United States

Nuclear Waste Technical Review Board (NWTRB)

Transcript

DOE Research and Development Activities Related to the Geologic Disposal Safety Assessment Framework

Fall 2021 Board Meeting

VIRTUAL PUBLIC MEETING – Day One

Wednesday

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NWTRB BOARD MEMBERS

Jean M. Bahr, Ph.D.

Steven M. Becker, Ph.D.

Allen G. Croff, M.B.A.

Tissa H. Illangasekare, Ph.D., P.E.

Kenneth Lee Peddicord, Ph.D., P.E.

Paul J. Turinsky, Ph.D.

NWTRB EXECUTIVE STAFF

Daniel Ogg, Acting Executive Director

Neysa Slater-Chandler, Director of Administration

NWTRB SENIOR PROFESSIONAL STAFF

Bret W. Leslie

Roberto T. Pabalan

Chandrika Manepally

Hundal Jung

NWTRB PROFESSIONAL STAFF

Yoonjo Lee

NWTRB ADMINISTRATION STAFF

Davonya S. Barnes

Jayson S. Bright

Sonya Townsend

Casey Waithe

PROCEEDINGS

>> BAHR: Hello, and welcome to the U.S. Nuclear Waste Technical Review Board's Fall Meeting. I'm Jean Bahr, Chair of the Board. This meeting will focus on the U.S. Department of Energy's research and development activities related to the geological disposal safety assessment software framework. Due to the Covid-19 pandemic, we're holding this meeting in a virtual format. Mr. Jake Swenson of Precon Events will serve as host of the meeting. If we can go to the next slide.

First I'll introduce the other board members and then briefly describe the board and what we do. I'll then tell you why we're holding this meeting and summarize the meeting's agenda. So at this point, we want to switch to the panel view so that I can introduce the board members. I'll ask that as I introduce the board members, the board members activate their cameras and come online and say hello so that the audience can see who they are. So are we in panel view? Yes. Okay. So I'll begin. I'm Jean Bahr, the board chair. All of the Board members serve part time and we all hold other positions. In my case, I'm Professor Emerita of Hydrogeology in the Department of Geoscience at the

University of Wisconsin-Madison. Our first two board members are only able to join us today by audio. The first of these is Dr. Steven Becker. And so you'll see a little slide with Steve's, with the board's logo there. Steve is Professor and Chair of Community and Environmental Health in the College of Health Sciences at Old Dominion University in Virginia. And then we have Mr. Allen Croff. And Allen is a nuclear engineer and Adjunct Professor in the Department of Civil and Environmental Engineering at Vanderbilt University. Next is Dr. Tissa Illangasekare. Tissa is the AMAX Endowed Distinguished Chair of Civil and Environmental Engineering, and the Director of the Center for Experimental Study of Subsurface Environmental Processes at Colorado School of Mines. Next is Dr. Lee Peddicord. Lee is Professor of Nuclear Engineering at Texas A&M University. Next we have Dr. Paul Turinsky. Paul is the Board's Deputy Chair. He will take over if I somehow lose connectivity today. And he is a Professor Emeritus of Nuclear Engineering at North Carolina State University.

So I've just introduced five boards members, plus myself. Not the full complement of 11. Our other board

positions are currently vacant. As I usually do at board meetings, I want to make clear that the views expressed by board members during the meeting are their own and not necessarily board positions. Our official positions can be found in our reports and letters available on the board's website. If we can go back to the slides and get to the next slide I'll say a little bit about the board and what we do.

As many of you know, the board is an independent federal agency in the executive branch. It's not part of the Department of Energy or any other federal department or agency. The board was created in the 1987 amendments to the Nuclear Waste Policy Act to perform objective ongoing evaluations of technical and scientific validity of DOE activities related to the management and disposal of spent nuclear fuel and high-level radioactive waste. Next slide.

Board members are appointed by the President from a list of nominees submitted by the National Academy of Sciences. And the next slide.

We're mandated by statute to report board findings, conclusions, and recommendations to Congress and to the Secretary of Energy. The board provides objective and

technical scientific information on a wide range of issues related to the management and disposal of spent nuclear fuel and high-level radioactive waste that will be useful to policy-makers in Congress and the administration. And all of this information can be found on the board's website, www.nwtrb.gov, along with board correspondence, reports, testimony, and meeting materials, including archived webcasts of recent public meetings. If you'd like to know more about the board, a 2-page document summarizing the board's mission and presenting a list of board members can be found on the board's website.

We will have a public comment period at the end of each day's meeting. Because of the virtual format of this meeting, we can only accommodate written comments. So as you join the meeting, on the right of your screen is a comment for the record section where you can submit your comments. If you're viewing the presentation in full screen mode, you can access the comment for the record section by pressing the escape key. A reminder on how to submit comments will be displayed during the break.

Comments received during the meeting will be read by

staff member Bret Leslie in the order that they're received. Time for each comment may be limited, depending on the number of comments we receive, but the entirety of submitted comments will be included as part of the meeting record. Comments in any other written materials may also be submitted later by mail or e-mail to the points of contact noted in the press release for this meeting, which is posted on our website.

There also will be -- these also will become part of the meeting record and will be posted on the board's website, along with the transcript of the meeting and the presentations you'll see today. This meeting is being recorded and the archived recording will be available a few days -- after a few days on our website. The meeting agenda and presentations have also been posted on the board's website and can be downloaded.

So why are we holding this meeting? This meeting is part of the board's continuing review of DOE activities related to the management and disposal of spent nuclear fuel and high-level radioactive waste. Over the past several years, DOE has been developing a modeling capability for evaluating the post closure performance of potential repositories for spent fuel and high-level

waste. The modeling capability includes different host types and different disposal options. According to the Department of Energy, this work is part of its efforts to develop a sound technical basis for multiple geological disposal options in the United States and the tools needed to support disposal concept implementation.

The board sees this effort as one that has the capability to address several of the recommendations we made in a report we issued last Spring, namely, to anticipate the required high-performance computing and data management infrastructure required for a multi decade waste management program, and to facilitate application of iterative and adaptive approaches to development of a geologic repository.

In 2013, the Department of Energy established a computational framework different from what was used in the previous repository program. This new computational framework is called the Geologic Disposal Safety Assessment Framework or GDSA framework. Our meeting will examine DOE's research and development activities related to this GDSA framework.

Today's meeting will start with opening statements by William Boyle and Alisa Trunzo from the DOE Department

of Nuclear Energy, who will provide an update on DOE's Spent Fuel and Waste Disposition program, including interim storage activities. Then we'll hear from the National Laboratory researchers who are conducting the work for DOE Emily Stein will give an overview of research and development activities related to the GDSA framework, including the objectives, research priorities, technical challenges, and recent accomplishments. After a 20 minute break, starting at 1:45 p.m. Eastern Time, we'll hear a presentation on the development of the GDSA framework, its capabilities, and applications. Then in the following three talks and in the first talk tomorrow, we'll hear about the details of several subcomponents of the GDSA framework, including multiphase flow and reactive transport code called PFLOTRAN, a discrete fracture network model called dfnWorks, and the Fuel Matrix Degradation Model and the biosphere model. As I mentioned earlier, we'll have a public comment period, during which staff member Bret Leslie will read the public comments as we receive them.

We'll adjourn day one of the meeting at about 5:00 p.m. Eastern Time. We'll resume the meeting tomorrow at 12:00 p.m. Eastern Time, starting with a presentation on

the biosphere model, then Tim McCartin and Dave Esh from the U.S. Nuclear Regulatory Commission will tell us their perspective on developing and applying performance assessment codes based on their collective experience in these activities at the Nuclear Regulatory Commission and their participation in international programs.

Following that, Sara Vines from the United Kingdom's Radioactive Waste Management organization will describe the development and environmental safety case models supporting geologic disposal in the United Kingdom's radioactive waste management program.

After a 20 minute break, starting at 2:15 p.m. eastern, we will have three presentations. One on uncertainty and sensitivity analysis tools being applied in the GDSA framework, and another describing the implementation of the GDSA framework to generic repository reference cases for bedded salt, shale and crystalline host rocks. The third presentation, which is the last of the meeting, will describe a case study in integrating insight and experience from the international community into geologic disposal safety assessments.

So now if we can go back to the camera view, thank you, I just would like to mention in closing that much effort

went into planning this meeting and arranging the presentations. I want to thank our speakers for making presentations at the meeting today. And I also want to thank board member Tissa, who is my co-lead for the meeting, and the board staff, particularly Bobby Pabalan and Chandrika Manepally, for putting this meeting together.

So now it's my pleasure to turn on the meeting over to William Boyle, who will get the meeting started, and if we can bring William up on the screen and get him unmuted, then I will leave.

>> BOYLE: Okay. I'm William Boyle. I'm the Department of Energy manager for research and development related to the disposal, storage, and transportation of spent nuclear fuel high-level waste. In meetings over the next two days, you'll hear some presentations related to disposal research and development.

As to the update related to those R&D activities, there's not really much to say. We're in a continuing resolution. The Funding we get from Congress through the first week of December and it's the same amount as last year. Just prorated for the shorter period. So

we're executing the plan we came up with for this year. There have been no major surprises, good or bad, and so we're just doing the work that we've set out to do. And if you have any questions for me related to this update, I request that you hold them until after my colleague, Alisa Trunzo, gives her update on another portion of the Department of Energy's efforts to help assure she has enough time, which I think she will. I think both Alisa and I can take questions afterwards. And I would, following onto Chair Bahr, I would also like to thank the presenters from the national labs for all the work they've put in to help support this meeting as well. Over to you, Alisa, if it's up to me.

>> Alisa Trunzo: Thanks, Jean and thanks, Bill. I'm Alisa Trunzo. I want to thank you for the opportunity to speak with you today. Just to give you a bit of background on me, I'm the strategic communications specialist for the Department of Energy's Office of Nuclear Energy. I'm housed in the immediate Office of the assistant secretary, but I work hand in hand with my colleagues in the offices of Spent Fuel and Waste Disposition, specifically on consent based siting.

As the board well knows, nuclear energy is absolutely

essential to our ability to achieve a 100% clean electricity sector and net zero emissions by 2050, but to make nuclear truly sustainable, we have to manage the back end of the fuel cycle, and of course management of the nation's spent nuclear fuel and high-level radioactive waste is the department's responsibility. This includes finding the sites to store and dispose of spent nuclear fuel. Our ultimate goal is, of course, permanent disposal and the technical R and D work that Bill and my other very smart colleagues do is in support of that goal, but obviously, science doesn't happen in a vacuum, and we need to make progress on identifying the sites for waste management facilities in willing host communities.

Given congressional appropriations and direction to move forward with the federal interim storage capability, that's where a lot of our focus currently is. Interim storage will enable near term consolidation of temporary storage of spent nuclear fuel, which will allow for the removal of spent nuclear fuel from reactor sites, reduce liability to taxpayers, provide increased R&D opportunities, and build trust and confidence with stakeholders and the public.

And as we begin that work to identify potential sites for federal interim storage facility, DOE is committed to a consent based approach to siting and a waste management system that enables broad participation and centers equity and environmental justice.

We believe that a consent based approach driven by community well-being and community needs is both the right thing to do and honestly our best chance for success. So in the very near term, we plan to issue a request for information on using a consent based siting process to identify sites to store the nation's spent nuclear fuel. We'll be asking questions of the public on a range of issues on the consent based siting process itself, removing barriers to meaningful participation, especially for groups and communities who have not historically been well represented in these conversations. And interim storage is a component of the nation's waste management system.

As I mentioned, we have special focus on ensuring issues of equity and environmental justice are built into the consent based siting process itself, as well as the waste management system as a whole. We plan to use the feedback we receive through that RFI to inform our next

steps on updating the consent based siting process, developing an interim storage capability, in our overall strategy for integrated waste management. Our communications with stakeholder engagement strategies, including developing the tools intended to help communities with their own decision-making and potentially a funding opportunity for interested groups and communities.

Organizationally, we're also incorporating expertise in the social sciences to help us move forward. That includes bringing in expertise through the national lab system in social sciences, as well as the currently open integrative research project that's up to three years and $3 million per university led team to perform research that will inform how we implement consent based management process. And actually, I'm the federal manager for that.

As we prepare to re-engage on consent based siting and interim storage, we'll be building on the work that NE [DOE Office of Nuclear Energy]] has been doing for years to prepare for integrated waste management system. My colleagues in the Office of Spent Fuel and Waste Disposition continue to prepare for the large-scale

transportation of spent nuclear fuel and high-level radioactive waste. As the board, I'm sure, knows, they're developing purpose-built railcar equipment, assessing transportation infrastructure and transport options at nuclear power plant sites, analyzing future transportation system elements and dependencies, actively engaging with state and tribal government representatives through the Department of Energy's National Transportation Stakeholders Forum and the associated work groups, and coordinating with appropriate federal agencies on safety and security considerations.

NE is also developing preliminary design concepts for interim storage facilities and continues to develop passive storage solutions that take advantage of recent advances in technologies. And NE is performing system integration and analysis activities that help us model varying system architectures and configurations, including options for the storage of spent nuclear fuel. And in addition to just helping us plan for an integrated system, those activities are also going to inform our engagement with interested groups and potential host communities as we move forward.

With all of that, I should note that we believe our thinking on these next steps is really aligned to the board's six over arching recommendations for how to move the nation's nuclear waste management program forward. In particular, my hope is that you'll see us fully embracing openness, transparency, and engagement as we move forward on consent based siting. And in fact, a successful approach to siting waste management depends on those principles. And the RFI which we plan to issue as soon as possible represents our commitment to public participation in our decision-making from the outset. We plan to take the feedback that we receive from the public through the RFI really seriously, so some of our next steps are going to be dependent on what we hear back through the RFI.

With that in mind, we really hope that the board will consider responding to the RFI when it becomes available and of course although I noted we are looking at the recommendations you've already provided, the other reports to Congress and the secretary.

With that, I thank you again for the opportunity to speak with you, and I think Bill and I can at least attempt to answer questions.

>> BAHR: I see Steve Becker's hand up. Go ahead, Steve.

>> BECKER: Good Afternoon, Alisa. I enjoyed your presentation very much and I'm very pleased to see that communication and stakeholder engagement are right at the center of what you're doing. As you're thinking about your communication strategy, are there lessons regarding communication, stakeholder engagement, and bringing in under-represented communities that have been learned from the experiences of other countries that you think that we may be able to learn from here in the U.S. as we move forward?

>> TRUNZO: Absolutely. I mean, obviously, there are some countries that are further along with the consent based approach, and it's really valuable experience to learn from them. In particular, the experience in Canada, I know it informs a lot of my thinking on the approach and the way that they have been able to really sustain a very long term and very productive communication and outreach strategy. I think it's really a helpful experience for us.

>> BECKER: Just to follow up, are there plans to sort of systematically look at experiences of other countries

regarding communication stakeholder engagement and bringing in under-represented communities as part of your data gathering effort?

>> TRUNZO: Yeah, absolutely. I think in addition to sort of like the literature review approach, there's also -- we intend to meet and engage with the people that did the work directly. I think there's a lot of value to being able to talk directly and ask questions. That moves kind of beyond what you can sort of doing from the lit review aspect.

>> BECKER: Thank you.

>> BAHR: Steve, thank you.

TURINSKY?

>> TURNINSKY: A lot of buttons to push. Along the same line of questions that Steve had, we had that experience with the deep bore hole trying to site an experiment. Let's say it didn't go well, but one can always learn when things don't go well. Are you planning on examining what happened there to get a better -- and there you're working with, you know, U.S. citizens. There's no cultural differences, so it would seem like a very valuable exercise to go back and look at that

experience and learn, you know, why did it get this way? Couldn't be carried out?

>> TRUNZO: That's a really good point. I don't know if we had formally put that, you know, in any work scope, but it's relevant experience. And certainly, you know, certain people on our team were in the area, working in the area at the time, so it's definitely worth investigating and taking a look at some of that.

Bill, looks like you have something to say?

>> BOYLE: Yeah. It's just to -- there's another way to look at the experience with the deep borehole field test, other than it didn't go well, is to look at it as it did go well. If you believe in listening to the local population, they expressed a view in North Dakota and South Dakota that they didn't want the test. And the government probably possesses the legal authority to have gone ahead anyway and chose not to. So to me, it's a good example of working to get the consent of the people involved. So in that sense I would say it did go well.

>> TRUNZO: Yeah. That's a good point to add onto that. As we begin to talk more closely with potentially

interested communities, success of a consent-based siting process is both, yes, we identify sites in willing host communities and we achieve consent agreements. Another possible successful outcome is the community decides, not interested after all. And that's also a successful use of the consent based siting process. So it's a really good point.

>> TURNINSKY: But eventually, the success is you could have carried out the experiment. And I agree. The government reacted appropriately to the citizens' concerns. I don't disagree with that.

Bill, I have a question for you. What is the person year effort involved in performance assessment? Developing the software? Do you have any idea how big it is?

>> BOYLE: I do not, but Emily may, you know, but I don't.

>> TURNINSKY: The budgets that we see are at a higher level and it's hard to decipher you know, talking about two person years here or --

>> BOYLE: Well, I haven't done this for a while, but if you have the dollars and it's mainly labor, you know,

they're not buying planes or, you know, rail cars or that sort of thing, all you need to figure out the FTEs is to take a stab, make an assumption that all national lab staff and all labs are essentially the same FTE cost per year. Well, the reality is they're not. You just make a few assumptions. And whether you make that $400,000 a year or whatever it is, you can get a rough idea, you know, of the number of full-time equivalents.

>> TURNINSKY: Okay. Thank you.

>> BAHR: Emily, did you want to add to that? Do you have harder numbers?

>> STEIN: I'm looking for harder numbers. I'm going to conjecture and I can be more specific later if you like, that it's about ten or so people per year at this point. Budgets were not that large earlier in the program.

>> TURINSKY: Say again. I missed the number.

>> STEIN: I think it's around ten.

>> TURINSKY: Ten person years?

>> STEIN: Yeah.

>> BAHR: Thanks, Emily. I see Lee with his hand up?

>> PEDDICORD: Thank you, Dr. Bahr. I'd like to come back and maybe expand a little bit on Dr. Becker's comments as well too. We have had the good fortune of the board to do some interactions with the other countries and so on. A couple things, to my mind, emerge from those. So one is there's not one size that fits all, and I would say I was really impressed with the nuances of the different approaches we saw in these countries. And so as you're kind of peeling the layers of the onion back, I think some of the deeper dives on each of the national approaches, because there's quite a bit of difference in the ones that are having success have taken a lot of I would say innovative ways of engaging with the public, so I think there's a lot to be learned there, and I encourage you to think about that as well, too.

The other part of it is we found through a couple of trips to almost get out on the ground with some of these and meet not only with those carrying out the program with some of the key stakeholder groups, and actually, that proved to be very interesting to hear what they had to say back in response to what their either ministries or the organizations handling the waste doing.

So these are just kind of some thoughts. I would have to say I was really impressed. Virtually all of these countries have gone through what I would say is a similar history that we are experiencing -- well, to this, launching and identifying priorities, endeavoring to move forward, and finding, as Dr. Boyle points out, the oppositions and so on, and they really modify what they are doing and how they are doing it. And as we know, some of these countries are now having pretty good success with this. So my message is really to encourage you, but really take I think some pretty deep looks, in-depth looks. And as you mentioned, engage with the people doing it and engage with the people who are the recipients or objects of the way they went about their consent based siting and communication strategies.

I apologize for the lengthy stream of consciousness, but I really applaud what you're doing. I think this is excellent and I commend DOE for what you're undertaking. I think it's going to be critical to the ultimate success.

>> TRUNZO: Well, thank you so much. I know I personally will take your advice to heart. And I know that our acting assistant secretary is really interested

in learning from other countries. Obviously, you know, there's different political setups, but there's really valuable experience and expertise to be learned from everybody who is undertaking a similar process.

>> PEDDICORD: If we can and it's appropriate, I would like to suggest the board hear from you periodically as this all progresses. There's always the questions about our mandate and so on, but I think all of us are keenly interested in what you're endeavoring to do.

>> TRUNZO: Well, as far as I'm able, I'm happy to be very responsive to the board and to keep lines of communication open.

>> PEDDICORD: Thank you.

>> BAHR: Tissa?

>> ILLANGASEKARE: Thank you. This question is for Ms. Alisa Trunzo. Thank you for your presentation. I sort of wanted to pick up on your idea of funding consent based research at the universities, and my assumption is that this research is multi-disciplined in bringing social scientists and technical people together. But in part of this, my question is that, you know, in these types of waste problems, we have to deal

with human capacity building, we have to train future scientists and engineers to do this type of work. So is part of this funding program includes some graduate student support of building the human capacity?

>> TRUNZO: The one that I specifically addressed, the integrated research project on consent-based siting is more on what you mentioned first, which is an integrated team with social scientists and people with nuclear engineering experience, it could be a multi-discipline team specifically looking at consent based siting itself, as well as with a focus of integrating issues of environmental justice and equity. That's more of like the research project.

I think, you know, we do have, I believe, I'm not the federal manager on it, so I can't really speak to the scope as well, but I think we have something that's looking at, you know, Human Capital issues and things like that, but I honestly would have to double-check what's publicly available on that. But it's a really good point, and we are looking -- actually, I think maybe Bill can talk a little bit more about this, but we're doing a lot of knowledge management within our organization in this area, because, you know, a lot of

people that work in this area are more towards retirement age and we risk losing some really valuable expertise, so bringing the next kind of generation along in the nuclear, the spent nuclear fuel management space is really important.

>> ILLANGASEKARE: Thank you.

>> BAHR: Steve again.

>> BECKER: It's really a positive comment about your presentation, that it has stimulated so much discussion. So kudos for that.

Just a quick follow-up. As you're developing your communication and engagement approach, including environmental justice, I'm glad to hear that you are looking to tap expertise in social science. Have you thought about expanding the expertise base that you draw on to include fields such as behavioral science, public health, and economics? Because as I understand it, there's a great deal of potentially relevant work in those disciplines as well.

>> TRUNZO: Yeah. That's a really good point. In nuclear in general, I think there's a tendency to think that we're really unique, and we are in many ways, but

in other ways, we're not. There's a lot of experience that we can learn from other fields and people that are dealing with similar issues and have run similar stakeholder engagement campaigns. So I think that's a really good point. It's on our minds. I don't know how much we're doing right at this moment as we build our early stage activities, how much we've incorporated that, but I think we should.

>> BECKER: I'm glad to hear that. Particularly with respect to topics such as environmental justice, I think you'll find that there's a great deal of work in public health and behavioral science and some of those other fields. So good to hear that you're thinking broadly about this. Thank you.

>> BAHR: Thanks, Steve.

I had a couple of questions. I realize that your initial work on consent based siting is going to be focused on interim storage, but are you going to be looking more broadly at issues that might relate to siting a repository? And do you think that there will be a significant difference in how one might approach a consent-based siting program for a repository as opposed to interim storage?

>> TRUNZO: Yeah. I mean, obviously, it's essential that we continue to work on permanent disposal pathway. And that will influence, quite honestly, how consent based siting process works for interim storage, because it's just that, it's interim, so there has to be a permanent solution eventually.

The reason that we're focused on interim storage first is we have congressional appropriations and authority to look at this, to look at federal interim storage facilities, but we expect the outline of the consented based process would be similar. It has to be phased and adaptive, as you all well know, to be responsive to potential host communities and to how things work through the consent based siting process itself, and there could be differences.

I think a primary difference could be the time that it takes as consent agreement for a permanent repository versus an interim storage facility. But I do expect experience with one would affect the other. And any experience and any progress moving forward I think is positive at this point.

>> BAHR: Okay. And then I'm just curious about how you're going to be distributing this request for

information? Who do you see as the stakeholders? How are you going to get the request out to them? How are you going to incentivize participation from the groups that you'd like to get feedback from?

>> TRUNZO: It's a really good question, because we want to be as inclusive as possible, and we want to bring groups that have been under-represented in the conversation into the space, but that is very much easier said than done. And so we plan to publish the request for information in the Federal Register as the first and easier step. And then we will be engaging in an outreach campaign first for the rollout, which that's one piece, just to share it with the media. And we have a list of stakeholders, those who have engaged previously on this issue. We want to make sure that they hear from us again now that we're asking more questions and we want to be respectful of the fact that a lot of people have put a lot of time and a lot of thought into consent-based siting. And we want to make sure that we reach them again.

And then as far as reaching new groups, we are working really hard to come up with a plan to make sure that we reach more groups. We are trying to be proactive and

reach out to environmental groups and communities and people that might be tangentially or think they're tangentially related to the issue, but that they, in fact, have a stake. I mean, you could argue everybody in the United States has a stake in this issue. They're all our stakeholders. So I don't want to say too much about our plans before we even launch it, but we are looking carefully at making sure that we do that.

>> BAHR: Okay. Thank you.

Are there any other questions from board members or staff, either for Alisa or for William Boyle? William, you have your hand up?

>> BOYLE: Yeah. I was thanking the lab staff earlier. I should have also thanked Tim Gunter for all of his efforts in making this meeting happen. So I just wanted to put that in.

>> BAHR: Okay. Any other points for this discussion? Okay. Well, I think we can probably go ahead and move on to our next presentation, which is Emily Stein, who is going to be talking about the GDSA, geologic disposal safety assessment framework. She's going to give us an overview that will set the stage for a lot of the rest

of the work that we're going to hear about over the next two days. Take it away, Emily.

>> STEIN: Okay. Thank you. I am going to share my screen first. The screen sharing is behaving differently than it did during rehearsal. So just give me a minute here. Okay. And then please tell me whether you're seeing full screen or presenter view?

>> BAHR: I'm seeing presenter mode. There. That's good. Thank you.

>> STEIN: Okay. Good. So my name is Emily Stein. I am a geoscientist and a manager at Sandia National Laboratories. I've worked within the geological disposal safety assessment program for several years now. I also have experience of working on the Waste Isolation Pilot Plant performance assessment. And I'm the control account manager for the GDSA work scope within DOE's Spent Fuel and Waste Science and Technology program.

I'd like to first ask and answer a question, what is GDSA? We sometimes throw that term around with ambiguous meaning. And then I'm going to tell you about the objectives of the geologic disposal safety

assessment work scope within the program, how we prioritize activities within GDSA, what some of the challenges are that we've run into over the last several years, and how those objectives, priorities, and challenges that have shaped our current 5-year plan.

First, what is GDSA? I will give you three different definitions. The first is a control account within the Spent Fuel And Waste Science And Technology Campaign. The second meaning that is sometimes implied is the process of safety assessment itself and finally it is our software framework or software toolkit that we use for generic safety assessments.

So within the SFWST Disposal Research program, there are several control accounts. These include control accounts related to research development within three different host rocks, argillite or shale, crystalline, and salt host rocks; engineered barriers; waste forms; international collaborations; direct disposal of dual purpose canisters; and technical support for underground research laboratory activities. So much of this R&D is aimed at developing understanding of how the features within a repository evolve. And that’s through laboratory experimental work, participation in large

scale experiments and demos in underground research laboratories and development of coupled process models.

The GDSA control account then, integrates concepts understanding and models developed in other control accounts to advance generic reference case concepts and our simulation and analysis capabilities needed for safety assessment.

And within GDSA itself, then, there are several different sub-work scopes, and these include development of GDSA framework, which is a comprehensive software toolkit for post closure safety assessment. You will hear plenty about it over the course of this meeting. Application of that toolkit to simulation and analysis of generic reference cases and concepts. Development and demonstration of uncertainty and sensitivity analysis methods. Development of multiphysics simulation capabilities within PFLOTRAN. Development of specific process model capabilities for integration into GDSA framework. And geologic modeling.

Generally speaking, the work that occurs in these lower four areas supports capability development within the overarching software framework and helps advance generic reference cases and reference case simulation.

The second definition that is sometimes implied when people say GDSA is the process of post closure safety assessment. Post closure safety assessment is a primary component in the overall demonstration that a deep geologic disposal facility will be safe. It includes a systematic analysis of the features, events, and processes or FEPs, that may affect the post closure evolution of a disposal facility. It includes a quantitative analysis of the post closure performance of the system, and an evaluation of the level of confidence, take into account uncertainties in the estimated performance of the system. And then a comparison of that performance to applicable safety standards.

The term performance assessment is often used interchangeably with the term safety assessments, and you'll hear both of those terms within this talk and over the course of the meeting. So construction of the models and the simulation and analysis tools for a quantitative analysis requires making some assumptions about what the safety assessment strategy should be and what the post closure technical bases are. So these are these other boxes above the post closure safety

assessment box that feed it. And we'll take a closer look at the assumptions made for development of GDSA capability in the next slide.

So I want to call your attention first to the two boxes at the top, the safety assessment strategy, and the post closure technical basis. The safety assessment depends on both of these. So the safety assessment strategy comprises performance goals and safety criteria, which are promulgated in regulations. GDSA assumes that future safety criteria are likely to include an individual performance standard, such as a dose to the reasonably maximally exposed individual, similar to the standards promulgated for the Yucca Mountain project in agreement with recommendations in the international community.

Caitlin will say more about this when she talks about the biosphere model.

Within the safety assessment strategy, there also needs to be an awareness of safety functions of the multiple barriers within the repository system. The degree of reliance on different variants varies among different host rocks and different design concepts.

And then the assessment strategy also needs to specify how uncertainty will be treated. GDSA assumes uncertainty should be assessed using a probabilistic risk assessment consistent with a methodology developed by the nuclear regulatory agency since about the mid-seventies for nuclear power plants and implemented for the Waste Isolation Pilot Plant and for the Yucca Mountain project.

Additionally, GDSA presumes separation of aleatory and epistemic uncertainty consistent with a probabilistic risk assessment methodology. So aleatory is random, stochastic or irreducible uncertainty, and epistemic is state of knowledge uncertainty. We don't know what the exact value of a parameter is – let’s give it a range. And Laura Swiler will talk more about this in her presentation on uncertainty and sensitivity analysis.

So the post closure technical basis comprise characterization of features of the waste, the engineered barrier system, the natural barrier system, and the biosphere, and also, of the processes acting upon these features. You'll notice that aleatory and epistemic uncertainty are called out as part of that characterization for the waste, the engineered barrier,

and the natural barrier, and not for the biosphere. And that's because it is possible that the representation of the biosphere will be prescribed by a future regulation.

So finally, if we look down at this last box, looking at the elements of the safety assessment, GDSA is going to prioritize development of simulation capability for the FEPs, the features, events, and processes that are likely to occur, regardless of site and design specifics. And that's because we're in a generic R&D environment right now. And we also want our GDSA software to be a capability that can provide a quantitative estimate of the performance of the disposal system for comparison to regulatory analysis.

As part of that quantitative estimate of the performance, sensitivity analysis is often performed, and this is a capability which helps you understand behavior of the system and also a tool that can be used to inform prioritization of future R&D. So that also loops back to your safety assessment strategy.

Okay. And then the third meaning of GDSA, that phrase, simply those four initials, GDSA, are times used as shorthand for GDSA framework, which is the software toolkit developed within the GDSA control account for

the purpose of post closure safety assessment. Within GDSA framework, PFLOTRAN is used to simulate the coupled processes affecting the source term, the engineered barrier, and flow and transport in the geosphere. Dakota is used for uncertainty and sensitivity analysis. We have a variety of pre and post processing tools. And workflow is controlled using Dakota's next gen workflow graphical interface. Over the next couple of days, you'll hear more about GDSA framework and its components, including PFLOTRAN, Dakota, the fuel matrix degradation model, which is integrated into PFLOTRAN. DfnWorks, which is a preprocessor used to set up fractured rock model domains and a brand new biosphere model that takes PFLOTRAN output as input.

Okay. Objectives. These objectives apply to the GDSA control account as well as to some extent to the GDSA software framework itself. Our primary objectives are to develop and demonstrate the capability necessary for quantitative safety analysis. We want those capabilities to be transparent, accessible, responsive, and adaptable.

So we need this simulation and analysis capability to be -- let me think about this. So we're going to use

the simulation analysis capability potentially to inform decisions at all stages of a deep geologic disposal program and that includes generic research, development, and demonstration in the concept evaluation phase, use within the site selection and characterization phase, and potentially use within a licensing and repository development phase.

So right now, the U.S. program is in the generic stage, and what we are primarily doing is developing and demonstrating technology. Analysis that assess the safety of any specific site or design would be developed and refined as site and design specific information becomes available.

We want to be able to apply this simulation and analysis capability to generic disposal concepts in three different host rocks, and these were chosen as the basis for the generic R&D program. From experience in the international community and also some early site identification efforts in the U.S. So these three different host rocks are fractured crystalline rock, which, for example, is the host rock being pursued in Sweden and Finland. And argillite or shale rock, which is being pursued in France and Switzerland. And a salt

host rock, which is also under consideration in Germany and the Netherlands.

So finally, we want that simulation and analysis capability to be flexible enough to account for the multiple barriers that may play different roles in different disposal systems. So at a very high-level, these barriers are the natural barriers, which prevent or delay water from reaching the waste form. Engineered barriers may also prevent or delay water from reaching the waste form. Slow degradation of the waste form will limit exposure of radionuclides to water, actual release of radionuclides.

In the near field, the water chemistry at depth will limit aqueous concentrations of radionuclides. And finally, both natural and engineered barriers, depending on the design concept and the host rock may play a role in preventing or delaying the transport of radionuclides to the accessible environment.

And I'll just note here that salt disposal concepts rely primarily on the first and last boxes. Fractured crystalline rock disposal concepts rely very heavily on these three middle boxes. And shale or argillite concepts rely on all of these barriers, including the

ability of that low permeability/high sorption capacity shale host rock to delay transport of radionuclides to the accessible environment.

So given those objectives and the generic state of the program, a list of very high-level requirements for a software toolkit or software framework were developed early on in 2012 and these requirements are listed here. The first is, and must be flexible to changes in design, geometry, or geology. We'd like to be able to represent three-dimensional geometry to facilitate two way coupling between processes to integrate process models transparently in a way that is easy to understand and explain and then leverage high-performance computing to allow more detailed representation of engineered and geologic features to reduce computational cost given that we're going to be doing all of the above and to enable probabilistic calculations, given the computational cost.

Finally, at this time around 2012, the international community was beginning to recognize the power of parallel processing for safety assessment modeling, and this use of high-performance computing is really a way to make sure that the software will carry us forward

through an extended repository program.

So several high-performance computing simulators and run controlled frameworks were evaluated, and eventually PFLOTRAN and Dakota were chosen as the basis for what then later game GDSA framework. They are both developed to run well and efficiently in a high-performance computing environment. They're both open source, lending them transparency and accessibility. PFLOTRAN came with the ability to couple flow and transport, as well as reaction and transport. And Dakota came with established uncertainty analysis methods previously used in U.S. repository programs, including Latin hypercube sampling and the ability to separate aleatory and epistemic uncertainty.

Today when you think about the high-level GDSA objectives, we are working to develop and demonstrate capability and geologic modeling, multi physics simulations, uncertainty and sensitivity analysis, and workflow that is and will be responsive to advances in process understanding, computer hardware and software, simulation and analysis methods. We want it to be adaptable to the generic site and design constraints that we're working with now, as well as future site and

design specific technical bases and possible evolution of the safety assessment strategy.

We'd also like our product to be transparent, so it's developed and distributed in an open source environment with publicly available documentation and accessible. So all of this software can run on a laptop or work station or in a high-performance computing cluster.

Okay. Priorities. So in meeting these objectives, how do we prioritize development efforts? There have been three main prioritization efforts that have contributed to prioritization of specific activities within the GDSA control account and those include an initial program wide road mapping exercise in 2012. A generic FEP screening that was performed at the same time those requirements for the software framework were being developed, and an update to that roadmap that was performed in 2019.

I'm going to tell you a little bit more about all of those. First, I'll just give you a flavor of the activities that have occurred within the GDSA control account over the last ten years. And these activities chosen here mark some of the milestones and the evolution of GDSA framework and our reference pieces.

So in 2012, the program wide road mapping exercise occurred. Requirements for the safety assessment software framework were developed and a generic FEPs screening was done.

In 2013, the first reference case, a salt reference case was performed using PFLOTRAN and Dakota.

In 2014, multiphase flow capability was added to PFLOTRAN. In 2015, we added a shale reference case to our repertoire, integrated the fuel matrix degradation model into PFLOTRAN, as well as a glass waste form dissolution model.

In 2016, the crystalline reference case came onboard, and this involved adding dfnWorks into the GDSA framework and the workflow for safety assessment. We also implemented an isotope partitioning model and a modular waste form process model within PFLOTRAN.

In 2017, a simple biosphere capability with water ingestion was added to PFLOTRAN. We started to develop a somewhat formal -- not formal QA, but a formalized software framework for quality assurance testing and analytical derivatives were implemented to improve the performance of our multiphase flow model.

In 2018, we really started to investigate state-of-the-art uncertainty and sensitivity analysis methods. We added variants based sensitivity analysis and step wise linear regression to the list of our capabilities. And also, initiated an alluvial reference case.

In 2019, that roadmap update occurred. We started looking at high temperature systems with some high temperature shale simulations and also integrated reduced order model, looking at the effect of bentonite swelling stress on permeability of the disturbed rock zone.

So we are nearing the present here. Surrogate models for the fuel matrix degradation model were begun. That work was begun a couple years prior, but reported out on in 2020. You'll hear more about that later today. We implemented advanced linear and nonlinear solvers, began working on creating a traceable workflow. We joined and were leading DECOVALEX task F, which I will not explain now, but you'll hear about it tomorrow, and began laying out the requirements for a biosphere model, which you will also hear about.

And then in this past year, we have advanced some of our

process modeling capabilities, including a dual porosity model for fracture matrix interaction, waste package criticality model, and we've also published a report summarizing a large collaboration on the topic of sensitivity analysis.

Okay. So that was kind of the flavor of GDSA activities. How have those been prioritized or how do they reflect priorities?

So the program has conducted the large disposal research program has conducted two program wide prioritization exercises since 2012. The 2012 roadmap and then the 2019 roadmap update. Both of these exercises have then influenced the development of the current disposal research five-year plan. Dave Sassani spoke about all of these exercises and documents a year ago in the fall 2020 meeting. And for the remainder of this presentation, I'm going to speak more specifically about the relationship of these activities to GDSA.

Okay. So that 2012 roadmap exercise identified two cross-cutting issues that became the foundation for the work scope and what is now the GDSA control account. And the first of that was high priority cross-cutting issue. We needed a disposal system modeling capability.

And that capability should enable risk informed probability based performance assessment, provide a capability for evaluating disposal system performance to inform research and development prioritization, and it also needs to support simple to complex integrated generic disposal system models.

And the second cross-cutting issue that was identified with medium priority was site screening and selection tools, so the ability to incorporate, catalog, and visualize geospatial data.

Also, in the early days of the program, in 2012 and more specific to development of simulation capability within GDSA framework, a generic FEPs screening was performed to identify the FEPs that are likely to be relatively independent of site and define specifics. So these are the list of FEPs that are prioritized for capability development within our generic safety assessment software framework. And I will just run down this list quickly.

Some of those FEPs involve inventory and waste forms, so effect the source term. We need to be able to model heat generation and decay and in-growth associated with the radionuclide inventory. We want to be able to model

waste form degradation, gas generation, and radionuclide release and transport.

In the near field, we are worried about waste package degradation, corrosion processes, possible mechanical damage or early failures. Evolution of the engineered barrier system components and the disturbed rock zone. Effects from rock fall or a drift collapse, which might be particularly important in a salt repository. Fluid flow and radionuclide transport. Of course, chemical interactions that are going to affect some of these other processes, like waste package degradation, waste form degradation, and radionuclide speciation and solubility.

Thermal effects, on flow and chemistry and effects from disruptive events, such as seismicity or human intrusion. In the far field, of course we need to be able to model fluid flow and radionuclide transport. We'd like to be able to understand the effects of fracture flow on radionuclide transport, as well as the effects of groundwater chemistry.

And finally, in the biosphere, in just a very simple biosphere goals were identified, so it should be able to handle dilution due to mixing contaminated with

uncontaminated waters, and it needs to have some kind of basis for converting radionuclide concentrations in groundwater to a dose.

In 2019, a roadmap update exercise was performed, and this identified several high impact R&D topics relevant to multiple control accounts within disposal research. These topics include high temperature impacts, buffering in field studies, coupled processes in salt, gas flow in the engineered barrier system, criticality, waste package degradation, in-package chemistry, generic performance assessment models, and radionuclide transport.

Over the past couple of years, GDSA implementation and simulation efforts have focused on those things highlighted in bold.

Okay. And then as we begin undertaking the tasks and begin implementing process models, doing generic repository simulations, what are some of the challenges that we have run into? I've listed three challenges here, but I'll just move right on to the next slide where the challenges are listed again.

The first challenge really is the generic nature of the

problem, which requires maintaining flexibility to substitute one process model for another, depending on the repository concept and the host rock.

For instance, you might want to be able to model glass dissolution or spent nuclear fuel dissolution. You might also want to have a simple representation of your fuel dissolution model versus a more complex mechanistic representation of your fuel dissolution model.

The size of the problem is definitely a challenge that we are kind of continuously dealing with, so we've moved into three-dimensional comprehensive model domains that include resolution of the repository of individual waste packages and then kilometer scale flow to look at transport within the far field. So it's a very large model domain. Many grid cells. We're running these simulations for a long time out to 1 million years, which may eventually, in the future, be required by safety regulations. We're looking at a large number of radionuclides so that increases the number of knowns in the problem. And then we want to be able to perform uncertainty propagation. We need to be able to do hundreds of realizations of any given problem.

And another challenge has been resolution of near field

processes, which is related to this size of the problem domain. Smaller grid cells in the near field require smaller time steps and increase the number of degrees of freedom in the problem. So it makes resolving in 3-D what's happening in the near field, increases the size of the problem again. So far, the approach within GDSA has been to embed 0D and 1D models, like our waste package degradation model or fuel matrix degradation model into the larger 3-D simulation.

And then sometimes we've found that specific modeling capabilities have presented a challenge. One of those is high temperature multiphase flow. Performance issues were experienced when saturations dropped below the residual liquid saturation. And these issues really are what motivated improvements to capillary pressure curves and also the development of advanced linear and nonlinear solvers that you saw in that timeline a few slides ago.

And then finally, the workflow to run a probabilistic performance assessment is complicated, and in the past year or so, we've invested in developing a reproducible, traceable workflow that provides a record. It can reduce human error, and also facilitate stakeholder

engagement at some point in the future.

Okay. And then how have these objectives, priorities, and challenges, how do they shape the current 5-year plan? So there are five research thrusts in the GDSA portion of the disposal research 5-year plan, and these include advancing simulation capability, advancing state-of-the-art uncertainty and sensitivity analysis methods and their application to deep geologic disposal. Developing a traceable user friendly workflow, repository systems analysis and geologic framework modeling.

Over the course of this meeting we're going to talk about the four that are in bold font.

So the need for continuing to advance simulation capability is motivated by continuing to implement the capabilities related to that initial 2012 generic FEPs screening, as well as the challenge of improving software performance and computational efficiency. So recently, some of the things that we've accomplished include implementation of the advanced solvers, implementation of a waste package criticality model, consideration of high temperature effects in our reference cases, the fracture matrix, diffusion, the

dual porosity model, implementing really efficient surrogate models for the fuel matrix degradation model, and developing a prototype biosphere model.

Over the next couple of years, we expect to continue to expand our simulation capability for high temperature disposal concepts, to implement material specific waste package degradation models, to continue to consider buffer and backfill evolution models, to add more pathways to the biosphere model. To improve capability within dfnWorks, our fracture generation software, and to tackle improving our ability to mesh geologic futures.

And you are going to hear about some of these simulation capability efforts in talks by Paul Mariner, Michael Nole, Jeffrey Hyman, and Caitlin Condon.

So our uncertainty and sensitivity analysis work scope seeks to identify methods that are going to leverage high-performance computing to increase computational efficiency and also to increase understanding of the system behavior.

Some recent accomplishments in this field include advancing the uncertainty and sensitivity analysis of

the crystalline reference case. Leading an international comparison of sensitivity analysis methods as applied to deep geologic disposal. And demonstrating the potential of multi fidelity methods to really extract information about the system while minimizing the computational expense.

And over the next couple of years, we expect to continue to apply methods that have the potential to increase computational efficiency and understanding assistive behavior. We'd like to implement metrics for assessing the goodness of the various surrogate models that we're using and continue to lead and participate in international collaborations to establish consensus on best-practices for certain uncertainty and sensitive analysis. And Laura Swiler is going to tell you more about all of this when she speaks tomorrow.

Workflow. So workflow has been let's say in the works only recently, and a couple of accomplishments in the last year include bringing the Next Generation Workflow online and expansion of our software verification testing suite.

In the next couple of years, we expect to continue to increase the number of components of the workflow that

are automated through that Next Generation Workflow interface. We will release our QA test suite publicly and work on developing a geologic meshing workflow.

So you will hear more about those things in talks by MARINER and Michael Nole.

And finally, in repository systems analysis, we are seeking additional breadth and depth in our disposal system understanding and also to address the needs of the U.S. program while contributing to and benefiting from the concepts and understandings developed in the wider international community. So some accomplishments here in the past couple of years include developing conceptual models and simulations that account for high-temperature impacts. Initiating the 4-year international performance assessment comparison under the DECOVALEX collaboration group. And growing a collaboration with Germany, the Netherlands, and the United Kingdom regarding features, events, and processes that could occur in a salt repository, together with scenario development.

In the next couple of years, we expect much of the effort in the repository systems analysis work scope to rest in simulation and analysis of the salt and

crystalline reference cases being developed under that DECOVALEX collaboration, which you'll hear about tomorrow, and those simulations are likely to drive further development of process models, including models for bentonite evolution, waste package degradation, and salt consolidation. So you'll hear more about that from Tara LaForce and I'll be back on the screen again tomorrow as well.

So I'll just leave you with a list of upcoming GDSA topics for this meeting. And open it up for questions.

>> BAHR: Thanks very much, Emily.

Do we have questions from board members? I see Paul's hand up, so go to him first.

>> TURINSKY: That was an excellent overview of the activity. It was very, very informative. It raises some more detailed questions and I have about a half dozen until Jean cuts me off here. Is the software NQA1 compliant?

>> STEIN: No, it's not.

>> TURINSKY: My experience is the sooner you get it NQA1 compliant, the easier it is, because I think at the

end, it will have to be. Is that not correct with the NRC?

>> STEIN: I will leave that question, maybe I would like to refer that to the NRC. I suspect so, yes. But I'm not the right person to answer that.

>> TURINSKY: It's a lot easier if you do it early on rather than try to do it at the end. It just becomes part of the workflow.

>> STEIN: Uh-huh.

>> TURINSKY: Regarding NRC, are you interacting with them now to sort of bring them up to speed?

>> STEIN: No. Through this program, I am not aware of interactions with the NRC.

>> TURINSKY: And how about stakeholders? I know this is very technical work. Are there folks out there who have been let's say critics in the past that would benefit from sort of being brought along with this? So you'll get their feedback and they would get more knowledgeable?

>> STEIN: Yeah. That is an interesting question, and I think that is a good -- I would actually like to put Tim

Gunter on the spot for answering that question. Right? It would be up to DOE whether and how much we interact.

>> TURINSKY: Okay. And have you actually used the code to make decisions? Is it mature enough that we can do a UQ or sensitivity analysis and decide, oh, this phenomena here, we really need to do some experimental work on it? I see Tim is on.

>> STEIN: Well, yeah. Maybe we go back to your previous question first.

>> GUNTER: So regarding the stakeholder interaction, we haven't really done a whole lot with that to date. It's interesting, like she said, an interesting thought. It may have some merit. We certainly could look at it to see how we could bring some of the people that may have an interest in it, you know, try to head to it early to see what thoughts they may have.

>> TURINSKY: Yeah, okay. Thanks, Tim.

Back to the subsequent question. Is the software mature enough that you can actually do some UQ and SA sensitivity analysis?

>> STEIN: So we typically do with every reference case

we are running probabilistic performance assessment or PA. So we are doing uncertainty analysis. We are doing sensitivity analysis. We can identify using those methods, which uncertainties in the input contribute most to uncertainty in the output. And you will see some of those results in both Laura's and Tara's talk later. Whether the uncertainty that is identified, you know, whether the uncertain input that is identified as having the most impact on output depends on a lot of things. So it depends on whether you are capturing all relevant processes in your model. It depends on the range of uncertainty over which you're sampling each of your uncertain parameters. So I would say that in specifically identifying topics for further R&D, there are a lot of caveats on the results that we've generated so far.

>> TURINSKY: And one more if you'll bear with me, and that is, you know, in contrast to Yucca Mountain, its assessment, there are some key conservative assumptions in there. The fuel was one of them. The state of the fuel. Are there other areas where you're trying to remove some of those key conservative assumptions, major conservative assumptions that have been made in the

past?

>> STEIN: Well, there are areas where we are working toward implementing more mechanistic models, which then given sufficient data would help eliminate the need for conservative assumptions. But also, in the process of setting up a performance assessment, there may be places where a conservative assumption is appropriate and adequate. And one example I will give of that is the waste package longevity in a salt host rock. There is, essentially, no reliance on the integrity of that waste package. So a simple conservative assumption that you can make is that it doesn't provide any containment, rather than trying to model a mechanistic degradation of the waste package in the salt host rock. So there are places where one approach is appropriate and other places where I think the other approach is completely adequate.

>> TURINSKY: Okay. Again, a very nice presentation. Thank you.

>> OGG: Looks like we lost Jean momentarily. Maybe Tissa can go ahead with his question.

>> ILLANGASEKARE: Thank you very much. I learn every

time you do a presentation, and I really appreciated the vision you have, because I think the reason for that is that eventually, it can be coupled with the biosphere, and then you go to larger and larger systems. I like the idea eventually you had to deal with issue of surface water interaction, because eventually these things are going to meet the surface systems.

Saying that I asked this question in the past but I'll ask it again. So your model, how well the model works depends on how good the process works. Eventually, the process models had to be captured accurately. So the process models, a lot of history in the other labs you mentioned in your slides that you are still working with other groups. So there are two ways you can look at these – the process models which are validated, and the experience which come with the process models. They have a lot of experience and I have been to many of their workshops and that. So how do you plan to bring those into the model? Your analysis [Indiscernible] of my statement. And the second question is when you are developing the PFLOTRAN, is it going to be more like a platform? Or are you going to integrate these process models into some coupled way, and the third question had

to do with the issue of efficiency. Because the challenges you have has to do with, when you integrate fully, the models become very, very inefficient. And you have to deal with this situation. So I like your thinking on your plans on how do you bring the accuracy of the process models and put into a large scale PFLOTRAN type of framework, and then eventually how to deal with this in simulating larger systems.

>> STEIN: Yeah. So I think one thing that we need to keep in mind when talking about software for performance assessment or safety assessment is that the purpose of that model is really to enable a decision. And in order to enable that decision, and it will sometimes be done in comparison back to safety standards, like quantitative safety standards, and it is not, in fact, always necessary to integrate a completely mechanistic and fully coupled process model in order to have enough understanding of the system that you can make a decision. So I think the key here is to develop really -- I'm not sure of modular is the right word Michael can correct me later if it’s not. It's to develop this capability where you can easily substitute one process model for another so that you end up with an

overall system model that is appropriate for the system at hand and the decision at hand.

So I guess I would say in terms of integrating process models that there is no one right answer, and it really needs to be use case specific.

>> ILLANGASEKARE: Sort of brings another question. So you mentioned, especially the capillary pressure saturation type of curve, because these are the traditional multi-phase problem, people really don't work at the extremes of these curves. They don't look at the very dry part of the curve. So are you funding more basic research, is it done internally or are you funding basic research in this area to look at? Because I think it's a good point you made here. I work with these things all the time. The capillary pressures are really really unknown particularly when it comes to simulating the large scale processes. So are you investing in outside research on these topics?

>> STEIN: I am not aware of any research within the program on developing those very tail ends of the capillary pressure curves. I do agree with you that that would be an interesting area to look into. What we've done for development within PFLOTRAN is mostly

refer to TOUGH and to FEHM to look what they had done to enable the simulations that were necessary for Yucca Mountain, and then implemented those options, also, in PFLOTRAN. And they're just making the tail end of the curve better behaved and easier to deal with numerically.

This is a little bit of literature out there, just generally out there, not generated by our program, that would point you toward some of those curve behaviors being better grounded in the physical theory of what's happening at those very low saturations than others.

>> ILLANGASEKARE: Okay. Thank you. I'm glad to hear your thoughts on that.

>> BAHR: I see Lee's hand up. If you can activate your camera? There you go.

>> PEDDICORD: Thank you. Just a couple of quick things. One is a more contextual question, I think. Back at the beginning, you talked about GDSA being a post closure safety assessment, then you said it might be a post closure performance assessment and maybe those are the same things. But I'm wondering if maybe they're not. So is it really just semantics or are there some

nuances in there between those two different descriptors? And I had the impression there ought to be.

>> STEIN: It's a really good question. And in fact I was asking myself the same question as I was --

>> PEDDICORD: Good for you.

>> STEIN: -- developing those slides. And for the purposes of what we're talking about in these next couple of days, we can use those terms interchangeably. I know there are other programs where somebody would distinguish a safety assessment is looking at, like, the answer to a safety assessment is something like a dose or risk to an individual. It's really assessing what is the safety of the system, whereas they might use that term performance assessment to go look at what is the permeability of the buffer and how is it performing within the larger system. Right? So there are definitely people out there who would distinguish between the two.

>> PEDDICORD: I had the impression in the performance characterization it would be a tool that could be used for optimization, whereas safety you're going to be

meeting requirements, regulatory and so on. But at any rate, I just wanted to thank you. That was very good. And again, your presentation was very good.

Let me ask another question --

>> BAHR: Thank you. I see Bill Boyle's hand up. Maybe he wanted to see something about safety assessment versus performance assessment.

>> William Boyle: No. Actually, I wanted to go back to one of TURINSKY's questions. So I can wait.

>> BAHR: Okay.

>> PEDDICORD: Okay. Well, let me just try this other one, too. I recently heard a presentation on kind of the interaction or the intersection, let me put it, of nuclear with petroleum, the petroleum field. And a new piece of information for me is the fact that they've been doing well logging for, like, 80 years now in the petroleum industry with cesium encapsulated sources, single encapsulated sources. And early on, there was big issues, a lot of these failed. Now they have double encapsulated and triple encapsulated capsules and so on.

Coming back to PFLOTRAN, and I'll be really impressed if

you say you've talked about a lot of data from these and you can see how cesium would migrate in a substrate, probably fractured rock and such things, so let me just pull the string, that sounds like something that might be accessed to pull out data and you could look at the performance of PFLOTRAN for actual cases in which radionuclides are now in the substrates and see if you could use it to assess some of the outcomes, the calculations from the code. Is that feasible? Maybe it's already being done, but I think it sounds really intriguing.

>> STEIN: As far as I know, that particular thing has not been done. It is an intriguing idea. When Michael gives his talk about PFLOTRAN, he has one slide that will show you some of the other uses that PFLOTRAN has been put toward, and one of those is use at the Hanford site in Washington to model uranium transport and speciation. So it has been used to model the fate of radioisotopes in the environment.

>> PEDDICORD: Cesium sounds like an interesting one, of course, because of its chemical properties. I suspect we may have a lot of locations in Texas where we could go look at some of these things. I don't know. I just

wanted to toss that out, because I was really struck in this presentation of maybe an opportunity of interests coming together.

Thank you, Dr. Bahr.

>> BAHR: Okay. William Boyle, who wanted to get back to one of Paul's questions.

>> William Boyle: Yes. It was a very good question about in NQA1 level quality assurance for the GDSA. And first of all, I want to assure everybody that the department does have a QA program for all the R&D work, and it's a graded program, and so the activities are looked at and very few of them reach the rigor of NQA at this time, but there is a quality assurance program.

And I agree wholeheartedly with Professor Turinsky's remarks. If you're an organization that is imminently starting on what is going to be an NRC licensed facility, you ought to have QA quality assurance starting day one. There is no doubt about it. And to show that the department takes it seriously, when the Obama Administration was considering a defense waste only repository and the various plans that were developed related to that activity, the plans had a QA

was going to start right away. It's not just software. Not just sciences. The quality assurance program reaches across procurement, records, resources. So it's important to get it in at the beginning.

I've also made that recommendation to my colleagues that are working on federal interim storage. And again, what sets those two apart from the GDSA is the plans were to actually pursue those. The GDSA exists for a potential repository and here it is, 11 years now the United States, the Congress and the country have been really not pursuing a definite repository. So if you're not going to be imminently in licensing for an NRC facility, quality assurance does cost money, and for some people, it costs them emotionally and, you know, if you don't have to have it, then perhaps it is okay to avoid it for a time. I just don't have a crystal ball to know when the U.S. will be imminently back in licensing for a repository in the United States and the NRC.

In general, it is recognized by the department that if you are going to be really pursuing an actual licensed facility, start QA early. Habits stability. You want them to be good habits, not bad habits.

>> BAHR: Tim Gunter, did you want to add to that in

>> Timothy Gunter: Actually, I didn't want to add to that, but I wanted to add to my previous response to the question about stakeholder involvement. I would point out that we may not be actively soliciting stakeholder comments on GDSA, but we do put that out in various conference presentations like upcoming American Nuclear Society waste management conferences in Phoenix and I'm sure there's lots of others, we could probably spell out several others where they present their work. So it is out in public forums. So that's all. I just wanted to add that point.

>> BAHR: I saw a hand up from Bobby Pabalan, one of the staff.

>> PABA LAN: the PFLOTRAN code has been applied to performance assessments for the Waste Isolation Pilot Plant Site, and you mentioned in your introduction that you've done some performance assessment work related to it. Are there any lessons learned from applying PFLOTRAN for the WIPP performance assessments that have taken into account for, for example, developing the conceptual model for the generic salt repository reference case and also in applying GDSA framework to that reference case, as well as the reverse part of

that, are there lessons learned from applying GDSA framework to PA calculations for the WIPP site?

>> STEIN: Yes. There definitely are. So our vetted salt reference case is heavily dependent on the conceptual model developed around the Waste Isolation Pilot Plant. So that is one thing. It is likely that I think in developing PFLOTRAN for use in the WIPP problem, one capability that needed to be added to it was the ability to simulate creep closure. Another capability that we added for that project was a gas generation model that depends on the chemistry within the repository. The chemistry for spent fuel repository would be different than what is in WIPP and likewise creep closure would occur differently when you have a backfilled drift. But I think the experience of implementing those models for WIPP is very likely to inform how we implement models in the future as we continue to develop processes for our salt reference case. So that's one set of lessons learned. Just how to couple ways of coupling those processes that work.

I'm sorry. Then you asked -- can you say the second part of your question again?

>> Roberto Pabalan: Is there lessons learned from

applying GDSA framework to the salt generic reference case to WIPP? I don't know if there's any back and forth between, you know, those two applications.

>> STEIN: Were there lessons or things the GDSA to WIPP? I know, I think I may have answered both of them already. Basically, what the team really got out of it was how to couple these processes that maybe are not an inherent capability of PFLOTRAN. And we know that we coupled them in in an acceptable way, because we had a way to benchmark them. Right? We had a goal of how our model should behave and we met that goal. I think that's the primary lesson. I'm actually wondering if -- not to put him on the spot. If Michael Nole might have something else to say about lessons learned in that effort?

>> NOLE: Yeah. Can you guys see me and hear me? One thing I would probably point out, especially since we discussed it a little bit earlier with Tissa's comments, was the idea of improving our representation of capillary pressure, which we used in our GDSA work. We've had numerical issues or I don't know if I call them issues, but just numerically, these problems could take a long time, simulating on WIPP. And in

particular, we saw a lot of performance issues where we had a lot of gas generation or where we were pushing gas saturations closer to those limits of the ends of the capillary pressure curve, and so we've actually been using a lot of what we learned on GDSA as far as better, more physically realistic representations of capillary pressure, more smooth representations. We've been looking at applying those to the WIPP problem as well. So that's kind of an example of going back.

And then I would also say we have learned a lot between -- we've learned a lot from WIPP to apply to GDSA in the QA realm. We've just recently finished QA in the flow portion of the code of PFLOTRAN for WIPP in a very rigid kind of QA structure. So we've learned a lot about what it takes to put all of those documents together, what it takes to actually really formally qualify PFLOTRAN for that specific application which we are definitely applying to our GDSA QA.

>> BAHR: Thanks, Mike. We are at the time where we're scheduled to take a break. So I think we'll go ahead and do that. And we are scheduled to reconvene in about 20 minutes. That will be 2:05 p.m. Eastern Time, one 11:05 on the West Coast. And other times in between.

So thank you and we will come back in about 20 minutes.

[BREAK]

>> BAHR: Okay. Welcome back from the break. Before we get started, some instructions to those who are asking questions. If you put your camera on at the same time that you raise your hand, you won't show up on the screen until Jake actually moves onto the screen, but that will speed the transition a little bit. So that's a little bit different from the instructions that we are given at the very start, but that's what's gonna work best.

Our next speaker is Paul Mariner, who’s going to talk a bit more in detail about the GDSA framework, and Paul is a researcher at Sandia National Laboratories. Thank you, Paul.

>> MARINER: All right. Thank you, Jean. Am I sharing my presentation mode?

>> BAHR: Yes, you are. Looks good.

>> MARINER: Okay. Very good. This presentation is about the advanced simulation capability GDSA framework.

The main topics I will be discussing are GDSA framework,

what it is, its purpose, what capabilities it has at this point, and I'll point out features, events, and processes that are not yet implemented in GDSA framework. Second, I'll discuss our GDSA framework applications. They include the reference cases we are developing and subsystem models. Next I'll discuss the performance metrics capabilities we have, both for total system performance and for multiple barriers. And last, I'll talk about our model capability development process. I'll point out the types of capability development we do, the influence of the roadmap and 5-year plans, and additional considerations that factor into whether a potential model capability is added to the framework.

GDSA framework. To be very clear, I'll read the objectives of our GDSA framework development work. The objective is to develop a disposal system and modeling analysis capability that supports the integrated modeling of detailed coupled processes controlling disposal system performance of deep geologic repositories, including uncertainty.

The system-level modeling capability will integrate updated conceptual models of subsystem processes and

couplings. Interface with site characterization data organized in a geologic framework model. Develop and apply uncertainty quantification and sensitivity analysis methods. Leverage existing computational capabilities, including meshing, visualization, and high-performance computing where appropriate. And be developed and distributed in an open source environment.

This slide shows the conceptual scope of the GDSA framework capability. The source term is in red on the left. It primarily consists of spent nuclear fuel and high-level radioactive waste glass. On the right is the biosphere. Each component in between, along with the waste form itself, acts as a barrier to some degree to inhibit the movement of radionuclides from the waste package to the biosphere. For any releases, the waste package must breach. The waste form inside the waste form will slowly degrade over time. Many of the radionuclide released from a failed waste package will precipitate or sorb to corrosion products or to buffer materials.

Intact buffer may greatly inhibit the extent of waste package corrosion due to its low permeability. The possibility of buffer erosion under certain

circumstances must be considered. It's an important process in international performance assessments. Alteration of smectite to illite in the buffer may also degrade the performance of the buffer.

Seals and liners may affect water flow that may affect the chemistry in the drift. In turn, the altered chemistry could affect radionuclide transport, waste package corrosion, and buffer performance. The disturbed rock zone around the drift tunnels may provide a radionuclide pathway, but buffer swelling may reduce its permeability.

Transport in the host rock and other geologic units will be affected by the permeabilities of these formations and the presence of fractures and fracture zones.

Finally, exposure in the biosphere depends on processes such as well water dilution, which occurs due to the convergence of contaminated and uncontaminated groundwater at the well. It will also potentially depend on other exposure pathways. All along the way, there may be important interactions and feedbacks. The engineered barrier system, what we call the EBS, includes many potentially important chemical reactions, including waste package corrosion, hydrogen generation,

fuel degradation, radiolysis, buffer alteration, and others. The extent and speed of these chemical reactions can be bounded and constrained by material mass balances, thermodynamics, and basic coupling relationships.

The alternative to including and coupling these various chemical reactions in the GDSA framework is to exclude them from GDSA framework. Exclusions, of course, require sound logic backed by supporting calculations. At this point in our program, our approach has not been to develop exclusion arguments. Rather, our approach is generally to proceed with developing new capabilities based on the possibilities of how important that can be. Without a site and without constraints on repository design, it is more difficult to justify that exclusion.

I will talk more later about the various factors we considered in our selection process for new model capabilities to implement in GDSA framework.

One last point I'd like to make here is that the relative importance of each of these components depends on the host rock and the repository design. For example, a repository embedded salt achieves much of its performance from the salt itself. In salt, the

engineered barriers were not as important to performance. We see that in our simulations. In contrast, for a repository in crystalline rock, the engineered barriers are much more important. Simulating the overall systems, the performance of each barrier in the system, and how each component interacts allows us to identify components and processes important to overall performance so that we can appreciate them, study them further, and consider design modifications to enhance overall performance.

GDSA framework is built around PFLOTRAN. PFLOTRAN does all the multi physics calculations. It simulates the source term, engineered barrier system, natural barrier system, and the various coupled processes within. PFLOTRAN also includes a biosphere model with several capabilities. In addition, a comprehensive biosphere model is under development and it will be discussed later by Caitlin.

Key attributes of PFLOTRAN include its parallel processing architecture or high-performance computing and its ability to scale. This high-performance architecture allows us to add model capabilities without terribly bogging down the simulations.

The code Dakota, shown in two places in this diagram, is an uncertainty quantification and sensitivity analysis software used by GDSA framework. It's used as a preprocessor and a post processor. One of Dakota's tasks is to sample uncertain inputs. Dakota can execute simple random sampling, Latin hypercube sampling, and other sampling schemes.

Second, Dakota's Next Generation Workflow is used to initiate and monitor performance assessment simulations, post process results, and documents all the steps of a simulation.

Third, Dakota's sensitivity analysis capabilities are used to identify inputs and quantities of interest important to performance metrics, reveal important interaction effects, and quantifying important sources of uncertainty in performance metrics and other quantities of interest.

Other components of GDSA framework include input parameter databases, including geologic framework model data that help characterize important stratigraphy. Python scripts that do a lot of preprocessing and post processing data. dfnWorks for stochastically generating discreet fracture networks. Meshing codes, such as

Cubit and Vorocrust, and visualization codes, such as Paraview. These visualization codes generate horsetail plots, 3-D figures, cross-sections, and animations.

With this framework, we simulate and assess the performance of our reference cases and their subsystems. At this point, I'd like to emphasize that we are well connected in many ways with the international working groups and we regularly consult the available literature released by leading international programs. International working groups include DECOVALEX, the international group working on DEvelopment of COupled models and their VAlidation against EXperiments. The Salt and Crystalline Clubs of the Nuclear Energy Agency. An informal international joint sensitivity analysis group, we call JOSA. And membership in international underground research laboratory programs. We also regularly participate in international activities, like conferences, journal publications, and manuscript reviews.

In the next few slides, I'll highlight the major modeling capabilities we've implemented in GDSA framework. I'll point out features, events and processes we have yet to implement. For the source

term, we can simulate the waste form radionuclide inventory over time. Decay and in-growth over time. And instant release fractions for certain radionuclides upon waste package breach.

Several models that have been implemented include the ones to simulate degradation of spent nuclear fuel after waste package breach. The fuel matrix degradation process model has been implemented in GDSA framework using surrogate models. Fuel matrix degradation involves radiolysis, electromagnetic reacts, alteration layer growth and diffusion of reactants through the alteration layer. I'll be giving a separate presentation on those surrogates later today.

Another spent fuel degradation model implemented in GDSA framework is the fractional dissolution rate model. It is a model that has been implemented in international performance assessments. And we also have an instantaneous degradation rate model that we can use for rapidly degrading waste.

For the degradation of high-level radioactive waste glass, we have implemented two models from the literature: The traditional transition state theory model and the Kinzler dissolution model. We have also a

custom waste form degradation model where we can do things like add surface area functionality.

With the implementation of the fuel degradation surrogate models, we have identified no other major source term FEPs that are not yet implemented in GDSA framework.

On this slide, the figure shows the evolution of the waste package, waste form, radionuclide inventory, and radionuclide release rates over time as affected by decay and in-growth, general waste package corrosion, and the fuel matrix degradation model. In these figures at about 1,000 years, the waste package breaches and the fuel matrix degradation begins. As indicated in the center figure, decay and in-growth occur continuously within the waste form. It occurs prior to and after waste package breach, causing significant changes to the radionuclide inventory in the waste form over time.

Decay and in-growth have important effects on relative radionuclide release rates over time, as shown in the bottom figure. After about 2 million years in the simulation, the waste form is fully degraded.

For the waste package and engineered barrier system, we

have implemented waste package objects, waste package degradation models, buffer behavior models, and disturbed rock zone behavior models.

The waste package object allows simulation of each waste package individually. This allows us to track each waste package's inventory, outer barrier degradation, and radionuclide releases. We have implemented two simple waste package degradation models: The general corrosion model, that is temperature-dependent, and a breach time specification model. More could be done here with other types of corrosion models.

Buffer and disturbed rock zone behavior models include temperature-dependent characteristic curves. Radionuclide absorption and diffusion. Water imbibition and swelling, smectite-to-illite alteration, and buffer swelling effect on disturbed rock zone permeability.

The photomicrograph in the figure shows alteration of buffer materials to sericite. The light-colored refractive material is the sericite and the dark material is a smectite rich clay chip. This sample was collected from an 18 year heater test at the Grimsel test site, an international underground research laboratory in the Swiss Alps. The Grimsel test site is

used to test repository concepts and component behavior in crystalline rock.

The Smectite alteration model implemented in GDSA framework can be used to slowly convert some of the smectite to illite as a function of temperature and time. In the implemented model, as the relative amount of illite increases, the permeability of the buffer increases.

Again, this slide lists the major model capabilities we have implemented in GDSA framework for the engineered barrier system. There are many features and processes in this domain that are not yet implemented. They include localized corrosion, stress corrosion cracking, cladding degradation, in-package chemistry, microbial reactions, seal degradation, and colloid formation and transport.

The importance of many of these not yet implemented features and processes is highly dependent on the waste package and engineered barrier system designs. Of course, there are no EBS design decisions at this time, so that makes it more difficult to justify deciding to implement a model that depends on, for example, the waste package outer barrier material or seal material.

Flow and transport capabilities. PFLOTRAN came well equipped to model flow and transport and thermal hydrological and chemical processes in full three dimensions. PFLOTRAN can model multiphase flow in water or gas. Recent advances have allowed PFLOTRAN to model complete dry out adjacent to a hot waste package without causing convergence issues. PFLOTRAN is not fully equipped to model mechanical processes. As a result, features, events, and processes involving mechanical processes have mostly been excluded at this point. However, many mechanical effects can be incorporated into GDSA framework.

For example, the buffer swelling model capability that was implemented in GDSA framework simulates mechanical pressure that pushes against the tunnel walls and effectively reduces the permeability of the damaged rock zone around the tunnels.

Fractured rock. For fractured rock, we stochastically generate discreet fracture networks using dfnWorks, and then we map these DFNs to our equivalent continuous porous medium mesh. This approach has been extensively tested and works quite well. We also have the ability to model fracture-matrix interaction as a multi

continuum.

Solute transport. Solute transport is one of the core capabilities of PFLOTRAN. Solutes, such as radionuclides, undergo advection, diffusion, decay, ingrowth, and partitioning between phases. Solutes can precipitate and dissolve in accordance with elemental solubility limits or their reactions can be represented in full reactive transport chemistry mode.

GDSA framework includes several biosphere capabilities. PFLOTRAN can currently simulate well water capture and dose from water ingestion. The well water capture model includes a model that includes mobility enhancement factors for short-lived radionuclides, like radon-222. In addition, as I mentioned earlier, there is a much more comprehensive biosphere model under development. The biosphere model will initially act as a post processor for performance assessment.

A key component of GDSA framework is its uncertainty capability. There are several uncertainty capabilities we have implemented in GDSA framework. There are also several we continue to develop.

For our probabilistic analysis, we propagate uncertainty

by using random sampling or Latin hypercube sampling to sample the uncertain distributions of our input parameters. We can also implement aleatory and epistemic uncertainty loops.

For post processing, we statistically characterize our outputs and quantities of interest in terms of means, medians, percentiles, variances, and other statistics. And we continue to develop sensitivity analysis tools to look at. That includes things like correlation, interaction, variance analysis, identification of input importance, and ranking of sources of uncertainty. These sensitivity analysis help us understand the effects of features and processes on quantities of interest and on performance metrics.

The figure here shows the results of a sensitivity analysis that examines the effects of uncertain parameters and quantities of interest on the peak iodine 129 concentration in the aquifer. For this crystalline reference case analysis, the number of fractures intersecting the repository and the average degree of intersecting factors in the host rock are the best predictors of peak iodine 129 concentration in the aquifer. In this case, the large uncertainty in the

spent fuel degradation rate has a much smaller effect on the peak iodine 129 concentration in the aquifer and the random number of fractures intersecting the repository.

What this simulation does not do, however, is tell us what would happen if we avoided emplacing waste packages in areas where intersecting fractures are found. In a real underground operation, we would identify these fractures on excavation, or at least we would try to, and we would not allow waste packages to be placed there. In future simulations, we will identify these intersecting fractures, simulate waste exclusion zones, and observe how the simulation exclusion zones affects repository performance.

These types of sensitivity analysis are informative and can help guide future research, but they are also quite specific to the application. For example, this particular simulation has a lot of failed waste packages. Many of these waste packages fail during the first 10,000 years. If the simulation had thick copper waste packages or a different receptor point, the sensitivity results might be much different. Because we don't have a specific site or a constrained repository design, it can sometimes be challenging to use

sensitivity analysis like these to guide future research and development.

Other GDSA framework capabilities include meshing and generating discrete fracture networks. Typical mesh generators, such as QBIT, are used to build structured and unstructured meshes. The Voronoi meshing capability is being developed to improve feature rendering without making the simulations too expensive to simulate.

dfnWorks, the stochastic DFN generator we use, allows us to study the effects of spatial heterogeneity in the host rock on performance assessment. As indicated in the previous slide, in many of our crystalline reference case simulations, the random spatial heterogeneity caused by stochastic DFN generation can be the largest contributor to uncertainty in the peak iodine 129 concentration in the overlying aquifer. Also, PFLOTRAN has a multi continuum model and can simulate the effects of diffusion from fracture into the matrix.

Here is a version of the generic FEP screening slide that Emily presented earlier. Highlighted in red are the features, events, and processes included at this point in GDSA framework, at least to some degree.

The FEPs in black are those where capability is lacking or where they are excluded at this point in our simulations. This assessment generally indicates that the majority of the excluded FEPs or yet to be implemented FEPs in our reference case simulations are chemical, mechanical, and disruptive FEPs.

Finally, in addition to the FEP capabilities of GDSA framework, the Next Generation Workflow capability of GDSA framework autonomously executes all of the major components of GDSA framework. It has a graphic interface and shows exactly how all components are linked and it shows the status of each component during each simulation. It executes post processing calculations and this workflow facilitates transparency and reproducibility.

The workflow is very flexible and can be easily modified by the user. So far, this workflow capability has greatly improved the reliability, documentation, and development of the crystalline reference case.

This diagram shows at a very general level the processing steps executed by the workflow. The workflow in the center is the deterministic simulation. Model simulation with one set of inputs. This deterministic

simulation is nested inside an epistemic uncertainty loop where epistemic uncertainties are sampled from established distributions.

In this case, the epistemic loop is nested inside an aleatory or spatial uncertainty. This nesting is done so that the contributions of these various types of uncertainty can be parsed out, evaluated separately, and quantitatively compared to each other.

Now I will talk briefly about our general applications of GDSA framework. The three primary host rocks we have been studying are crystalline, argillite, and salt. These reference cases are simply hypothetical generic constructs. These reference cases are not actual sites associated. These do not represent actual sites. Each reference case has its own repository design, based on conceptual models developed several years ago. Each of these reference cases has in-drift emplacement. The argillite reference case assumes shale host rock. The salt reference case is for bedded salt and has run-of-mine salt as back fill. The shale and crystalline reference cases have buffers surrounding the waste packages in the drifts. The main purpose of these reference cases is to study and assess total system

performance and the performance of included features, events, and processes.

The purpose of these reference cases is not to compare the performance of the reference cases to each other. Our objective is simply to develop the modeling capability that can be used to assess performance of a repository design, regardless of host rock type. In a later presentation, Tara LaForce will go into later detail where these reference cases.

GDSA framework is also used to simulate subsystems. By focusing on subsystems, higher fidelity meshes -- well, and their interactions can be simulated. This can improve our understanding of localized processes. In turn, this can tell us whether the full scale model implementation is acceptable.

These figures are from a higher fidelity near field simulation of the evolution of buffer surrounding a hot waste package in a shale repository reference case. The refined mesh shows a permeability increase near the waste package due to simulated alterations of smectite to illite This effect cannot be captured well in a full scale reference case simulation. The full scale simulation has a mesh that's too big for this.

To measure performance in our applications, we have different types of performance metrics. Performance metrics are used to compare to regulatory limits and to assess effectiveness of repository design and the natural barriers on waste isolation. A likely regulatory performance metric is mean annual dose to a receptor, as shown on the left. Here the dose is from a well in a sandstone aquifer above a shale repository reference case. The dose is expressed in units of sieverts per year. The red line is the mean of all probabilistic realizations. The dotted line shows the 90% confidence interval. And the gray lines show the computed annual doses for the individual realizations.

Over the years as we've developed model capabilities for GDSA framework, we've focused on engineered barrier system and the geosphere. Because of that, an acceptable indicator of the combined performance of the engineered barrier system and geosphere has often been the peak iodine 129 concentration in the aquifer. Iodine 129 is consistently the dominant contributor to radioactivity in the aquifer in our reference case simulations. The figure on the right is from a monitored location in the limestone aquifer in the shale

repository reference case simulation. The red line in that figure shows the mean peak iodine 129 concentration at that observation point overtime. For this particular system and observation point, the lower 5% quantile is below the scale of the figure.

Performance metrics for multiple barriers typically involve comparison to the total inventory activity. In this figure, total inventory activity over time is indicated by the upper blue line. Activity release to the host rock is indicated by the red line and release to the biosphere is indicated by the green line. The difference between the red and blue lines indicates the performance of the engineered barrier system. The difference between the green and blue lines indicates the combined performance of the engineered and national barrier systems. This capability for evaluating performance allows us to parse out the engineered and natural system contributions so that we can clearly show the relative performance of these two general barriers in our simulations.

The final topic of this presentation has to do with our decision process for choosing model capabilities to implement in GDSA framework. The scope of potential

model implementation is guided by the roadmaps, FEP analysis, and 5-year plans that Emily spoke about. That scope identifies FEPs that have been deemed important to include, if possible, in GDSA framework. Importance is further guided by simulations, subject matter experts, and the available literature. The feasibility of including a FEP is guided by a codeveloper's analysis of inputs, outputs, and code constraints. Readiness of the model for implementation is another important consideration. I'll present a list of the major readiness screening questions in a moment.

Finally, decision to proceed with model implementation depends on the results of readiness screening and consideration of priorities.

When we talk about capability development for GDSA framework, there are many different types of capabilities to develop. In addition to new physics based features and processes to add as model capabilities, there are solvers, preprocessors, post processers, verification and maintenance testing and other capabilities and attributes that are useful in enhancing reproducibility, transparency, and user friendliness. Here, though, I will simply address the

process for selecting new model capabilities to add in order to address not yet implemented FEPs.

To assess whether a model capability is ready for implementation, we have a set of questions to consider. They include will the model have significant effects on important repository performance metrics and/or provide important answers to key questions? Are all model assumptions affecting the validity of the model acceptable for the intended use? Does the model cover the necessary ranges of input values? Is there a better model or approach with more defensible assumptions that covers the necessary range of applicability? And does the standalone model converge and produce sensible, defensible results for the entire multi-dimensional sample space of the application? If the answer to these questions affirm that the model is ready and it's important to implement, then the model can be prioritized.

Prioritization depends on the importance of the proposed model capability to the five-year plan and to the roadmap, the importance of the model to the reference cases, and the prioritization depends on the balance of the required level of effort and the available

resources. If the resulting priority prioritization for the proposed model capability is high enough, it will be assigned for implementation.

Summary. This presentation shows that the GDSA framework capability is evolving at a strong and steady pace. Each year, we add new model capabilities and we improve current capabilities, all with the aim of improving our ability to include the effects of important FEPs in the performance assessment of repository designs. GDSA framework development is guided by the roadmap, FEP analysis and five-year plan. It's also guided, in part, by international influences, including available literature, international FEPs lists and analysis, and engagement in the international working groups and activities.

It's important that we stay focused on model development as a high likelihood of enhancing our ability to assess total system performance for potential future sites. For this reason, the final decision to adding model capability to GDSA framework relies on important readiness and prioritization considerations, in addition to the interests of the roadmap and 5-year plan.

And with that, I will briefly show the reference slide.

And I will end my presentation.

>> BAHR: Okay. Thank you, Paul. And we have a hand from Paul Turinsky of the board. If you can get your camera on, Paul? There you go.

>> MARINER: The other Paul.

>> MARINER: There you go.

>> TURINSKY: With regard to verification where you're comparing analytics solutions of available or looking at the order of the error how it behaves if the numerics are correctly implemented, and likewise, this question also goes into validation, do you have an automated system that does that for you? I'm used to big codes, having that sort of capability. You sort of run it overnight to make sure that whatever has been added recently passes all the verification tests developed and validation is a little more subjective, but it sort of gives you a scoreboard of where you're at.

>> MARINER: Right. That's a good question. That kind of automated verification that the code is running correctly, we often call it regression testing. Mike Nole is going to talk more about that in his presentation. That certainly is a quality assurance

procedure that we run to make sure that the code isn't broken, that we're not breaking the code.

As far as validation goes, we do have quite a few validation experiments for the flow and transport parts of the PFLOTRAN code ready to go. So what happens there is because those are primary components of the PFLOTRAN code, we do do some validation there against analytical solutions, against benchmarks, things like that. And a lot of that has been automated already.

In terms of the other parts of GDSA framework, when we're adding new capabilities for PFLOTRAN that are specific to nuclear waste repositories, things like corrosion of the waste package or fuel matrix degradation, those are separate process models that are developed usually separately from us in performance assessment. They're developed at the process model level, and they are validated there with experimental data and so forth.

By the time we get it in performances assessment, what we do is work on verifying that our implementation adequately reproduces their validated process model.

>> TURINSKY: And related to that, when someone develops

a new model, who is the gatekeeper who decides that this can go in the approved production version of the code? Is that a collective process?

>> MARINER: Well, there is a process that we have. I showed you the screening questions that we go through.

>> TURINSKY: Right.

>> MARINER: At this point, we're in R&D mode. It's not a formal process where we're signing things off, but we certainly get the right people involved. We get project managers involved. We make sure that they understand why we may want to add a specific model. So we do do quite a bit of work to make sure that everyone is onboard and the model is ready to be implemented and that it's important to implement.

>> TURINSKY: And how often do you do a formal new release? New version of the code? Is that once a year process? Twice a year? Because you have external users who have this code. Right?

>> MARINER: Yeah. Well, Michael, again, will talk probably more about this. The code itself is open source, and anybody that can download it anytime. As far as upgrades? It's every couple of years or so. And

there's some maybe major announcement. That's just a real rough estimate.

>> TURINSKY: Okay. Thank you.

>> MARINER: Uh-huh.

>> BAHR: I see Tissa's hand up?

>> ILLANGASEKARE: Thank you for a very clear presentation. So I have a few questions. In your slide five, between the biosphere and your rock, there you have “other”, so the “other” I assume that looking at your biosphere on the slide that “other” includes surface systems. Is that correct? Surface water bodies.

>> MARINER: I think you're referring to that conceptual diagram?

>> ILLANGASEKARE: Yeah. Slide number 5. It had like an orange box between -- yes.

>> MARINER: Right. So you're asking if we have included surface processes in the biosphere model in our current GDSA framework?

>> ILLANGASEKARE: Yeah. Your orange box between the

biosphere and the rock. You said other. So that other, I assume that basically it includes surface water systems and what will become input to the biosphere model?

>> MARINER: That is our conceptual model. And at this point, our GDSA framework is working on that connection now.

>> ILLANGASEKARE: Okay.

>> MARINER: It's just in the past year or two where we built the plan to pull in this biosphere code that's going to be developed. But until now, it's mostly just been focusing on moving through the host rock and then our biosphere has been actually just very simple aquifer to this point.

>> ILLANGASEKARE: So the next question is --

>> BAHR: Can I ask for clarification? My interpretation of the box that I think Tissa is referring is that you have, in a geologic system, you have the host rock. For example, in a salt repository, the salt is the host rock, but you have other geologic units through which transport would occur prior to reaching it.

>> ILLANGASEKARE: Yeah.

>> BAHR: Carbonate or a sandstone. I was interpreting that as what you meant by other beyond host rock.

>> MARINER: I can try to pull up that slide if you like.

>> BAHR: Yeah.

>> MARINER: I assume you are looking at this other units box? So in this case, the other units are like an aquifer, an overlying aquifer that we have simulated so far. So the host rock might be salt or granite and then the radionuclides travel through that host rock into an aquifer, where there might be a well. And it's the concentrations in those aquifers or in the well that we have been focusing on up 'til now.

[Talking at the same time]

>> ILLANGASEKARE: My question had to do with the units. I think that clarifies, the units that exist, you are looking at the aquifer subsurface formation, but my question has to do with a slide you have later where the biosphere cartoon shows that there is a surface system. You gave the answer earlier, at this time you are

looking at just the subsurface of the units.

>> MARINER: That's true. That's true. We've just been looking at subsurface processes.

>> ILLANGASEKARE: Can I continue?

>> BAHR: Yeah. My understanding of what Paul just explained, so thank you.

>> ILLANGASEKARE: So next question is in your transport simulation, you assume the water is at steady state?

>> MARINER: No.

>> ILLANGASEKARE: No?

>> MARINER: No. It's fully transient. You can see that quite dramatically. And the main reason is we have a thermal system that's causing some of the flow to happen. And so overtime as the thermal pulse subsides, you see that the flow rates and even sometimes the flow directions are changing over time.

>> ILLANGASEKARE: So my question is sort of related to that. So that nonsteady state is created by thermal. How about the boundary conditions which are climate driven? For example, precipitation? Rainfall? So then

it brings the question, are you looking at the climate concern in GDSA framework?

>> MARINER: That certainly is going to be important. That is on our radar, but we, no, have not been working on that part of it.

>> ILLANGASEKARE: And then your multiphase improvements you are making, capabilities, you mention that you are looking at unsaturated flow. In unsaturated flow, you are not looking at a Richard's equation. It's a full two phase flow problem. You are not assuming that there are phases free to move. Is that correct?

>> MARINER: I'm not as familiar with that. We do have the capability of doing both modes. I would think that there's someone on the line who could answer that question if you're real curious.

>> ILLANGASEKARE: You mentioned gas flow. When you have gas generation, you cannot make the assumption in the Richard's formulation, you assume that everywhere the pressure is constant. And I think I know the answer, but I just want to clarify in a multiphase flow formulation. You need to make sure that it's a truly, fully multi phase flow. You should not use the soil

physics approximations in this type of model. That's the point I'm trying to.

>> NOLE: I can just pipe in.

>> BAHR: Mike, maybe he can come on screen?

>> NOLE: We do have a full multiphase immiscible flow option. Depending on what the needs of the system are, you can certainly simulate multiphase in those instances where you have gas generation or high heat input and you're boiling off water, for instance.

>> ILLANGASEKARE: The last question for Paul. The verification, so in your process models, they're verified using experimental data, but ultimately, the larger model, integrated model where you're looking at all of these coupled processes. I'm very aware that you don't have data to validate, but have you looked at other data since coming from other earth science applications where you can verify existing data sets to sort of verify your coupled behavior in your model? Because you'll never get data to verify your model at this stage. Have you looked at other data sets that you could use to look at this coupled behavior? In other environmental subsurface, remediation applications?

>> MARINER: Right. And it's very important to do. Our job with GDSA framework for the total system performance assessment is really to pull the models from our process modelers. And so it's really our process modelers that are working on those various processes and also thinking about the couplings that go on for those process models. They are the ones that are participating in the underground research laboratory experiments. They see that data. They try to model it. They develop process models that can be verified by that data, and then once they can do that, then our job in PA is to represent, you know, somehow implement those validated process models in ours.

>> BAHR: I see Dave Sassani with his hand up. Is this a clarification of an answer, Dave? I need you to unmute yourself and be brought on.

>> Dave Sassani: Yeah. It was just an addition to Paul's answer to get after the validation and verification aspects for the system model, for the GDSA model. We're relying on the process model validation where the process models show they're valid against independent data sets and give a range of validation conditions, and then bring them into the GDSA into the

system model. And as Paul, I think, discussed earlier, verify that the implementation reproduces the process models accurately. But then it's the coupling aspects. Right? And it's also the extended duration time for estimating performance for safety in the future. Those aspects are done by two parts: Verifying that the actual couplings are functioning the way they're supposed to among validated process models and then in a less quantitative fashion in many cases, looking at things like natural analogues and data sets for natural analogues, and I believe Michael Nole spoke earlier about having the system being applied to something like perhaps radionuclide transport at Hanford, much smaller time scales, but demonstrating the process function. That's kind of the whole ball of wax for looking at verification or validation of a system model, the GDSA or Total System Model that Paul referred to.

>> ILLANGASEKARE: That's what I was getting at, because you can do that using other data sets. So those are good examples. Thank you.

>> BAHR: Okay. Bret Leslie had his hand up. Bring him on stage.

>> Bret Leslie: Okay. Paul, good talk. I did have a

question, which is so how do you assess disposal options if you're right now not focusing on material-specific things that are really design options? So for instance, you know, you really can't assess a disposal option. You can assess sites generically, but unless you include those FEPs, what is a disposal option?

>> MARINER: Well, that's a good question. Could you give me an example of a disposal option? Are you talking, like, in certain waste package material?

>> Bret Leslie: Yeah. And the various degradation processes. So you've identified that you haven't included specific FEPs associated with specific corrosion processes and those would be the things that distinguish between different design options for a particular rock type.

>> MARINER: Yeah. And that is a conundrum right now. We do not have an EBS design at this time. We do not have a site at this point. That makes possibilities a little bit endless and hard to get our minds around. If we go ahead and spend a lot of time on a copper corrosion model and then find out that we're not going to use copper and have we wasted our time on that? No, maybe but it would be much better if we had more

direction on, you know, what the likely EBS designs are going to be. So all we can do is really just look at the international community, look at what is being developed, and just make decisions based on what we think are very important FEPs to include in our model capabilities, in our toolbox.

>> Bret Leslie: Thank you. That's sufficient.

>> BAHR: Dave Sassani, did you have a comment on this point?

>> Dave Sassani: It sounds like Bret got his answer. That's generally what it is, those specific engineered system evaluations are down the road a bit, because they tend to be more site specific.

>> BAHR: Okay. Lee Peddicord has his hand up and this will be the last question.

>> PEDDICORD: This is maybe an extension of what Dr. Leslie was focusing on and along the same lines. You know, yours was a good point if you do copper. I think the Swedes are going to use up all the copper in the world for their system, so there may not be any more available. But I wanted to come back on your slide 17 you had, of course, the three principal options. And

you rightly made the point, as we just discussed, you can't look more specifically really, because you wouldn't want to give the impression that you have picked out some place in the U.S. where there's going to be a repository. But as Emily Stein pointed out, other countries are looking at these. So my question is along the following lines. Is PFLOTRAN fairly unique among all the national programs looking as this challenge and given the fact that each of these three cases have countries looking at them, does this give you a chance to benchmark what you're doing against maybe what they've done, or there is a collection of countries, the Clay Club or the Salt Club, what the IAEA is doing? How much can you look at all of these and kind of get some validation of what you're doing coincides, at least, with what's going on in other countries in the international community?

>> MARINER: Right. Well, yeah. So PFLOTRAN, because of its HPC capabilities and it's really kind of state of the art in a lot of ways, it's far more advanced than what some countries are using. Now, what we do do is we do look at the other programs' data. For example, for the crystalline case, we look at Forsmark and we look at

Olkiluoto and we look at their characterization of fracture zones and fracture networks and we make sure that we can implement those types of data into our codes and we test them against them, and we actually communicate with them, just to make sure that we've got it right. So yes, we definitely leverage a lot of that information from other programs.

>> PEDDICORD: That's good to hear. And I appreciate the fact that probably the computational capabilities you're using for these within, you know, the DOE complex far exceeds what other countries have available to themselves, too. So good. Thanks very much. Appreciate that.

>> BAHR: Thank you. I think we need to move on now to our next speaker. That's Mike Nole, who's going to tell us a bit more specifically about PFLOTRAN. If we can get Mike up?

>> NOLE: Are you seeing the presentation or is it in presenter mode?

>> BAHR: Uh-huh.

>> NOLE: Okay. Great. Thank you. So my name is Michael Nole. I lead the PFLOTRAN development team at

Sandia National Labs. Today I'm going discuss what PFLOTRAN is, as well as our software development process.

So in my talk today, I want to hit on three main topics. First, I'm going to give an introduction to the code PFLOTRAN. I'll discuss what the code is designed to do and what kinds of projects use its capabilities. And one key component of the code and the GDSA framework in general is that it's open source, so we'll talk about the benefits of an open source approach to the framework and then get into the details of our open source software development process, which includes version control, task management, and code verification.

And then finally, I'll talk about process modeling in PFLOTRAN. Specifically we'll look at where PFLOTRAN fits into the GDSA framework and then discuss PFLOTRAN's approach to coupling multiple process models together flexibly. And then to end, I'll go over some recent advancements made to the code over the last eight years as they pertain to GDSA related applications.

So what is PFLOTRAN? PFLOTRAN is a scalable finite volume reactive, multiphase flow and transport code for simulating subsurface processes. So I really want to

emphasize here PFLOTRAN's scalability. It's written in parallel from the ground up and we're frequently testing scalability. That graphic in the bottom right shows PFLOTRAN's strong scaling as compared to ideal one-to-one scaling.

So what this means is for a fixed problem size, the time to solve the problem decreases as you increased number of computational nodes across which you distribute the problem on a high-performance computing cluster.

PFLOTRAN really shows industry leading scalability in this regard, and this is critical for GDSA, because as others will and have shown you, the code is being used on really large scale problems with upwards of tens of millions of degrees of freedom. So the code really means this level of parallelism.

Another key aspect of the code is that it's open source, meaning that anybody can access the code and contribute to it. It also has a modular design and it's written in modern object-oriented Fortran 2003. And it's built on a number of very well established and well supported open source libraries. For example, solving the linear systems of equations in parallel, parallel input and output to files, and load distribution on each PCs.

So the overarching goal of the simulator design and software development infrastructure is to really be developing capability that can innately involve in response to advances in his numerical methods and computing and process models.

So how is PFLOTRAN used? It's used extensively in the nuclear waste disposal realm. Specifically, the performance assessment team at the Waste Isolation Pilot Plant in Carlsbad, New Mexico, is qualifying the code for use as one of their official PA codes. The flow portion of the code recently underwent a rigorous QA as part of a qualification process, which I kind of touched on a little bit earlier today. And then in addition to WIPP, it's used across the DOE SFWST campaign of which GDSA is a part. It's being used in international model comparison study on the Development of Coupled Models and Validation against Experiments or DECOVALEX, which Emily mentioned. She'll go into detail tomorrow, I believe.

And this project brings together an international set of teams across North America, Asia, Europe. It's also used by Amphos 21 for nuclear waste repository performance assessment at Forsmark. Outside of the

nuclear waste disposal area, it's been used for all sorts of applications, including climate modeling in the Arctic and through the DOE systems modeling program. And as Emily mentioned earlier today, it's also used to model biogeochemical transport phenomena at Hanford and other sites across the U.S.

So as I mentioned before, a key component of the software in GDSA in general is its open source framework. Open source brings a variety of benefits, and the four that I'm highlighting here include enhanced collaboration across institutions to code development, code deployment, and testing, as well as code debugging. Open source offers pretty much complete transparency, which is increasingly being demanded by the broader scientific community in general. Transparency provides the important details necessary for reproducibility.

Additionally, open source provides a significantly lower barrier to entry for an institution. There are no financial barriers or gatekeepers, and since it's source code, a user can compile the code on their own machines themselves. And finally, open source promotes code fitness and robustness, which ensures its survivability.

So when I talk about an open source framework, what do I

actually mean? Our open source framework for PFLOTRAN development consists of five major components. Our public code repository, our documentation, our continuous integration, task manager, and a quality assurance test suite.

So the public repository is where version control happens, where our coding standards and development philosophy are set, where merge request requirements are specified, and where we'll do our code versioning.

The documentation site contains all the relevant information on the theory behind certain process models, as well as a user guide for developing input decks. We use continuous integration to do all of our regression testing, which tests any updates to the code made by developers so that it can ensure quality code before merging the changes into the main version of the code.

So what we do with regression testing is we take outputs from these small mechanistic simulations and compare them to gold standards so we can identify if there are any unintended behaviors resulting from recent changes.

And then on the flip side is unit testing, which those tests test individual function output over a predefined

range of input values. And so the combination of regression testing and unit testing are what we use to ensure that we can confidently merge any changes made by developers. And then besides the repository, our code development team manages and prioritizes our development tasks using a Jira task manager. We also have a QA test suite, which is designed to be modular and adaptable to evolving process model capabilities.

So our code is hosted in a public repository on Bitbucket, which is where we do all of our version control. Version control is how we keep track of any changes that have occurred to the code, and this repository keeps a history of all code the changes since the repository was begun. Version control uses the Git protocol, which makes it extremely easy to move backward in time and recreate the code as it was in an earlier point in history. And in addition each code change is labelled with each author, with a unique identifier and brief description of the change, as well as a check that verifies that it passed all of our tests.

We've been working with this system since PFLOTRAN was initially included in GDSA. It's been working very, very well for us.

Task management is similarly approached using an agile paradigm with openness and transparency in mind. We use JIRA as our task manager, which allows us to align issues to particular developers, as well as identify stages of development associated with each issue. And prioritize and categorize all of our issues, so its categories include bugs, and these are just kind of getting technical, but we call them bugs, stories, epics, or tasks, which kinds of delineate the different type of issue that we might be going after. And then we identify how much of a development effort for a given issue represents.

Our development team works in bi-weekly sprints where we evaluate our issue scoping every other week, and this image down on the right is just a recent snapshot of what this development sprint board looks like where we have color-coding of our issues by category, and then we assign them to developers, and we slot them into different phases of development, like to do, in progress, under review, and done.

We have a GDSA-specific quality assurance test suite, which is built off of the PFLOTRAN QA toolbox, which we're developing to perform code verification in a way

that is consistent with DOE's graded QA requirements. This is currently developed in Gitlab which is similar to the Bitbucket repository but it's internal for now while it's being developed before it's released to the public.

The idea with the QA test suite is to benchmark the code against analytical solutions where those solutions exist and to have modularity and extendability for testing PFLOTRAN results against other simulators designed for similar purposes, such as the TOUGH family of codes.

And this image on the bottom right shows the steady state three-D pressure distribution comparison against an analytical solution, which is one of our suite tests.

So then finally, I want to touch on process modeling in PFLOTRAN. PFLOTRAN is the multi physics simulation engine of the GDSA framework. So it runs the multi physics simulations over a given performance period of interest, which can typically be tens of thousands of years. The simulator is designed to accommodate heterogeneity in length and time scales associated with lots of different process models that it's able to consider. And these models are generally dropped into one of three categories for either the source terms,

flow and transport models, or biosphere model, which at this point, the biosphere model is mostly a post processor on the flow and transport solutions.

So GDSA makes use of a number of different combinations of what we call flow and transport modes. It makes use of three different fluid flow modes. The first is Richards mode, which solves conservation of water mass to model variably saturated flow problems. Second is TH mode, which couples Richards mode with an energy balance to solve conservation of water mass and conservation of energy. And then finally, general mode, which solves conservation of water mass, air mass, and conservation of energy to model immiscible multiphase flow.

These formulas are all sequentially coupled to solute transport where we have three different transport mode options. The first is global implicit reactive transport which contains PFLOTRAN's standard set of reactive transport libraries. The second is a GDSA specific UFD decay process model, developed specifically to study radionuclide sorption, partitioning, decay, and in-growth. And then finally our newest transport mode is nuclear waste transport mode, which is similar to global implicit reactive transport, but is formulated with

different primary variables so it can be useful in situations where for instance you get dry out occurring.

So PFLOTRAN has a distinct approach to process modeling. Process model coupling, which I want to elaborate on with a few slides here, because it demonstrates a key component of the GDSA framework, which is its modularity. So the traditional approach to time stepping, which you can see on the left, is so when you're time stepping through a solution to a nonlinear system of equations, you start with initialization of all the variables and then in the case of sequential flow and transport solution, coupling. You then enter inside of a time stepping loop where you solve the flow solution. And then the reactive transport solution, and then you check your criteria for achieving convergence before declaring that you're done with a given time step. And then you cycle for all the time steps and finalize all the outputs when you reach the end time.

PFLOTRAN, on the other hand, was conceptualized, it conceptualizes the first and last stages of the process the same. But in the middle, the middle part is thought of as more of a flexible execution stage where process models can be flexibly coupled in at the will of the

modeler so you don't necessarily have to take that strictly linear approach.

So what does this coupler look like? A given process model coupler is associated with the process model. Like for instance, multiphase flow, and the numerical method for solving that associated system of partial differential equations. And then from there, the process models can be coupled to each other through either a peer to peer relationship or a parent child relationship. And if those two process models are considered peers, they sync up at the same prescribed time intervals. But if the process models have a parent/child relationship, then the process model proceeds in subintervals and catches up to the parent at a specific time where they exchange relevant information.

The parent/child sequential coupling is useful when there's a difference in timescale associated with different processes and the peer to peer relationship is useful when decoupled processes act at similar time scales.

So when we stack these up, we can get a series of parent/child relationships. For instance, process model

A takes a given time step and then process model B can take smaller time steps and syncs back up with an A time step. Similarly, process model C can sub-step B.

And as we add on more and more process models, these relationships can be extended for each combination of different types of process models. So specific to our radioactive waste process modeling workflow, one example of a potential execution phase can generally include maybe multiphase flow as the parent processes model with transport as a child process model and then the waste form source term can include the waste package degradation model and would be a child of transport. And then the isotope decay partitioning growth model would be evaluated as a peer of waste form.

So the benefits of this process model coupling approach align with a few of the really essential requirements of GDSA framework, which include customizable linkages between process models describing flow, transport, source and sink terms and reactions, as well as flexible time stepping which allows each individual process model to run at its own relevant time scale. And modularity for incorporating new process models into the execution phase without needing to impact the other models.

So over the last eight years or so, GDSA has pushed forward many new significant advancements to the code, which include fully coupled modeling and multiphase fluid flow and heat flow. Radioactive sorption partitioning decay and in-growth modeling through the UFD decay process model. Soil matrix compressibility. And flexible models for thermal conductivity and anisotropy. The code has been tested on massive domains with lots of heterogeneity and various degrees of spatial resolution, which I think is captured pretty well by the figure in the top right, which shows the repository at high resolution with an heterogeneous layered geology. And then some of our recent advancement in thermal modeling for multi phase anisotropic systems are summarized in a figure in the bottom right and included in our recent PFLOTRAN development report this year.

The figure on the bottom right shows an anisotropic thermal conductivity and the resulting temperature distribution.

And so now on top of those recent advancements, we've also added the generalized sorption iso-therms, advanced fuel matrix degradation models which Paul will discuss.

The biosphere well model. Multi continuum transport for modeling. Fracture matrix diffusion through dual porosity model. Advanced Linear and nonlinear solvers. High temperature equations of state. And reduced order geo-mechanics models. So some highlights, that figure on the top right comes from use of PFLOTRAN on that international DECOVALEX project where multi continuum transport capability has been developed to model solute exchange between matrix and fracture networks. And then that figure on the bottom right illustrates some of our recent work looking at integrating some reduced order geo-mechanics models to study near field re-saturation behaviors.

And that's all I have. I'm happy to take any questions that anybody has at this point. Thank you.

>> BAHR: Okay. Thank you, Michael. Do we have some questions? I see Tissa's hand up. Go ahead, Tissa.

>>ILLANGASEKARE: Again, thank you, Michael. Nice talk. And I have a related question. I have a little question. Early on, you answered my questions saying that the PA model doesn’t need, that level of demand. I don't know what the term means. But at the same time, I listened to your talk about PFLOTRAN is not only

developed for this framework. It can be used for a lot of other different applications. Is that correct? Where you need that level of refined simulation. Is that correct? I mean, you're using it in this framework, but at the same time, it is much higher capability model to many other things. Is that correct?

>> NOLE: Yes. It is applied to other projects besides the GDSA framework. And so, I mean, coordination and communication across development teams can actually be really useful across projects. So something that works on a different project could potentially be useful for GDSA framework and vice versa. Yeah.

>> ILLANGASEKARE: I want to talk about your earlier discussion mentioned about working on the retention functions. Is that what you are mentioning in your slide? Dry out? Is that the situation you are looking at? Low saturation capillary pressure type of curves?

>> NOLE: Yes. That's exactly what we're talking about. So with I guess I would say traditional kind of capillary pressure or saturation relationships like the van Genuchten function, for instance, as you approach residual saturation of water, your capillary pressure tends to infinity, and we know that's not realistic.

You can't have an infinite capillary pressure. So we have run into instances where we get dry air simulation, either through boiling or gas generation, various types of mechanisms, and we've been pushing our liquid saturations toward that residual saturation, and in the past, what we've done and what other simulators do is just impose a cap on a maximum capillary pressure. But that introduces a cusp in the capillary pressure curve, so that can be really difficult numerically to solve. It can slow down the simulator, because the simulator has trouble converging. And so what we've worked on recently is looking into literature to find kind of physically based ways to come up with just better, smoother capillary pressure functions that are physically realistic, that also can help us with our convergence issues that we're seeing during dry out. So yeah, that's what we're talking about.

>> ILLANGASEKARE: My observation is exactly that. I work with both [Indiscernible] and I think the one mistake we are doing in this type of modeling is trying to model this equation to these models. These are fitted models for, you know, basic soil physics applications. My advice is your thinking is correct

that you should go through more physically based approaches not only low saturation, but both the high saturation and the low saturation, in between, you know, they fit these curves. I think it is a good idea to look at the fundamental physics at the low saturation – we thought that relying on these constitutive models which are fitted for, probably those cases which probably have nothing to do with the types of things you are looking at.

>> NOLE: Right. And they're fitted for -- I mean, really, it's like a drainage problem that gets used to create these equations, these curves. And so the processes that we are modeling like boiling and gas generation, it really actually isn't the same as what these experiments are used to generate these equations. So yeah, there are ways to get the water out past residual that doesn't involve just pushing it through like with a mercury injection capillary pressure measurement or something.

>> ILLANGASEKARE: Advection dispersion in unsaturated flow actually is not done very well. Like some of the tortuosity effects are not actually done [Indiscernible]. These are detailed and I like your

approach and I think you are making very good progress.

>> NOLE: Thank you.

>> BAHR: I see Paul's hand up, if we can bring him on stage?

>> TURINSKY: So the curiosity. Have you folks had any luck with using GPUs? A lot of people challenge that.

>> NOLE: That's actually something we haven't really deeply looked into at this point, but we are preparing to explore GPU compatibility. So the solver library we use is called PETC, portable extensible solver toolkit. And they actually have put in a concerted effort over the last couple of years to look at whether GPUs can be efficiently utilized for their solver library. And since Fortran is heavily reliant on PETC. We're looking into whether or not we can use GPUs, but we don't have anything to show for that at this point.

>> TURINSKY: Okay. How many cores do you usually execute on?

>> NOLE: Thousands. Yeah. We throw it to a cluster. It's a big PA skill simulation.

>> TURINSKY: And turnaround time? I know that's

machine-dependent.

>> NOLE: It's machine-dependent and it's problem-dependent. If you're talking about a multi-phase flow simulation, those can be numerically challenging. So those can take a week. But if we're just talking saturated flow, I mean, those can take a matter of half a day. If it's a really big simulation, if this is incorrect some of the process modelers can --

>> STEIN: Michael, I can give a few numbers based on my experience running the PA simulation. So most of those are run depending on the problem size between 500 and 2,000 cores. And again, depending on the complexity of the problem and how many radionuclide species we're tracking, it will take anywhere between half an hour and four hours for a typical run. And then there may be some outliers that take longer than that.

>> TURINSKY: Okay. An example you showed of basically the different models, you didn't show any feedback loops in there, nonlinearities, in other words. Having raised two kids, I know that the children will impact the parents substantially. How is that handled numerically?

>> NOLE: So the way we split up the coupling is we do

sequential coupling between flow and transport. Within the flow and within the transport, you solve nonlinear systems of equations using Newton-Raphson iteration. And so sequential coupling, if it's a parent/child relationship, so for instance, between flow and transport, flow will take one time step and then transport will sub-step flow. So it will take as many time steps as it needs to converge adequately. And then at the sync point, they'll exchange relevant information, like for instance a velocity field from flow will get exchanged to transport, which then transport will use. It is a sequential coupling between process models.

>> TURINSKY: It's what I would call explicit coupling rather than a more implicit where you would go back and repeat that time step?

>> NOLE: Yeah, yeah. It's just a sequential, yeah.

>> TURINSKY: Okay. All right. Thank you.

>> BAHR: Do we have any other questions at this point? Tissa has his hand up again.

>> ILLANGASEKARE: I want to touch on another question. When you say couple, in my view, coupling and

integration are two things. Coupling you do for the process. So do you think coupling becomes most important close to the source or the barriers, but when you go further and further away, its more for integration? So for the integration, some of these issues, like time lagging and all, may not be a problem, because you are looking at very large time steps. So you're coupling is really needed close to the source. Is that correct? Or is the process coupled?

>> NOLE: Yes I would say you need tighter coupling where the outputs from one model affect the other model more. Right? So those are instances where like you were saying, maybe you have more heat generation going on. Also, higher concentrations are spatial variation of radionuclide concentrations. There's definitely more going on closer to the waste forms in terms of heat and radionuclide generation and stuff like that. Gas generation potentially. So, I mean, we don't apply separate coupling schemes by -- we don’t apply them differently spatially. So we just apply the same one across the board, but convergence is determined dynamically. Right? If you have really small grid cells in the repository with a lot going on, the time

step that the simulator will have to necessarily take -- the time stepping will have to take appropriate steps in order to properly converge with all the process models.

>> ILLANGASEKARE: My point is when you go larger integrated behavior of the system, the coupling may not be important, like when you go farther and farther away advection and dispersion basically takes over in the source area is where most of the coupling [Indiscernible] this is my thinking. I may be wrong of the reason I'm saying this, this is a computation, the challenge is finalized still. Most of the high-level computing, you need that closer to the source. You go further and further away. Your time steps can be much larger. When you're looking at million-year simulations.

>> BAHR: Maybe just to clarify, though, there are going to be processes going on in the source area at the same time as transfer is occurring in the far field, particularly when you go out to long time steps. You still have the processes, and it's not a pulse source. It's a --

>> ILLANGASEKARE: Yes, yes, yes.

>> BAHR: So you have some parts of the system that can take long time steps, but at the same instant in time, you have processes occurring that require short time steps.

>> ILLANGASEKARE: I see. GP, like all of the GPUs, we use GPUs in the ability to [inaudible] process model very, very efficient. The question is maybe if computing power become a problem for a million years, maybe you should look at the strategy of time stepping in a different, like, decompose the system into different regions, looking at different coupling in some areas and coupling in other areas. Rather than trying to write the equations for the whole system in a coupled way.

>> NOLE: That's a good thought and it's definitely a challenge that we kind of wrestle with, challenges of scale and where the interesting phenomena are happening with times and lengths and all that.

>> BAHR: Michael, thank you. I think we need to move on to our next speaker. Thanks to everyone. And I see Jeffrey Hyman's camera is on. So I think he's keyed up, if we can bring him on stage. And he's going to give the first of three talks on some of the specific process

model integration that we have.

>> HYMAN: All right. Can everyone hear me and see my slides?

>> BAHR: We can hear you, but I don't see your slides yet.

>> HYMAN: Okay. There we go. Sorry. It's moving a little slow for me today.

>> BAHR: It's okay. I see it, but it started screen sharing. Oops. If you're having too much trouble, do you want Jason to project the slides?

>> HYMAN: Jason, could you bring them up for efficiency?

>> BAHR: Can you do that, Jason? Okay.

>> HYMAN: All right. My name is Jeffrey Hyman, I'm a staff scientist at Los Alamos National Laboratory in the Earth and Environmental Sciences division. I'm going to be talking about the first process model that we will be working with GDSA, which is dfnWorks, which is LANL's discreet fracture network modeling suite. I'm going to be going through what it is, why we chose to use it for GDSA and why we chose dfnWorks and what are the specific

capabilities that we're utilizing for this project.

From a high-level there's a number of different computational models to flow and transport in fractured media. This is at a higher level than choosing PFLOTRAN. This is conceptually how do you want to represent fractured rock. So let’s say there in the middle you have an actual fractured rock, this is actually quartzite, about two hours north of me in the Ortega mountains of New Mexico, and you have different options of how you want to represent flow within the fractures and the rock matrix along the fractures.

So on the top left, you have a thing called a channel network. These are conventional pipe networks where each one of those edges kind of represents flow between individual fractures. So you can see you're in a structure there, but it's not necessarily really giving geometry of the system. Down below that in the lower left corner you have discreet fracture network models where each fracture is represented by a planar distance face. And they connect together and it results in flow and transport on them. On the bottom right corner you have discreet fracture matrix models where you have the fractures are represented as planar disks, but then you

have the rock matrix surrounding it as kind of this continuum volume. And then in the upper right corner you have more conventional equivalent continuum methods. So what I'm going to be talking about today are the bottom left and upper right and how we're using those two models within GDSA. Next slide.

So we're going to begin with something called discreet fracture network. So the conceptual idea here is that crystalline rocks where most of the flow and associated transports is really happening within the fractures themselves. Those are the primary conduits. You can represent just that piece of the system and not explicitly represent the surrounding rock matrix. Clearly, this breaks down if you have higher permeability rocks, like a sandstone, for example. But for crystalline rocks, short timescale, it seems to be an okay assumption. So conventional or kind of classical dfn networks we have two examples. On the left is [Indiscernible] example. Each one of these lines represents an individual fracture. They get placed into the domain based on the site characterization, so you get the orientation, the length, and aperture. And they form up to connect a

network. You discretize these and solve your flow equations on the resulting linear system.

On the right side you have how you would derive that channel network, that pipe network. In this case, the fracture is a planar disk. We're only resolving flow along the dotted lines, in between the connections between different fractions. Next slide.

Next slide. So modern -- back one, please. So within the past ten years or so, there's been quite a lot of development within discrete fracture network modeling, and a lot of that has been propped up by advances in both theoretical developments and HPC capabilities. Modern three dimensional DFN modeling, we have fractures are explicitly represented as disks and rectangles. We have a mesh on each fracture of a hydraulic properties that vary between fractures so you can get spatially variable hydraulic properties, aperture permeability. You still use the site characterizations to inform the descriptions of each fracture family. So on the right side here, we have a network that contains 350,000 fractures. You can see those three different stratigraphic layers in there. And there's a different families within each one of those layers. So once we

construct that network in the mesh, we'll have flow and transport through it and keep asking any questions we want to know about how the network structure is affecting the flow.

That's kind of the overview of where dfn modeling is specifically at this point. Next slide.

And what I'm going to be talking about is a specific software called dfnWorks. dfnWorks is LANL's 3D DFN software. It's a modular built code similar to kind of these process models in PFLOTRAN where we have four different pillars. And I'm going to walk through each one of those today and describe how we're using it for GDSA. You have dfnGen, which is our generation and meshing, dfnFlow, which is our flow solution, dfnTrans, which is transport, and dfnGraph, using graph theory to analyze these networks and try to understand their system a little bit better. Next slide.

We're going to start with dfnGen. Next slide. So dfnGen, this is our network generation. Specific attributes we're using in dfnGen, are stochastically generated fractures because we don't know specific location of every fracture in the subsurface and we never will, these networks are developed stochastically,

essentially what we do is we take distributions that describe attributes of the fractures and their families and we sample fractures according to those distributions that are based on the site characterization. I'm not going to talk about the site characterization part. That's more for structural geologists to take in the data and give dfnWorks as an input. For a lot of our data, we're relying on what's kind of SKB, with relation to the [Forsmark site or Posiva with their potential site as well. So you have these different fractures that are generated randomly, and we can place them by different families, so here we have a synthetic repository system. This is about 7,000 fractures here, and again, we can see these three different stratigraphic layers. You have high density in the stop and those fractures are colored red. Medium-density in the middle and those are blue and green. And low density in the bottom and those are orange and purple. So each color represents a different fracture family.

In addition to the stochastic families, we can put in deterministic features. Say for example, faults, we would be able to detect in the subsurface, or repositories and potential repository sites that we

could put in.

A feature with dfnWorks as well, you can get detailed geological output to make sure what you put in is actually the geology that you wanted to see. Next slide.

All right. So the next thing is after we've generated our network, we have meshing capabilities. So we actually have to go and create something that is something like PFLOTRAN or FEHM can actually solve on. The key feature with dfnWorks is we can create these conforming Delaunay triangulations. Why is that important? They're dual mesh and I can explain that if you want is essentially optimal for these 2 point flux finite volumes of codes, such as PFLOTRAN. What it gives us the is the ability to have local mass conservation throughout the entire system on the fractures. You can see if you look closely, each one of those fractures, you have a triangular mesh that's now representing the fracture itself and computationally that's what the solver sees. We can make the mesh a little coarser to save on computational expenses.

We also have upscaling models, which is the next thing we'll talk about, where we'll take this network and

incorporate both properties of the rock matrix and the fractures into a single continuum volume that we could hand off to PFLOTRAN as well.

Next slide. So a big piece of our workflow that we are doing for GDSA is mapping a DFN to an equivalent porous media. There's a few different ways to do this. Right now where we're heading, previous slide, please. Right now, we're using something where we have uniform hexes. We can also do more refined meshes so we can pick up the details of the fractures, and those aren't lost to upscaling, which can cause false connections and erroneous early travel times and deviations from effective permeability. Next slide, please.

So the next piece is called dfnFlow, which encapsulates how we're doing all of our flow within the system. And the way we set this up, we have access to multiple flow solvers. Next slide.

And the main one that we're using right now is PFLOTRAN and we have seamless integration. If you set up an input card, say Michael sets you up, you can set one up yourself you can use that on one of these discreet fracture networks. Here we have a network composed of about 17 fractures, and what we've done here is we're

running a reactive transport simulation, where we are dissolving quartz out of the system and letting permeability evolve. We're injecting just water on the left side, and you can see the red areas are where essentially the fractures that are dissolving out and you're having higher permeability. The key thing, back to what we talked about with DFN Gen, is the mesh refinement which allows us to pitch up the steep gradients in the flow. In addition to reactive transport, we have access to radionuclide decay tracer transport, multiphase flow, and waste form process models that we're using in GDSA. We also have back ends analysis of PFLOTRAN runs. You can look at your effective permeability, look at breakthrough curves, all of that piece coming out of the dfns. Like I said before it's also modular. You can also use additional solvers such as FEHM and AMANZI, developed at Los Alamos. If you want to look at new processes that we are putting into PFLOTRAN, they already exist over those solvers. We can use an identical domain, an identical mesh to compare and do some benchmarking with previous codes. Next slide, please.

The third pillar of dfnWorks is dfnTrans. If you look

at the image on the right, you see orange lines. Those are particle trajectories coming in from a point source. The way dfnTrans works, it's the LaGrangian transport where we are looking at particles through the system. Next slide.

The particle tracking is essentially just an internal path line tracking. You have the Velocity field that is established within the network and you essentially have stream lines that you're setting a particle on and watching it go through the system. We have ability to have matrix diffusion, so a particle can go along its trajectory, diffuse into the matrix and come back to the fractures. We also have a low fidelity pipe network that's very quick to run so you do a large ensemble of transport going through quickly. We have a flow topology graph analysis toolkit associated with this. So you can query where is your primary flow channeling happening and part of your geology is influencing your flow and transport. In the future, we're going to have tight integration with the Migration Analysis of Radionuclides in the Far Field, known as MARFA. This is something that SKB has used extensively in the past. It's something that we're most likely going to integrate

with the DECOVALEX Task F in the future, which Emily is going to talk about I think tomorrow. Next slide.

In terms of transport for GDSA, we're mostly relying on the upscaling methods and advection-dispersion equation. One thing we are doing is we always benchmark to make sure if we run transport with particles in ADE they at least look similar. So clearly you're going to have some numerical dispersion effects from your advection dispersion equation and we're just making sure our particles are at least matching the general trend of that. Like I mentioned before with development of DECOVALEX simulations, we're working at using more dfn's and particle tracking in that aspect. Next slide, please.

The last piece is called dfn graph. Next slide. Dfn graph takes a graphical representation or a network science representation of the fracture network. You can think about this like something like Facebook. Each person in Facebook is a node in graph. If you're friends with somebody, there's an edge between them. You can have fractures representing individual nodes and if they intersect there is an edge between them in the associated graphs. So these graphs become very

complicated, but the nice thing is then we have our hands around them and we can start asking kind of key mathematical questions about what is the structure of the network and how is it dictated? So from that, you can see if I put a repository in this realization of the network, is there even a path from the repository to the surface going through fractures? And that's something you can run without a single flow simulation or meshing. And you can know that there's either a very fast path or not a path at all between your repository and the surface. Okay?

In addition to that, we can ask all sorts of questions about global and local topological attributes and run low fidelity pipe network models to get to kind of flush out our ensembles for uncertainty quantification. Next slide.

So just to put everything in context with dfnWorks in GDSA. We're using the network generation stochastic fractures, multiple families, layers, deterministic features. We're using the graph-based dfn analysis. Laura will talk about that tomorrow morning. We're using transport in our dfn's to benchmark our porous media transport simulations, just to make sure that

we’re not wildly off base due to our upscaling procedures. Things we're looking forward to including in the future are depth and stress dependent aperture and permeability measurements or permeability. This is in dfnWorks but we have yet to put it in GDSA. That's coming up in the future. And then as I mentioned before, doing more dfn particle tracking simulations with DECOVALEX task app.

How does dfnWorks fit into the GDSA workflow? On the right, you have the general sampling workflow where we’re looking at uncertainty quantifications. dfnGen, is the inputs. It generates the network based on our statistical description of a site and then we create the equivalent porous media and that all gets plugged in and runs through PFLOTRAN, Dakota, the whole workflow goes through there, but it's all based on that initial realization of the fracture network. Any uncertainties we have there kind of propagates itself through. All right? So as Laura will talk about tomorrow, we need to generate a large number of these network samples to start covering that uncertainty space. Next slide, please.

Additional applications that are outside of GDSA, but I

just wanted to mention them, in addition to repository science, we're using it for carbon sequestration. We looked at unconventional hydrocarbon. Enhanced geothermal energy, something that we are getting very interested in. And fundamental research science about kind of how does network structure and aperture variability within a fracture affect flow? So I've already mentioned the matrix diffusion piece we can look into. We can look at scaling of breakthrough curves. How does having a stress dependent aperture, and if you change your background stress fields, how does that affect your flow and transport? And then also, discrete fracture matrix models where you have this tight coupling between the fractures and the matrix. Next slide.

So from the technical side, dfnWorks is also open source. We really looked at PFLOTRAN, how they build their community and we're modeling what we are doing after them. It's open source. We're trying to keep very robust online documentation. We have had a few workshops. We'll have one hopefully in 2022. Covid willing. Website dfnWorks.com swing by and check it out. If you have specific questions about it, just

email dfnWorks@lanl.gov. We're happy to point you around.

Last slide, please. And dfnWorks has been supported by a number of different entities, in addition to Nuclear Energy, the Office of science, NSF, and of course internal funding from Los Alamos and LDRD. And thank you for your time.

>> BAHR: Okay. Thank you, Jeffrey. And I see Paul's hand up. So I'll go to him first.

>> TURINSKY: I'm doing better remembering to turn on my mic. To get sort of a high confidence level, let's say, in evaluating the variance of some quantity. How many samples would you actually have to take of the network?

>> HYMAN: Of the one for the GDSA what we've had now or just kind of a general network?

>> TURINSKY: What you're doing now, basically the fractures.

>> HYMAN: Laura is going to touch on this a little bit more tomorrow. She has more quantitative pieces of it. She might actually -- I'm not sure the exact number that they've ran, but a ballpark, I wouldn't start with

anything less than 20 or 30. Laura wants to take it.

>> Laura: Yeah. We've been running 20 to 30 dfns for these kinds of analysis. But then for each dfn, we sample large -- we generate samples on the other epistemic parameters. So I'll talk about that nested kind of sampling tomorrow.

>> TURINSKY: Okay. What sort of confidence level are you at, then? I mean, are you up in it the 95% confidence level?

>> Laura: I'll show some results tomorrow, but we have typically very broad ranges on some of our quantities of interest. We do have accurate estimates for means, of course, but we're trying to look at whole ensembles of results for these kinds of analysis.

>> TURINSKY: Where I'm getting at, I'm on the reactive side of the business and I'm so used to 95% probability, 95% confidence level. So to give you background of the basis of my question. Thank you.

>> BAHR: I see Tissa with his hand up.

>> ILLANGASEKARE: Yes. Thank you. I have a question maybe to the PFLOTRAN question. [Indiscernible] the

computation power needs to run with discreet refinement, so your grid system is not adaptable when you ask a question, adaptability, so you have reverse diffusion, say you have reverse diffusion and you have a forward diffusion, then that would be the [Indiscernible] push the particles by diffusion into the rock and it's going to come back slowly. As the plume spreads, it was diffusion, your gradients are much, much lower, because it's going to get diluted. So what happens, you now have a very high resolution grids for the diffusion in, but reverse diffusion which is a very slow process and is covering a large area. So is your grid system adaptable based on the process or are you stuck with the one grid system, which you have to run for a million years?

>> HYMAN: Right now there's no AMR. It's all static. And so, you know, if you have -- the other thing there, so as far as for the actual coupling of the fractures into the matrix and having the matrix cells, that is all static at this point as far as its resolution. The whole thing is just uniform size hexes. So that would be nice if you could see gradients going into the future. I don't believe PFLOTRAN can take adaptive

meshes where it would change overtime, and we don't have the feedback loop between, say, like [Indiscernible] our meshing tool and the flow solver. I think it would be fairly intrusive to build that in actually. Right now kind of build your first mesh and you're kind of stuck with it.

>> ILLANGASEKARE: The reason for my question, people are working on this type of problem, but in your problem, the nuclear problem, there's some very specific, very fundamental differences, because you have a source. The source is starting in an area that is more an area [Indiscernible] as it moves. Then the plume is going to get dispersed and then in that case, then you're going to million years in this type of simulation, having a high resolution like you have, will take a major, major computational effort.

>> HYMAN: Yes. We do have -- there is [INDISCERNIBLE] capabilities we can start with, and then you can run unstructured within PFLOTRAN. You can stay close to the repository and be refined or you can go downstream from that as well and say your lateral and kind of against the flow, you could coarsen up. As far as actual feedback of knowing kind of riding your plume front and

actually refining right along that plume front, I've worked on that for other problems, but it's not built into this. But yeah, that would be nice if you have your plume release and you're just only walking along with a very tight grid as it moves. That would be fantastic.

>> ILLANGASEKARE: Thank you.

>> BAHR: Do we have any other questions for Jeffrey? Okay. If not, then I think we can move on to our next speaker. We're going to hear from -- let's see. Did I miss anybody? Paul Mariner again.

>> MARINER: Yes. You've got me again. Okay. So now I will share my screen. Am I sharing?

>> BAHR: Looks good.

>> MARINER: Very good. Well, this talk is about integrating the fuel matrix degradation model into GDSA framework. I'll first talk about the process model, the fuel matrix degradation model, what it is and what it does. Next I'll explain the motivation for developing surrogate models for it. I'll then go through the approach used to develop the surrogates. And finally, I'll show the results of the work and talk about future

plans.

The fuel matrix degradation process model is a combination of a complex set of components and interacting processes. The components include the spent nuclear fuel, the chemical composition of the fuel, noble metal particles in the fuel. Fuel corrosion products. Water contacting the fuel and contacting corrosion products. And the dissolved chemical species in the water.

The major processes include radiolysis, chemical reactions within and between aqueous surfaces and chemical phases, oxidation of hydrogen via a noble metal particle catalyst. Growth overtime of an alteration layer on the fuel surface. The alteration layer that grows on fuel surface is composed primarily of uranium oxide corrosion products. And the other processes involved are one dimensional reactive transport and diffusion through the corrosion layer.

Most important thing this process model can do for our reference case simulations is to estimate the rate at which the fuel matrix degrades for a given waste package at a given time. This process model is coded in MATLAB and requires many thousands of Newton-Raphson iterations

for each simulation. The high number of iterations causes the process model to be much too expensive to run for each breached waste package in a repository simulation.

Calculation of the fuel matrix degradation rate for a given waste package using this process model depends heavily on local conditions. Specifically, it depends on temperature, fuel burnup, dose rate, and the concentrations of hydrogen, oxygen, ferrous iron, and carbonate. They all affect the degradation rate. Spent fuel degradation rates can vary by several orders of magnitude, depending on these variables.

Consequently, radionuclide release to the host rock and to the biosphere is highly sensitive to these degradation rates. For these reasons, it potentially can be highly important that we calculate fuel degradation rates for each exposed waste form over time based on the local conditions of each breached waste package.

Because the process model is complicated and slow and it can actually be unstable under certain conditions, development of a rapid surrogate model trained by the process model was a logical way to include the effects

of the specific features and processes of the process model in full scale.

Before I go into detail about our surrogate models, I'd like to make clear the differences between process models and surrogate models. A process model simulates individual system components and the physical processes that govern system component interactions and behavior. I just went through a long list of components and processes included in the MATLAB process model. In contrast, a surrogate model does not simulate individual system components and physical processes. Rather, the surrogate model simply predicts system output values based on its learned knowledge of the relationship between system input values and output values.

Another way to say this is that the surrogate models are methods for mapping inputs to outputs. The surrogate model can be trained with experimental data, simulations of a process model, or both. The surrogate models in this presentation are simply trained by the MATLAB process model. A very simple form of a surrogate model is a lookup table. For a lookup table, a process model is used to calculate the system output for many combinations of input conditions and input values. The

surrogate model then typically uses these tables to interpolate the output response. A more advanced lookup type surrogate is the K-nearest neighbors search. K-nearest neighbors is more advanced than a typical lookup table, because it can more easily handle very large data sets, multi dimensional systems, and additional data when they become available.

The other two examples listed here, polynomial regression and artificial neural network, are parametric surrogates. They look for patterns in the data and use that information to build a continuous multi-dimensional response surface over the sample domain. The four surrogates listed here are examples of machine learning, from very simple machine learning to complex machine learning. Whether complex or simple, the accuracy of these surrogates is easily and directly quantifiable. All one has to do is compare surrogate predictions to independently derived test data.

Three different surrogates were developed and tested for the MATLAB process model. Artificial neural network regressor, k-nearest neighbors regressor, and polynomial regression. The polynomial regression surrogate did not perform as well as the other two, so it was dropped.

The primary difference between the neural network surrogate and the nearest neighbors surrogate is the neural network regressor uses the training data to generate a continuous response surface described by the set of equations and coefficients. The K-nearest neighbors surrogate, on the other hand, retains all the training data in a multi-dimensional lookup tree. It simply interpolates the response based on the set of data points nearest the interrogation point. Which approach will end up being better for the fuel matrix degradation model is yet to be determined. It will likely depend on how the process model evolves. In the meantime, maintaining both approaches is expected to help us prepare for other potential surrogate applications.

Development and integration of the surrogate models began with the generation of training and testing data using the MATLAB process model. Using Latin hypercube sampling, approximately 30,000 realizations of the MATLAB process model were run. This resulted in about 3 million training data points, because each simulation produces about 100 data points through time.

For test data, an additional 3,000 random realizations

of the process model were run to generate 300,000 data points. These test data are kept completely independent and are not used for training the surrogates. The ranges of the various inputs are shown in the table. Temperature and fuel burn up ranges were sampled, assuming a uniform distribution. Environmental concentrations of hydrogen, oxygen, ferrous iron, and carbonate were sampled assuming log uniform distributions.

Once trained and tested, the surrogates were implemented in PFLOTRAN. The neural network surrogate requires PFLOTRAN to read the training fitted coefficients from a file for direct calculation of the fuel degradation rate. The k-nearest neighbor surrogate requires PFLOTRAN to scan a search tree of all the training data to find the data points nearest the combination of values for the six different input parameter values. In this case, the k-nearest neighbor surrogate searches for the 250 nearest neighbors, then it uses an inverse distance rule to weight the closer neighbors more heavily than the more distant neighbors.

For the round of surrogate model development presented here, the artificial neural network surrogate provided

the more accurate results. In this figure, 100 randomly generated test simulations are compared to the results of the trained neural network surrogate. The surrogate predictions are light-colored and dotted. The black lines are the true process model results. Notice that the surrogate does quite well at predicting the degradation rates over the orders of magnitude changes in the degradation rates. You might not be able to see it very well, but the degradation rates on the Y-axis vary over a range of five orders of magnitude from values below ten to minus six to values above 10 to the minus two moles per meter squared per year.

The time on that X axis is also in log scale. It goes from less than one year to 100,000 years.

The speed of the surrogates is thousands of times faster than the process model. In 2015, the speed of the process model coupled to PFLOTRAN was measured for a test problem. The test problem involved 52 breached waste packages in a flow field. In 2020, the simulation was repeated using the newly developed surrogates. The 2020 flow and transport parts of the simulations were approximately twice as fast as in 2015. And that's due to differences in in computers and computer settings.

However, the fuel matrix degradation calculation was over 30,000 times faster for the neural network surrogate and over 2,800 times faster for k-nearest neighbor surrogate. Clearly the surrogates run very fast and the coupled process model runs very slowly.

The fidelity of the neural network surrogate is demonstrated here in a shale reference case simulation. Prior to this demonstration, only the fractional dissolution rate model was available to simulate fuel degradation in a reference case simulation. The top figure shows the deterministic value of the fractional dissolution rate model for every failed waste package in the simulation as soon as it breached, as soon as the waste package is breached. In these simulations, the specific surface area is constant, so the fractional dissolution rate in units of moles per meter squared per year never changes for each failed waste package over time.

The neural network surrogate demonstration is shown in the lower figure. This deterministic simulation accounts for the burnup, local chemical conditions and dose rates over time. The rates are quite high at first, primarily because the dose rates are high at

early times and the hydrogen concentration is assumed to be low in this demonstration. Because the neural network surrogate emulates the fuel matrix degradation process model, the degradation rates it calculates are a function of temperature, local chemical conditions, and the changing dose rate over time. These figures show that the degradation rates calculated by the neural network surrogate, unlike the simpler model, are of higher fidelity.

In summary, surrogate modeling has allowed us to emulate the effects of fuel matrix degradation processes in full scale reference case simulations. Modeling each breached waste package allows us to account for the local concentrations of multiple dissolved species, individual burnups, and changing dose rates overtime.

Second, the artificial neural network surrogate and the k-nearest neighbors surrogate are extremely fast. They are also quite accurate for this application.

Key to acceptance of these surrogate models is the fact that we can directly test surrogate outputs against process model outputs. As for the next steps, future work on these surrogates is paused for now. We expect surrogate work to resume after the next major upgrade of

the process model. And that is my presentation.

>> BAHR: Thank you, Paul. Quick question. When is the next iteration of the process model expected to be completed?

>> MARINER: We are working on it. We've got a really good start on it. I have an integration meeting actually set up in a week or two that involves some of the key players from two or three of the different labs that are also involved in this project, people from Argonne and from Oak Ridge and from PNNL who are all experts in fuel matrix degradation. And we're just going to make sure that we're doing it right and we're hopefully at least going to get something within a year, something new in a year. Maybe even this fiscal year.

>> BAHR: And are you the one who's actually responsible for the process model itself taking inputted advice from these other researchers or is there a separate team that's working on the process model?

>> MARINER: The process model right now is the fuel matrix degradation model as defined by other process models over time. Jim Jerden and others, those folks. They put that together and they've defined it. We are

right now just making sure we can implement it in Fortran, because once we can implement it in Fortran, it can be a lot more flexible when for dealing with different conditions and timings and things like that. So once we get that going, then I think we'll be ready to test it for some more conditions.

>> BAHR: Okay. I see Paul's hands up.

>> TURINSKY: I have a question about the detail in the model as far as heterogeneity and cracking is concerned. As fuel goes up and burn up, the fuel meat I'm talking about now, gets very heterogeneous. You get the rim effect on the outside with plutonium oxides building there. The grain sizes change. I would think that impacts dissolution rates. And then you have cracks, which is going to influence the water getting in, increases the surface areas, also. Is that sort of detail currently in the model?

>> MARINER: The MATLAB model, there's no cracking in there, but there is this buildup of the corrosion products and this diffusion through that corrosion layer that is in there. I am not the process model lead on this. That is precisely why we are putting together this integration team, so we can get people with

expertise like apparently you have to make sure that our next steps are real good ones.

>> TURINSKY: You're giving me too much credit for expertise. Thank you.

>> BAHR: Did you want to add to that explanation?

>> Dave Sassani: There is a surface area term in there, Paul, and it covers a range, but it is not explicit representation of cracking or rim effects or grain size at this point. But that surface area piece of the model which can be very important in terms of the overall dissolution rate can be worked on further. It was mostly the electrochemical portions and the drivers on the matrix grains, the dissolution themselves that was incorporated in that first round.

>> TURINSKY: And of course the composition is changing as well.

>> Dave Sassani: Sure.

>> BAHR: Dan Ogg has his hand up?

>> Dan Ogg: My question also has to do with the dissolution of the fuel and assumptions that are made about the condition of the cladding. Maybe I missed it.

Is there any credit given to the fuel cladding? I know you mentioned corrosion layers. It wasn't clear to me if you were talking on the corrosion layer on the cladding or corrosion layer on the fuel matrix itself?

>> MARINER: Right. Right now this fuel matrix degradation model is only considering the corrosion of the UO2 fuel and their corrosion products. That's what builds up there. There has been some modeling, though, that includes a steel surface on the other side of it. So you have your fuel surface. You have this water in between. You have a steel surface, for example, on the other side. As it corrodes, of course, it's going to affect the hydrogen concentration, which is really important, for the degradation. That part of it is not part right now of this degradation model, but I know process modelers have been working on that.

Cladding itself, no. We have not included that.

>> Dan Ogg: Okay.

>> BAHR: Dave Sassani's hand is up again. Maybe he has something to add to this?

>> Dave Sassani: Sure. There is a cladding model that's under development. So Dan, no, that dissolution

is for failed fuel. There's no cladding protection at all. It's a degradation rate of the SNF pellets. But the cladding model that's being developed we're hoping to begin implementing sometime in the next year. Probably next fiscal year would be my guess.

>> Dan Ogg: Thank you.

>> BAHR: And I see Andy Jung has his hand up?

>> Andy Jung: This is Andy Jung. It's a very great presentation. It's very useful. I have two small questions. The first one, on your last slide, you say there's future work. You also mentioned that you need the collaboration with other labs, but for clarification, what kind of upgrades, considering experimental or so, has been included in the plan? Such as, like, your model, field matrix degradation model was based on the low temperature experiment. You don't know maybe some high temperature, you may have a different mechanism or behavior involving complex processes, so if that is the example. The second two questions, the first question is actually what type of aspect are you planning for the upgrade of the process model? The second could be very fundamental. And know that most European companies, the model also utilizes a chemical

dissolution model of the spent fuel in reducing environment. So they have a lot of this database having closed loop testing or a lot of this test data are present. So I know that the fuel by involving the radiolysis it can be the electrochemical process basis or the fuel. Maybe the fundamental question, is there any special motivation? Why do you consider this electrochemical mixed potential model instead of just a traditional chemical dissolution model as done from the many other European countries?

>> MARINER: Thank you. The fuel matrix degradation model is very much at the process model development stage. I work mostly at the other end. We try to implement these models in total system performance. My expertise is taking that process model and building a surrogate model that we can use in PA.

But to answer your question. I know that there is ongoing research on fuel matrix degradation. In fact, there's been a new push in our program to actually get more experimental data. I'm certain that there are process modelers that are working on building it. The key improvement that we can make this year, I think, in our process model is to allow these chemical

concentrations to change with time, because right now, in that MATLAB process model, you have to fix those four chemical species concentrations for the entire simulation period. Because we are reprogramming this in Fortran with some more flexible coding, we're going to be able to change those concentrations over time, and so once we have that ability, I think that's going to kind of revolutionize how we do the surrogate modeling work.

>> BAHR: And I see Dave Sassani's hands up again.

>> Dave Sassani: I want to add to this. It's outside the GDSA itself. We have in the process areas, we've collected together the work for the cladding modeling and for the waste form degradation modeling and testing and validation aspects and performance, and we're putting together a test plan to look at doing validation testing for the mixed potential model for the fuel matrix degradation model. It's a component of that. And also looking to expand that testing. And Andy, that's a great question, because the DISCO program over in Europe has looked specifically at some of the degradation processes. This model itself was based originally and it was an expansion of Dave Shoesmith's model. And the electrochemical aspect was the potential

coupling of the noble metal particles, the five metal particles cathodically coupled to the UO2 pellets and the grains to reduce and affect its cathodic potential. So there was always a question about is it a cathodic coupling or a catalytic effect of these noble particles? That question is up in the air, but the hydrogen over-pressure is the main feature this responds to, this model, and as that gets higher in the system, which is due to corrosion of things like iron, it reduces it down to that chemical dissolution model. That's the lower limit. Basically, it's then based on the solubility of the UO2 fuel particles at that point. So it's consistent with those chemical models, but it looks at some other features. It may increase the degradation rates as well.

>> Andy Jung: Okay. My question was basically, I agree that there hydrogen generation can decrease the dissolution rate and many processes can involve. Just my simple question was that there is a lot of [Indiscernible] the data already done from the European researchers and you know, even though this potential -- this mixed potential model could have been more [Indiscernible] and can accommodate many processes, but

my point was that is the major advantage use of this model as compared to just the traditional chemical dissolution model that was done for the other countries?

>> Dave Sassani: Sure. The major advantage is the coupling to the radiolytic phenomena.

>> Andy Jung: Thank you.

>> BAHR: I see Bret's hands up?

>> Bret Leslie: Thanks. Paul, good talk. And Dave, also, you've brought up kind of gas generation, which Paul's earlier talk said was not part of what's been incorporated so far. And so to me, it sounds like there's some sort of disconnect that you guys started to work on the FDM or the fuel matrix dissolution model, which has as an input hydrogen. Right? So if you're not generating and doing gas generation as part of your GDSA, isn't that a disconnect? And I'll stop there and I have a follow-up question.

>> MARINER: For the fuel matrix degradation model, it's not a high concentration of hydrogen that would actually create a gas phase. So we're talking about dissolved hydrogen in this case, that results. So that isn't related to creating bubbles and to that other process

that you mentioned.

>> Bret Leslie: Sure. So the follow on question is really now that you're modeling every waste package, things like defense fuel, uranium metal, behaves very fundamentally differently than uranium oxide and in fact it creates hydrogen gas. So while your model right now for a defense spent nuclear fuel is instantaneous, it's not necessarily capturing the processes that are applicable to repository performance. And what aspects will you go back or are you planning to further look at, processes that are relevant to the waste forms that can be disposed?

>> MARINER: You raise important points there. Those are good points. We have been focusing on spent nuclear fuel at this stage. As soon as we discover any kind of FEP that we think can have a significant effect on performance, we are going to go after that FEP and see what we can do to either hopefully include it in our capability.

>> Bret Leslie: Thanks.

>> BAHR: Okay. Are there any other questions for Paul? If not, then I think we can go on to the final segment

of our meeting, which are going to be the public comments. And I'm going to turn it over to Bret Leslie. Again, these are comments that came in in written form and Bret is going to read them into the record. We also have opportunities to submit comments after the fact that we will also include in the meeting transcript. Bret needs to unmute himself.

>> LESLIE: Yes, I'm unmuted. Jean, remind me, I have one last public comment that just came in. I've copied them all into another document and one that came in as you were talking. Thank you, Jean. I am Bret Leslie, member of the board staff. Before I begin with the submitted public comments, I would like to let those who are listening know that the meeting transcript will be available on our website by January 3rd. I'll be reading the comments in the order they were submitted. I will identify the approximate timing of the comments. I will identify the commenter and any affiliation they gave before I read their comment. The transcript will include the following public comments: During the update on DOE's program, there were several comments submitted. The first comment: By Phil Plevoric, Clark County Nuclear Waste. He stated, what does as soon as

possible timeline mean regarding the RFI? Is this months? Years? Et cetera.

The next comment was submitted by Ken Bahr from Metatomic, Incorporated, and he states, I am technical Director of our company. We are established for two prime objectives: 1, process spent nuclear fuel to molten salt fuel. Two, reduce the footprint of spent nuclear fuel by 90%. What would be our chance of being allowed to perform this process? Of course with safety and security.

The next comment. By Sara Fields from Uranium Watch. She states, I'm offended by DOE's claim that nuclear energy is a zero emissions source of energy or clean energy. The nuclear fuel chain involves several types of operations and facilities from uranium exploration to the long-term care and storage of spent nuclear fuel. All these operations require energy that for the most part is provided by fossil fuel. Nuclear energy also produces radioactive and toxic and hazardous waste and emissions that are not produced by other methods of energy generation. Nuclear energy is anything but a, quote, clean or zero emission source of energy.

The last comment during the DOE program update was by

Gordon Edwards from the Canadian Coalition for Nuclear Responsibility. He stated, the Canadian experience is hampered by the selective and one-sided nature of the communication. Communities are only told things which are promotional in nature, so when hitherto unreported snags, for example, releases from repackaging used fuel are revealed, the trust is tarnished.

The next set of comments came during Emily's overview talk, and we received these comments. First comment by Barbara Warren, RNMS from Citizen's Environmental Coalition. How are potential local climate change impacts evaluated in this research?

The next comment was by Shin U. Pong from the U.S. Environmental Protection Agency. Are there comparison studies between the performance assessment results from this generic modeling and the performance assess used for the Waste Isolation Pilot Plant?

Moving on, during Paul's first presentation on GDSA, there were a couple of comments. First, by Karen Bonome with no affiliation. She states, I have concerns about the thickness of the steel cask being manufactured and proposed by Holtec International for use in centralized interim storage in New Mexico. This cask made of 5/8th

inch thick steel when used for dry storage at San Onofre have experienced denting and scratching during placement in concrete silos. I believe the U.S. Navy uses casks made of steel that is 8 or 10 inches thick. Does the model address cask thickness? If so, is a recommendation for using thicker-walled casks for centralized interim storage a possible outcome of the modeling? Also, the storage cask at Fukushima are, I believe, at least 8-inch thick and withstood the 2011 tsunami without damage. If stakeholder buy-in is a goal of centralized interim storage, then thicker steel requirements might go a long way toward inspiring public confidence.

Karen had another comment. This is again Karen Bonome with no affiliation. I see three reference cases. Argillite, crystalline, and salt. What about karst? The proposed centralized interim storage site is situated over extensive karst formation. What about sinkholes? Migration of water through karst is well-documented. How does GDSA address these factors?

During Michael Nole's presentation, there were also a couple of comments. John Busher from Sierra Club, New Mexico, had two comments. His first, excellent summary

by Emily Stein. His second, given the long time scales for permanent repository processes versus the much shorter scales for interim repositories, it would seem valuable to look at failure modes of current commercial cask systems in the 100 to 500 year timeframe as the probability of mechanical failures, which would preclude or make future transport very difficult to a permanent repository. Would the models currently presented be useful for interim repository assessment? In parenthesis, [Holtec], New Mexico, site has been approved by NRC, for example, closed parenthesis.

The next comments was by Karen Bonome. Again, no affiliation. She states, my previous two questions, I realize, are about centralized interim storage rather than deep geologic disposal. However, there is a very real concern in New Mexico and West Texas about the possibility of interim storage facilities becoming de facto permanent disposal sites. This concern is mentioned in lawsuits against the NRC by New Mexico and Texas Attorney General. Since your first speaker talked about centralized centralized interim storage, I felt that these questions were germane to today's discussion.

So Jean, I need to check the in-box again to see if

there are additional comments, and there are.

The next comment, I'm going to read anyway. It was submitted. Richard Andrews, president Boulder Innovative Technology Incorporated. You may wish, and I recommend, that you do not make public these comments by automatic posting. Please do heed them in your duties as public servants. Overall big picture does not seem to be present in functioning and scope of NWTRB, nor does DOE or NRC, the agency, NWTRB is charged to conduct oversight. By that, I mean the basic assumption that our nation should even be continuing to produce more and more spent nuclear fuel and high-level waste does not seem to be questioned by your organization. Our nation has been accumulating these wastes since the dawn of nuclear age, now more than 80 years, and there's still no safe or engaged and functional management of these wastes and one must actually question whether there's actually a safe disposal solution, particularly in light of the exceedingly long life of these radionuclides that have been created, almost all of which are not occurring from natural processes on earth with minor exceptions. So my question to NWTRB, why do you not focus and earnestly advise on the dangers from not shutting down

any additional waste generation that endangers we occupants of the biosphere? Is this institutional failure to provide advice and oversight not particularly shortsighted when the waste that we recent hominids are created incredibly hazardous materials, unlike any other wastes, given the 100,000 plus to millions of years timeframe, even when expressed as half-lives? Longer than our species and even our ancestors have existed. I actually see no valid or rational reason to continue down the path of nuclear energy and certainly not the undeniable intimate connections with nuclear weapons. Within the purview of the other DOE functions of alternative energy sources, should it not be entire clear that we have options for energy generation that are actually clean and far less costly? When those costs are legitimately measured in full life cycle analysis? Other truly clean and renewable energy systems are actually available to meet existential dangers of planetary climate disruption, not like the inherent dangers of the radioactive materials and waste of nuclear power.

Again, why are we scientists and engineers and citizens, including the NWTRB, continuing to promote in any

fashion the false path that nuclear power is safe. Moving on to the last paragraph. Admittedly, we have already created large amounts of dangerous nuclear waste and those materials must be disposed right away not many generations into the future. A key focus must be to shut down all of the existing nuclear power plants. No more waste should be produced. For many, hearing and testimony submissions to NRC, DOE, EPA, and previously to the NWTRB have personally conducted detailed computer modeling using data and computer codes readily available from the national labs of example cases of terrorist attacks on existing nuclear plants and in particular, attacks on the spent nuclear fuel. Such spent materials are still located at every nuclear power plant. Huge amounts in overall design basis cooling ponds. A single such attack with readily means can cause uninhabitable region of thousands of square miles with companion hundreds of thousands or millions of individual human casualties and deadly health effects and enormous economic, social, and cultural damages. All such materials are highly vulnerable actually to easily conducted attacks and these nuclear plants are even more dangerous with greater catastrophic large scale damages when attacked than even a typical fission weapon

explosion. In other words, a determined miscreant or malicious group does not need a nuclear weapon. We've provided such actors with targets of their choosing. Each nuclear plant is actually a de facto fixed location weapon and most plants are located near major population centers and financial and economic centers of our nation. I would also recommend that all NWT and others involved in nuclear technology to read similar accident models published by Professor Frank Von Hipple, Princeton University, and his colleagues, plus many other scientists at other highly credible institutions. Enough said for now. What I'm asking of NWTRB is a refocus on face the reality of the big picture of nuclear technology overall and its unique, unacceptable hazards to life.

And Jean, I have a couple more comments that came in. The next comment is from Sven Bader from Orano Federal Services. For the FMD model, does it matter if the spent nuclear fuel is oriented in the vertical or horizontal direction?

And then the last question I have is also from Sven Bader from Orano Federal Services. For the FMD model, is the impact of higher burnup fuels deleterious to the

degradation of the failed fuel?

And Jean, that is the last of the public comments that were submitted today.

>> BAHR: Okay. Thank you. I don't know if I'm on. There, I'm on. Okay. Thank you, Bret, for reading those, and we will have another opportunity for public comments tomorrow. And thanks to all the speakers today for doing timely presentations. We're finishing just right about on time. And we look forward to seeing everyone again tomorrow at noon Eastern Time, 9:00 Pacific. And have a good rest of your day.