters that has been corrected, and unfortunately, I cannot repost them during this webinar presentation. So, be advised that they will be uploaded, the proper ones will be uploaded to the GIF website at www.gen-4.org following the presentation. It is recorded and that webinar recording will also be made available.

Okay Jiri, I have elevated you so that you can read the questions also. The first one, is the end-to-end reaction with these ions-containing beryllium should affect neutron economy there?

Jiri Krepel
No. If you speak about the neutrons based on beryllium, no. It's not in the balance. In the actual simulation, it may be there, but not in the balance, of post-processing the balance.

Berta Oates
Thank you. Have you also quantified neutron balance and other characteristics for MSRs and the hypothesis of using thorium-plutonium as startup fuel, could be generic plutonium vector similar to that of fresh MOX fuel?

Jiri Krepel
We did some analysis how to start thorium fuel cycle and to use, for instance, reactor-grade plutonium, but I didn't show it much in this presentation. You may have a look on the previous presentation 2-1/2 years ago. But in this presentation, it was mainly focusing on the equilibrium vector because the beauty of the equilibrium vector is that it's only one. If you give me a reactor design, I can calculate this vector and its Eigen value of the system. Knowing this Eigen value, I can assess the performance of the reactor, and it's only one kind of set of data. Transition from different plutonium vectors, it's published, we did it, Boris Homburger did it and co-authoring the paper, so you can try to find it. You have many options how to do it, if you will keep the material in the reactor or if you put it in blankets, and you will cumulate the material somewhere outside. There might be many other options, so I didn't include it in this presentation. But of course, if you have plutonium, you profit from almost renewed transfer fission, it's much easier, so to say, to breed new fuel with thorium material.

Berta Oates
Thank you. What condition needs to be achieved for complete burnup of transuranic elements in the fast reactors?

Jiri Krepel
Okay, this is equally good question as how to define the transmutation performance. In fast spectrum, you have the advantage that if you start to burn, for instance, the plutonium-242, ultimately, you will gain neutrons from its transmutation. But it does not tell you how many daughters you will generate and how long it will take to burn it. But roughly speaking, I mean, if you think about efficiency of burning, you can say I have reactor with installed power, this rector will burn in one year X tons of actinides. The question is only how many persons from this mass will be the material I want to burn and how many percent will be the material, which was bred and I didn't want actually it to be burned. There is no generic answer, but for any system you can say, okay, how many percent of the material I loaded was burned from the mass each was burnt in total.

Berta Oates
Thank you. That's all the questions I see that have come in. Again, there are several dealing with whether or not the webinar was recorded and available, and again it is, it has been recorded, it is recording now. The recording and the slide deck will be posted to the GIF's website. Just give us a couple days to get that rendered and uploaded.

Jiri Krepel
Yeah, I don't know. I see also a raised hand, but I don't know if this is still actual, maybe – it was 78 minutes ago, so probably not actual anymore.

Berta Oates
Yeah. I don't see one now.

Jiri Krepel
Yeah. If there should be not another question, I will just repeat that there are three sources of literature you can have a look. One is the IAEA report. The second one is the second edition of Thomas Dolan's book. The third one, which probably I didn't stress enough, is a set of three chapters in [Unclear] encyclopedia dedicated to self-sustaining breeding. If you Google or if you have a look on the references, I mentioned on my slides, there are three parts of self-sustaining breeding documents where many things, which I presented are described.

Berta Oates
Great. Thank you for sharing that. Thank you again for sharing your expertise and presenting all of this information. It's very interesting, and you can tell from the number of participants and the interactive

questions and answers the level of interest. Patricia, do you have any closing thoughts?

Patricia Paviet
I think it was a very good webinar. I would love to thank Jiri again for the presentation. Like Berta said, we have a YouTube channel give education and training working group, so you will have the presentation available on the YouTube channel as well as the GIF portal. I would like to thank all the participants, and we will see you in a month.

Berta Oates
Thank you.

Jiri Krepel
Thank you.

Berta Oates
With that, we will close. Bye-bye.

Patricia Paviet
Yeah. Bye-bye everyone. Bye.

END